Lectures on Applied

André Bakker

2008

Contents

Overview

Welcome!

- This document contains the lectures for the Computational Fluid Dynamics (ENGS 150) class that I taught at the Thayer School of Engineering at Dartmouth College from 2002-2006.
- These lectures are provided – at no charge - for educational and training purposes only.
- You are welcome to include parts of these lectures in your own lectures, courses, or trainings, provided that you include this reference:

  Bakker A. (2008) *Lectures on Applied Computational Fluid Dynamics.* www.bakker.org.

About the author

- I received my Doctorate in Applied Physics from Delft University of Technology in the Netherlands in 1992. In addition, I obtained an MBA in Technology Management from the University of Phoenix. From 1991 to 1998 I worked at Chemineer Inc., a leading manufacturer of fluid mixing equipment. In 1998 I joined Fluent Inc., the leading developer of computational fluid dynamics software. Since 2006 I have been with ANSYS, Inc.
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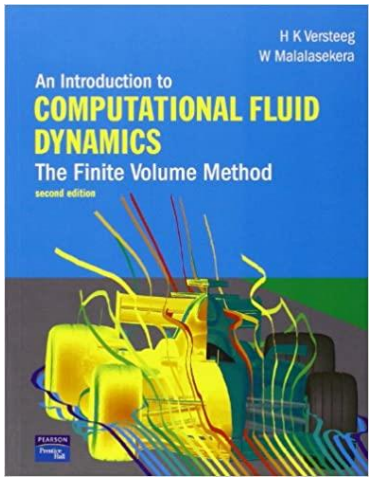
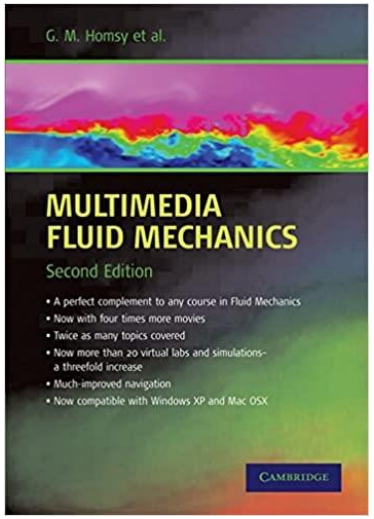
  - ResearchGate: https://www.researchgate.net/profile/Andre_Bakker
  - Personal web page: www.bakker.org

André Bakker

Course materials

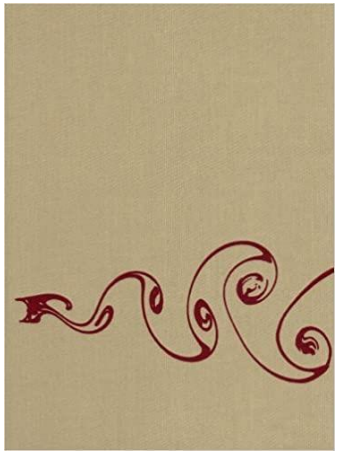
- This class uses the book *An introduction to Computational Fluid Dynamics: The Finite Volume Method* by Versteeg and Malalasekera, Longman Scientific & Technical.
- It also uses the *Multimedia Fluid Mechanics* CD-ROM by Homsy et al., Cambridge University Press.
- These lectures contain some materials from that book and the CD-ROM.
- I therefore recommend that users of these lectures purchase those.
- Additional references used in these lectures are provided below.



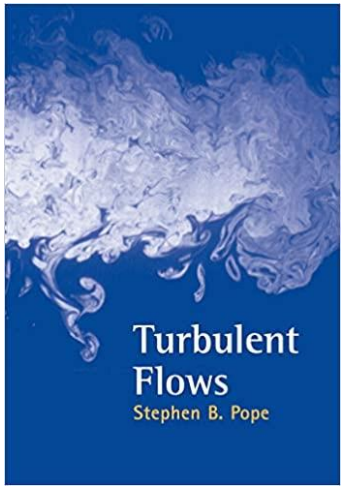


Additional recommended reading

- A classic: *Album of Fluid Motion* by Milton Van Dyke (1982) showcases photographs of many different flow fields. These lectures also include photographs from this book.



- *Turbulent Flows* by Stephen B. Pope (2000) provides a comprehensive, mathematical, overview of the theory of turbulent flows.



References (1/2)

[1] Barnes H.A., Hutton J.F., and Walters K. (1989) “An introduction to rheology,” Elsevier Science Publishers B.V. ISBN 0-444-87140-3 and 0-444-87469-0.

[2] Homsy G.M. et al. (2000) “Multi-Media Fluid Mechanics 1st Edition.” Cambridge University Press. ISBN 0521787483.

[3] Homsy G.M. et al. (2008) “Multi-Media Fluid Mechanics 2nd Edition.” Cambridge University Press. ISBN 978-0521721691.

[4] Pope, Stephen B. “Turbulent Flows.” Cambridge University Press 2000.

[5] Launder B. E. and Spalding D.B. (1974) “The numerical computation of turbulent flows.” Comp. Meth. In Appl. Mech. Engng. 3, pp. 269-289.

[6] Richardson L. F. (“Weather Prediction by Numerical Process.” Cambridge University Press, 1922)

References (2/2)

[7] Tennekes H., Lumley J.L. “A First Course in Turbulence.” The MIT Press 1972.

[8] Van Dyke (1982), “An Album of Fluid Motion.” The Parabolic Press. ISBN 0-915760-03-7

[9] Versteeg H.K., Malalasekera W. (1995) "An introduction to Computational Fluid Dynamics: The Finite Volume Method" 1st Edition by, Longman Scientific & Technical. ISBN 0-582-21884-5.

[10] Versteeg H.K., Malalasekera W. (2007) "An introduction to Computational Fluid Dynamics: The Finite Volume Method" 2nd Edition by, Longman Scientific & Technical. ISBN 978-0131274983.

[11] D. Gidaspow. Multiphase Flow and Fluidization. Academic Press, Boston, MA. 1994.

[12] Baldyga J., Bourne J.R. (1984) “A Fluid Mechanical Approach To Turbulent Mixing And Chemical Reaction.” Chemical Engineering Communications, Volume 28, 1984 - Issue 4-6

Student Projects (1/3)

- Students completed projects of their choosing as part of this class using the CFD software package FLUENT.
- These articles highlight some interesting student projects:
  - Bakker A. (2003) *Ivy League CFD Simulations*, Fluent Newsletter, Fall 2003, page 38-39.
  - Bakker A. (2005) *Having Fun While Studying CFD*. Fluent Newsletter, Summer 2005, page 26-27.

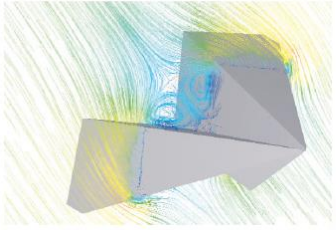
Student Projects (2/3)

academic news

Ivy League CFD Simulations

By André Bakker, Fluent Inc. and Dartmouth College, Hanover, NH

The Thayer School of Engineering at Dartmouth College has used FLUENT for many years. Until recently, its primary use was for research and development projects. For the past two years, however, a graduate class on applied computational fluid dynamics has been offered. The course covers the fundamentals of CFD, including numerical methods, turbulence models, mesh generation, and solution strategies. During the class, the students work on a CFD project of their own choosing. The projects have led to a number of interesting CFD results. Examples include modeling the flow through Antarctic firn (compressed snow) layers, heat transfer and phase change in a Southpole hot water drill used to collect micrometeorites (cosmic dust) at different depths, flow in a hydrogen-water separator, free surface flow around boat hulls, shallow water modeling on the continental slope, flow through nozzles, flow in a beaker with a magnetic stirrer, a radial compressor, and airflow around an America's Cup yacht.

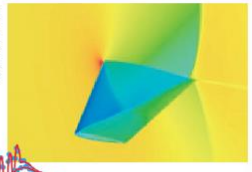


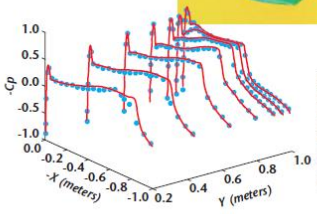
Pathlines illustrate the secondary flow surrounding a paper airplane in flight

Paper Airplane Competition

Students **Kyle Rick** and **Burkhard Lewerich** each folded a paper airplane, one that is commonly used in American classrooms and one that rules the sky in the German Schule. After extensive scientific experimentation, they concluded that the American design flew farther, but its flight was characterized by a destabilizing wobble. The German design, on the other hand, did not fly quite as far, but had a smooth and stable glide. What better way to analyze this than by using FLUENT?! Both designs were meshed in GAMBIT and flow field calculations were performed with FLUENT for a number of different angles of attack. From the flow fields they extracted drag, lift, and the torque on the plane. They then used this information to extract the flight path of each design, reproducing the experimentally found results. After visualizing the flow with pathlines, they found that the additional flap on the German folded design increased the drag (resulting in a shorter flight path), but resulted in a different vortex structure that stabilized the flight.

Contours of density show shocks formed by an ONERA M6 wing flying at Mach 0.93 and a 6 degree angle of attack





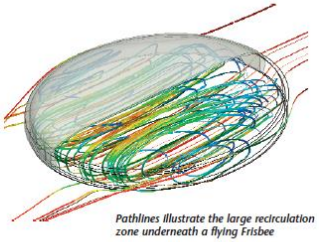
FLUENT predictions for the normalized pressure coefficient for the ONERA M6 wing at 0 degree angle of attack are in good agreement with data at several spanwise locations

ONERA Wing Modeling

Edward Hopkins took a different perspective to study airplane flight, by modeling the flow around a three-dimensional transonic airfoil, the ONERA M6 wing. He obtained the mesh from NASA and the experimental data for three flight conditions from ONERA (The French National Aerospace Research Establishment). The three conditions were for a zero-degree angle of attack at Mach numbers of 0.7 and 0.92, and a six-degree angle of attack at Mach 0.93. The data consisted of pressure tap data along a cross section of the wings at different spanwise locations. He calculated the flow fields using the coupled implicit solver, second order upwind differencing, and the Spalart-Allmaras turbulence model. FLUENT predictions for the pressure at the upper pressure taps for one set of conditions were found to be in very good agreement with data. Through contours of density, the CFD results were also used to illustrate the various shocks that form at a six-degree angle of attack and a free stream Mach number of 0.93.

Frisbee® Aerodynamics

An investigation of another type of flying object was performed was performed by **Ross Gortner**, who modeled the flow around a Frisbee. Ultimate Frisbee, or simply Ultimate, is a fairly recent sport with a long history that dates back to 1871 when the Frisbee Pie Company was founded. Frisbee pies became popular at Yale, and the students developed the habit of playing catch with the empty pie tins. Today, Frisbees are usually made from plastic resins, and the Ultimate Players Association organizes college tournaments in which Dartmouth College teams participate. Ross cut a Frisbee in half so that he would be able to accurately measure the cross-section. He then built the geometry and mesh in GAMBIT and modeled the flow with FLUENT. One interesting aspect of the flow around a Frisbee that was revealed in the simulation is that a vortex forms on the inside of the rotating disk. This recirculation zone may serve to enhance the lift.

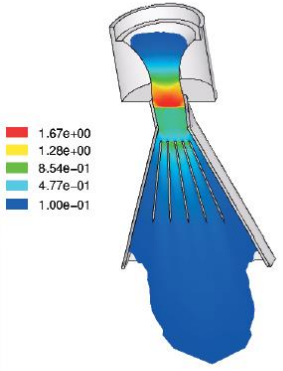


Pathlines illustrate the large recirculation zone underneath a flying Frisbee

SAE Formula Racecar Diffuser

A fourth example relates to an exciting application in land transport. **Diana Martin** and **Axel Schmidt** used FLUENT to design a new diffuser for the air intake of Dartmouth College's formula racecar. Formula racecars adhere to a certain formula involving design guideline parameters. They are open-wheeled, open-cockpit, single-seat racecars weighing between 400 and 500 pounds, with an engine less than 600 cubic centimeters in size, and are raced at the annual Formula SAE (Society of Automotive Engineers) racecar competition in Detroit. The rules limit the cross-sectional area of the air intake, so diffusers are used to get the maximum possible airflow to (and horsepower from) the engine. Using the coupled implicit solver, the students compared systems with three different diffuser designs to a system with no diffuser, and selected the system with the highest pressure recovery coefficient. The CFD results, as well as experiments performed earlier, indicated that using a diffuser is a lot better than not using one. The flow in the diffuser is choked, with a peak Mach number of 1.6. Only one diffuser design was successfully tested experimentally, but using CFD, the students tested multiple designs and identified the best one. A diffuser for this year's car was already built, but the new design may be used in next year's model.

All in all, the graduate CFD course at Dartmouth has been very successful, and the students have shown a great level of creativity in applying CFD to situations that are not commonly studied. ■



Contours of Mach number in one of the simulated diffuser designs shows choked flow

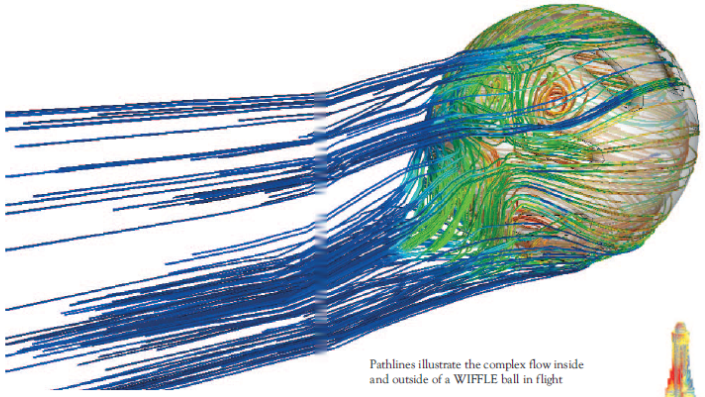
Baker Library, Dartmouth College

Student Projects (3/3)

Having Fun While Studying CFD

By André Bakker, Fluent Inc. and Dartmouth College, Hanover, NH

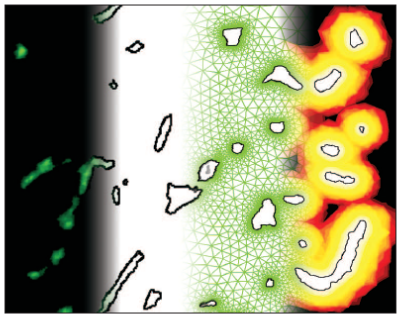
THE THAYER SCHOOL OF ENGINEERING at Dartmouth College has offered a graduate class on CFD for several years now. Students learn about the theory behind fluid flow and heat transfer, turbulence modeling, and numerical methods. The class ends with the students choosing a research topic of their own interest, and studying it using CFD. A wide range of topics is usually covered in the projects, and highlights from some recent projects are summarized below.



Pathlines illustrate the complex flow inside and outside of a WIFFLE ball in flight

WIFFLE® ball

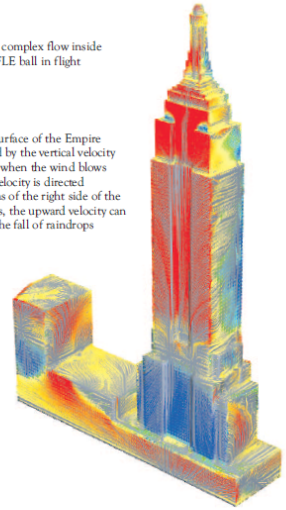
John Gagne and **Alex Tee** were interested in the flow field through and around a WIFFLE ball, a hollow plastic ball with several openings, popular for use in outdoor games. The ball can be thrown with very strong curves when the user gives it the right spin. This is thought to be due to the aerodynamic phenomena resulting from the flow through the spinning holes. John and Alex tried several options to model the flow around the ball. They found that in order to obtain good results they had to use the sliding mesh model to include the transient phenomena resulting from the rotation of the holes. A strong circulation flow was found to exist inside the ball, as well as vortices in the wake. The exact nature of the curved path the ball takes when thrown is most likely due to the interaction between these different vortex structures.



A sequence of tumor images shows (from left to right) the fluorescent image, the outline of the blood vessels, the computational mesh, and the drug volume fraction after a period of time has passed

Drug diffusion in a tumor

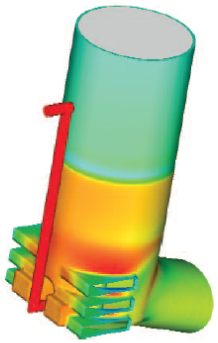
Xiaodong Zhou and **Rajeev Kumar** studied the diffusion of a drug inside a tumor. Their objective was to develop a model to better understand the physics behind this type of drug delivery. In order to obtain a realistic model of a tumor, the students took fluorescent images of a slice of a frozen mouse tumor to determine the locations of the blood vessels. These images were converted to contour images in MATLAB®. Edges and vertex data were extracted, and imported into GAMBIT, where a 2D mesh of the tumor cross-section showing the locations of the blood vessels was created. Transient calculations of the diffusion of the drug from the blood vessels into the solid part of the tumor were then performed using FLUENT. Drugs are active chemicals that are not just absorbed, but consumed because they are bound by the tumorous cells. The ratio between the rates of consumption and diffusion determine how deep a drug will penetrate into a tumor. It is important that the drug reach all regions of the tumor, and this process is controlled by preparing the drug in special ways, such as encapsulating the active drug in very tiny fat particles. This fat-encapsulated drug is absorbed better and its distribution to the tumor site is improved. Xiaodong and Rajeev developed user-defined functions (UDFs) for different consumption models and evaluated their effect on the distribution of the drug in the tumor. They found that realistic results could be obtained using a first-order model for the drug consumption.



Oil film lines on the surface of the Empire State Building, colored by the vertical velocity component show that when the wind blows from the left, the air velocity is directed upwards along portions of the right side of the building; in some cases, the upward velocity can be enough to reverse the fall of raindrops

Empire State Building

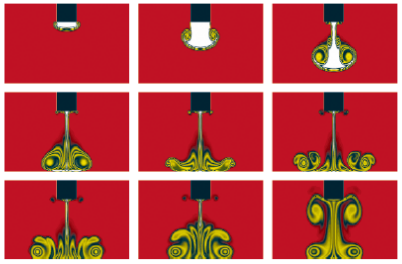
Exchange students from the University of Aachen in Germany **Philip Engelhardt** and **Daniel Wichmann** wanted to model an American icon: the Empire State Building (ESB) in New York. According to popular lore, during rainstorms there are windows in this building where people claim to see raindrops going up instead of down. Philip and Daniel concluded that CFD offered an excellent way to test this theory. They studied maps of New York, aerial photographs, and building drawings to create a GAMBIT model of both the ESB and the closest surrounding buildings. They also studied meteorological data to obtain realistic vertical profiles for the local wind velocity. They studied a variety of wind conditions and raindrop sizes. They concluded that it is indeed possible for the upward velocity of the wind flowing over the building walls and windows to exceed the falling velocity of raindrops. So, yes, it is possible that one day you will find yourself looking out over New York and wondering why the rain seems to be falling up instead of down!



Contours of static pressure on the surface of an inhaler equipped with a spirometer; the pressure sensor is shown in red

Pressure in an inhaler with a spirometer

Jordan Desroches analyzed a portable spirometer that is integrated into a standard medication inhaler. Millions of people suffer from asthma and rely on inhalers to dispense their medication. About 25% of them can not tell when they are becoming short of breath, however, a condition called "low perception of dyspnea." Spirometers allow them to assess how well their lungs are working by measuring the maximum volume of air that they can exhale. The user blows into the inhaler equipped with a spirometer; a pressure sensor picks up the resultant pressure pulse and determines the user's pulmonary status from this data. The inhaler has gills to vent excess pressure during exhalation. Jordan was interested in sizing the gills correctly so that the pressure sensor gives an accurate measure of the pressure pulse. This would allow the measured pressure to be correlated with the exhalation velocity. Furthermore, he wanted to prevent recirculation zones or other flow features that might result in inaccuracies in the pressure pulse measurement. Jordan created the geometry in Pro/ENGINEER, meshed it with GAMBIT, and performed transient simulations of the pressure at the sensor as a function of the exhalation velocity of the user with FLUENT. He found that there was a good correlation between the measured pressure and flow rate. This information can now be used to calibrate the electronics in the device.



Tracer concentration field in an impinging jet at a Reynolds number of 1600 as a function of time; the image sequence covers a total of 16.2 seconds

Impinging jet

Arthur Shaw and **Robert Haehnel** were interested in studying the flow field of impinging jets, particularly those in the downwash of helicopter blades. For validation purposes, they studied the spreading rate of a round jet, and also reproduced an experimental flow visualization study. In the experiment, the flow field of a pulsed jet at a Reynolds number of 1600 is visualized by means of fluorescent tracers and a laser sheet, showing the vortex rings that form, interact, and eventually break up. In the simulation, a tracer species was used to visualize that same flow field. They performed a detailed comparison between the experimental images and the FLUENT results, and concluded that all key flow field features were resolved. Satisfied with the results of the validation study, they studied the dispersion of dust and sand particles in an impinging jet, as it would occur below a helicopter, which is important because it affects the pilot's visibility during take-off and landing.

As always, the students were very creative and showed that CFD is not just a practical engineering tool but can also be fun to use! ■

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Lecture 1 - Introduction to CFD

Applied Computational Fluid Dynamics

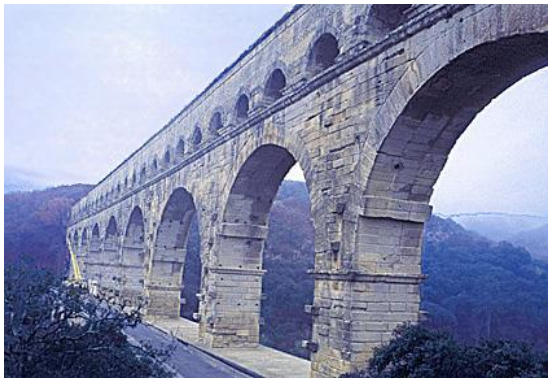
André Bakker

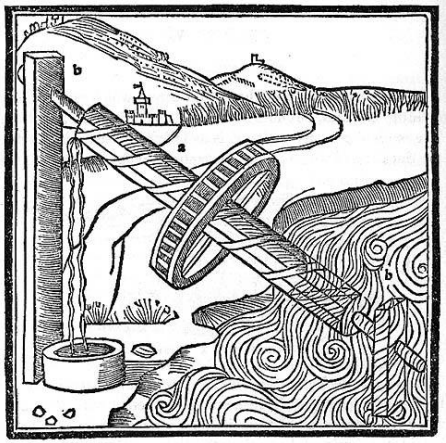
Fluid dynamics

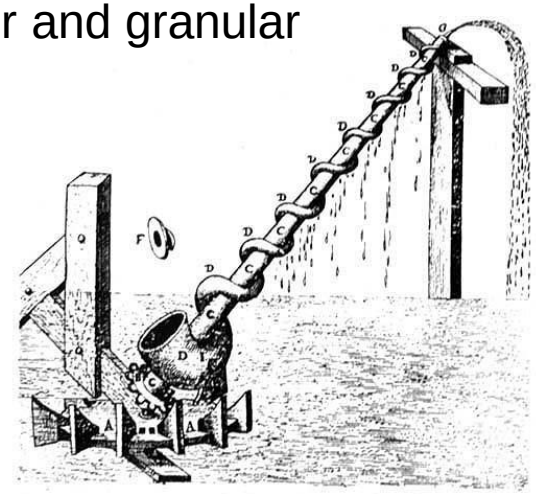
- Fluid dynamics is the science of fluid motion.
- Fluid flow is commonly studied in one of three ways:
  - Experimental fluid dynamics.
  - Theoretical fluid dynamics.
  - Numerically: computational fluid dynamics (CFD).
- During this course we will focus on obtaining the knowledge required to be able to solve practical fluid flow problems using CFD.
- Topics covered today include:
  - A brief review of the history of fluid dynamics.
  - An introductory overview of CFD.

Antiquity

- Focus on waterworks: aqueducts, canals, harbors, bathhouses.
- One key figure was Archimedes - Greece (287-212 BC). He initiated the fields of static mechanics, hydrostatics, and pycnometry (how to measure densities and volumes of objects).
- One of Archimedes' inventions is the water screw, which can be used to lift and transport water and granular materials.



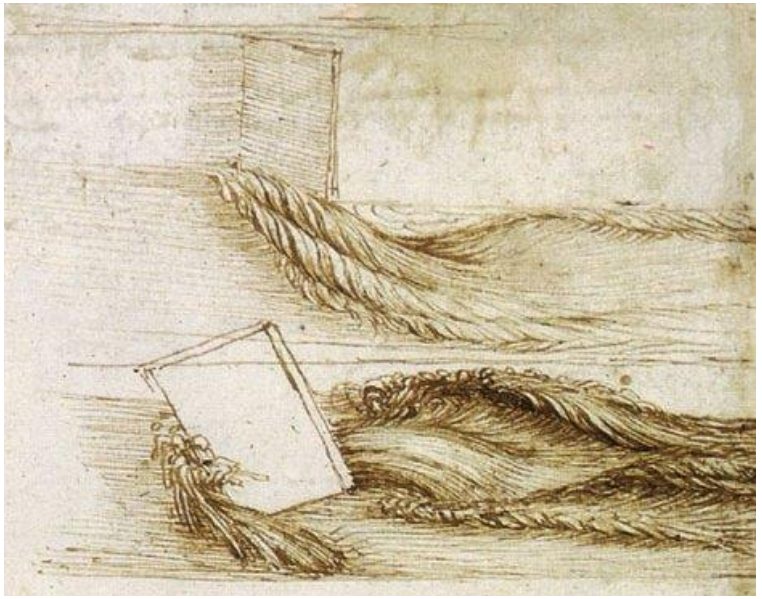




Images: Homsy et al. [2]

Leonardo da Vinci - Italy (1452-1519)

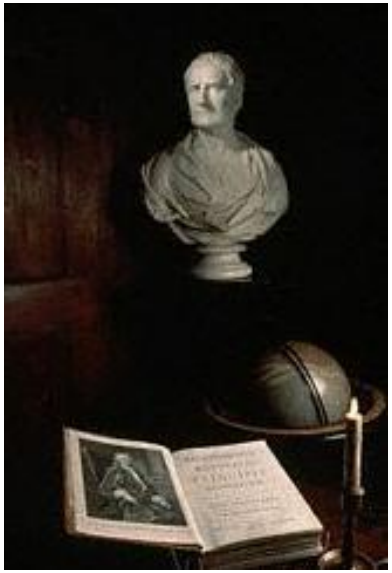
- Leonardo set out to observe all natural phenomena in the visible world, recognizing their form and structure, and describing them pictorially exactly as they are.
- He planned and supervised canal and harbor works over a large part of middle Italy. In France he designed a canal that connected the Loire and Saone.
- His contributions to fluid mechanics are presented in a nine-part treatise (*Del moto e misura dell'acqua*) that covers the water surface, movement of water, water waves, eddies, falling water, free jets, interference of waves, and many other newly observed phenomena.



Leonardo da Vinci *"A Gigantic Explosion"*

Isaac Newton - England (1643-1727)

- One of the most important figures in science.
- Most well-known for his three laws of motion.
- His key contributions to fluid mechanics include:
  - The second law: F=m.a.
  - The concept of Newtonian viscosity in which stress and the rate of strain vary linearly.
  - The reciprocity principle: the force applied upon a stationary object by a moving fluid is equal to the change in momentum of the fluid as it deflects around the front of the object.
  - Relationship between the speed of waves at a liquid surface and the wavelength.



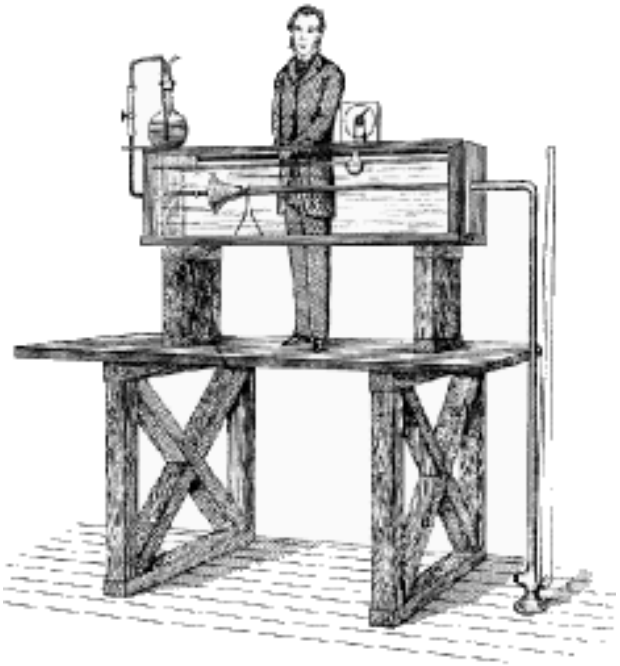
Images: Homsy et al. [2]

18th and 19th century

- During this period, significant work was done trying to mathematically describe the motion of fluids.
- Daniel Bernoulli (1700-1782) derived Bernoulli's equation.
- Leonhard Euler (1707-1783) proposed the Euler equations, which describe conservation of momentum for an inviscid fluid, and conservation of mass. He also proposed the velocity potential theory.
- Claude Louis Marie Henry Navier (1785-1836) and George Gabriel Stokes (1819-1903) introduced viscous transport into the Euler equations, which resulted in the Navier-Stokes equation. This forms the basis of modern day CFD.
- Other key figures were Jean Le Rond d'Alembert, Siméon-Denis Poisson, Joseph Louis Lagrange, Jean Louis Marie Poiseuille, John William Rayleigh, M. Maurice Couette, and Pierre Simon de Laplace.

Osborne Reynolds - England (1842-1912)

- Reynolds was a prolific writer who published almost 70 papers during his lifetime on a wide variety of science and engineering related topics.
- He is most well-known for the Reynolds number, which is the ratio between inertial and viscous forces in a fluid. This governs the transition from laminar to turbulent flow.

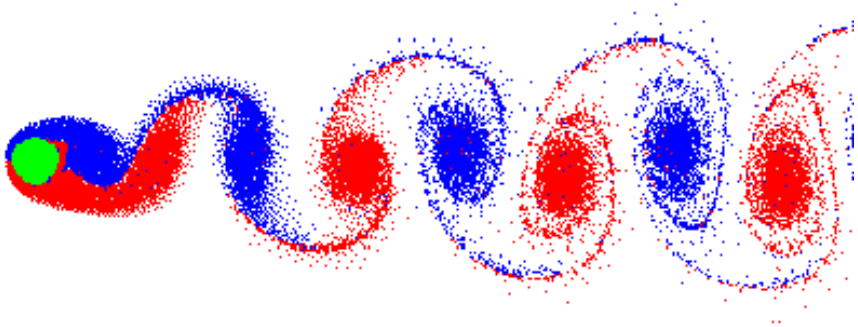


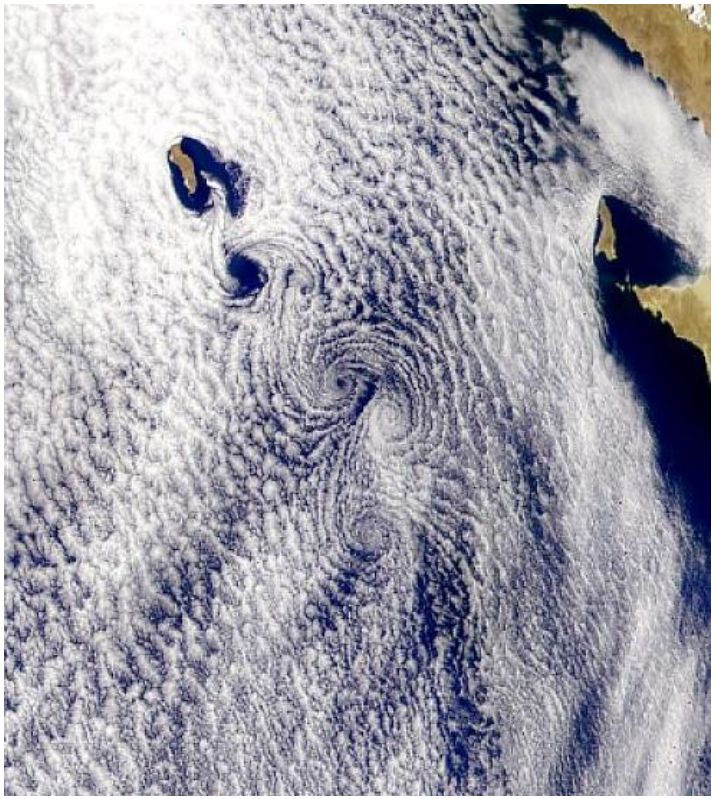
- Reynolds' apparatus consisted of a long glass pipe through which water could flow at different rates, controlled by a valve at the pipe exit. The state of the flow was visualized by a streak of dye injected at the entrance to the pipe. The flow rate was monitored by measuring the rate at which the free surface of the tank fell during draining. The immersion of the pipe in the tank provided temperature control due to the large thermal mass of the fluid.

Image: Homsy et al. [2]

First part of the 20th century

- Much work was done on refining theories of boundary layers and turbulence.
- Ludwig Prandtl (1875-1953): boundary layer theory, the mixing length concept, compressible flows, the Prandtl numbers, and more.
- Theodore von Karman (1881-1963) analyzed what is now known as the von Karman vortex street.
- Geoffrey Ingram Taylor (1886-1975): statistical theory of turbulence and the Taylor microscale.
- Andrey Nikolaevich Kolmogorov (1903-1987): the Kolmogorov scales and the universal energy spectrum.
- George Keith Batchelor (1920-2000): contributions to the theory of homogeneous turbulence.



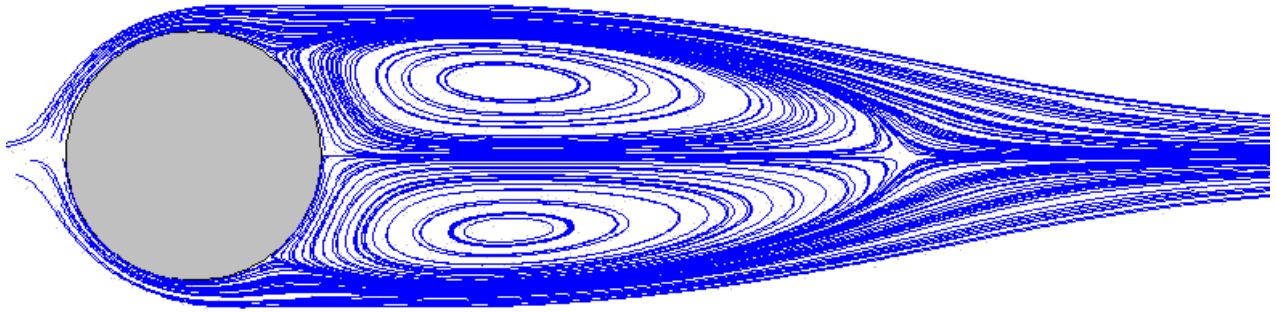


Lewis Fry Richardson (1881-1953)

- In 1922, Lewis Fry Richardson [6] developed the first numerical weather prediction system.
  - Division of space into grid cells and the finite difference approximations of Bjerknes's "primitive differential equations."
  - His own attempt to calculate weather for a single eight-hour period took six weeks and ended in failure.
- His model's enormous calculation requirements led Richardson to propose a solution he called the "forecast-factory."
  - The "factory" would have filled a vast stadium with 64,000 people.
  - Each one, armed with a mechanical calculator, would perform part of the calculation.
  - A leader in the center, using colored signal lights and telegraph communication, would coordinate the forecast.

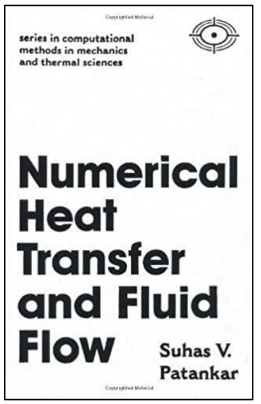
1930s to 1950s

- Earliest numerical solution: for flow past a cylinder (1933).
  - A.Thom, 'The Flow Past Circular Cylinders at Low Speeds', Proc. Royal Society, A141, pp. 651-666, London, 1933
- Kawaguti obtains a solution for flow around a cylinder, in 1953 by using a mechanical desk calculator, working 20 hours per week for 18 months.
  - M. Kawaguti, 'Numerical Solution of the NS Equations for the Flow Around a Circular Cylinder at Reynolds Number 40', Journal of Phy. Soc. Japan, vol. 8, pp. 747-757, 1953.



1960s and 1970s

- During the 1960s the theoretical division at Los Alamos contributed many numerical methods that are still in use today, such as the following methods:
  - Particle-In-Cell (PIC).
  - Marker-and-Cell (MAC).
  - Vorticity-Streamfunction Methods.
  - Arbitrary Lagrangian-Eulerian (ALE).
  - *k*-ε turbulence model.
- During the 1970s a group working under D. Brian Spalding, at Imperial College, London, develop:
  - Parabolic flow codes (GENMIX).
  - Vorticity-Streamfunction based codes.
  - The SIMPLE algorithm and the TEACH code.
  - The form of the *k*-ε equations that are used today.
  - Upwind differencing.
  - ‘Eddy break-up’ and ‘presumed pdf’ combustion models.



- In 1980 Suhas V. Patankar publishes *Numerical Heat Transfer and Fluid Flow*, probably the most influential book on CFD to date.

1980s and 1990s

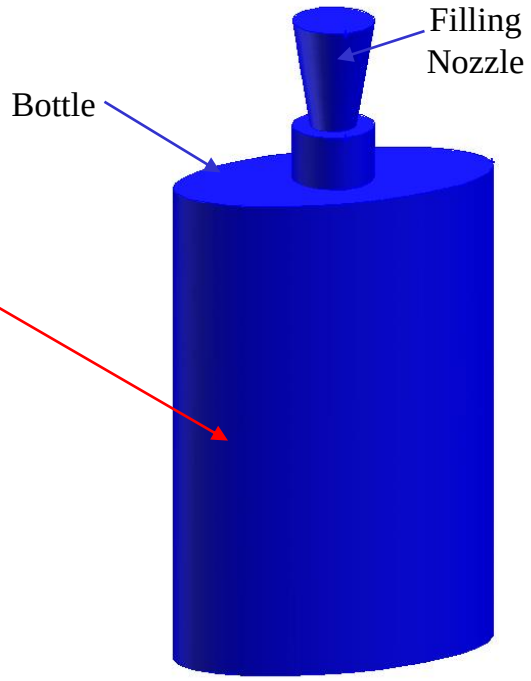
- Previously, CFD was performed using academic, research and in-house codes. When one wanted to perform a CFD calculation, one had to write a program.
- This is the period during which most commercial CFD codes originated that are available today:
  - Fluent (UK and US).
  - Fidap (US).
  - Polyflow (Belgium).
  - Phoenix (UK).
  - Star CD (UK).
  - Ansys/CFX (UK).
  - Flow 3d (US).
  - ESI/CFDRC (US).
  - SCRYU (Japan).
  - and more, see www.cfdreview.com.

What is computational fluid dynamics?

- Computational fluid dynamics (CFD) is the science of predicting fluid flow, heat transfer, mass transfer, chemical reactions, and related phenomena by solving the mathematical equations which govern these processes using a numerical process.
- The result of CFD analyses is relevant engineering data used in:
  - Conceptual studies of new designs.
  - Detailed product development.
  - Troubleshooting.
  - Redesign.
- CFD analysis complements testing and experimentation.
  - Reduces the total effort required in the laboratory.

CFD - how it works (1/2)

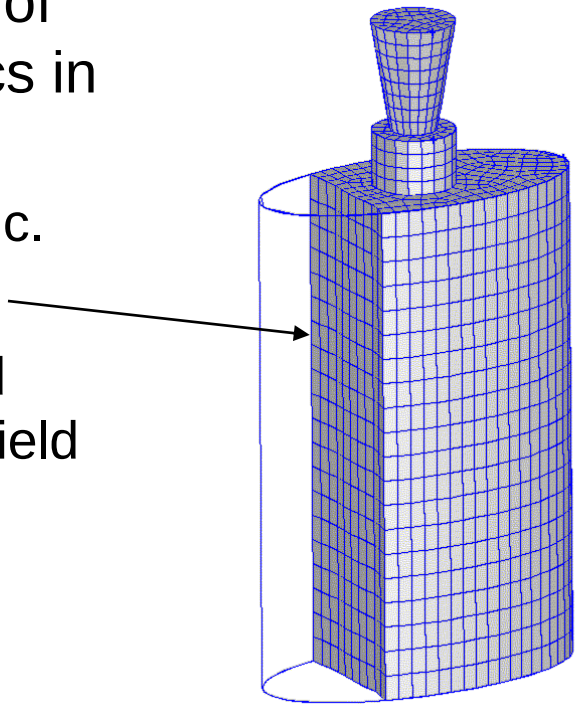
- Analysis begins with a mathematical model of a physical problem.
- Conservation of matter, momentum, and energy must be satisfied throughout the region of interest.
- Fluid properties are modeled empirically.
- Simplifying assumptions are made in order to make the problem tractable (e.g., steady-state, incompressible, inviscid, two-dimensional).
- Provide appropriate initial and boundary conditions for the problem.



Domain for bottle filling problem.

CFD - how it works (2/2)

- CFD applies numerical methods (called discretization) to develop approximations of the governing equations of fluid mechanics in the fluid region of interest.
  - Governing differential equations: algebraic.
  - The collection of cells is called the grid.
  - The set of algebraic equations are solved numerically (on a computer) for the flow field variables at each node or cell.
  - System of equations are solved simultaneously to provide solution.
- The solution is post-processed to extract quantities of interest (e.g., lift, drag, torque, heat transfer, separation, pressure loss, etc.).



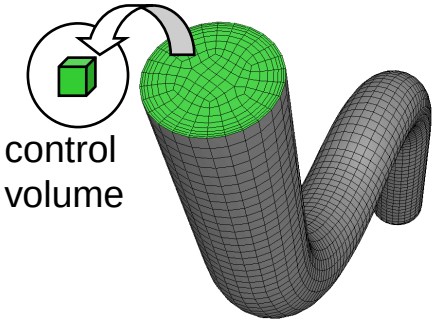
Mesh for bottle filling problem.

Discretization

- Domain is discretized into a finite set of control volumes or cells. The discretized domain is called the “grid” or the “mesh.”
- General conservation (transport) equations for mass, momentum, energy, etc., are discretized into algebraic equations.
- All equations are solved to render flow field.

$$\underbrace{\frac{\partial}{\partial t}\int_V \rho\phi dV}_{\text{unsteady}} + \underbrace{\oint_A \rho\phi\mathbf{V}\cdot d\mathbf{A}}_{\text{convection}} = \underbrace{\oint_A \Gamma\nabla\phi\cdot d\mathbf{A}}_{\text{diffusion}} + \underbrace{\int_V S_\phi dV}_{\text{generation}}$$

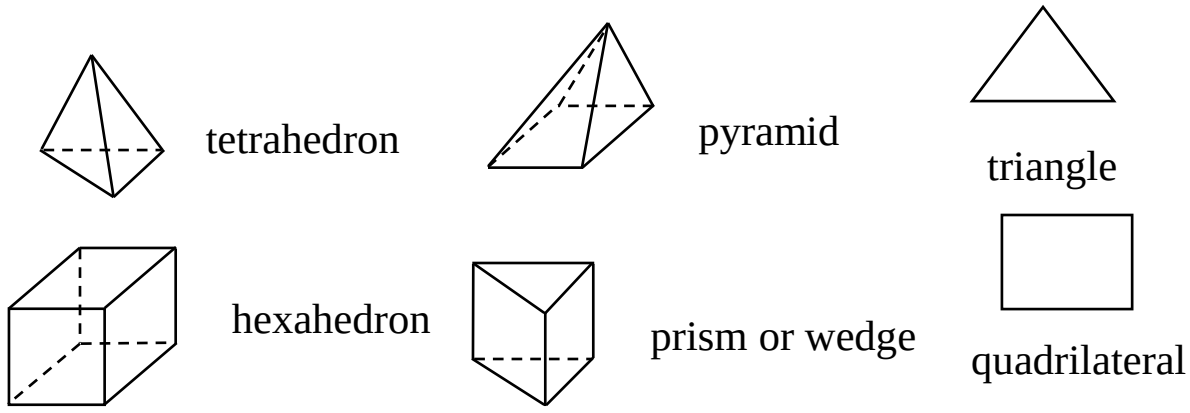
Eqn.	ϕ
continuity	1
x-mom.	u
y-mom.	v
energy	h



Fluid region of pipe flow discretized into finite set of control volumes (mesh).

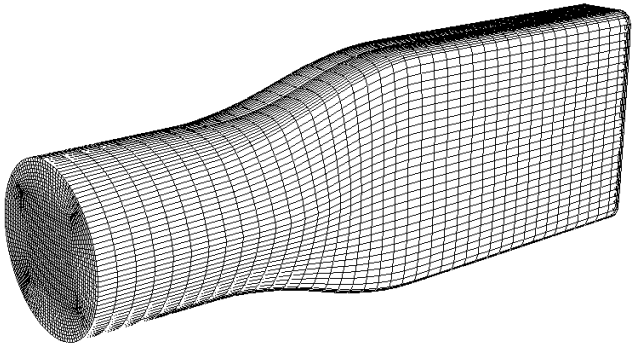
Design and create the grid

- Should you use a quad/hex grid, a tri/tet grid, a hybrid grid, or a non-conformal grid?
- What degree of grid resolution is required in each region of the domain?
- How many cells are required for the problem?
- Will you use adaption to add resolution?
- Do you have sufficient computer memory?

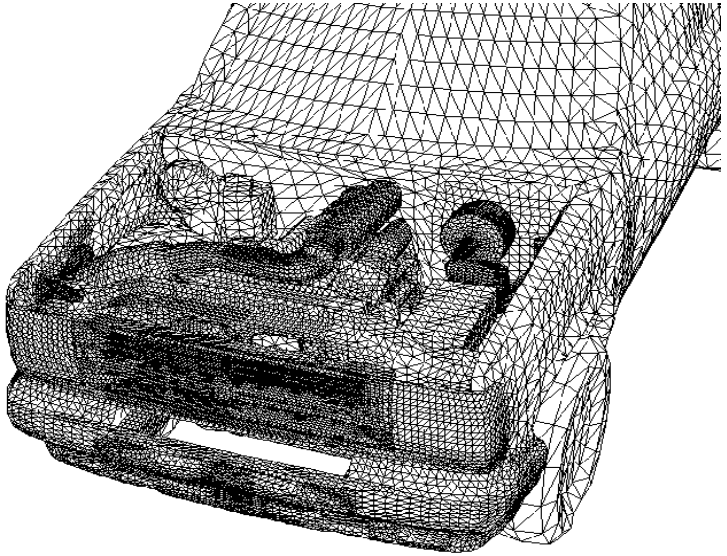


Tri/tet vs. quad/hex meshes

- For simple geometries, quad/hex meshes can provide high-quality solutions with fewer cells than a comparable tri/tet mesh.

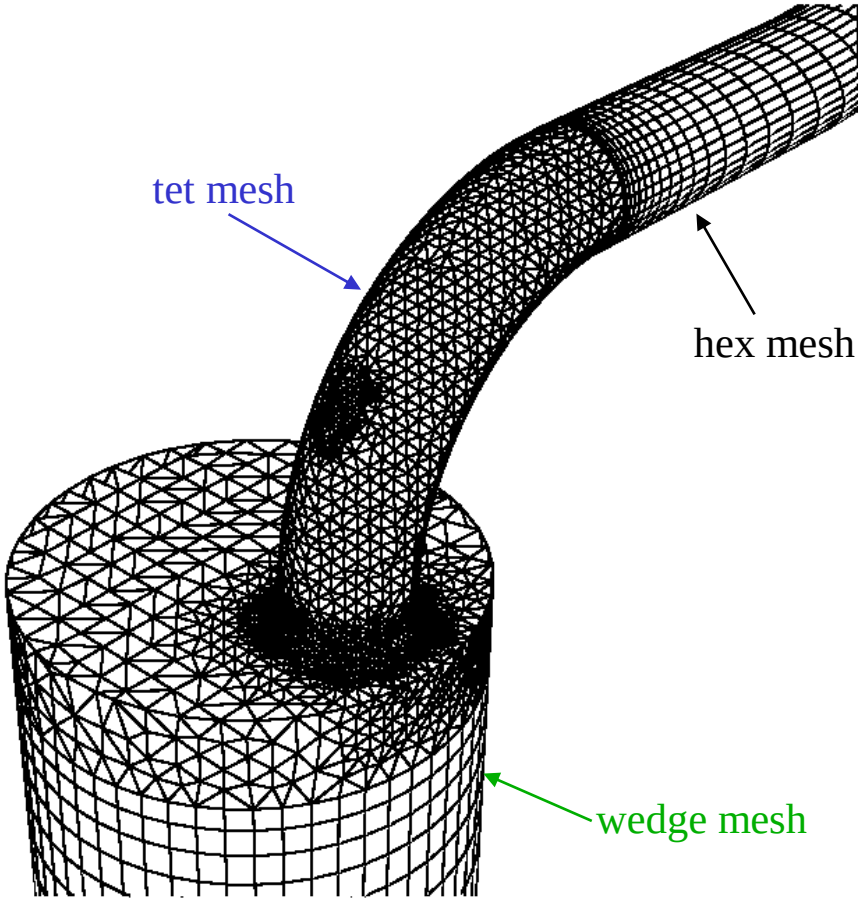


- For complex geometries, quad/hex meshes show no numerical advantage, and you can save meshing effort by using a tri/tet mesh.



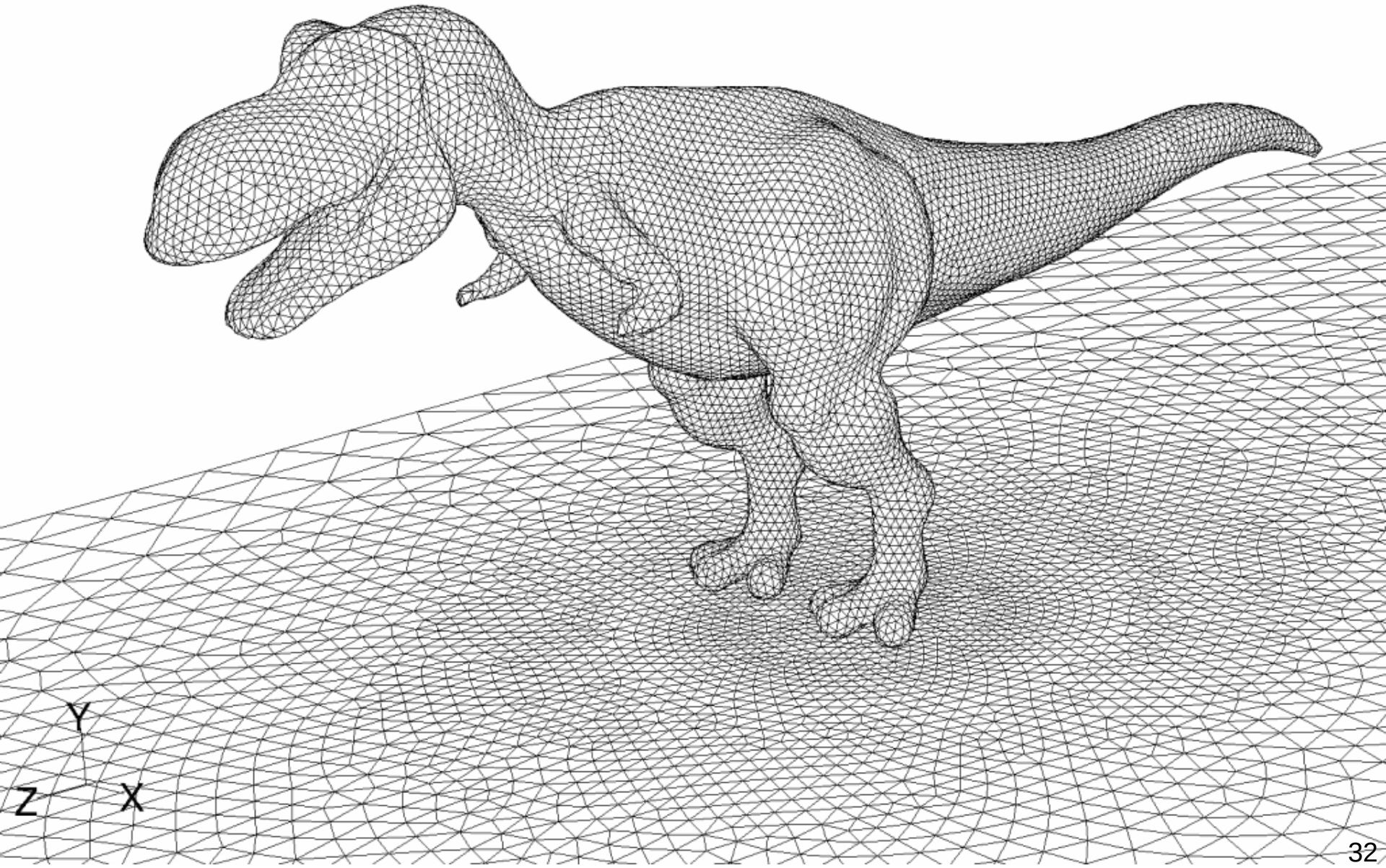
Hybrid mesh example

- Valve port grid.
- Specific regions can be meshed with different cell types.
- Both efficiency and accuracy are enhanced relative to a hexahedral or tetrahedral mesh alone.



Hybrid mesh for an
IC engine valve port

Dinosaur mesh example



Set up the numerical model

- For a given problem, you will need to:
  - Select appropriate physical models.
  - Turbulence, combustion, multiphase, etc.
  - Define material properties.
    - Fluid.
    - Solid.
    - Mixture.
  - Prescribe operating conditions.
  - Prescribe boundary conditions at all boundary zones.
  - Provide an initial solution.
  - Set up solver controls.
  - Set up convergence monitors.

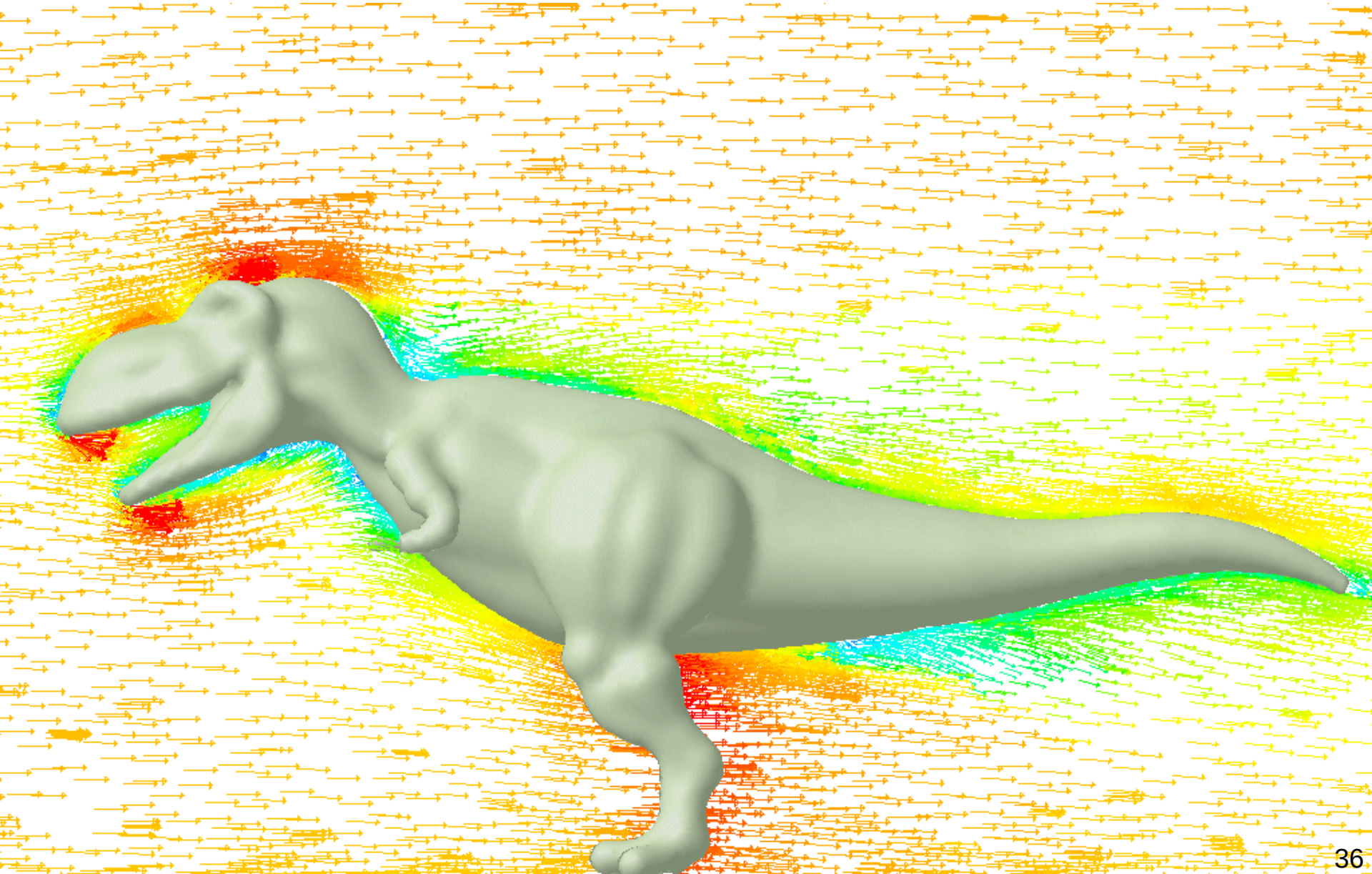
Compute the solution

- The discretized conservation equations are solved iteratively. A number of iterations are usually required to reach a converged solution.
- Convergence is reached when:
  - Changes in solution variables from one iteration to the next are negligible.
  - Residuals provide a mechanism to help monitor this trend.
  - Overall property conservation is achieved.
- The accuracy of a converged solution is dependent upon:
  - Appropriateness and accuracy of the physical models.
  - Grid resolution and independence.
  - Problem setup.

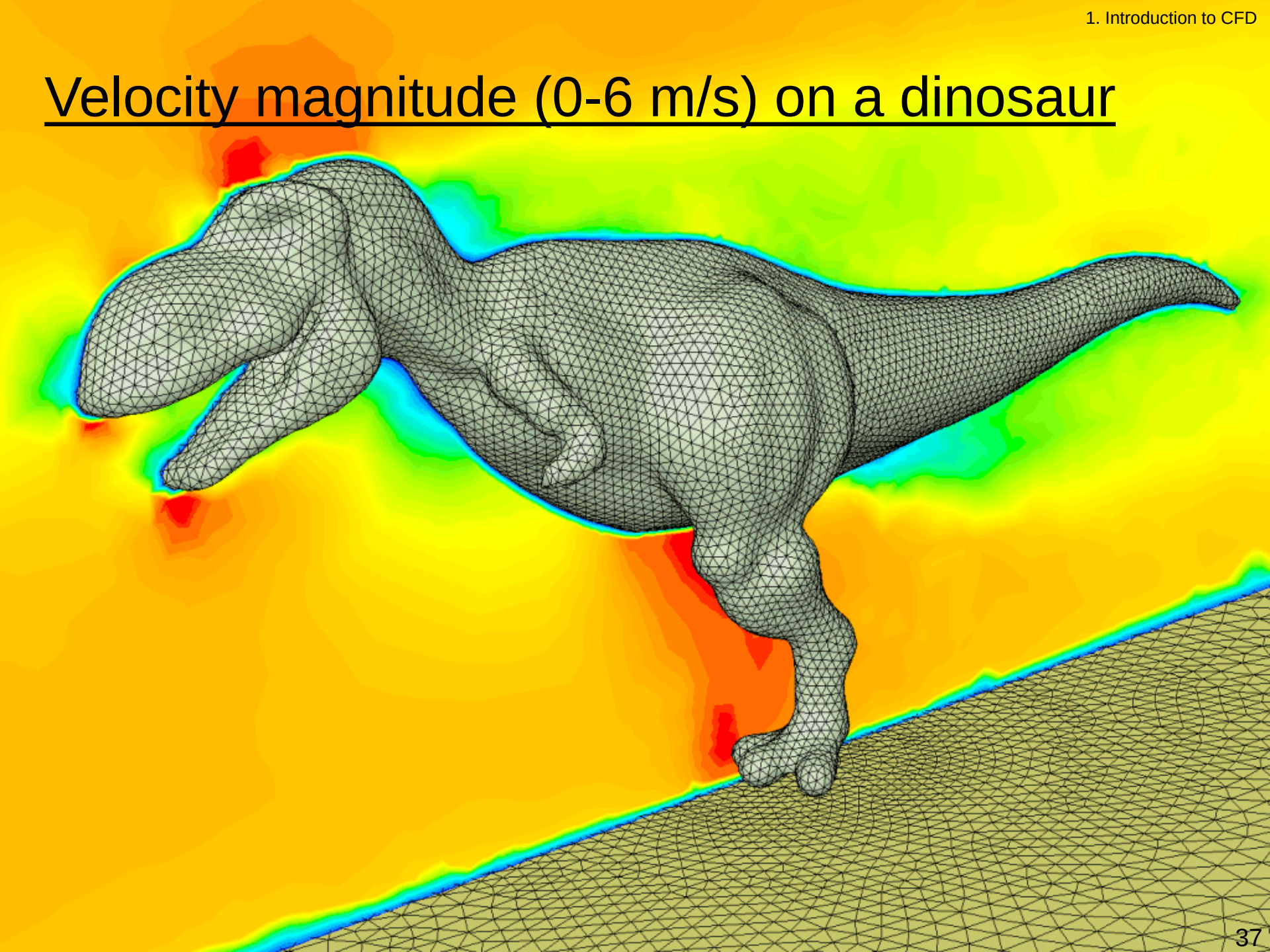
Examine the results

- Visualization can be used to answer such questions as:
  - What is the overall flow pattern?
  - Is there separation?
  - Where do shocks, shear layers, etc. form?
  - Are key flow features being resolved?
  - Are physical models and boundary conditions appropriate?
  - Numerical reporting tools can be used to calculate quantitative results, e.g.:
    - Lift, drag, and torque.
    - Average heat transfer coefficients.
    - Surface-averaged quantities.

Velocity vectors around a dinosaur



Velocity magnitude (0-6 m/s) on a dinosaur



Tools to examine the results

- Graphical tools:
  - Grid, contour, and vector plots.
  - Pathline and particle trajectory plots.
  - XY plots.
  - Animations.
- Numerical reporting tools:
  - Flux balances.
  - Surface and volume integrals and averages.
  - Forces and moments.
- The next slides show an example of a CFD analysis for an amusement park dinosaur.

Pressure field on a dinosaur

Forces on the dinosaur

- Drag force: 17.4 N.
- Lift force: 5.5 N.
- Wind velocity: 5 m/s.
- Air density: 1.225 kg/m^3.
- The dinosaur is 3.2 m tall.
- It has a projected frontal area of A = 2.91 m^2.
- The drag coefficient is:

$$C_D = \frac{F_D}{\frac{1}{2}\rho v^2 A} = \frac{17.4}{0.5*1.225*25*2.91} = 0.11$$

- This is pretty good compared to the average car! The streamlined back of the dinosaur resulted in a flow pattern with very little separation.

Consider revisions to the model

- Are physical models appropriate?
  - Is flow turbulent?
  - Is flow unsteady?
  - Are there compressibility effects?
  - Are there 3D effects?
  - Are boundary conditions correct?
- Is the computational domain large enough?
  - Are boundary conditions appropriate?
  - Are boundary values reasonable?
- Is grid adequate?
  - Can grid be adapted to improve results?
  - Does solution change significantly with adaption, or is the solution grid independent?
  - Does boundary resolution need to be improved?

Applications of CFD

- Applications of CFD are numerous!
  - Flow and heat transfer in industrial processes (boilers, heat exchangers, combustion equipment, pumps, blowers, piping, etc.).
  - Aerodynamics of ground vehicles, aircraft, missiles.
  - Film coating, thermoforming in material processing applications.
  - Flow and heat transfer in propulsion and power generation systems.
  - Ventilation, heating, and cooling flows in buildings.
  - Chemical vapor deposition (CVD) for integrated circuit manufacturing.
  - Heat transfer for electronics packaging applications.
  - And many, many more!

Advantages of CFD (1/2)

- Relatively low cost.
  - Using physical experiments and tests to get essential engineering data for design can be expensive.
  - CFD simulations are relatively inexpensive, and costs are likely to decrease as computers become more powerful.
- Speed.
  - CFD simulations can be executed in a short period of time.
  - Quick turnaround means engineering data can be introduced early in the design process.
- Ability to simulate real conditions.
  - Many flow and heat transfer processes cannot be (easily) tested, e.g., hypersonic flow.
  - CFD provides the ability to theoretically simulate any physical condition.

Advantages of CFD (2/2)

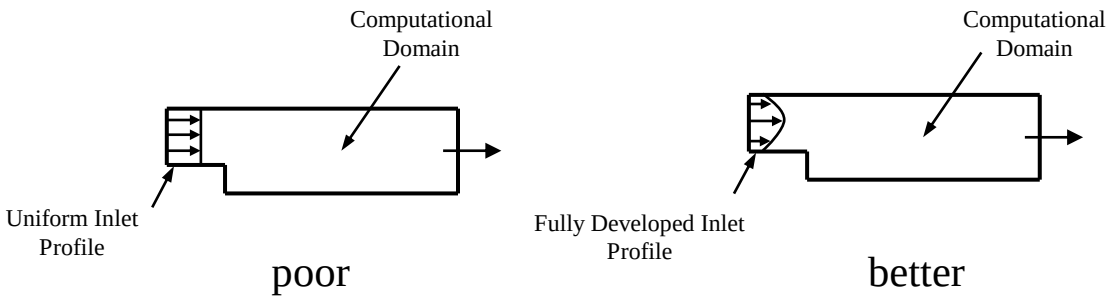
- Ability to simulate ideal conditions.
  - CFD allows great control over the physical process and provides the ability to isolate specific phenomena for study.
  - Example: a heat transfer process can be idealized with adiabatic, constant heat flux, or constant temperature boundaries.
- Comprehensive information.
  - Experiments only permit data to be extracted at a limited number of locations in the system (e.g., pressure and temperature probes, heat flux gauges, LDV, etc.).
  - CFD allows the analyst to examine a large number of locations in the region of interest and yields a comprehensive set of flow parameters for examination.

Limitations of CFD (1/2)

- Physical models.
  - CFD solutions rely upon physical models of real-world processes (e.g., turbulence, compressibility, chemistry, multiphase flow, etc.).
  - The CFD solutions can only be as accurate as the physical models on which they are based.
- Numerical errors.
  - Solving equations on a computer invariably introduces numerical errors.
  - Round-off error: due to finite word size available on the computer. Round-off errors will always exist (though they can be small in most cases).
  - Truncation error: due to approximations in the numerical models. Truncation errors will go to zero as the grid is refined. Mesh refinement is one way to deal with truncation error.

Limitations of CFD (2/2)

- Boundary conditions.
  - As with physical models, the accuracy of the CFD solution is only as good as the initial/boundary conditions provided to the numerical model.
  - Example: flow in a duct with sudden expansion. If flow is supplied to domain by a pipe, you should use a fully-developed profile for velocity rather than assume uniform conditions.



Summary

- CFD is a method to numerically calculate heat transfer and fluid flow.
- Currently, its main application is as an engineering method, to provide data that is complementary to theoretical and experimental data. This is mainly the domain of commercially available codes and in-house codes at large companies.
- CFD can also be used for purely scientific studies, e.g., into the fundamentals of turbulence. This is more common in academic institutions and government research laboratories. Codes are usually developed to specifically study a certain problem.

Lecture 2 - Flow Fields

Applied Computational Fluid Dynamics

André Bakker

Important variables

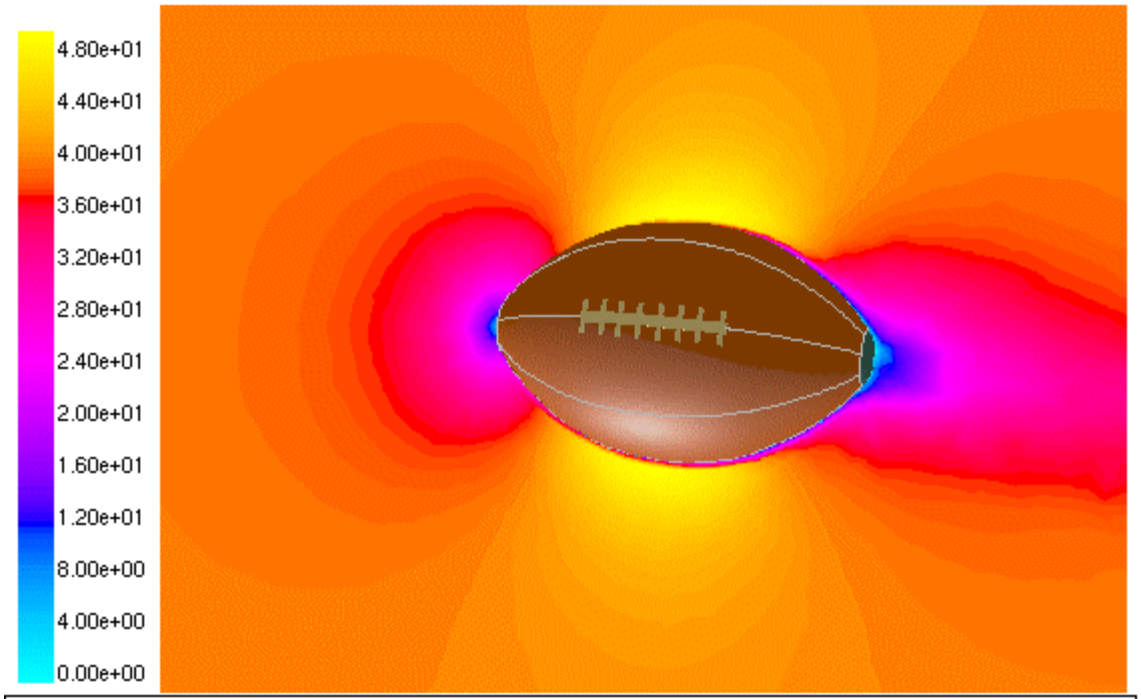
- Pressure and fluid velocities are always calculated in conjunction. Pressure can be used to calculate forces on objects, e.g., for the prediction of drag of a car. Fluid velocities can be visualized to show flow structures.
- From the flow field we can derive other variables such as shear and vorticity. Shear stresses may relate to erosion of solid surfaces. Deformation of fluid elements is important in mixing processes. Vorticity describes the rotation of fluid elements.
- In turbulent flows, turbulent kinetic energy and dissipation rate are important for such processes as heat transfer and mass transfer in boundary layers.
- For non-isothermal flows, the temperature field is important. This may govern evaporation, combustion, and other processes.
- In some processes, radiation is important.

Post-processing

- Results are usually reviewed in one of two ways: graphically or alphanumerically.
- Graphically:
  - Vector plots.
  - Contours.
  - Iso-surfaces.
  - Flowlines.
  - Animation.
- Alphanumerics:
  - Integral values.
  - Drag, lift, torque calculations.
  - Averages, standard deviations.
  - Minima, maxima.
  - Compare with experimental data.

A flow field example: the football

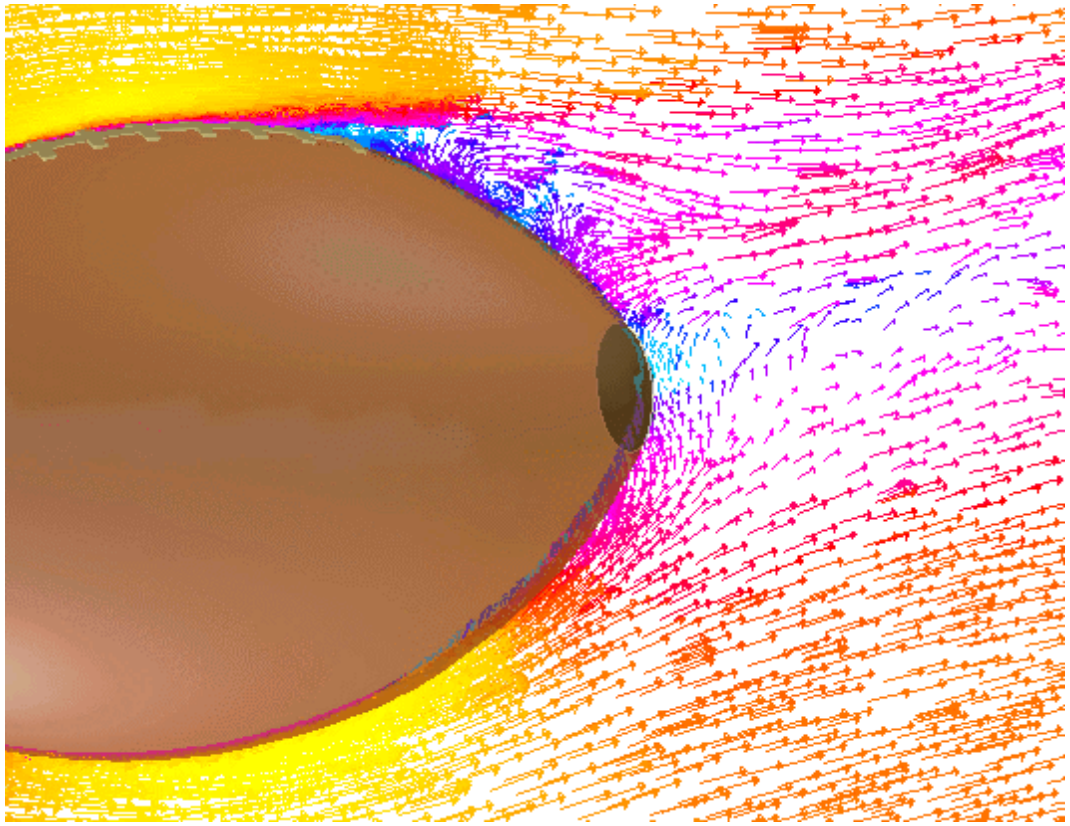
- Regulation size American football.
- Perfect throw. Ball is thrown from right to left.
- Flow field relative to the ball is from left to right.
- Shown here are filled contours of velocity magnitude (time averaged).



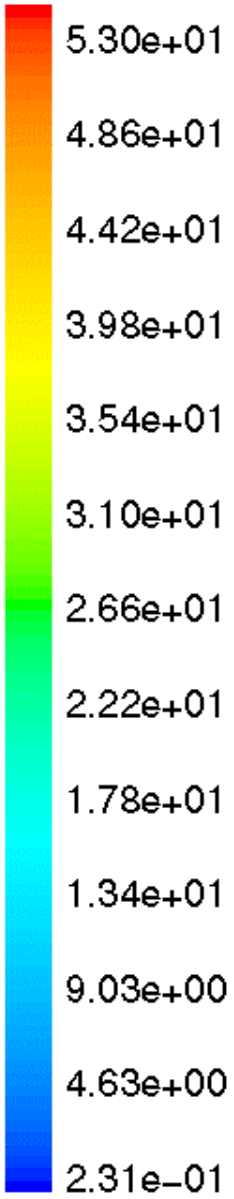
Regulation Size American Football – 300 RPM – Mach 0.052 – Perfect Throw
Contours of Velocity Magnitude (mph)

Football flow field

- Velocity vectors.
- Watch the flow separation behind the leather strips.

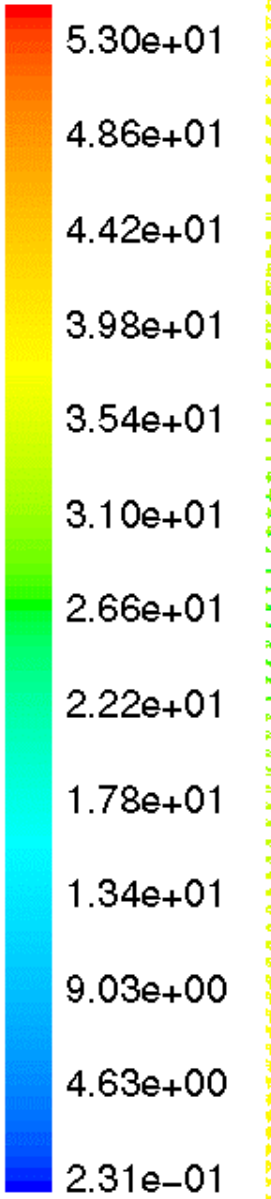


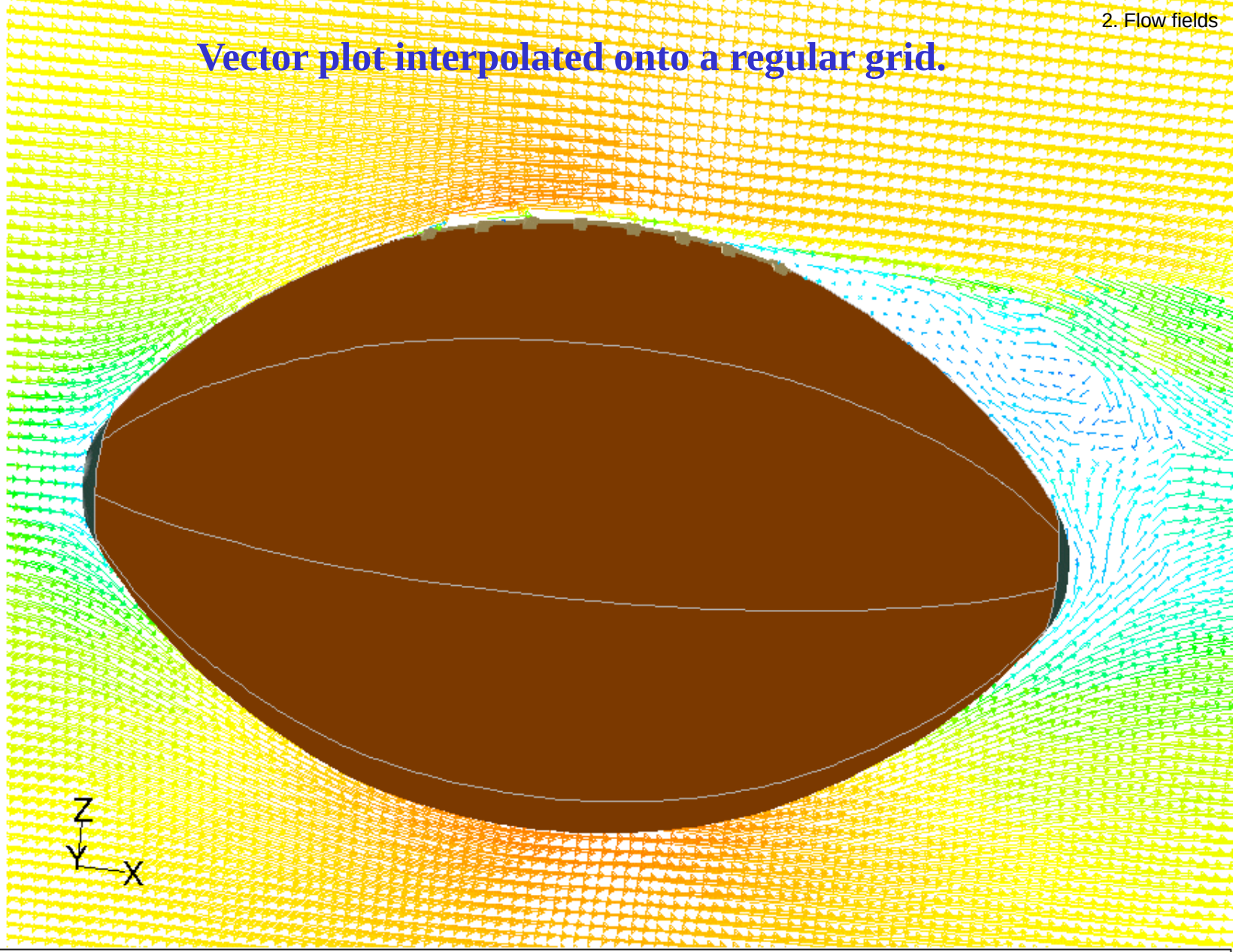
Vector plot on the grid nodes. Irregular looking.



Regulation Size American Football – 300 RPM – Mach 0.052 – Perfect Throw
Velocity Vectors Colored By Velocity Magnitude (mph)

Vector plot interpolated onto a regular grid.

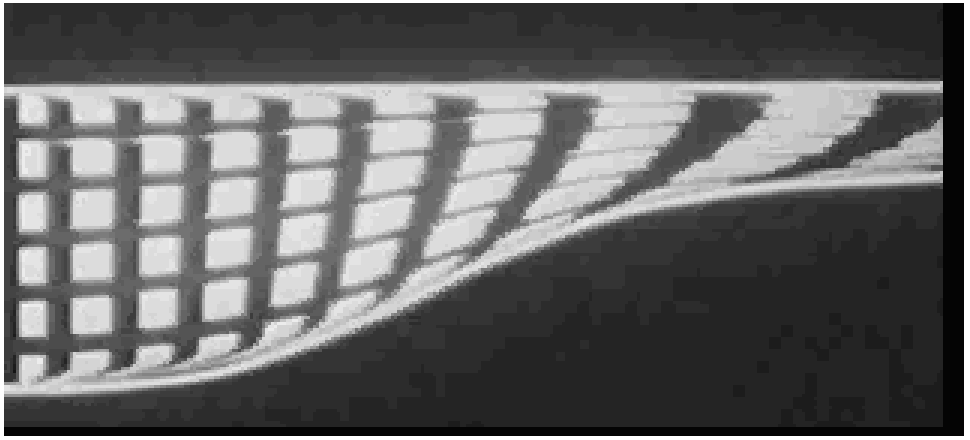




Regulation Size American Football – 300 RPM – Mach 0.052 – Perfect Throw
Velocity Vectors Colored By Velocity Magnitude (mph)

Fluid motion

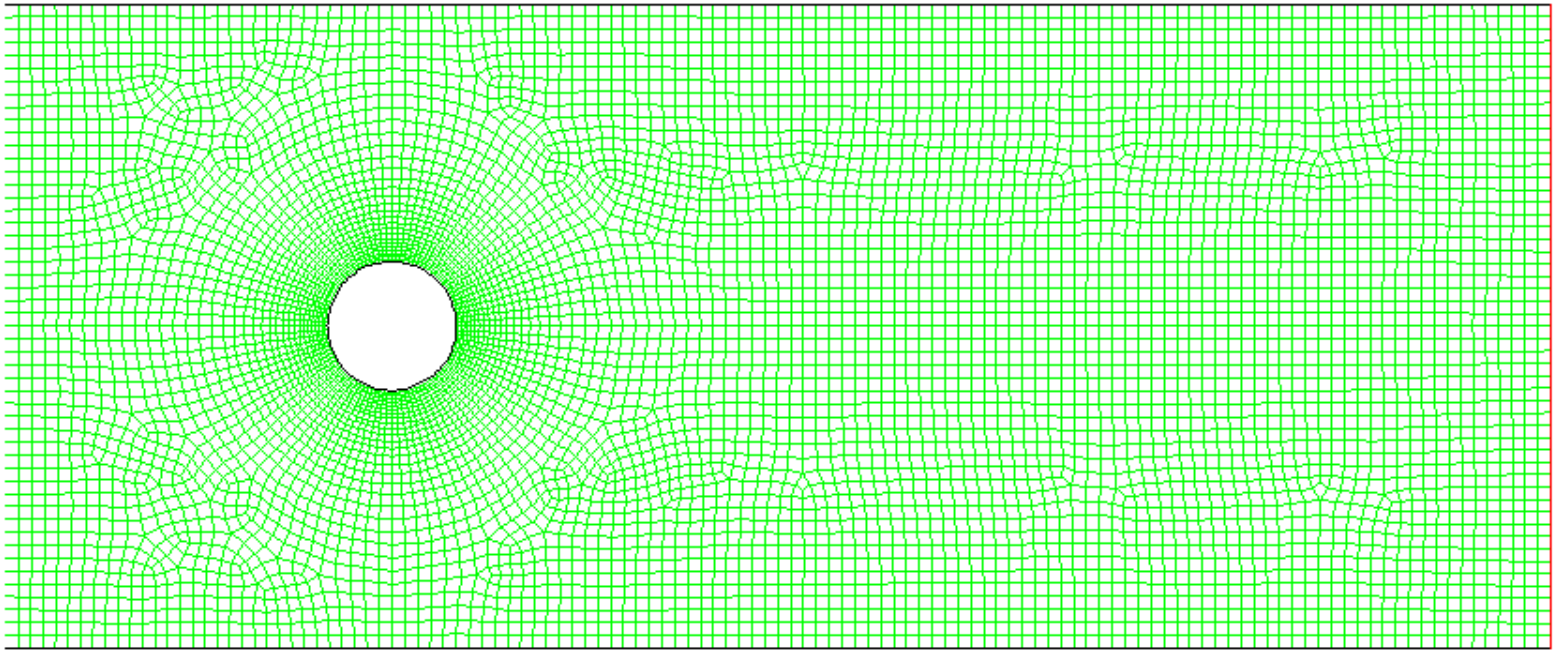
- In a fluid flow field, each fluid element undergoes three different effects:
  - 1. Translation.
  - 2. Deformation.
  - 3. Rotation.



Translation and deformation

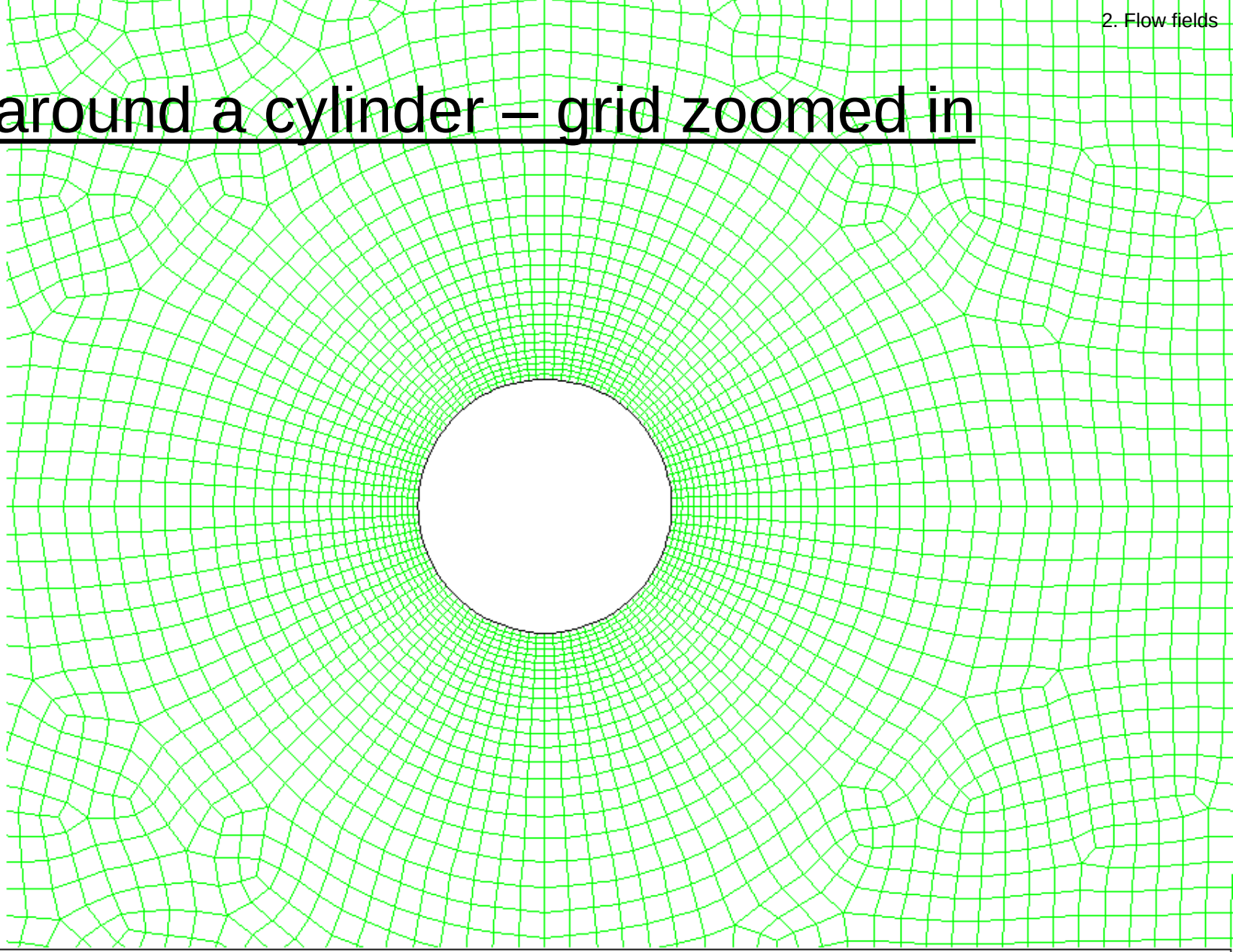
Image: Homsy et al. [2]

Example: flow around a cylinder - grid



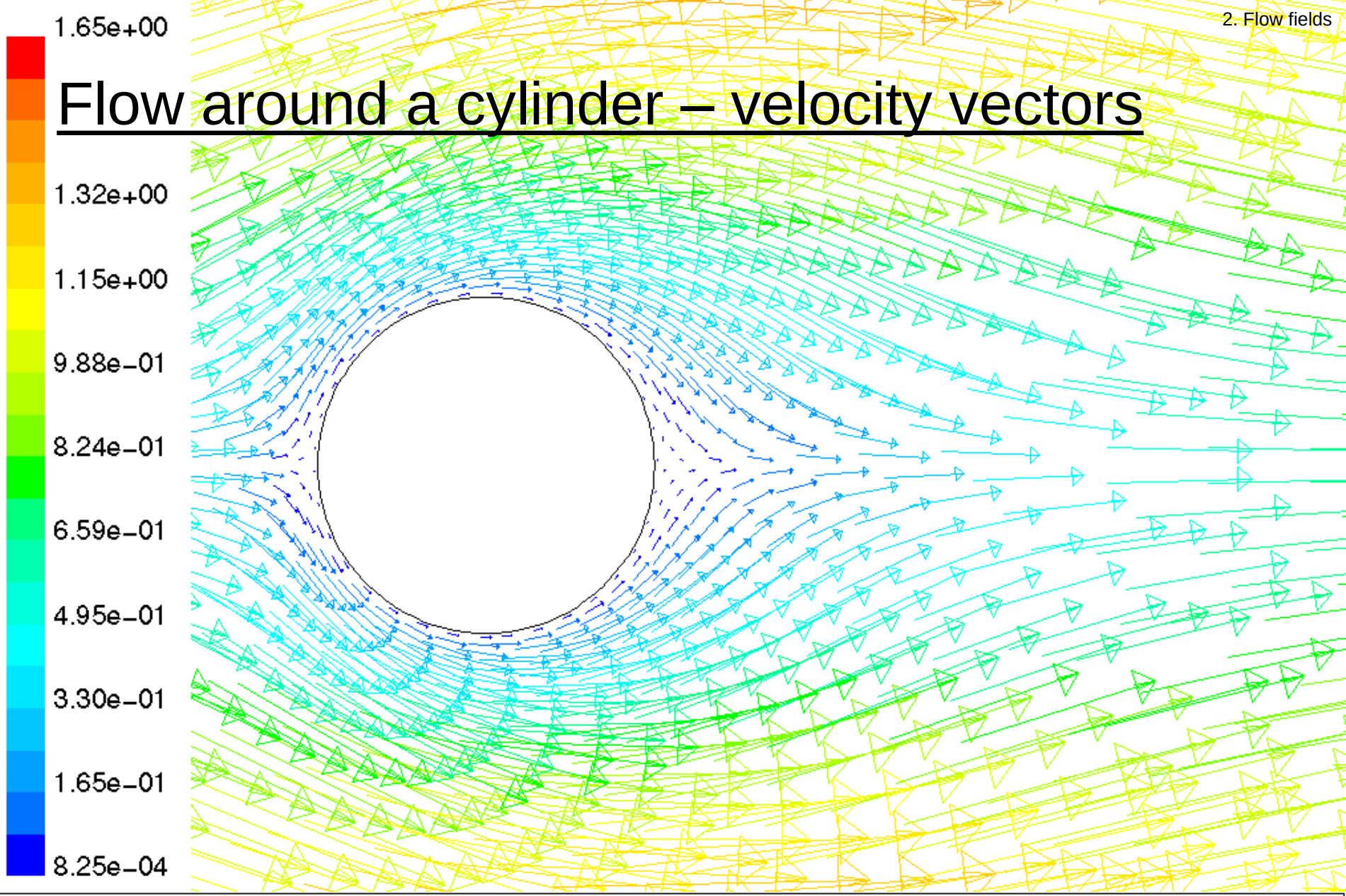
Grid

Flow around a cylinder – grid zoomed in



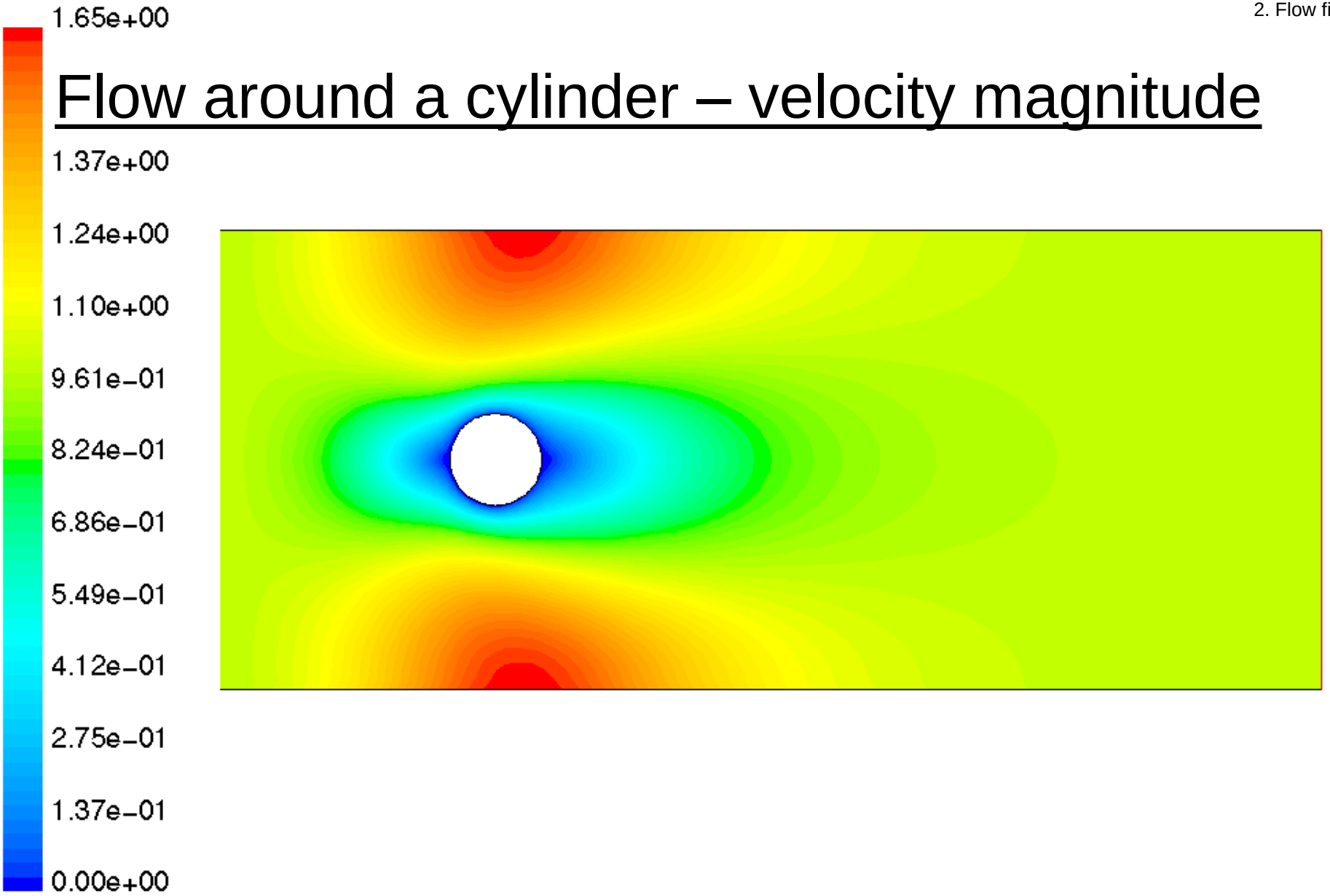
Grid

Flow around a cylinder – velocity vectors



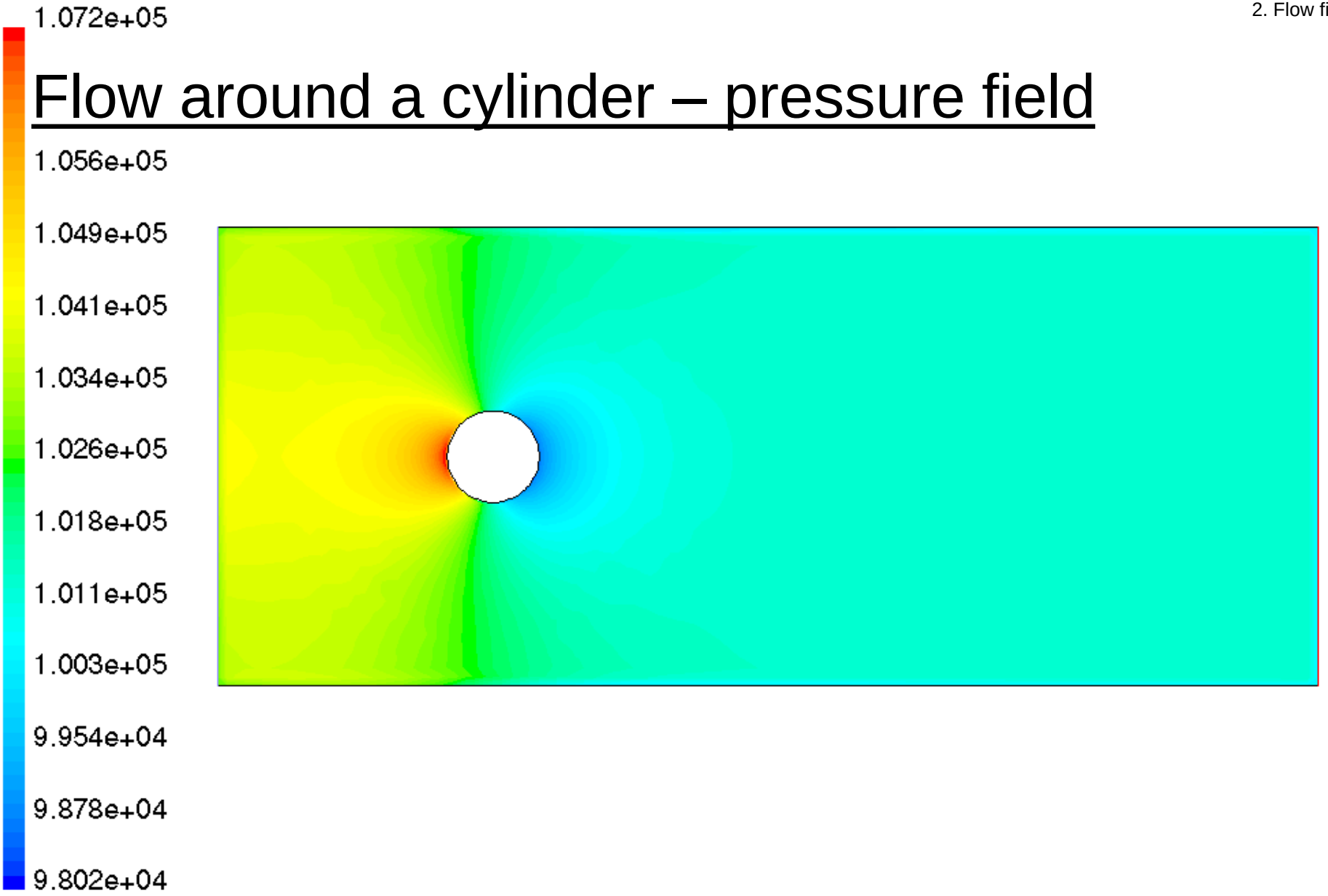
Re = 1
Velocity Vectors Colored By Velocity Magnitude (m/s)

Flow around a cylinder – velocity magnitude



Re = 1
Contours of Velocity Magnitude (m/s)

Flow around a cylinder – pressure field



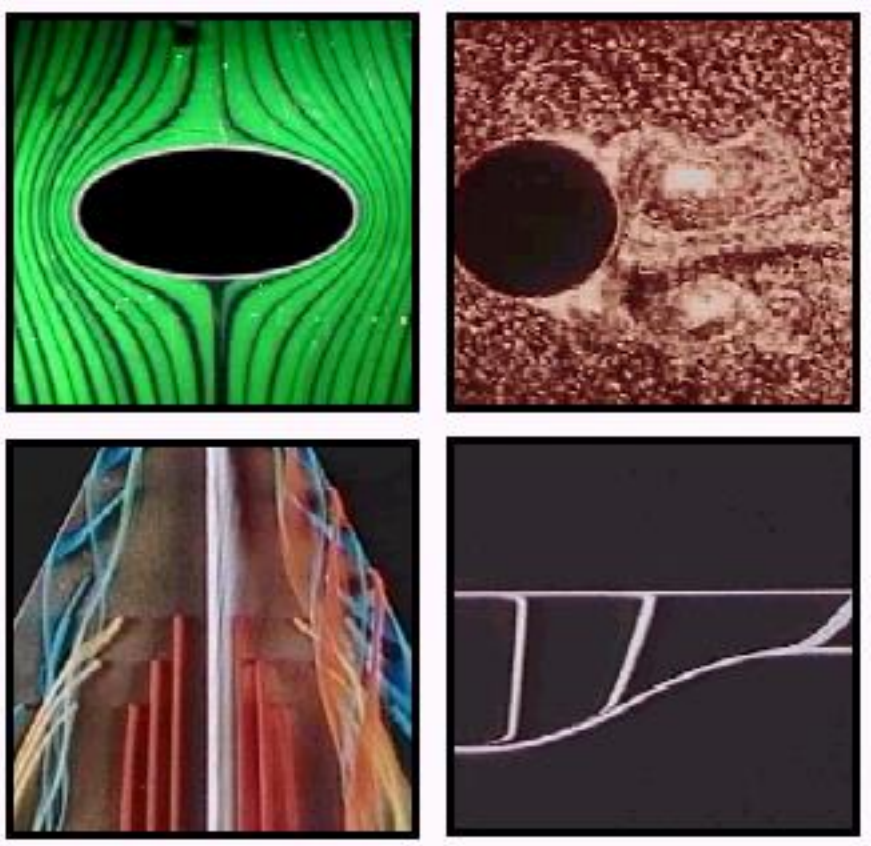
Re = 1
Contours of Absolute Pressure (pascal)

Pressure

- Pressure can be used to calculate forces (e.g., drag, lift, or torque) on objects by integrating the pressure over the surface of the object.
- Pressure consists of three components:
  - Hydrostatic pressure ρgh.
  - Dynamic pressure $\rho v^2/2$.
  - Static pressure p_s. This can be further split into an operating pressure (e.g., atmospheric pressure) and a gauge pressure.
- When static pressure is reported it is usually the gauge pressure only.
- Total pressure is the static pressure plus the dynamic pressure.

Methods to show translation

- Translation can be shown by means of:
  - Velocity vectors.
  - Flowlines:
    - Streamlines.
    - Pathlines.
    - Streaklines.
    - Timelines.
    - Oilflow lines.



Images: Homsy et al. [2]

Streamlines

- Streamlines are curves that are everywhere tangent to the velocity vector U.
- The animation shows streamlines for a steady state 3-D flow.
- For 3-D flow fields, instead of streamlines one usually visualizes streaklines or pathlines, which for steady flow are the same.
- For 2-D flow fields, a stream function Ψ can be defined:

$$u = \frac{\partial \psi}{\partial y}; \qquad v = -\frac{\partial \psi}{\partial x}$$

- In 2-D, lines of constant stream function are streamlines. Calculating the stream function and isolines is a more efficient way to calculate streamlines than by integrating particle tracks.

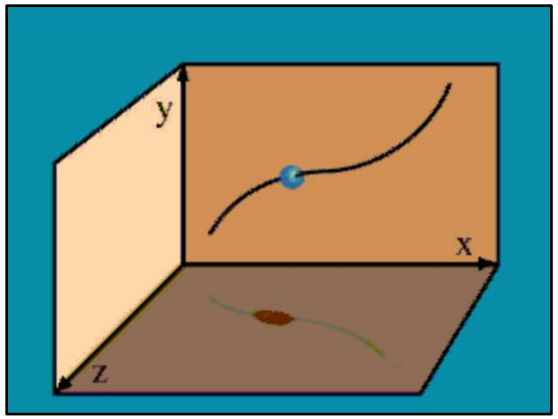
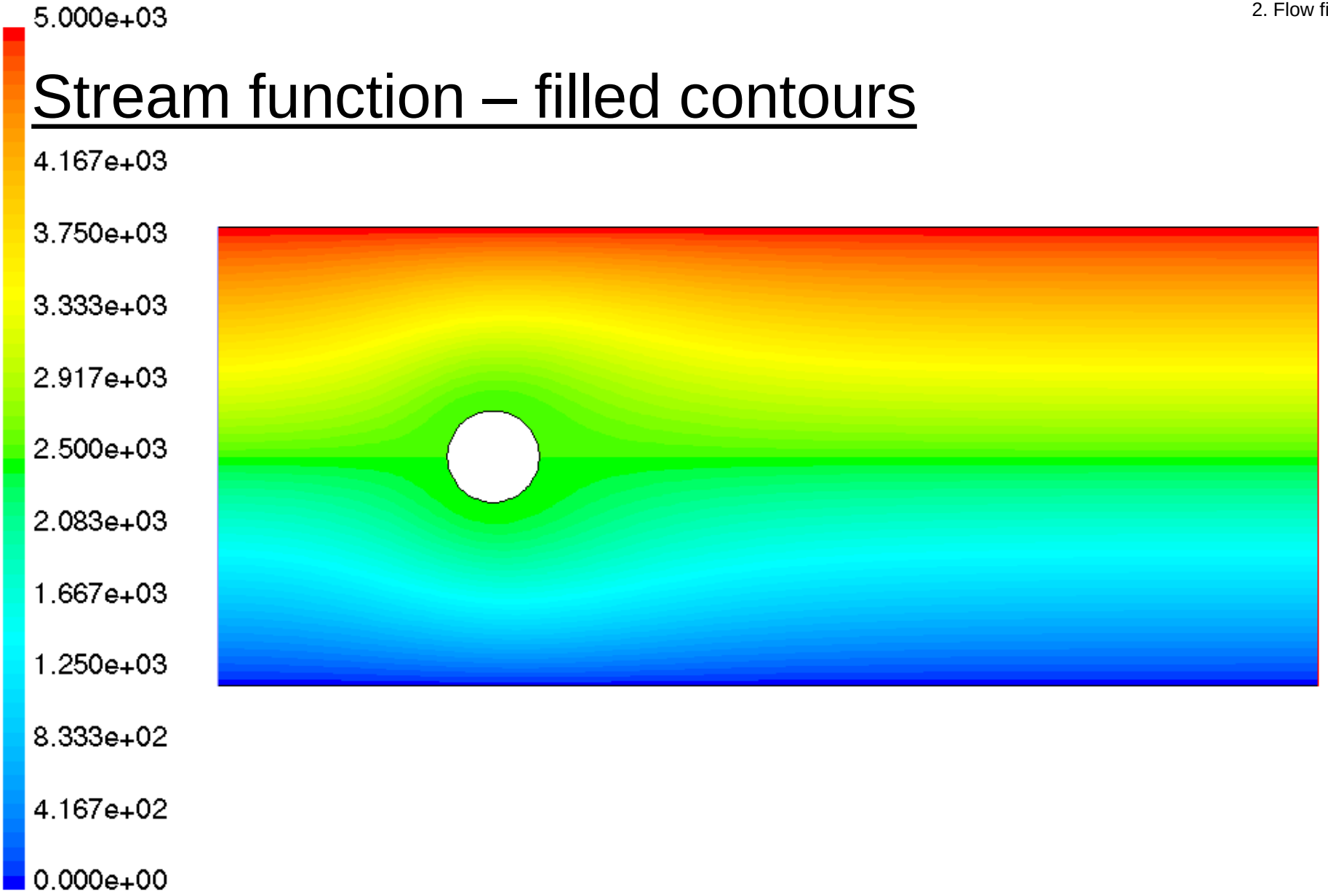


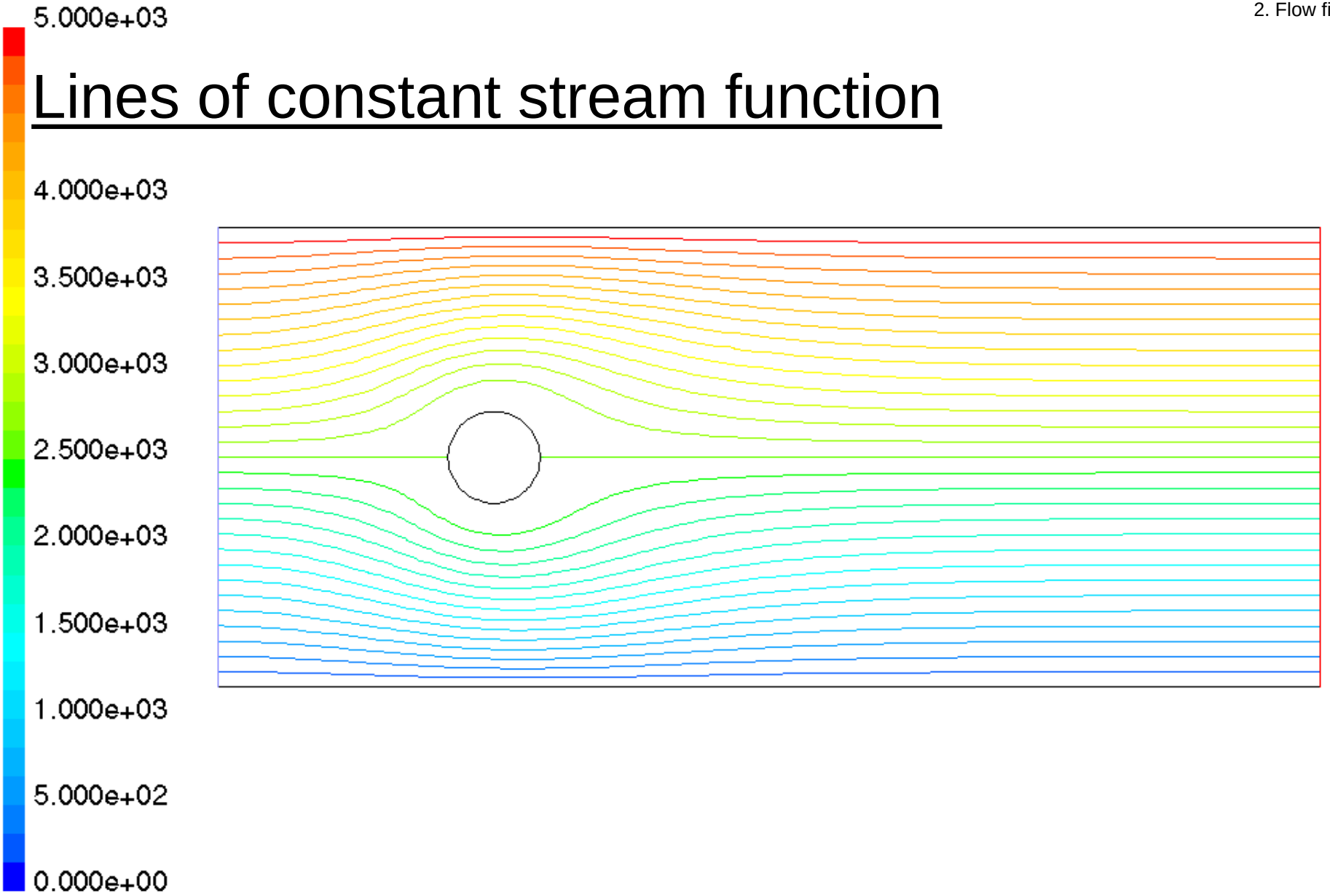
Image: Homsy et al. [2]

Stream function – filled contours



Re = 1
Contours of Stream Function (kg/s)

Lines of constant stream function



Re = 1
Contours of Stream Function (kg/s)

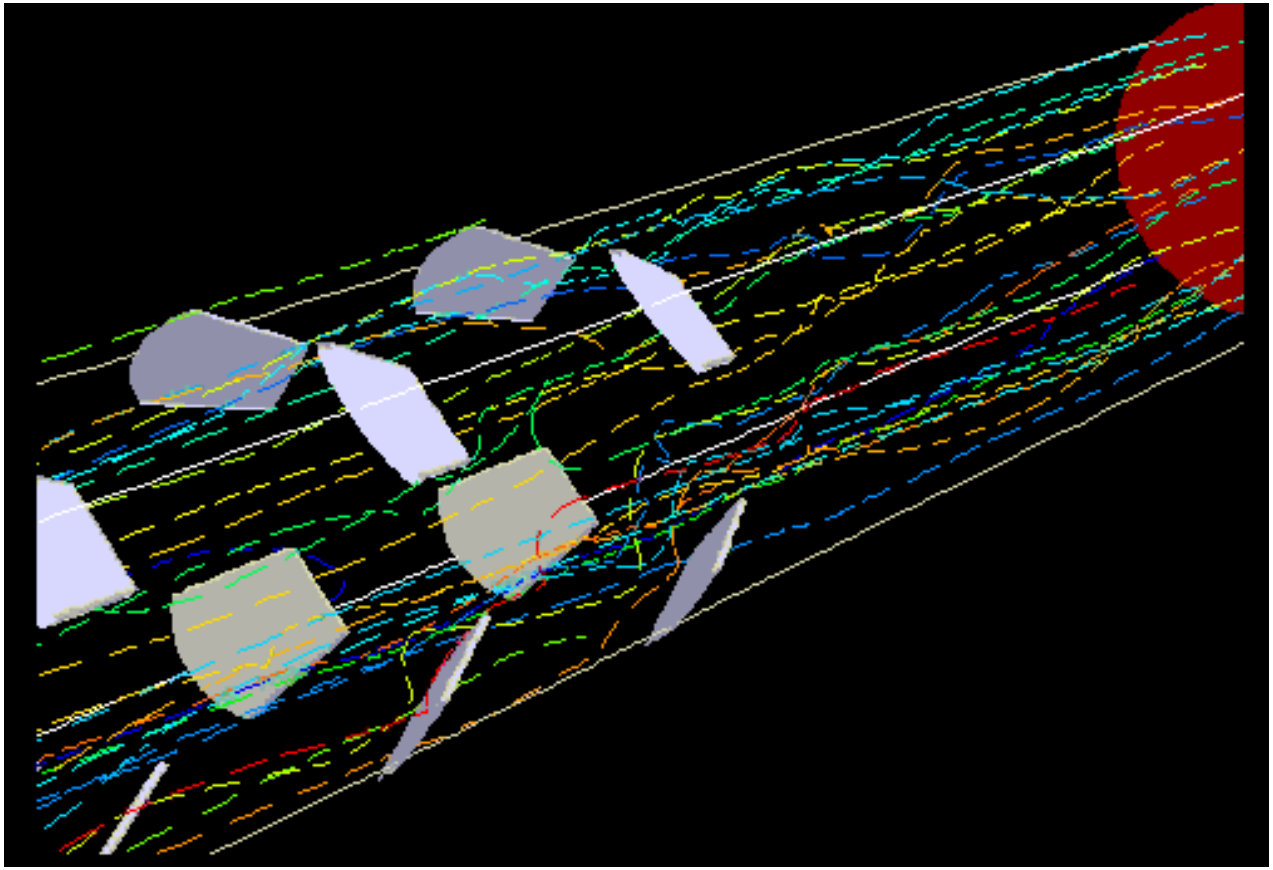
Pathlines

- A pathline is the trajectory followed by an individual particle.
- The pathline depends on the location where the particle was injected in the flow field and, in unsteady flows, also on the time when it was injected.
- In unsteady flows, pathlines may be difficult to follow and not easy to create experimentally.
- For a known flowfield, an initial location of the particle is specified. The trajectory can then be calculated by integrating the advection equation:

$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{U}(\mathbf{X}, t) \qquad \textit{with inital condition } \mathbf{X}(0) = \mathbf{X}_0$$

Pathlines

- Example: pathlines in a static mixer.



Pathlines and streaklines - unsteady flow (1/2)

- The animation shows a simple model of an unsteady flow coming from a smokestack.
- First, there is no wind, and the smoke goes straight up.
- Next there is a strong wind coming from the right.
- The yellow circles show the trajectory of a single particle released at time 0. The pathline is straight up with a sharp angle to left.
- The grayish smoke shows what happens to a continuous stream. First it goes straight up, but then the whole, vertical plume of smoke moves to the left.
- So, although for steady flows. pathlines and streaklines are the same, they are not for unsteady flows.

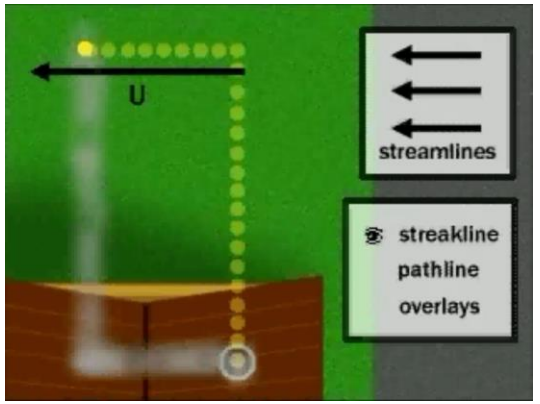
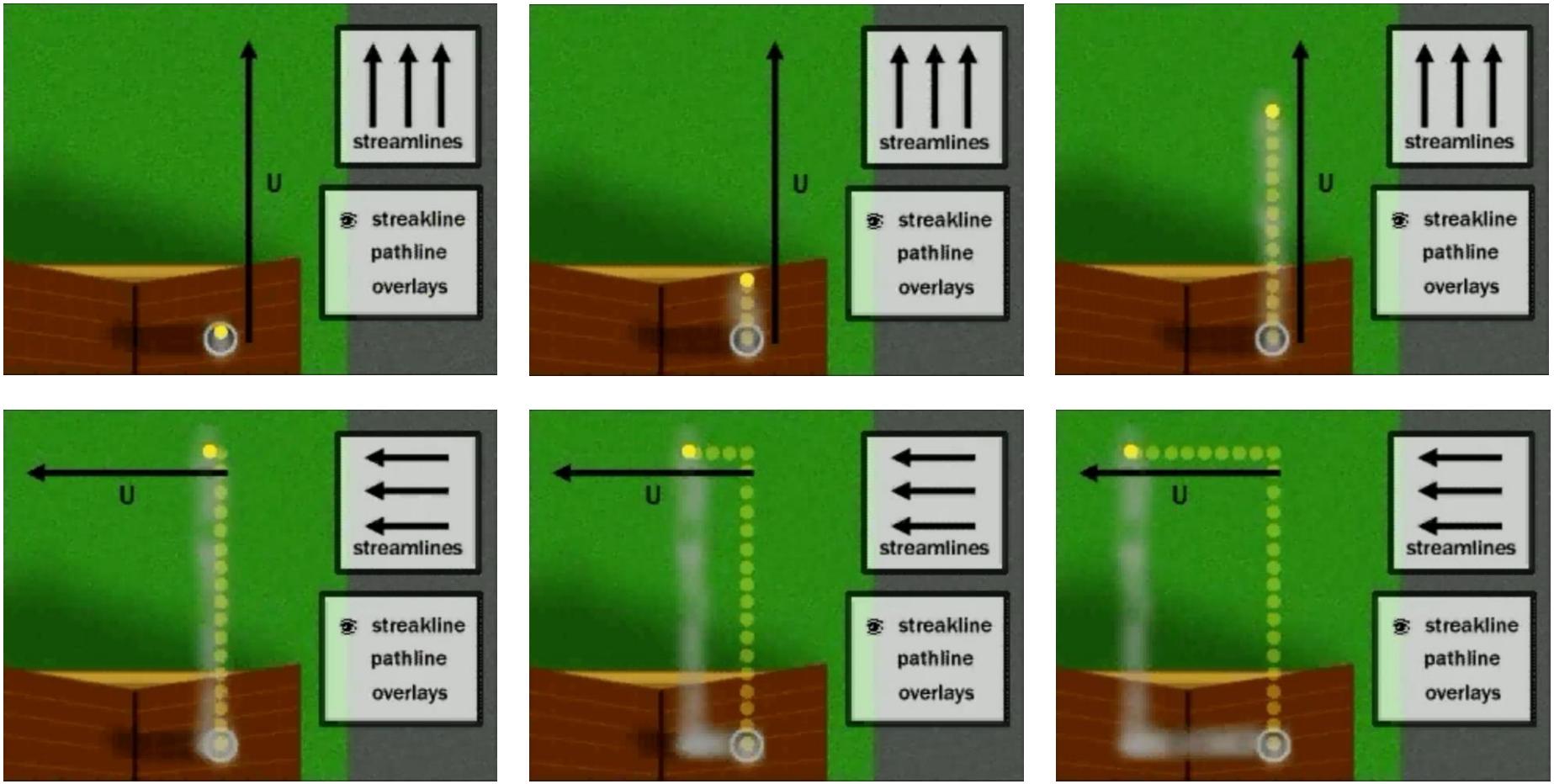


Image: Homsy et al. [2]

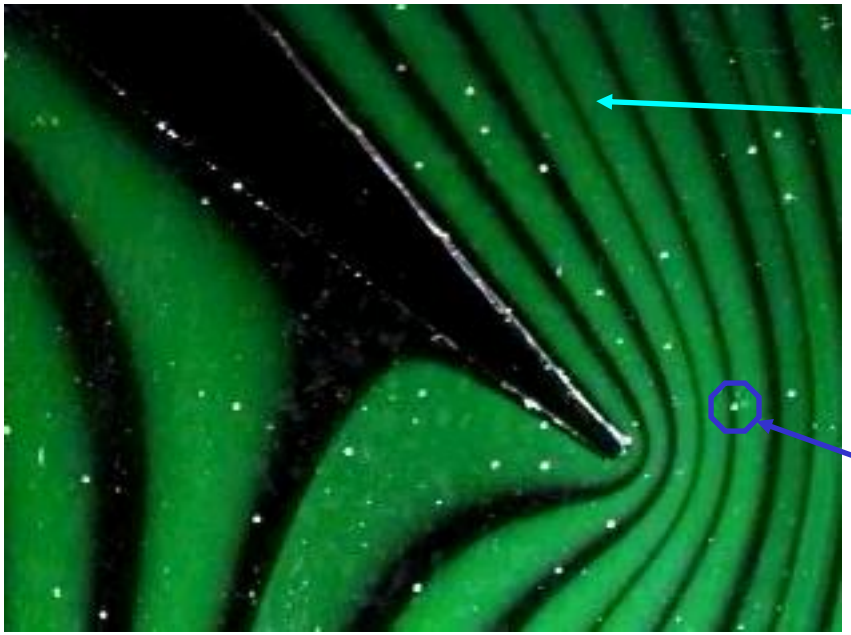
Pathlines and streaklines - unsteady flow (2/2)



Images: Homsy et al. [2]

Streaklines

- This is the flowline formed by a series of particles released continuously in the flow.
- Experimentally, this can also be done by continuous dye injections.
- In steady flows, streaklines and pathlines coincide.
- In unsteady flows, they may be very different.



The lines formed by the continuous injection of the green dye are streaklines.

The trajectories followed by individual particles are pathlines.

Image: Homsy et al. [2]

Timelines

- A timeline is the flow line that arises when we place a marker along a curve at some initial time and inquire into the shape of this curve at a later time.
- They are sometimes called material lines.
- Like streaklines they involve the simultaneous positions of many particles but unlike streaklines the particles of a timeline do not emanate from a single point but are initially distributed along a curve.
- They are relatively easy to produce experimentally, by placing lines of dyes in the flow field at time zero.
- In fluid mixing studies the deformation of material lines is studied in great detail.

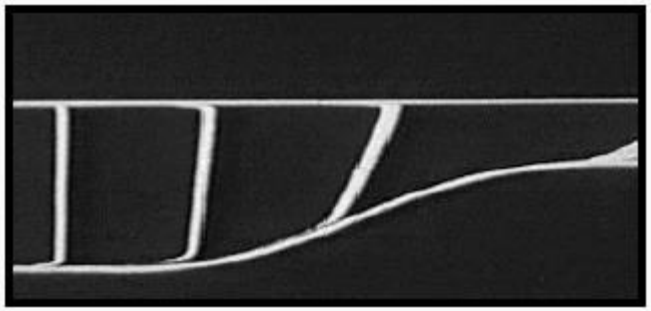
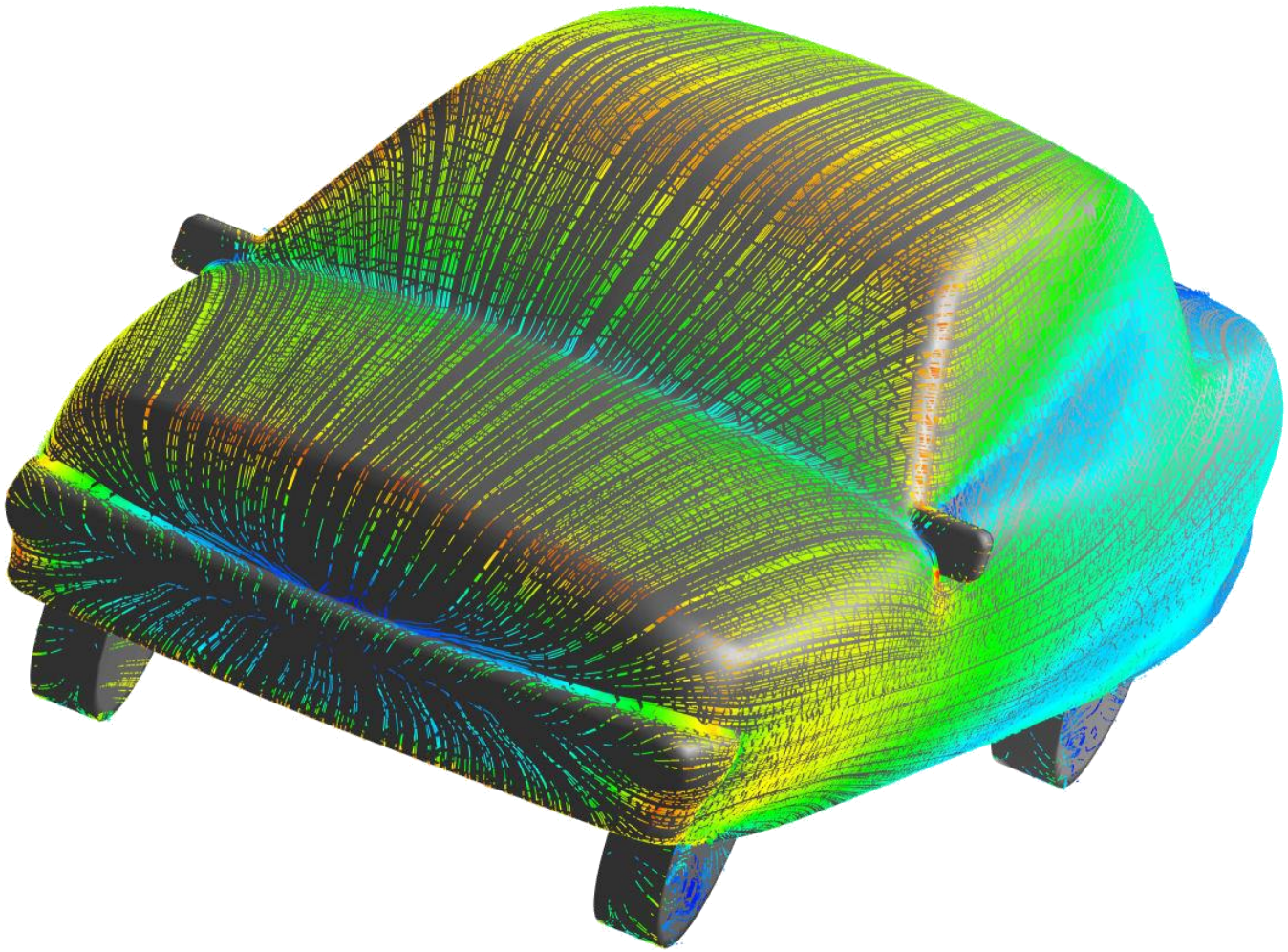


Image: Homsy et al. [2]

Oilflow lines

- Oilflow lines are pathlines that are constrained to a surface, e.g., the lines traced by droplets of water on a car windshield.



Deformation - derivatives

- An instantaneous flow field is defined by velocities u(x,y,z), v(x,y,z), and w(x,y,z).
- The derivatives are du/dx, du/dy, etc.

$$\nabla \mathbf{u} = \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} \partial u/\partial x & \partial u/\partial y & \partial u/\partial z \\ \partial v/\partial x & \partial v/\partial y & \partial v/\partial z \\ \partial w/\partial x & \partial w/\partial y & \partial w/\partial z \end{pmatrix}$$

- The tensor $\nabla \mathbf{u}$ is the gradient of the velocity vector.
- Each of the terms by itself is a gradient, e.g., du/dy is the gradient of the u-velocity component in the y-direction. These may also be called shear rates.

Decomposition

- For the analysis of incompressible flows, it is common to decompose the gradient in the velocity vector as follows:

$$\frac{\partial U_i}{\partial x_j} = S_{ij} + \Omega_{ij} \qquad S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \qquad \Omega_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i}\right)$$

- S_{ij} is the symmetric rate-of-strain (deformation) tensor.
- Ω_{lj} is the antisymmetric rate-of-rotation tensor.
- The vorticity and the rate of rotation are related by:

$$\omega_i = -\varepsilon_{ijk}\Omega_{jk} \qquad \Omega_{ij} = -\tfrac{1}{2}\varepsilon_{ijk}\omega_k \qquad \varepsilon_{ijk} \text{ is the alternating symbol}$$

Deformation tensor

- The velocity gradients can be used to construct the deformation rate tensor **S**:

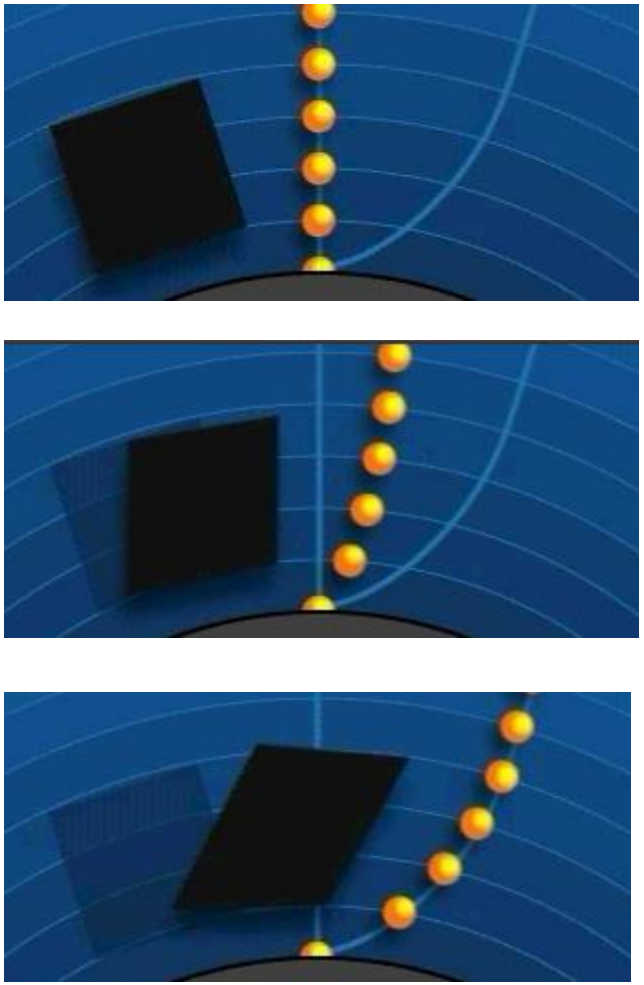
$$\mathbf{S} = \tfrac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right) \qquad S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\mathbf{S} = \begin{pmatrix} \dfrac{\partial u}{\partial x} & \dfrac{1}{2}\left(\dfrac{\partial u}{\partial y} + \dfrac{\partial v}{\partial x}\right) & \dfrac{1}{2}\left(\dfrac{\partial u}{\partial z} + \dfrac{\partial w}{\partial x}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial u}{\partial y} + \dfrac{\partial v}{\partial x}\right) & \dfrac{\partial v}{\partial y} & \dfrac{1}{2}\left(\dfrac{\partial v}{\partial z} + \dfrac{\partial w}{\partial y}\right) \\ \dfrac{1}{2}\left(\dfrac{\partial u}{\partial z} + \dfrac{\partial w}{\partial x}\right) & \dfrac{1}{2}\left(\dfrac{\partial v}{\partial z} + \dfrac{\partial w}{\partial y}\right) & \dfrac{\partial w}{\partial z} \end{pmatrix}$$

- This symmetric tensor is also called the rate of strain tensor.
- Instead of the symbol **S**, the symbols **D** and **E** are sometimes used.

Deformation illustration

- In an incompressible flow field, a fluid parcel may become distorted, but it retains its original volume.
- The divergence of the velocity field is zero: div u = 0. This is the continuity equation.
- De deformation is governed by the rate of strain tensor.



Images: Homsy et al. [2]

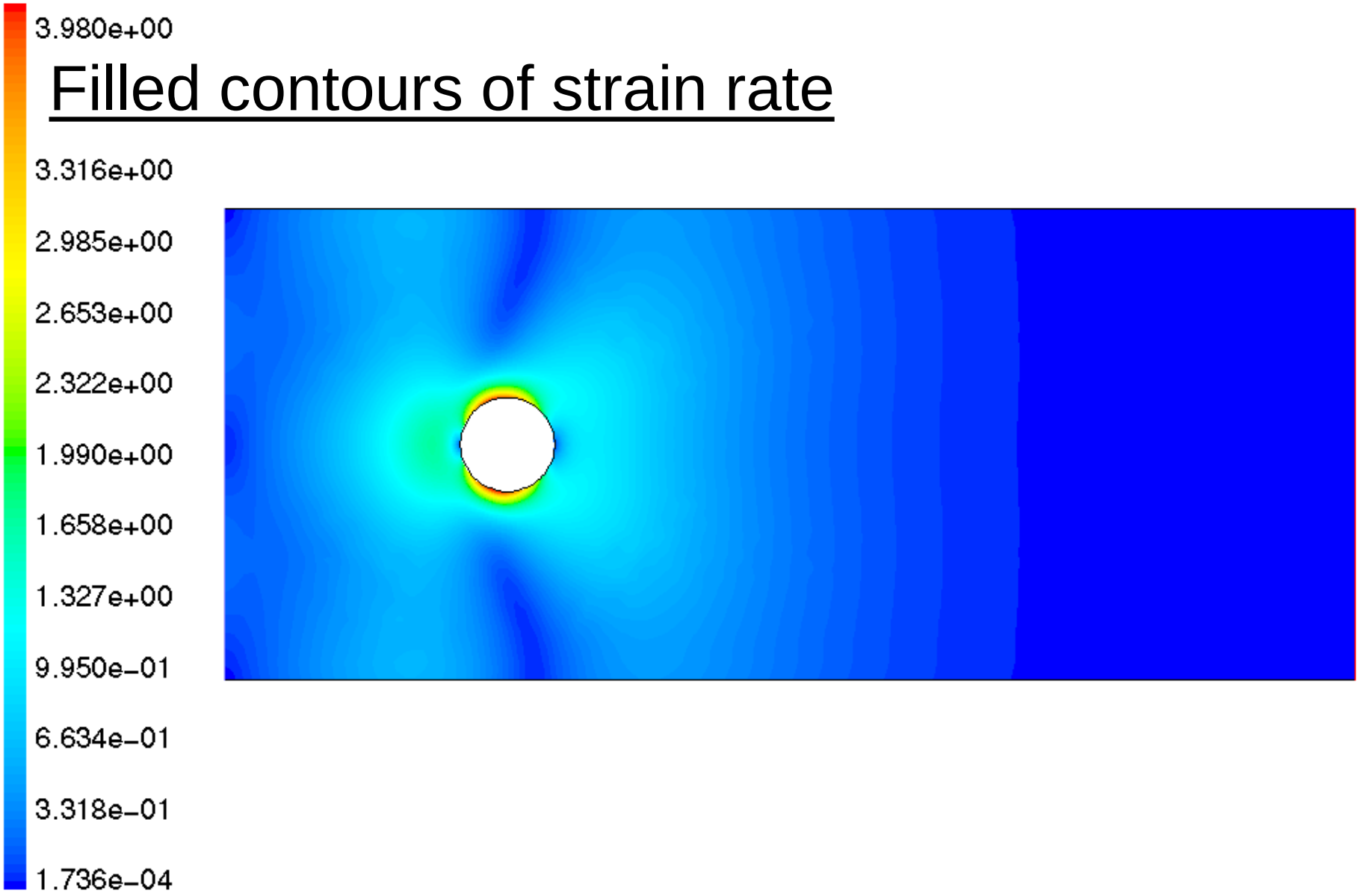
Strain rate

- The deformation rate tensor appears in the momentum conservation equations.
- It is common to report the strain rate S(1/s), which is based on the Euclidian norm of the deformation tensor:

$$S = \sqrt{2 S_{ij} S_{ij}}$$

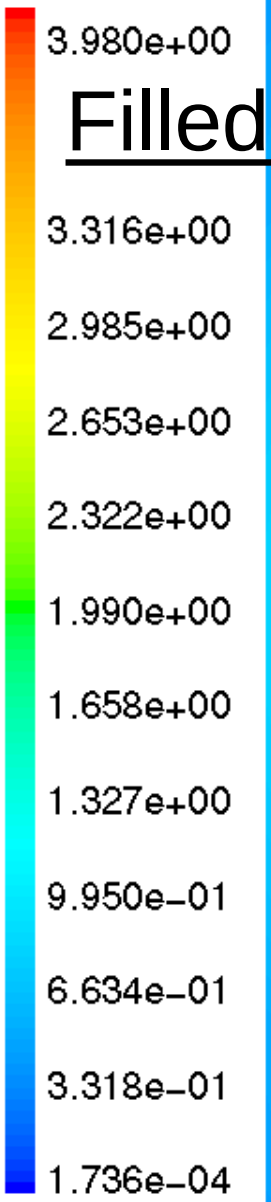
- The strain rate may also be called the shear rate.
- The strain rate may be used for various other calculations:
  - For non-Newtonian fluids, the viscosity depends on the strain rate.
  - In emulsions, droplet size may depend on the strain rate.
  - The strain rate may affect particle formation and agglomeration in pharmaceutical applications.

Filled contours of strain rate



Re = 1
Contours of Strain Rate (1/s)

Filled contours of strain rate – zoomed in



Re = 1
Contours of Strain Rate (1/s)

Rotation: vorticity

- As discussed, the motion of each fluid element can be described as the sum of a translation, rotation, and deformation.
- The animation shows a translation and a rotation.
- Vorticity is a measure of the degree of local rotation in the fluid. This is a vector. Unit is 1/s.
- For a 2-D flow this vector is always normal to the flow field plane.
- For 2-D flows, vorticity is then usually reported as the scalar:

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$$

- For 2-D flows, a positive vorticity indicates a counterclockwise rotation and a negative vorticity a clockwise rotation.

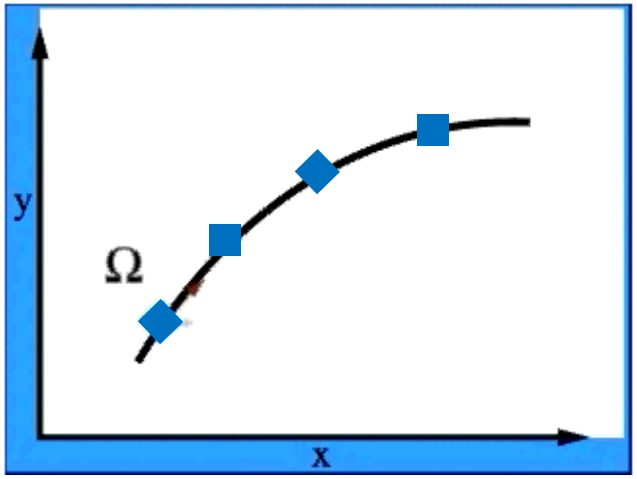


Image: Homsy et al. [2]

Vorticity - 3-D

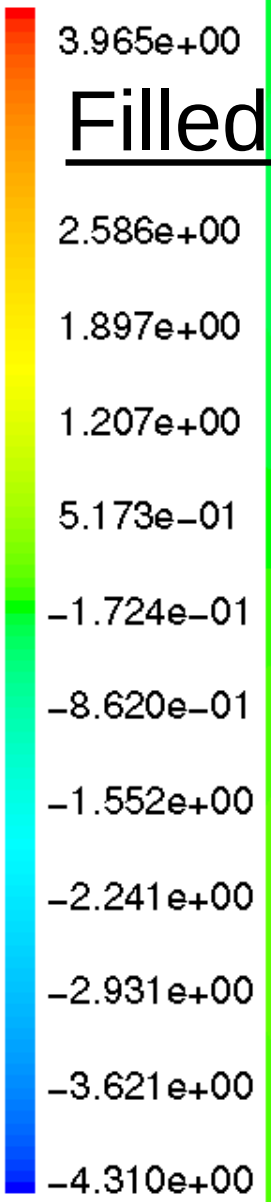
Three – dimensional velocity vector : $\mathbf{u} = (u, v, w)$

Definition of vorticity: $\boldsymbol{\omega} = \nabla \times \mathbf{u} = \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \ \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \ \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)$

Relationship between vorticity and angular velocity of a fluid element : $\boldsymbol{\omega} = \nabla \times \mathbf{u} = 2\boldsymbol{\Omega}$

Vorticity magnitude is calculated using the norm : $\omega(1/s) = |\boldsymbol{\omega}| = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$

Filled contours of vorticity



Re = 1
Contours of Vorticity

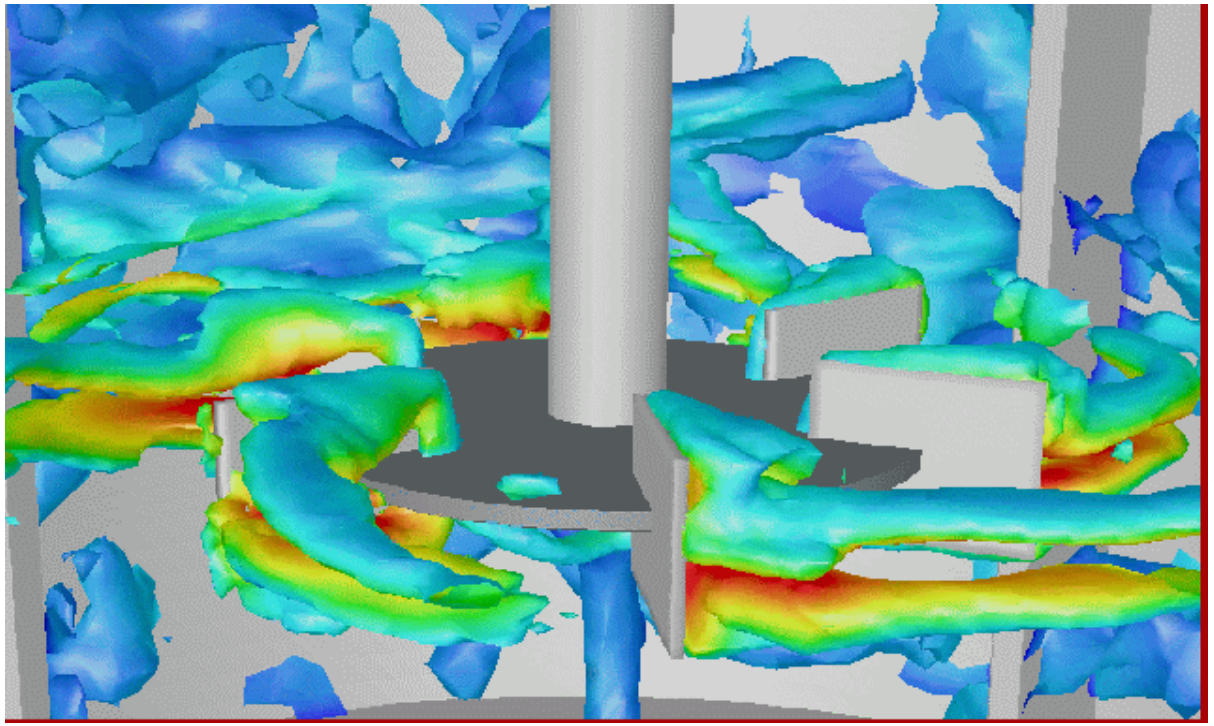
Vortexlines and helicity

- Iso-surfaces of vorticity can be used to show vortices in the flow field.
- Vortex lines are lines that are everywhere parallel to the vorticity vector.
- Vortex cores are lines that are both streamlines and vortexlines.
- The helicity H is the dot product of the vorticity and velocity vectors: $H = \boldsymbol{\omega} \cdot \mathbf{U}$
- It provides insight into how the vorticity vector and the velocity vector are aligned. The angle between the vorticity vector and the velocity vector (which is 0º or 180º in a vortex core) is given by:

$$\alpha = \cos^{-1}(H / (|\boldsymbol{\omega}| \, |\mathbf{U}|))$$

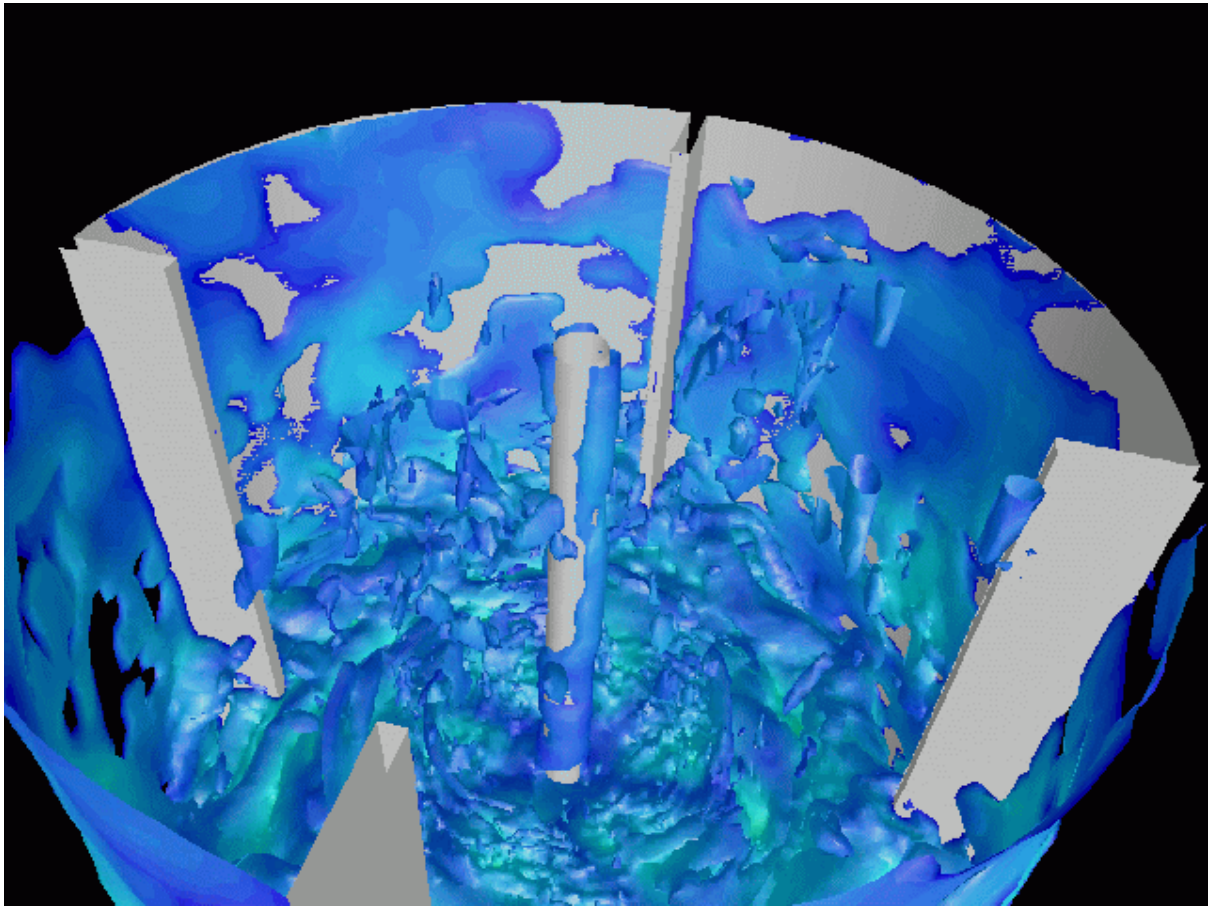
- Algorithms exist that use helicity to automatically find vortex cores. In practice this only works on very fine grids with deeply converged solutions.

Isosurfaces of vorticity magnitude



Iso-surface of vorticity magnitude colored by velocity magnitude.

Isosurfaces of vorticity magnitude

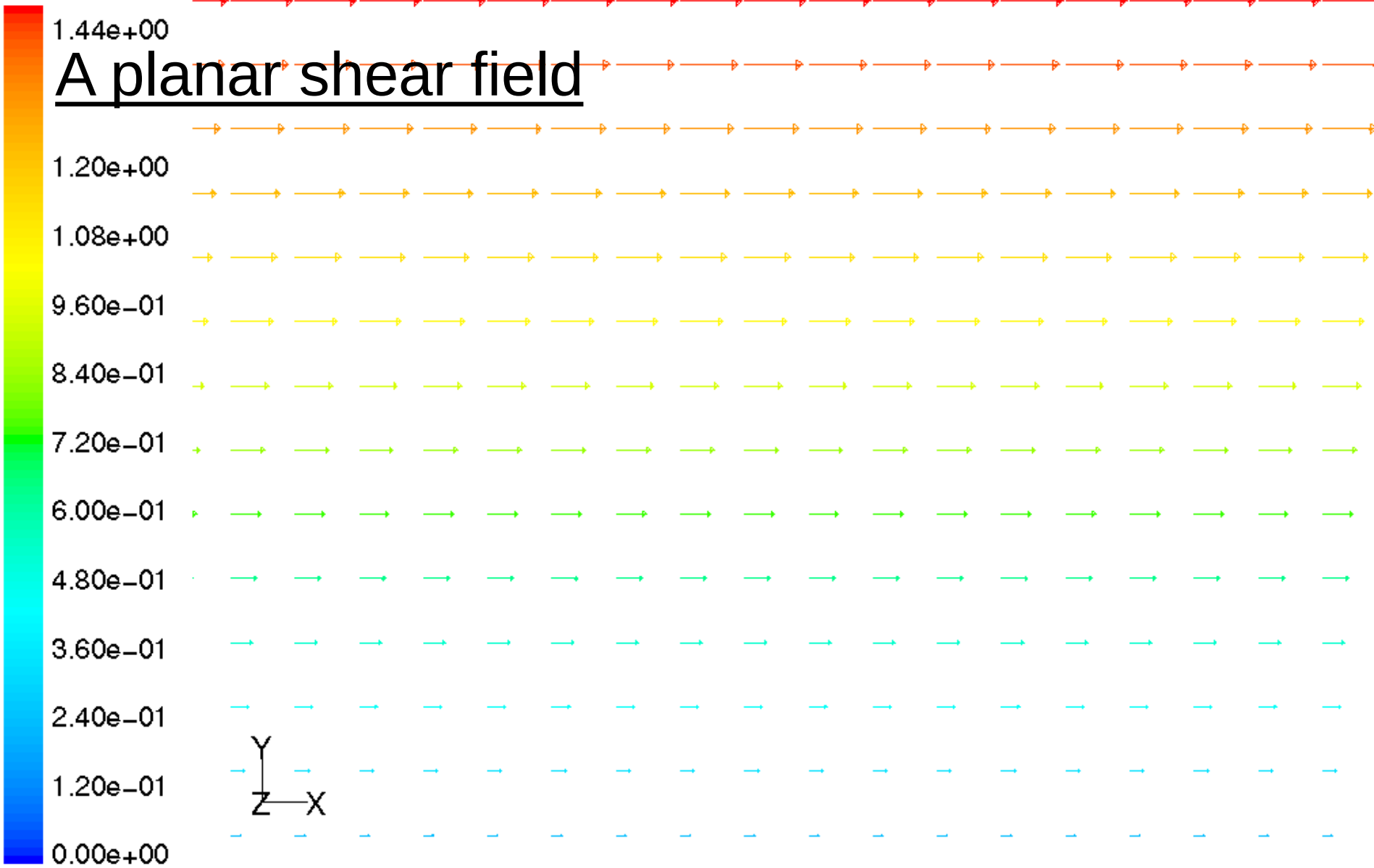


Iso-surface of vorticity magnitude colored by velocity magnitude.

Comparison between strain and vorticity

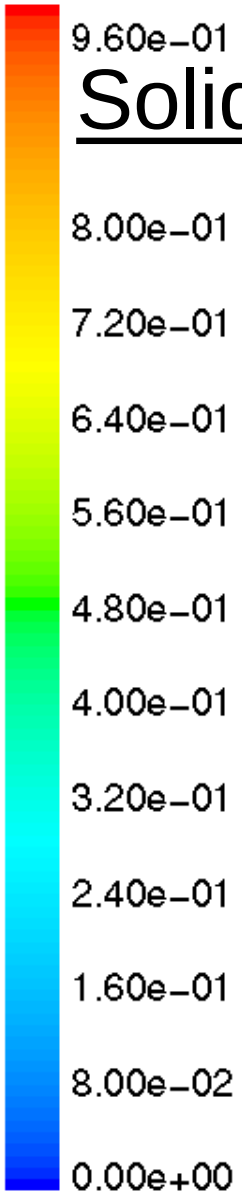
- Both strain and vorticity contain velocity gradients.
- The difference between the two will be shown based on three different flow fields:
  - A planar shear field: both the strain rate and the vorticity magnitude are non-zero.
  - A solid body rotation: the strain rate is 0(!) and the vorticity reflects the rotation speed.
  - Shear field and solid body rotation combined.

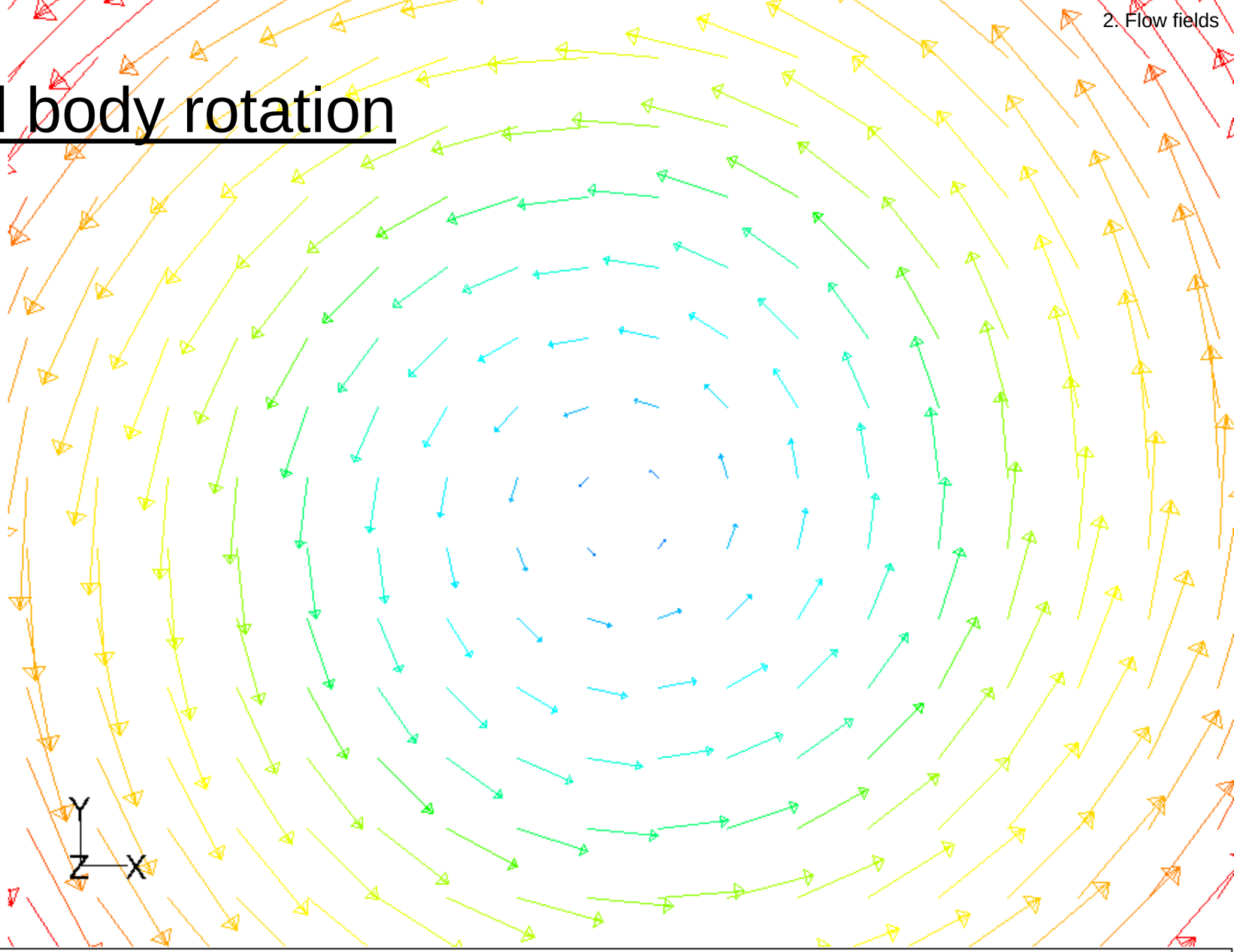
A planar shear field



u−velocity = y
Velocity Vectors Colored By Velocity Magnitude (m/s)
vorticity−magnitude=1 1/s; strain−rate=1 1/s; du/dy=1; other derivatives are 0

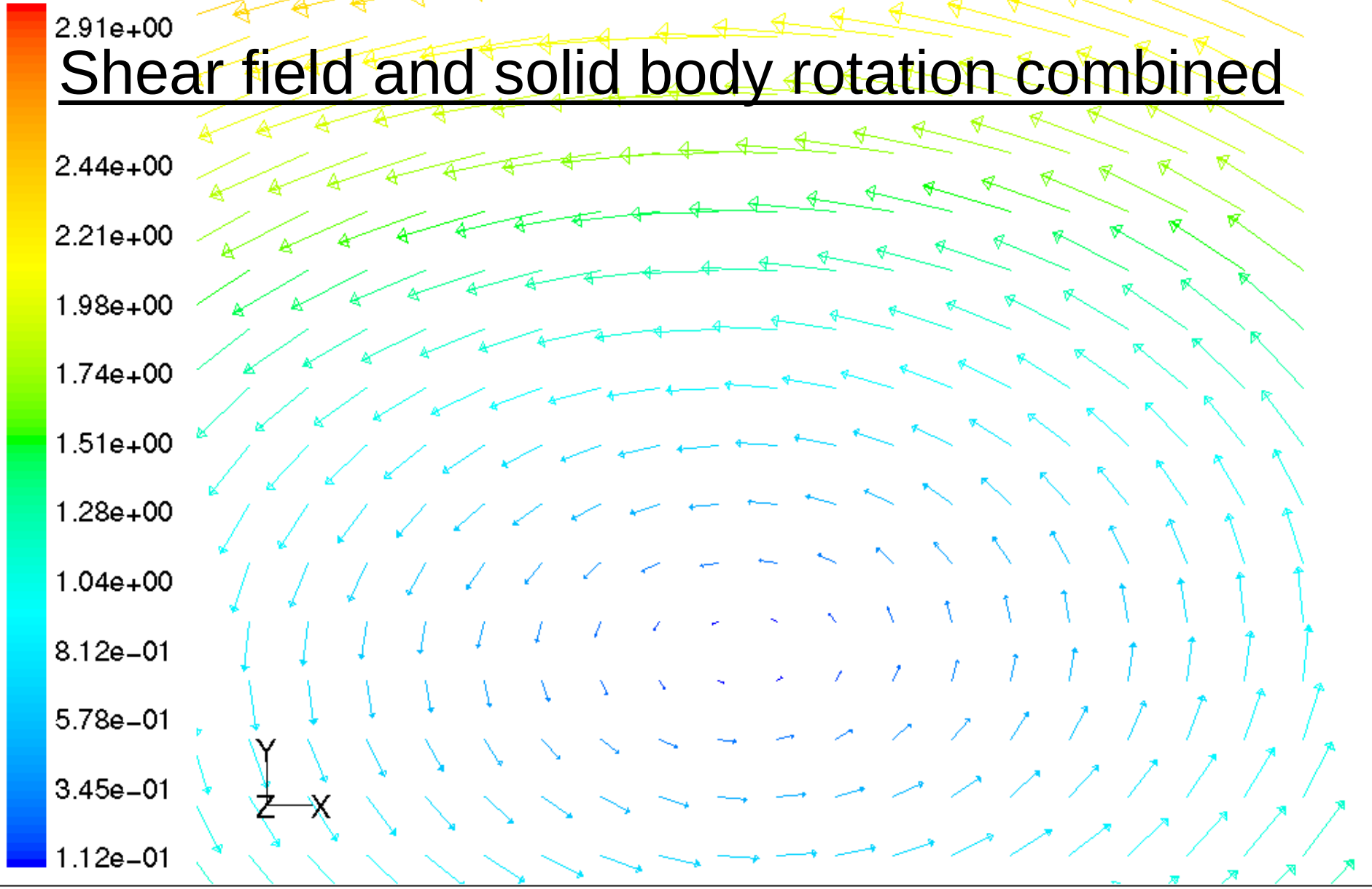
Solid body rotation





angular velocity is 1 rad/s
Velocity Vectors Colored By Velocity Magnitude (m/s)
vorticity-magnitude=2 1/s; strain-rate=0 1/s; dv/dx=1; du/dy=-1; other derivatives are 0

Shear field and solid body rotation combined



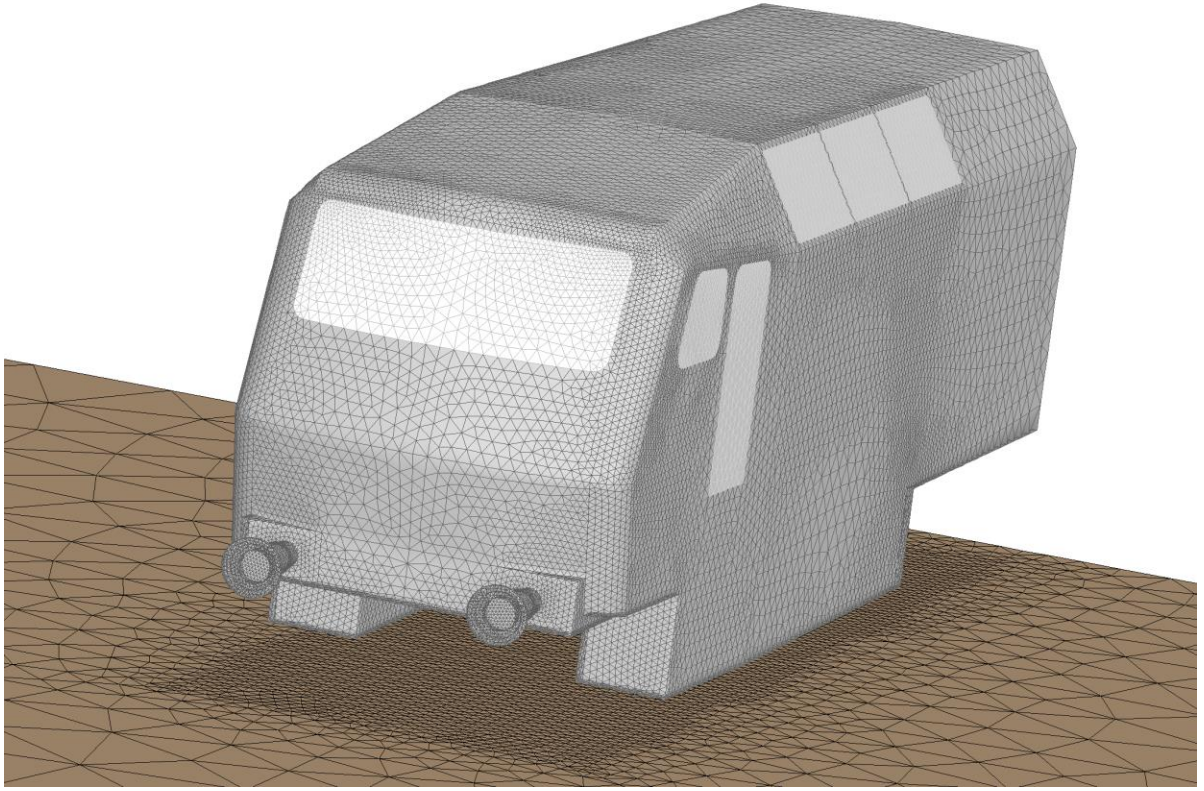
angular velocity is 1 rad/s + translational velocity u=−y
Velocity Vectors Colored By Velocity Magnitude (m/s)
vorticity−magnitude=3 1/s; strain−rate=1 1/s; dv/dx=1; du/dy=−2; other derivatives are 0

Flux reports and surface integrals

- Integral value: $\int \phi \, dA = \sum_{i=1}^{n} \phi_i \, | A_i |$
- Area weighted average: $\frac{1}{A} \int \phi \, dA = \frac{1}{A} \sum_{i=1}^{n} \phi_i \, | A_i |$
- Mass flow rate: $\int \phi \, \rho (\vec{V} . \vec{n}) \, dA = \sum_{i=1}^{n} \phi_i \, \rho_i \, (\vec{V}_i . \vec{n}) \, A_i$

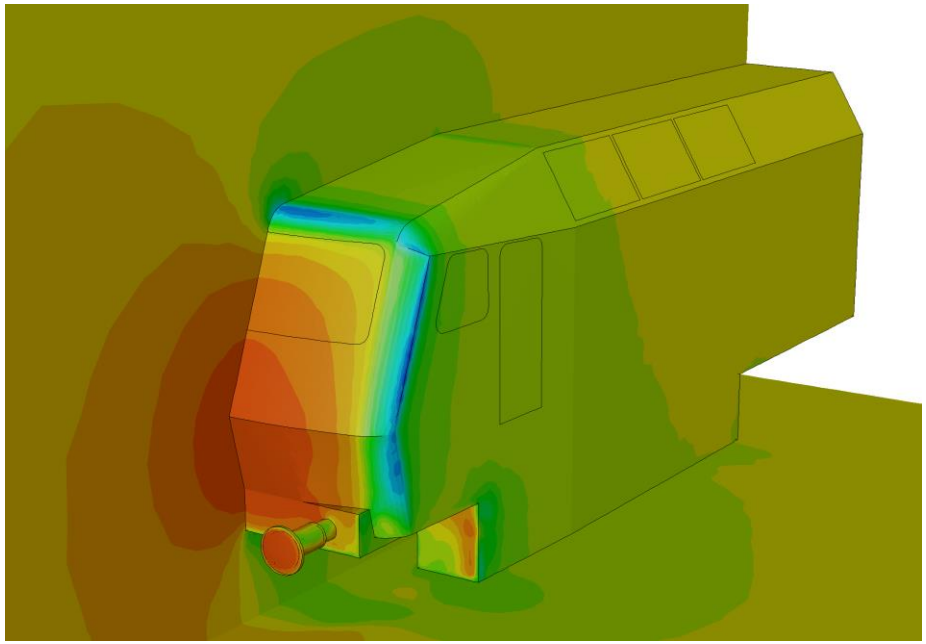
Quantitative validation - moving locomotive

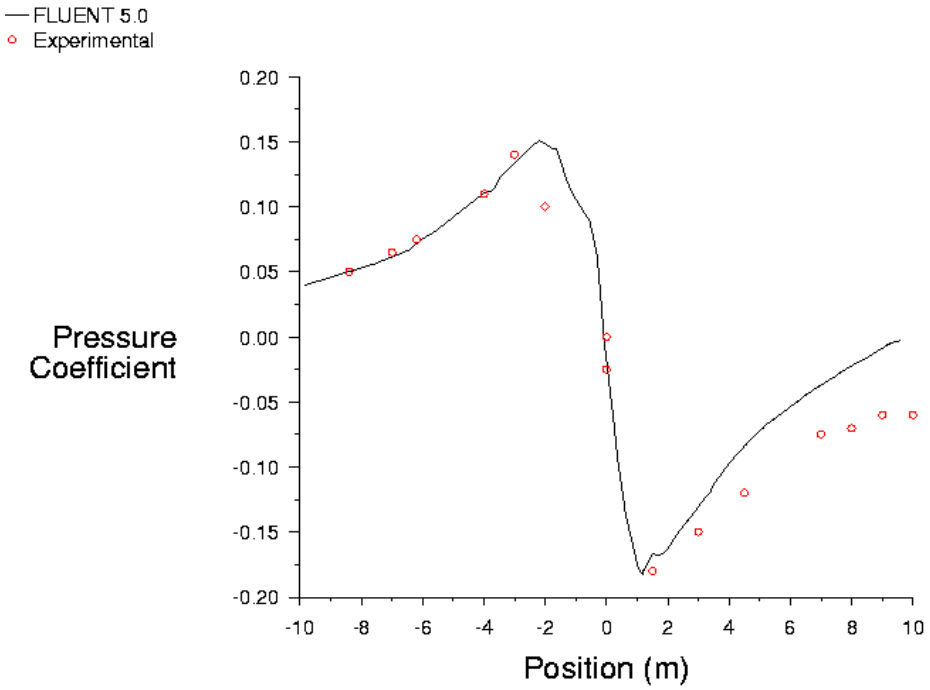
- Turbulent simulation (using k-ε RNG and 170,000 tetrahedral cells) is used to predict the near-body pressure field.



Flow over a moving locomotive

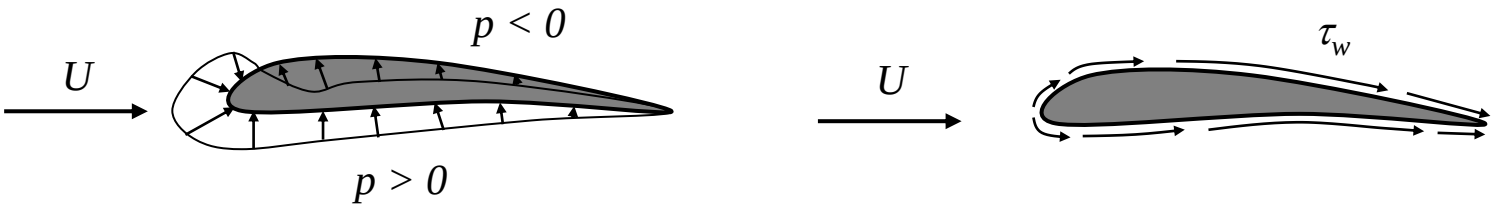
- Pressure contours show the disturbance of the passing train in the near field region.
- The figure on the left shows the pressure field over the locomotive.
- Predictions of pressure coefficient alongside the train agree reasonably well with experimental data.





Quantitative validation - NACA airfoil

- The surrounding fluid exerts pressure forces and viscous forces on the airfoil:



- The components of the resultant force acting on the object immersed in the fluid are the drag force and the lift force. The drag force D acts in the direction of the motion of the fluid relative to the object. The lift force L acts normal to the flow direction.

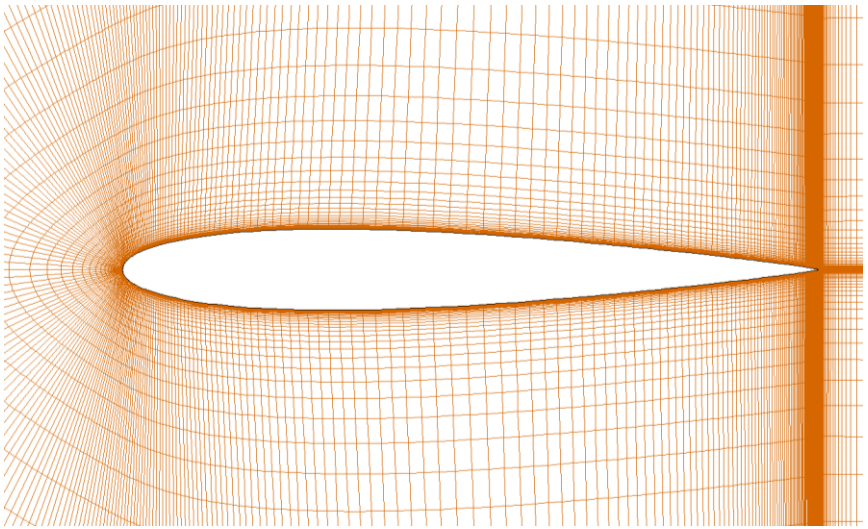
$$L = C_L . A . \frac{1}{2} \rho U^2 \qquad D = C_D . A . \frac{1}{2} \rho U^2$$

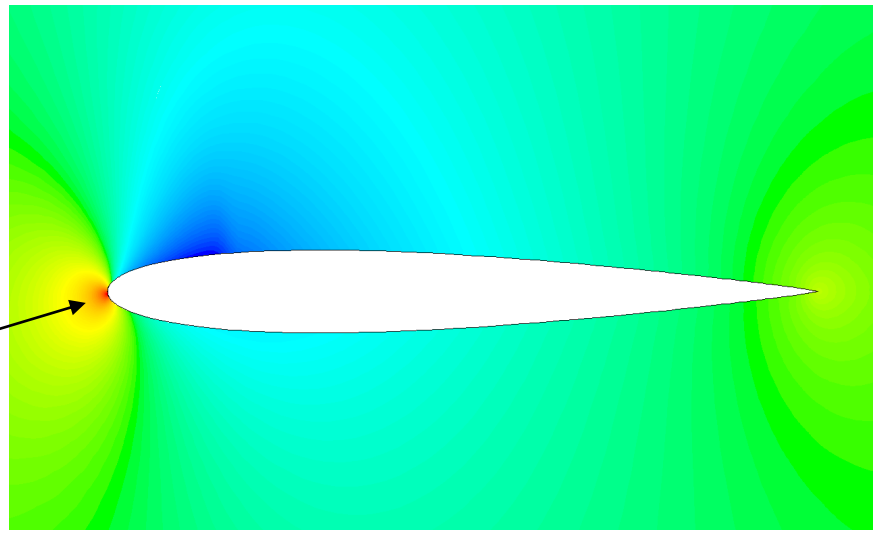
Lift *Drag*

- Lift and drag are obtained by integrating the pressure field and viscous forces over the surface of the airfoil.

Quantitative validation - NACA airfoil

- Transonic, compressible flow over the NACA 0012 airfoil is modeled using FLUENT.
  - Free stream Mach number = 0.7.
  - 1.49^{o} angle of attack.
- The realizable k-ε turbulence model with 2-layer zonal model for near-wall treatment is used.
- Pressure contours.



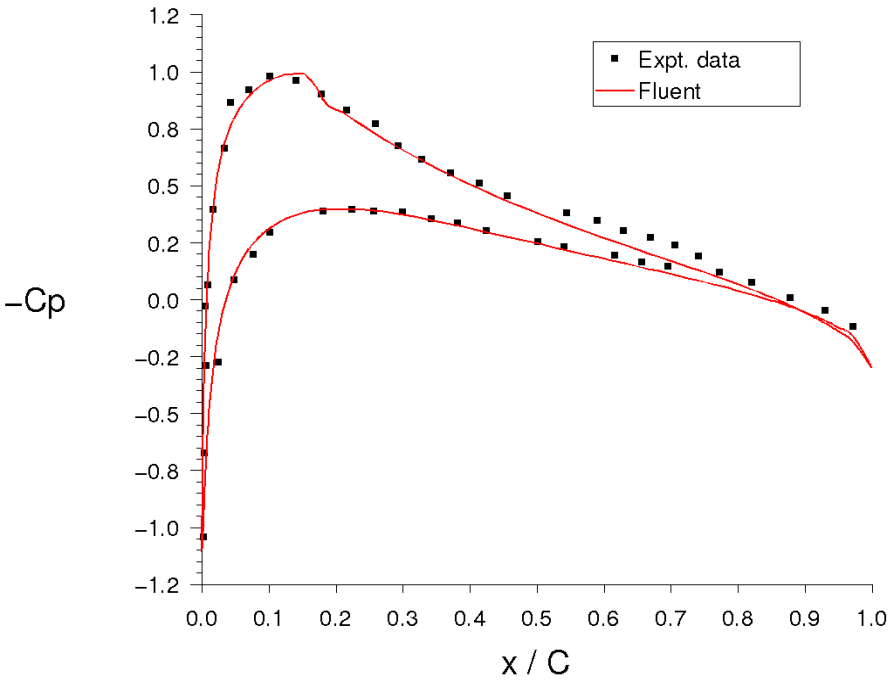


Transonic flow over NACA airfoil

- The pressure coefficient is calculated as follows:

$$c_p = \frac{p - p_0}{\frac{1}{2}\rho v_0^2}$$

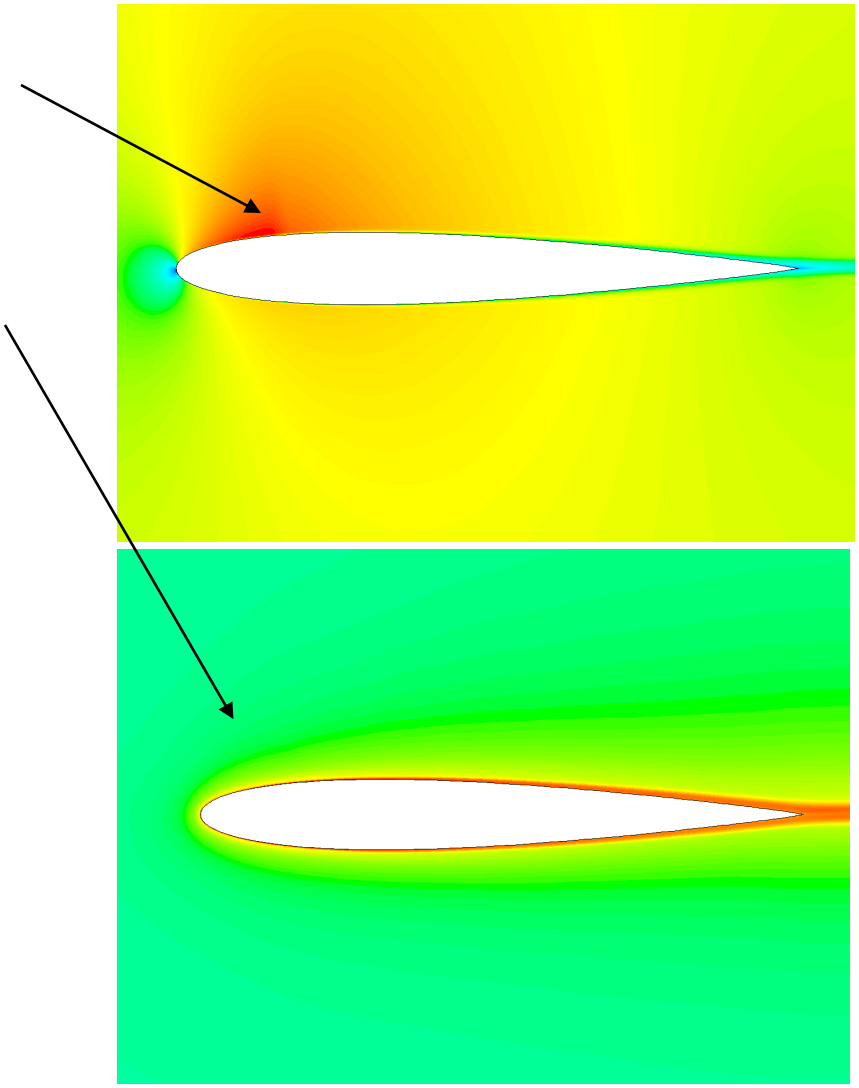
- Here p_0 is the far-field pressure and v_0 the free stream velocity.
- Pressure coefficient for upper (top) and lower airfoil surfaces shows very good agreement with data.
- Drag coefficient:
  - FLUENT: 0.0084
  - Coakley*: 0.0079



Thomas J. Coakley, "Numerical simulation of viscous transonic airfoil flows", AIAA-87-0416, 1987.

Transonic flow over NACA airfoil

- Mach number contours exhibit transonic flow, with maximum (red) of 1.08.
- Turbulence kinetic energy contours show generation primarily in boundary layer.
- Overall CFD can be very useful in validating lift and drag for airfoils.



Summary

- CFD simulations result in data that describes a flow field.
- Proper analysis and interpretation of this flow field data is required in order to be able to solve the original engineering problem.
- The amount of data generated by a CFD simulation can be enormous. Analysis and interpretation are not trivial tasks and the time it takes to do this properly is often underestimated.

Lecture 3 - Conservation Equations

Applied Computational Fluid Dynamics

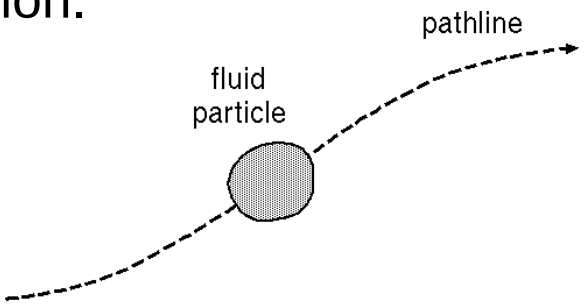
André Bakker

Governing equations

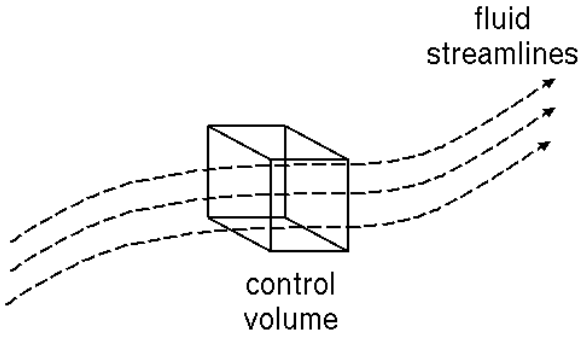
- This lecture largely follows Versteeg and Malalasekera [10].
- The governing equations include the following conservation laws of physics:
  - Conservation of mass.
  - Newton's second law: the change of momentum equals the sum of forces on a fluid particle.
  - First law of thermodynamics (conservation of energy): rate of change of energy equals the sum of rate of heat addition to and work done on fluid particle.
- The fluid is treated as a continuum. For length scales of, say, 1μm and larger, the molecular structure and motions may be ignored.
  - We treat all properties as averages over a suitably large number of molecules.
  - A small element of fluid, a fluid particle or fluid point, is the smallest element of fluid whose macroscopic properties are not influenced by individual molecules.

Lagrangian vs. Eulerian description

A fluid flow field can be thought of as being comprised of a large number of finite sized fluid particles which have mass, momentum, internal energy, and other properties. Mathematical laws can then be written for each fluid particle. This is the Lagrangian description of fluid motion.



Another view of fluid motion is the Eulerian description. In the Eulerian description of fluid motion, we consider how flow properties change at a fluid element that is fixed in space and time (x,y,z,t), rather than following individual fluid particles.

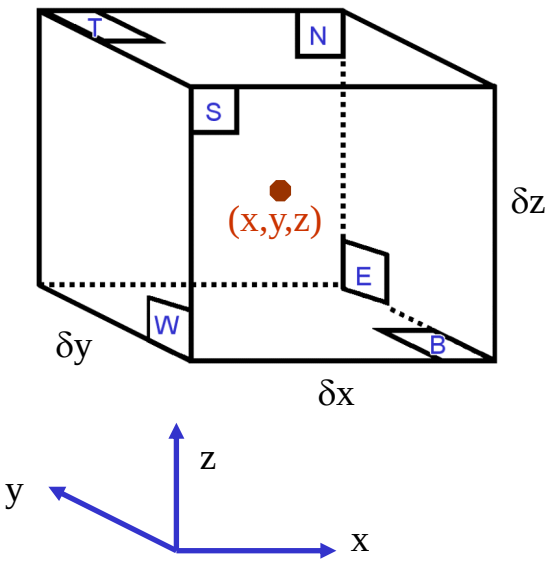


Governing equations can be derived using each method and converted to the other form.

Fluid element and properties

- The behavior of the fluid is described in terms of macroscopic properties:
  - Velocity **u.**
  - Pressure p.
  - Density ρ.
  - Temperature T.
  - Energy E.
- Typically ignore (x,y,z,t) in the notation.
- Properties are averages of a sufficiently large number of molecules.
- A fluid element can be thought of as the smallest volume for which the continuum assumption is valid.

Fluid element for conservation laws



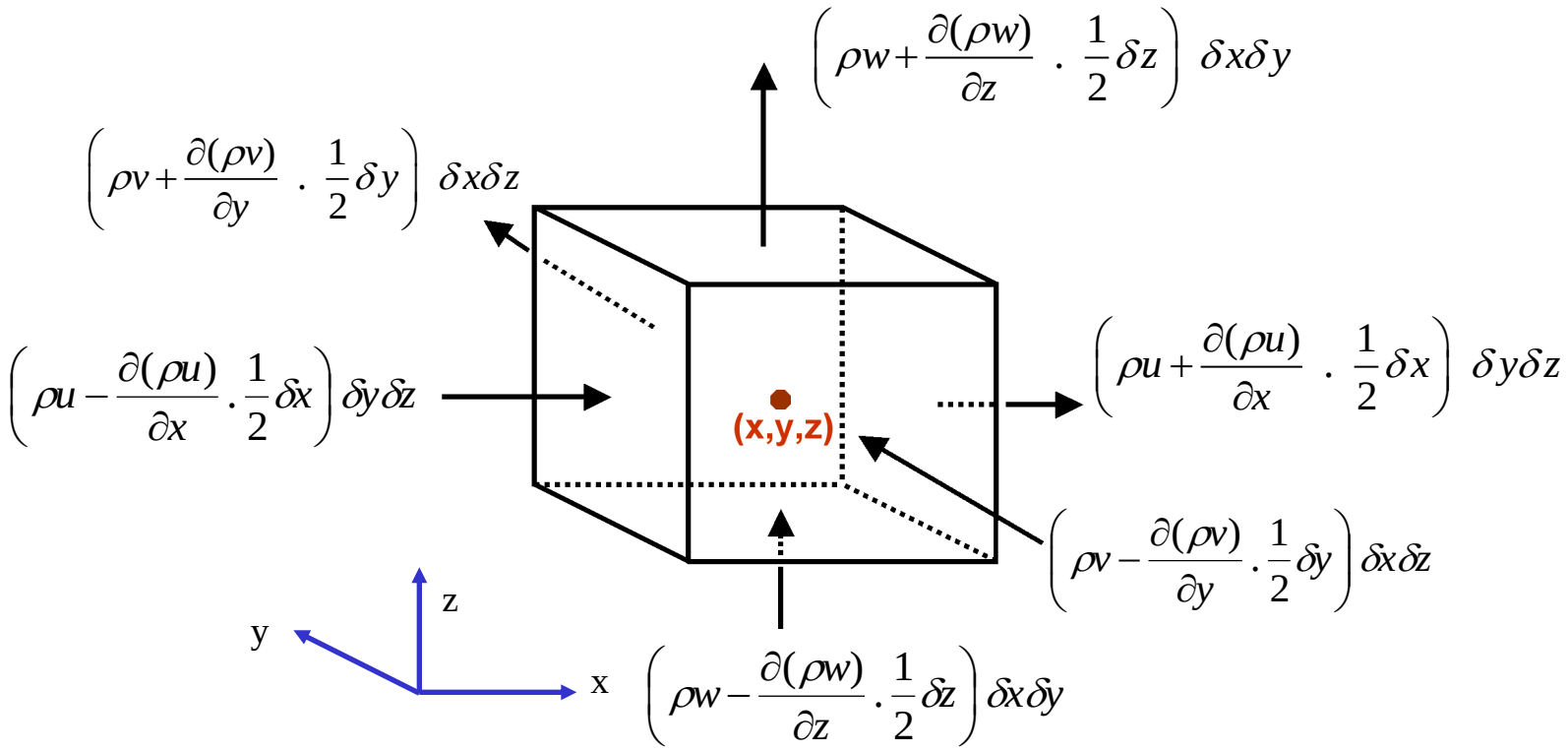
Faces are labeled North, East, West, South, Top and Bottom

Properties at faces are expressed as first two terms of a Taylor series expansion,

e.g. for p: $p_W = p - \frac{\partial p}{\partial x}\frac{1}{2}\delta x$ and $p_E = p + \frac{\partial p}{\partial x}\frac{1}{2}\delta x$

Mass balance

- Rate of increase of mass in fluid element equals the net rate of flow of mass into element.
- Rate of increase is: $\frac{\partial}{\partial t}(\rho \delta x \delta y \delta z) = \frac{\partial \rho}{\partial t} \delta x \delta y \delta z$
- The inflows (positive) and outflows (negative) are shown here:



Continuity equation

- Summing all terms in the previous slide and dividing by the volume $\delta x \delta y \delta z$ results in:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} + \frac{\partial (\rho w)}{\partial z} = 0$$

- In vector notation:

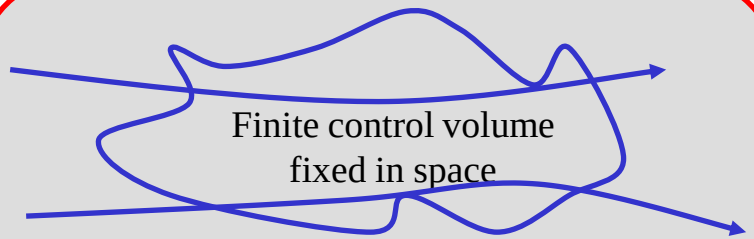
$$\frac{\partial \rho}{\partial t} + div\,(\rho\,\mathbf{u}) = 0$$

Change in density

Net flow of mass across boundaries
Convective term

- For incompressible fluids $\partial \rho / \partial t = 0$, and the equation becomes: $div\ \mathbf{u} = 0$.
- Alternative ways to write this: $\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$ and $\frac{\partial u_i}{\partial x_i} = 0$

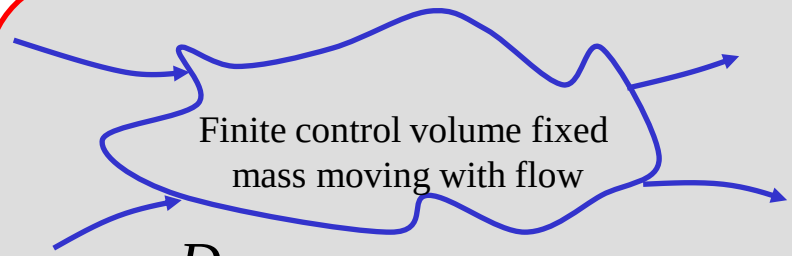
Different forms of the continuity equation



$$\frac{\partial}{\partial t}\iiint_V \rho\, dV + \iint_S \rho\, \mathbf{U}\cdot\mathbf{dS} = 0$$

Integral form

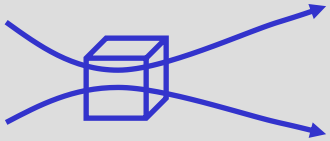
Conservation form



$$\frac{D}{Dt}\iiint_V \rho\, dV = 0$$

Integral form

Non – conservation form

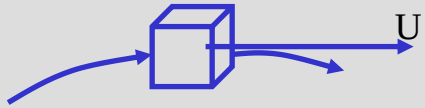


Infinitesimally small
element fixed in space

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{U}) = 0$$

Differential form

Conservation form



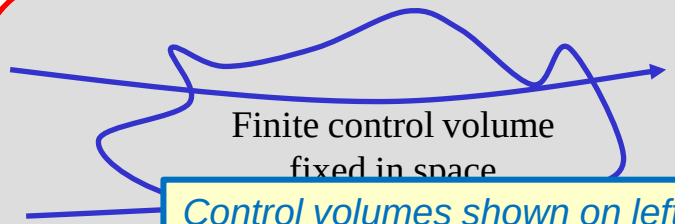
Infinitesimally small fluid element of fixed
mass (“fluid particle”) moving with the flow

$$\frac{D\rho}{Dt} + \rho\nabla\cdot\mathbf{U} = 0$$

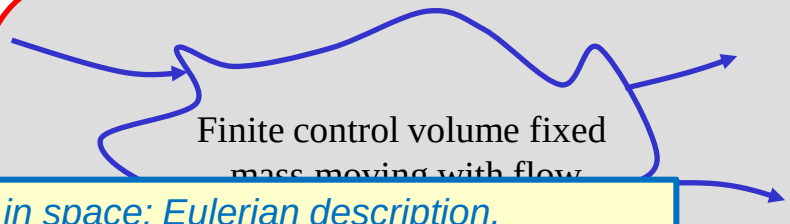
Differential form

Non – conservation form

Different forms of the continuity equation



Finite control volume fixed in space



Finite control volume fixed mass moving with flow

Control volumes shown on left are fixed in space: Eulerian description, also called the conservation form.

Control volumes shown on right move with flow: Lagrangian description, also called the non-conservation form.

Important: in Lagrangian description we look at fluid particles with FIXED MASS, so integral form does not contain a velocity surface integral since there is no net mass flux across the surface. But the volume and average density may still change.

The book also calls the differential – conservation form, the "divergence form".

Infinitesimally small element fixed in space

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

Differential form

Conservation form

Infinitesimally small fluid element of fixed mass ("fluid particle") moving with the flow

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{U} = 0$$

Differential form

Non – conservation form

Rate of change for a fluid particle

- Terminology: fluid element is a volume stationary in space, and a fluid particle is a volume of fluid moving with the flow.
- A moving fluid particle experiences two rates of changes:
  - Change due to changes in the fluid as a function of time.
  - Change due to the fact that it moves to a different location in the fluid with different conditions.
- The sum of these two rates of changes for a property per unit mass ϕ is called the *total* or *substantive* derivative $D\phi/Dt$:

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x}\frac{dx}{dt} + \frac{\partial \phi}{\partial y}\frac{dy}{dt} + \frac{\partial \phi}{\partial z}\frac{dz}{dt}$$

- With $dx/dt=u$, $dy/dt=v$, $dz/dt=w$, this results in:

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + \mathbf{u}.grad\ \phi$$

Rate of change for a stationary fluid element

- In most cases we are interested in the changes of a flow property for a fluid element, or fluid volume, that is stationary in space.
- However, some equations are easier derived for fluid particles. For a moving fluid particle, the total derivative per unit volume of this property ϕ is given by:

(for moving fluid particle) $$\rho \frac{D\phi}{Dt} = \rho \left(\frac{\partial \phi}{\partial t} + \mathbf{u}.grad\ \phi \right)$$ (for given location in space)

- For a fluid element, for an arbitrary conserved property ϕ:

$$\frac{\partial \rho}{\partial t} + div\,(\rho \mathbf{u}) = 0$$

Continuity equation

$$\frac{\partial (\rho\phi)}{\partial t} + div\,(\rho\phi\, \mathbf{u}) = 0$$

Arbitrary property

Fluid particle and fluid element

- We can derive the relationship between the equations for a fluid particle (Lagrangian) and a fluid element (Eulerian) as follows:

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\phi\,\mathbf{u}) = \rho\left[\frac{\partial\phi}{\partial t} + \mathbf{u}.grad\phi\right] + \phi\underbrace{\left[\frac{\partial\rho}{\partial t} + div(\rho\mathbf{u})\right]}_{\text{zero because of continuity}} = \rho\frac{D\phi}{Dt}$$

$$\underbrace{\frac{\partial(\rho\phi)}{\partial t}}_{\text{Rate of increase of } \phi \text{ of fluid element}} + \underbrace{div(\rho\phi\,\mathbf{u})}_{\text{Net rate of flow of } \phi \text{ out of fluid element}} = \underbrace{\rho\frac{D\phi}{Dt}}_{\text{Rate of increase of } \phi \text{ for a fluid particle}}$$

To remember so far

- We need to derive conservation equations that we can solve to calculate fluid velocities and other properties.
- These equations can be derived either for a fluid particle that is moving with the flow (Lagrangian) or for a fluid element that is stationary in space (Eulerian).
- For CFD purposes we need them in Eulerian form, but (according to the book) they are somewhat easier to derive in Lagrangian form.
- Luckily, when we derive equations for a property ϕ in one form, we can convert them to the other form using the relationship shown on the bottom in the previous slide.

Relevant entries for Φ

x-momentum	u	$\rho \frac{Du}{Dt}$	$\frac{\partial(\rho u)}{\partial t} + div(\rho u \mathbf{u})$
y-momentum	v	$\rho \frac{Dv}{Dt}$	$\frac{\partial(\rho v)}{\partial t} + div(\rho v \mathbf{u})$
z-momentum	w	$\rho \frac{Dw}{Dt}$	$\frac{\partial(\rho w)}{\partial t} + div(\rho w \mathbf{u})$
Energy	E	$\rho \frac{DE}{Dt}$	$\frac{\partial(\rho E)}{\partial t} + div(\rho E \mathbf{u})$

Momentum equation in three dimensions

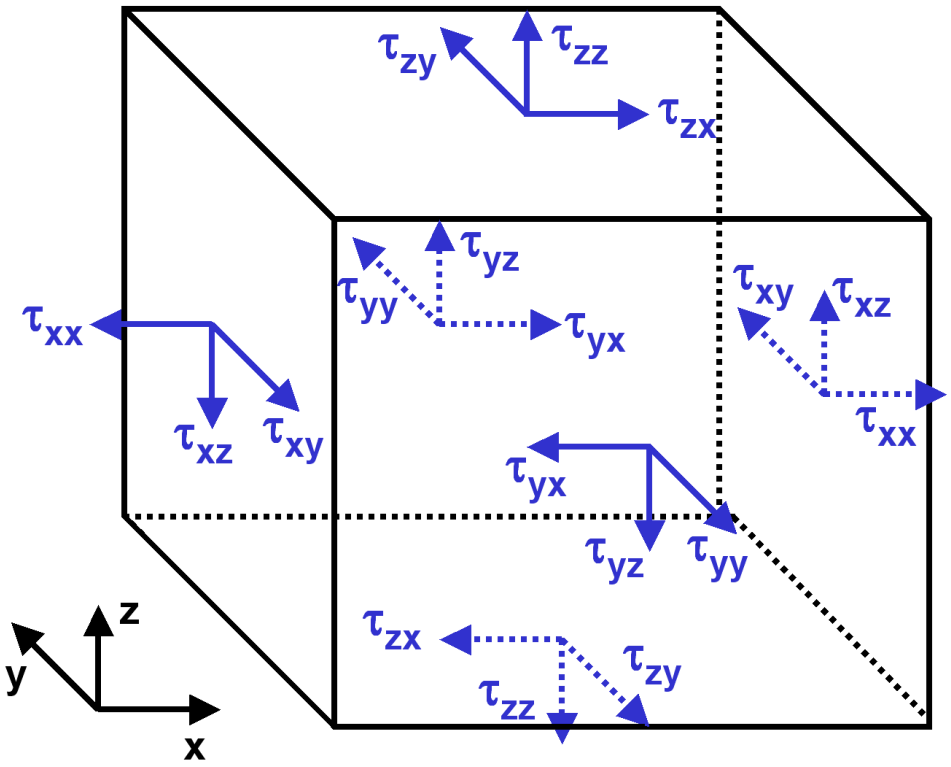
- We will first derive conservation equations for momentum and energy for fluid particles. Next, we will use the above relationships to transform those to an Eulerian frame (for fluid elements).
- We start with deriving the momentum equations.
- Newton's second law: rate of change of momentum equals sum of forces.
- Rate of increase of x-, y-, and z-momentum:

$$\rho \frac{Du}{Dt} \qquad \rho \frac{Dv}{Dt} \qquad \rho \frac{Dw}{Dt}$$

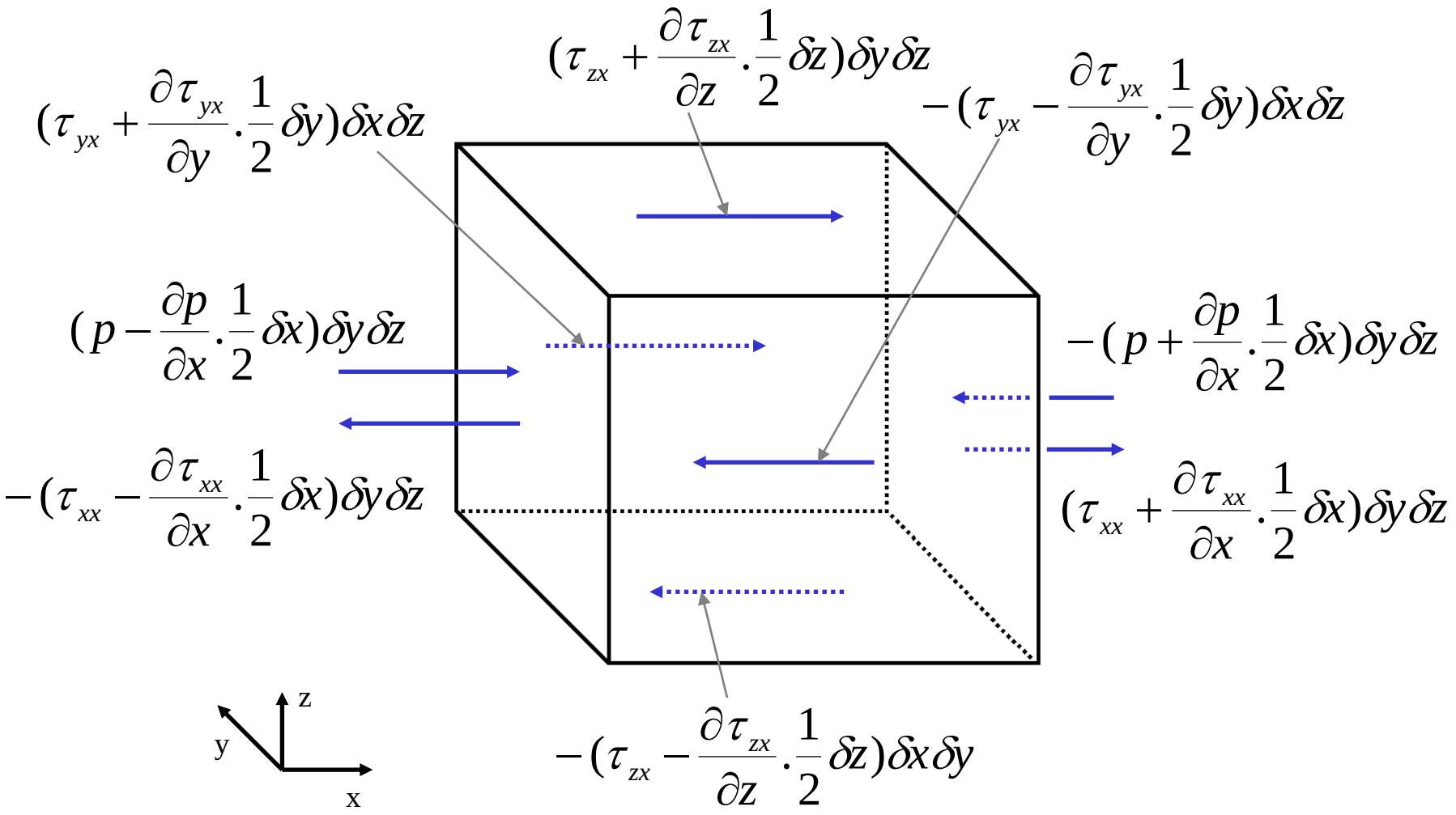
- Forces on fluid particles are:
  - Surface forces such as pressure and viscous forces.
  - Body forces, which act on a volume, such as gravity, centrifugal, Coriolis, and electromagnetic forces.

Viscous stresses

- Stresses are forces per area. Unit is N/m^2 or Pa.
- Viscous stresses denoted by τ.
- Suffix notation τ_{ij} is used to indicate direction.
- Nine stress components.
  - τ_{xx}, τ_{yy}, τ_{zz} are normal stresses. e.g., τ_{zz} is the stress in the z-direction on a z-plane.
  - Other stresses are shear stresses. e.g., τ_{zy} is the stress in the y-direction on a z-plane.
- Forces aligned with the direction of a coordinate axis are positive. Opposite direction is negative.



Forces in the x-direction



Net force in the x-direction is the sum of all the force components in that direction.

Momentum equation

- Set the rate of change of x-momentum for a fluid particle Du/Dt equal to:
  - the sum of the forces due to surface stresses shown in the previous slide, plus
  - the body forces. These are usually lumped together into a source term S_M:

$$\rho \frac{Du}{Dt} = \frac{\partial(-p+\tau_{xx})}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + S_{Mx}$$

  - p is a compressive stress and τ_{xx} is a tensile stress.
- Similarly, for y- and z-momentum:

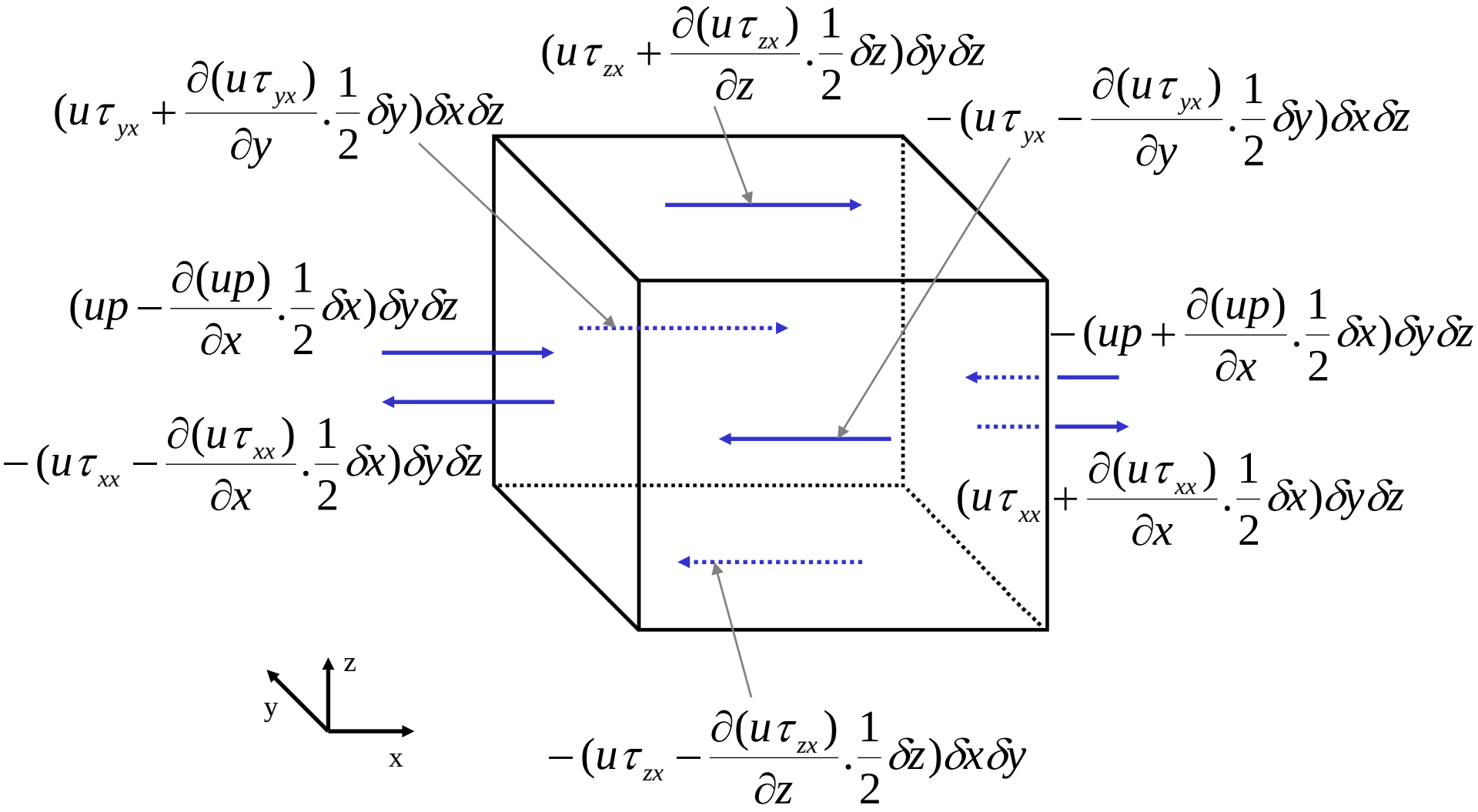
$$\rho \frac{Dv}{Dt} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial(-p+\tau_{yy})}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + S_{My}$$

$$\rho \frac{Dw}{Dt} = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial(-p+\tau_{zz})}{\partial z} + S_{Mz}$$

Energy equation

- First law of thermodynamics: rate of change of energy of a fluid particle is equal to the rate of heat addition plus the rate of work done.
- Rate of increase of energy is $\rho DE/Dt$.
- Energy $E = i + \frac{1}{2}(u^2+v^2+w^2)$.
- Here, i is the internal (thermal energy).
- $\frac{1}{2}(u^2+v^2+w^2)$ is the kinetic energy.
- Potential energy (gravitation) is usually treated separately and included as a source term.
- We will derive the energy equation by setting the total derivative equal to the change in energy as a result of work done by viscous stresses and the net heat conduction.
- Next, we will subtract the kinetic energy equation to arrive at a conservation equation for the internal energy.

Work done by surface stresses in x-direction



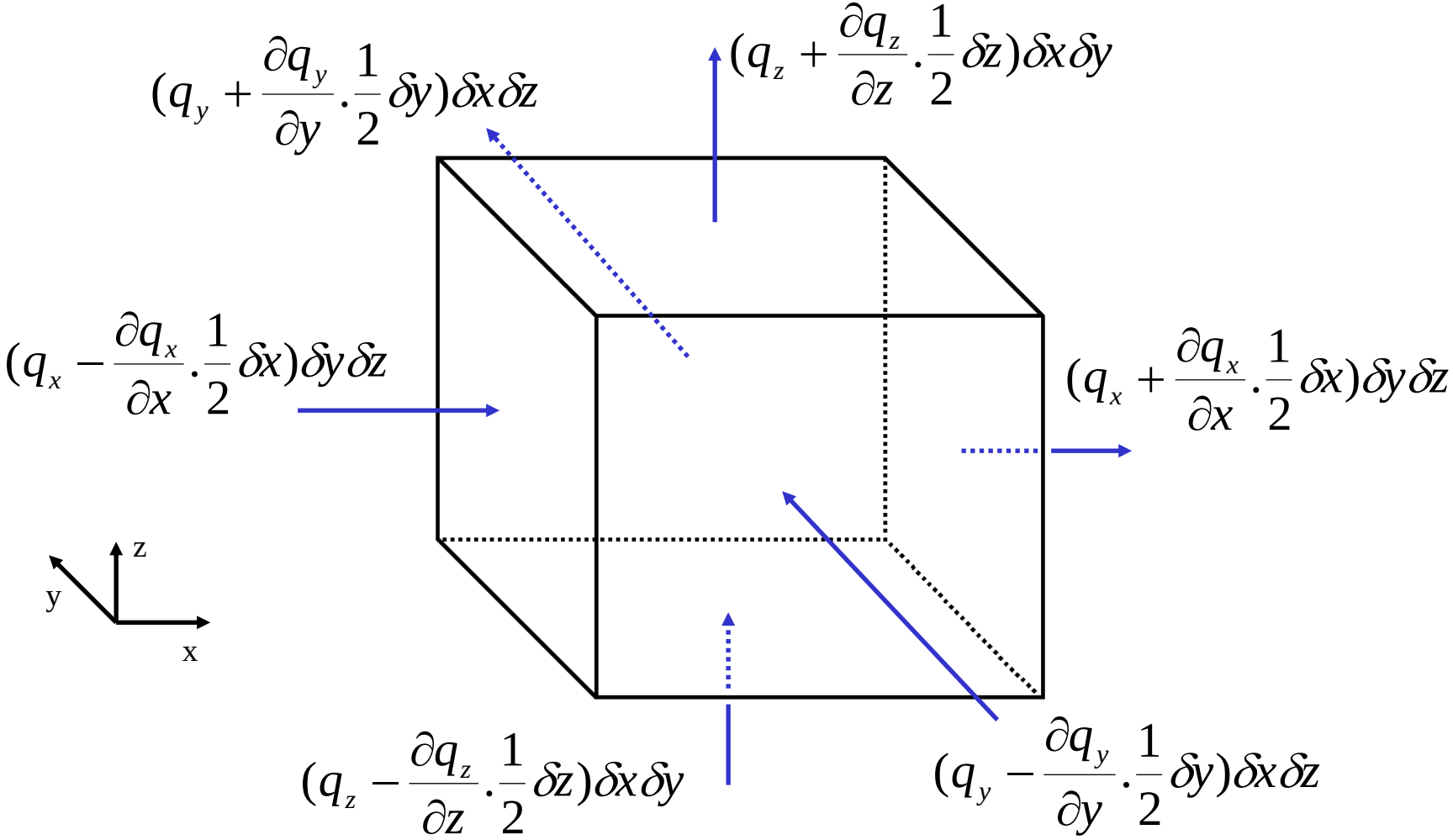
Work done is force times velocity.

Work done by surface stresses

- The total rate of work done by surface stresses is calculated as follows:
  - For work done by x-components of stresses add all terms in the previous slide.
  - Do the same for the y- and z-components.
- Add all and divide by $\delta x \delta y \delta z$ to get the work done per unit volume by the surface stresses:

$$-div(p\mathbf{u}) + \frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x}$$
$$+ \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(u\tau_{zz})}{\partial z}$$

Energy flux due to heat conduction



The heat flux vector q has three components, q_x, q_y, and q_z.

Energy flux due to heat conduction

- Summing all terms and dividing by $\delta x \delta y \delta z$ gives the net rate of heat transfer to the fluid particle per unit volume:

$$-\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} = -div\,\mathbf{q}$$

- Fourier's law of heat conduction relates the heat flux to the local temperature gradient:

$$q_x = -k\frac{\partial T}{\partial x} \qquad q_y = -k\frac{\partial T}{\partial y} \qquad q_z = -k\frac{\partial T}{\partial z}$$

- In vector form: $\mathbf{q} = -k\ grad\ T$
- Thus, energy flux due to conduction: $-div\,\mathbf{q} = div(k\ grad\ T)$
- This is the final form used in the energy equation.

Energy equation

- Setting the total derivative for the energy in a fluid particle equal to the previously derived work and energy flux terms, results in the following energy equation:

$$\rho \frac{DE}{Dt} = -div(p\mathbf{u}) + \left[\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(u\tau_{zz})}{\partial z} \right] + div(k\ grad\ T) + S_E$$

- Note that we also added a source term S_E that includes sources (potential energy, sources due to heat production from chemical reactions, etc.).

Kinetic energy equation

- Separately, we can derive a conservation equation for the kinetic energy of the fluid.
- In order to do this, we multiply the u-momentum equation by u, the v-momentum equation by v, and the w-momentum equation by w. We then add the results together.
- This results in the following equation for the kinetic energy:

$$\rho \frac{D[\frac{1}{2}(u^2+v^2+w^2)]}{Dt} = -\mathbf{u}.grad\ p + u\left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z}\right)$$

$$+ v\left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z}\right) + w\left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}\right) + \mathbf{u}.\mathbf{S}_M$$

Internal energy equation

- Subtract the kinetic energy equation from the energy equation.
- Define a new source term for the internal energy as $S_i = S_E - \mathbf{u}.\mathbf{S_M}$. This results in:

$$\rho \frac{Di}{Dt} = -\, p\, div\, \mathbf{u} + \left[\tau_{xx} \frac{\partial u}{\partial x} + \tau_{yx} \frac{\partial u}{\partial y} + \tau_{zx} \frac{\partial u}{\partial z} + \tau_{xy} \frac{\partial v}{\partial x} \right.$$
$$\left. + \tau_{yy} \frac{\partial v}{\partial y} + \tau_{zy} \frac{\partial v}{\partial z} + \tau_{xz} \frac{\partial w}{\partial x} + \tau_{yz} \frac{\partial w}{\partial y} + \tau_{zz} \frac{\partial u}{\partial z} \right]$$
$$+ div(k\ grad\ T) + S_i$$

Enthalpy equation

- An often-used alternative form of the energy equation is the total enthalpy equation.
  - Specific enthalpy $h = i + p/\rho$.
  - Total enthalpy $h_0 = h + \frac{1}{2}(u^2+v^2+w^2) = E + p/\rho$.

$$\frac{\partial(\rho h_0)}{\partial t} + div(\rho h_0 \mathbf{u}) = div(k \ \ grad \ \ T) + \left[\frac{\partial(u\tau_{xx})}{\partial x} + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(u\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{yy})}{\partial y} + \frac{\partial(v\tau_{zy})}{\partial z} + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} + \frac{\partial(u\tau_{zz})}{\partial z} \right] + S_h$$

Equations of state

- Fluid motion is described by five partial differential equations for mass, momentum, and energy.
- Amongst the unknowns are four thermodynamic variables: ρ, p, i, and T.
- We will assume thermodynamic equilibrium, i.e., that the time it takes for a fluid particle to adjust to new conditions is short relative to the timescale of the flow.
- We add two equations of state using the two state variables ρ and T: $p=p(\rho,T)$ and $i=i(\rho,T)$.
- For a perfect gas, these become: $p=\rho RT$ and $i=C_v T$.
- At low speeds (e.g., Ma < 0.2), the fluids can be considered incompressible. There is no linkage between the energy equation, and the mass and momentum equation. We then only need to solve for energy if the problem involves heat transfer.

Viscous stresses

- A model for the viscous stresses τ_{ij} is required.
- We will express the viscous stresses as functions of the local deformation rate (strain rate) tensor.
- There are two types of deformation:
  - Linear deformation rates due to velocity gradients.
    - Elongating stress components (stretching).
    - Shearing stress components.
  - Volumetric deformation rates due to expansion or compression.
- All gases and most fluids are isotropic: viscosity is a scalar.
- Some fluids have anisotropic viscous stress properties, such as certain polymers and dough. We will not discuss those here.

Viscous stress tensor

- Using an isotropic (first) dynamic viscosity μ for the linear deformations and a second viscosity λ=-2/3 μ for the volumetric deformations results in:

$$\boldsymbol{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix}$$

$$= \begin{pmatrix} 2\mu\frac{\partial u}{\partial x} - \frac{2}{3}\mu\, div\,\mathbf{u} & \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) \\ \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) & 2\mu\frac{\partial v}{\partial y} - \frac{2}{3}\mu\, div\,\mathbf{u} & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) \\ \mu\left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right) & \mu\left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right) & 2\mu\frac{\partial w}{\partial z} - \frac{2}{3}\mu\, div\,\mathbf{u} \end{pmatrix}$$

Note: div u = 0 for incompressible fluids.

Navier-Stokes equations

- Including the viscous stress terms in the momentum balance and rearranging, results in the Navier-Stokes equations:

$$x-momentum: \quad \frac{\partial(\rho u)}{\partial t} + div(\rho u \mathbf{u}) = -\frac{\partial p}{\partial x} + div(\mu\ grad\ u) + S_{Mx}$$

$$y-momentum: \quad \frac{\partial(\rho v)}{\partial t} + div(\rho v \mathbf{u}) = -\frac{\partial p}{\partial y} + div(\mu\ grad\ v) + S_{My}$$

$$z-momentum: \quad \frac{\partial(\rho w)}{\partial t} + div(\rho w \mathbf{u}) = -\frac{\partial p}{\partial z} + div(\mu\ grad\ w) + S_{Mz}$$

Viscous dissipation

- Similarly, substituting the stresses in the internal energy equation and rearranging results in:

$$Internal\ energy: \quad \frac{\partial(\rho i)}{\partial t} + div(\rho i \mathbf{u}) = -\,p\ div\,\mathbf{u} + div(k\ grad\ T) + \Phi + S_i$$

- Here Φ is the viscous dissipation term. This term is always positive and describes the conversion of mechanical energy to heat.

$$\Phi = \mu\left\{2\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2 + \left(\frac{\partial w}{\partial z}\right)^2\right] + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}\right)^2\right\} - \frac{2}{3}\mu(div\,\mathbf{u})^2$$

Summary of equations in conservation form

$$Mass: \quad \frac{\partial \rho}{\partial t} + div(\rho\, \mathbf{u}) = 0$$

$$x-momentum: \quad \frac{\partial (\rho u)}{\partial t} + div(\rho u \mathbf{u}) = -\frac{\partial p}{\partial x} + div(\mu\ grad\ u) + S_{Mx}$$

$$y-momentum: \quad \frac{\partial (\rho v)}{\partial t} + div(\rho v \mathbf{u}) = -\frac{\partial p}{\partial y} + div(\mu\ grad\ v) + S_{My}$$

$$z-momentum: \quad \frac{\partial (\rho w)}{\partial t} + div(\rho w \mathbf{u}) = -\frac{\partial p}{\partial z} + div(\mu\ grad\ w) + S_{Mz}$$

$$Internal\ energy: \quad \frac{\partial (\rho i)}{\partial t} + div(\rho i \mathbf{u}) = -\ p\ div\ \mathbf{u} + div(k\ grad\ T) + \Phi + S_i$$

$$Equations\ of\ state: \quad p = p(\rho, T) \quad and \quad i = i(\rho, T)$$

$$e.g.\ for\ perfect\ gas: p = \rho RT \quad and \quad i = C_v T$$

General transport equations

- The system of equations is now closed, with seven equations for seven variables: pressure, three velocity components, enthalpy, temperature, and density.
- There are significant commonalities between the various equations. Using a general variable ϕ, the conservative form of all fluid flow equations can usefully be written in the following form:

$$\frac{\partial(\rho\phi)}{\partial t} + div(\rho\phi\,\mathbf{u}) = div(\Gamma\, grad\,\phi) + S_\phi$$

- Or, in words:

Rate of increase of ϕ of fluid element	+	Net rate of flow of ϕ out of fluid element (convection)	=	Rate of increase of ϕ due to diffusion	+	Rate of increase of ϕ due to sources

Integral form

- The key step of the finite volume method is to integrate the differential equation shown in the previous slide, and then to apply Gauss' divergence theorem, which for a vector **a** states:

$$\int_{CV} div\,\mathbf{a}\,dV = \int_{A} \mathbf{n}\cdot\mathbf{a}\,dA$$

- This then leads to the following general conservation equation in integral form:

$$\frac{\partial}{\partial t}\left(\int_{CV}\rho\phi\,dV\right) + \int_{A}\mathbf{n}\cdot(\rho\phi\,\mathbf{u})\,dA = \int_{A}\mathbf{n}\cdot(\Gamma\,grad\,\phi)\,dA + \int_{CV} S_{\phi}\,dV$$

Rate of increase of ϕ	+	Net rate of decrease of ϕ due to convection across boundaries	=	Net rate of increase of ϕ due to diffusion across boundaries	+	Net rate of creation of ϕ

- This is the actual form of the conservation equations solved by finite volume based CFD programs to calculate the flow pattern and associated scalar fields.

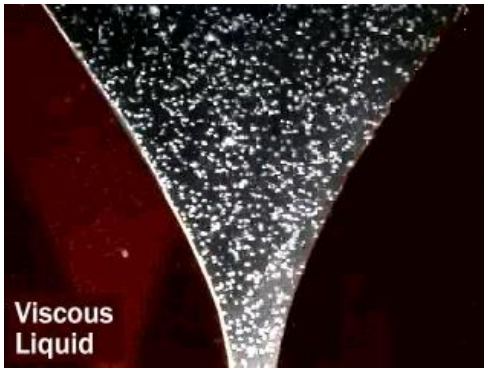
Lecture 4 – Classification of Flows

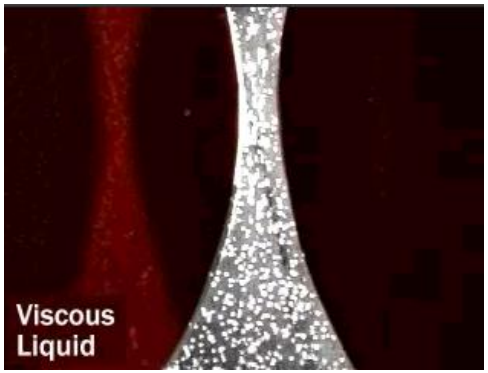
Applied Computational Fluid Dynamics

André Bakker

Classification: fluid flow vs. granular flow

- Fluid and solid particles: fluid flow vs. granular flow.
- A fluid consists of a large number of individual molecules. These could in principle be modeled as interacting solid particles.
- The interaction between adjacent salt grains and adjacent fluid parcels is quite different, however.





Images: Homsy et al. [2]

Reynolds number

- The Reynolds number Re is defined as: $Re = \rho V L / \mu$.
- Here L is a characteristic length, and V is the velocity.
- It is a measure of the ratio between inertial forces and viscous forces.
- If $Re >> 1$ the flow is dominated by inertia.
- If $Re << 1$ the flow is dominated by viscous effects.

Effect of Reynolds number

Re = 0.05 Re = 10 Re = 200 Re = 3000

Image: Homsy et al. [2]

Newton's second law

- For a solid mass: **F** = m.**a**
- For a continuum:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right] = \nabla.\sigma + f$$

Force per volume (body force)

Mass per volume (density)

acceleration

Force per area (stress tensor)

- Expressed in terms of velocity field u(x,y,z,t). In this form the momentum equation is also called Cauchy's law of motion.
- For an incompressible Newtonian fluid, this becomes:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right] = -\nabla p + \mu\nabla^2\mathbf{u}$$

- Here p is the pressure and μ is the dynamic viscosity. In this form, the momentum balance is also called the Navier-Stokes equation.

Scaling the Navier-Stokes equation

- For unsteady, low viscosity flows it is customary to make the pressure dimensionless with ρV^2. This results in:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right] = -\nabla p + \mu\nabla^2\mathbf{u}$$

with dimensionless variables:

$$(x^*,\ y^*,\ z^*) = (x/L,\ y/L,\ z/L)$$

$$\mathbf{u}^* = \mathbf{u}/V;\ \ p^* = p/\rho V^2;\ \ t^* = t/(V/L)$$

this becomes:

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^*.\nabla\mathbf{u}^* = -\nabla p^* + \frac{1}{\mathrm{Re}}\nabla^2\mathbf{u}^*$$

Euler equation

- In the limit of Re $\to\infty$ the stress term vanishes:

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^*.\nabla \mathbf{u}^* = -\nabla p^*$$

- In dimensional form, with μ = 0, we get the Euler equations:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla \mathbf{u}\right] = -\nabla p$$

- The flow is then inviscid.

Scaling the Navier-Stokes equation - viscous

- For steady state, viscous flows it is customary to make the pressure dimensionless with $\mu V/L$. This results in:

$$\rho \mathbf{u}.\nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u}$$

with dimensionl ess variables :

$$(x^*, y^*, z^*) = (x/L, y/L, z/L)$$

$$\mathbf{u}^* = \mathbf{u}/V$$

$$p^* = \frac{p}{\mu V / L}$$

this becomes :

$$\mathrm{Re}\ \mathbf{u}^*.\nabla \mathbf{u}^* = -\nabla p^* + \nabla^2 \mathbf{u}^*$$

In the limit of $\mathrm{Re} \to 0$ the convective term vanishes :

$$-\nabla p^* + \nabla^2 \mathbf{u}^* = 0$$

Navier-Stokes and Bernoulli

- When:
  - The flow is steady: $\partial u / \partial t = 0$
  - The flow is irrotational: the vorticity $\omega = \nabla \times \mathbf{u} = 0$
  - The flow is inviscid: $\mu = 0$
- And using: $\mathbf{u}.\nabla\mathbf{u} = \frac{1}{2}\nabla(\mathbf{u}.\mathbf{u}) - \mathbf{u} \times \nabla \times \mathbf{u}$

- We can rewrite the Navier-Stokes equation:

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}.\nabla\mathbf{u}\right] = -\nabla p + \mu\nabla^2\mathbf{u}$$

as the Bernoulli equation:

$$\nabla\left(\frac{p}{\rho} + \frac{\mathbf{u}.\mathbf{u}}{2}\right) = 0$$

Basic quantities

- The Navier-Stokes equations for incompressible flow involve four basic quantities:
  - Local (unsteady) acceleration.
  - Convective acceleration.
  - Pressure gradients.
  - Viscous forces.
- The ease with which solutions can be obtained and the complexity of the resulting flows often depend on which quantities are important for a given flow.

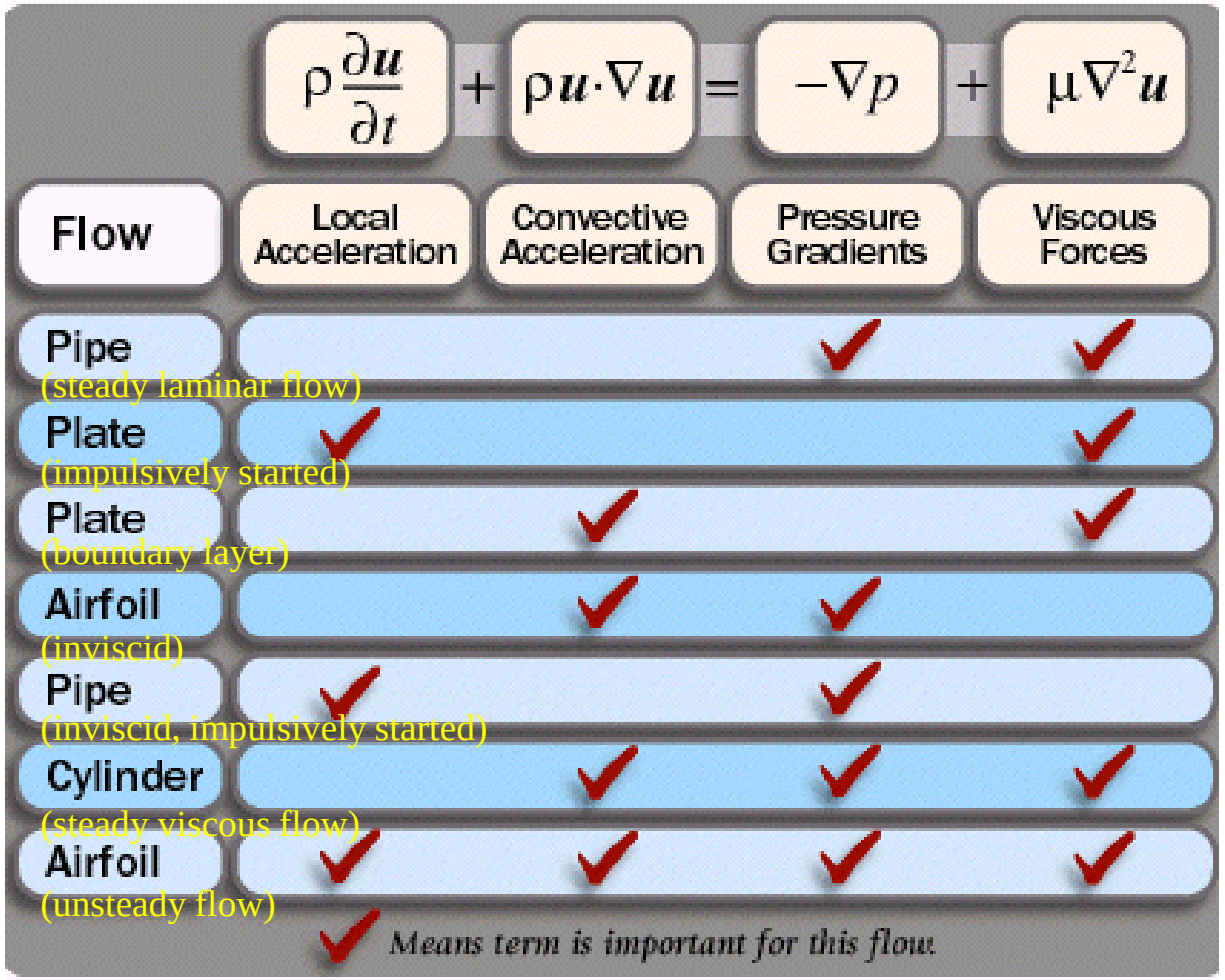
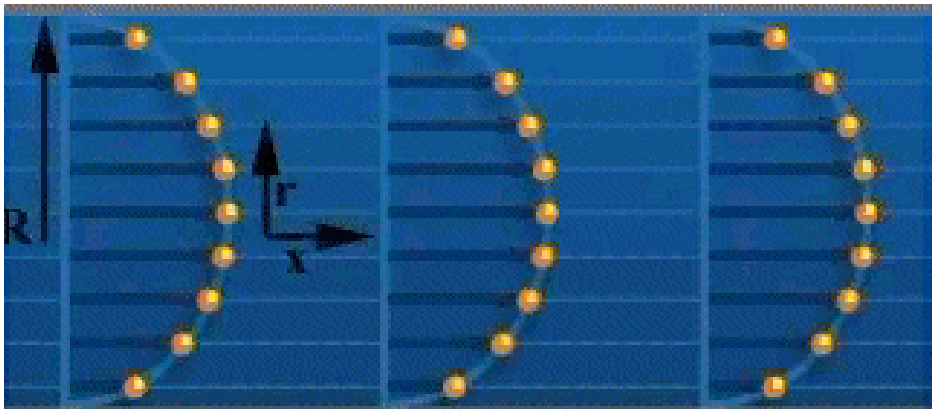


Image: Homsy et al. [2]

Steady laminar flow

- Steady viscous laminar flow in a horizontal pipe involves a balance between the pressure forces along the pipe and viscous forces.
- The local acceleration is zero because the flow is steady.
- The convective acceleration is zero because the velocity profiles are identical at any section along the pipe.



Pressure Gradients and Viscous Forces

$$0 = -\nabla p + \mu \nabla^2 u$$

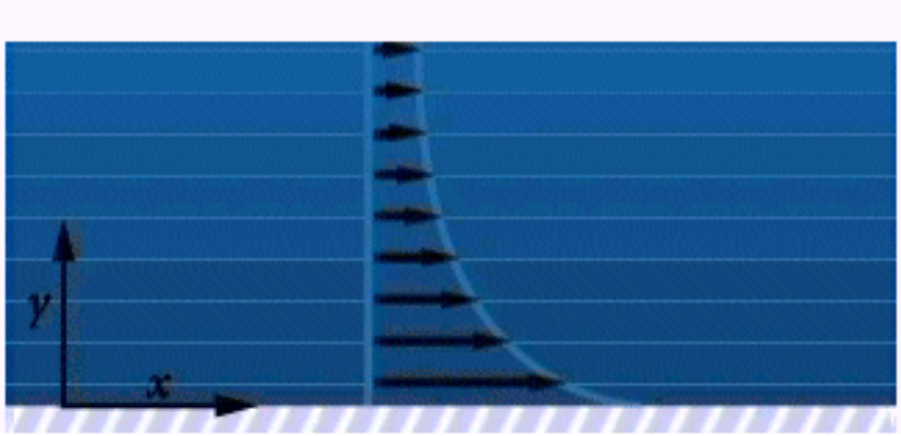
$$u = \left(-\frac{dp}{dx}\right) \frac{R^2}{4\mu} \left[1 - \left(\frac{r}{R}\right)^2\right]$$

velocity profile is independent of x

Images: Homsy et al. [2]

Flow past an impulsively started flat plate

- Flow past an impulsively started flat plate of infinite length involves a balance between the local (unsteady) acceleration effects and viscous forces. Here, the development of the velocity profile is shown.
- The pressure is constant throughout the flow.
- The convective acceleration is zero because the velocity does not change in the direction of the flow, although it does change with time.



Local Acceleration and Viscous Forces

$$\frac{\partial u}{\partial t} = \nu \nabla^2 u$$

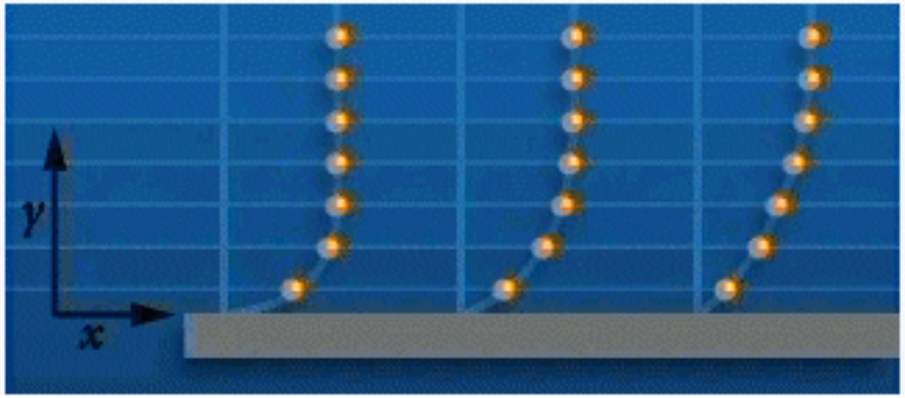
$$\nu = \mu/\rho$$

$$u = V_0 \left[1 - erf\left(\frac{y}{\sqrt{4\,\nu t}} \right) \right]$$

Images: Homsy et al. [2]

Boundary layer flow along a flat plate

- Boundary layer flow along a finite flat plate involves a balance between viscous forces in the region near the plate and convective acceleration effects.
- The boundary layer thickness grows in the downstream direction.
- The local acceleration is zero because the flow is steady.



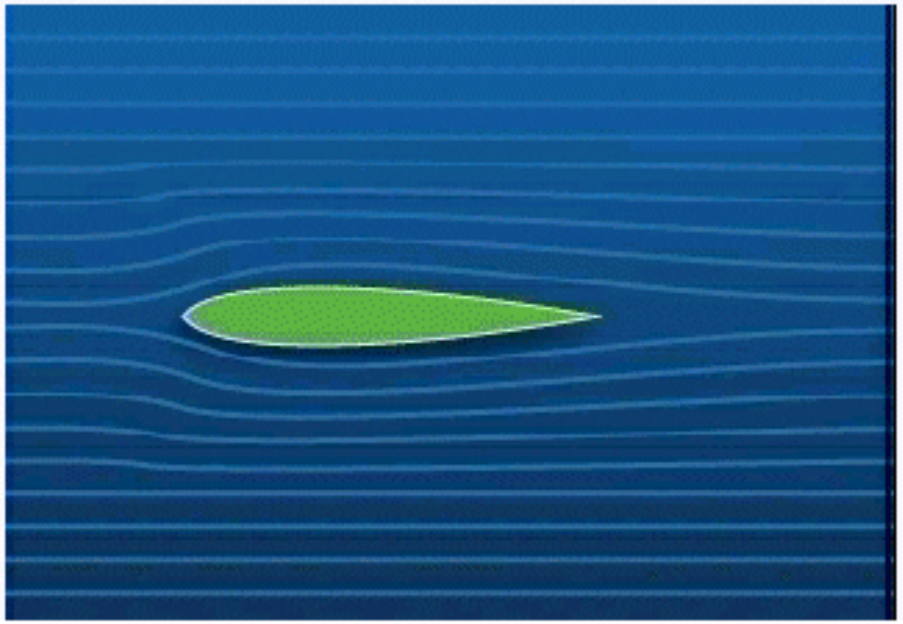
Convective Acceleration and Viscous Forces $\boldsymbol{u}\cdot\nabla\boldsymbol{u} = \nu\nabla^2\boldsymbol{u}$

$\boldsymbol{u} = \boldsymbol{u}(x,y)$

Images: Homsy et al. [2]

Inviscid flow past an airfoil

- Inviscid flow past an airfoil involves a balance between pressure gradients and convective acceleration.
- Since the flow is steady, the local (unsteady) acceleration is zero.
- Since the fluid is inviscid (μ=0) there are no viscous forces.



Convective Acceleration and Pressure Gradients

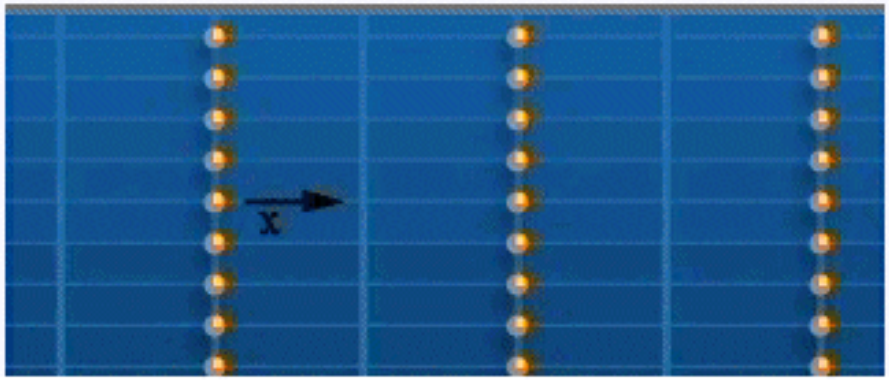
$$\rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p$$

$$\boldsymbol{u} = \boldsymbol{u}(x, y)$$

Images: Homsy et al. [2]

Impulsively started flow of an inviscid fluid

- Impulsively started flow of an inviscid fluid in a pipe involves a balance between local (unsteady) acceleration effects and pressure differences.
- The absence of viscous forces allows the fluid to slip along the pipe wall, producing a uniform velocity profile.
- The convective acceleration is zero because the velocity does not vary in the direction of the flow.
- The local (unsteady) acceleration is not zero since the fluid velocity at any point is a function of time.



Local Acceleration and Pressure Gradients

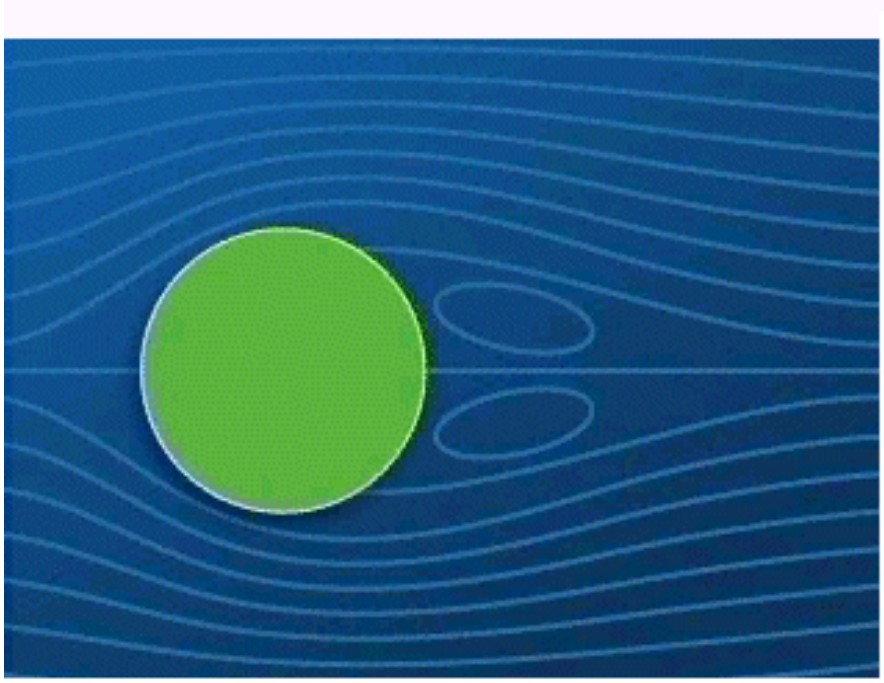
$$\rho \frac{\partial u}{\partial t} = -\nabla p$$

$$u = u(t)$$

Images: Homsy et al. [2]

Steady viscous flow past a cylinder

- Steady viscous flow past a circular cylinder involves a balance among convective acceleration, pressure gradients, and viscous forces.
- For the parameters of this flow (density, viscosity, size, and speed), the steady boundary conditions (i.e., the cylinder is stationary) give steady flow throughout.
- For other values of these parameters the flow may be unsteady.



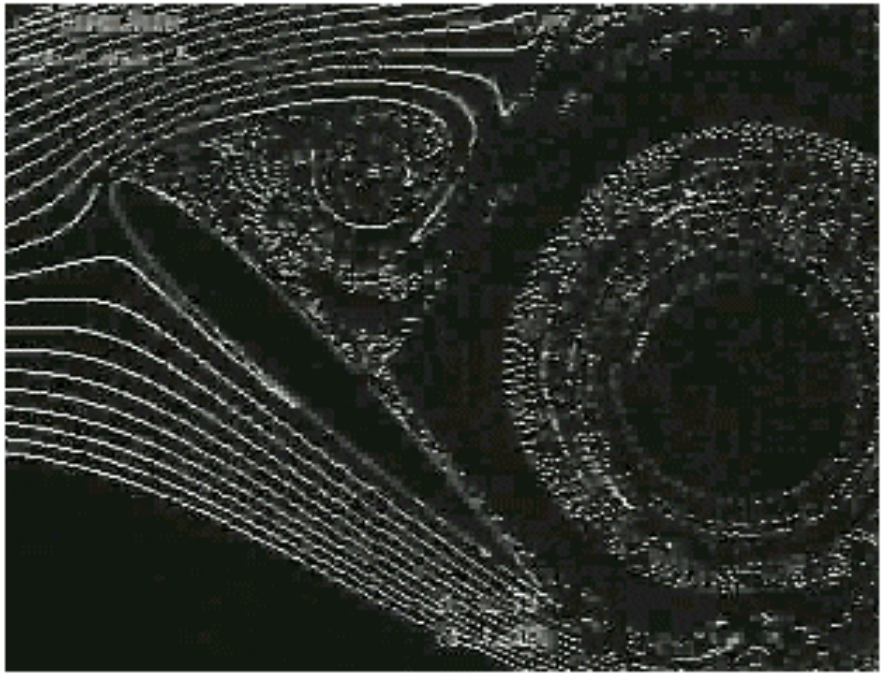
Convective Acceleration, Pressure Gradients and Viscous Forces

$$\rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \mu \nabla^2 \boldsymbol{u}$$

Images: Homsy et al. [2]

Unsteady flow past an airfoil

- Unsteady flow past an airfoil at a large angle of attack (stalled) is governed by a balance among local acceleration, convective acceleration, pressure gradients and viscous forces.
- A wide variety of fluid mechanics phenomena often occurs in situations such as these where all of the factors in the Navier-Stokes equations are relevant.



Local Acceleration, Convective Acceleration, Pressure Gradients and Viscous Forces

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \mu \nabla^2 \boldsymbol{u}$$

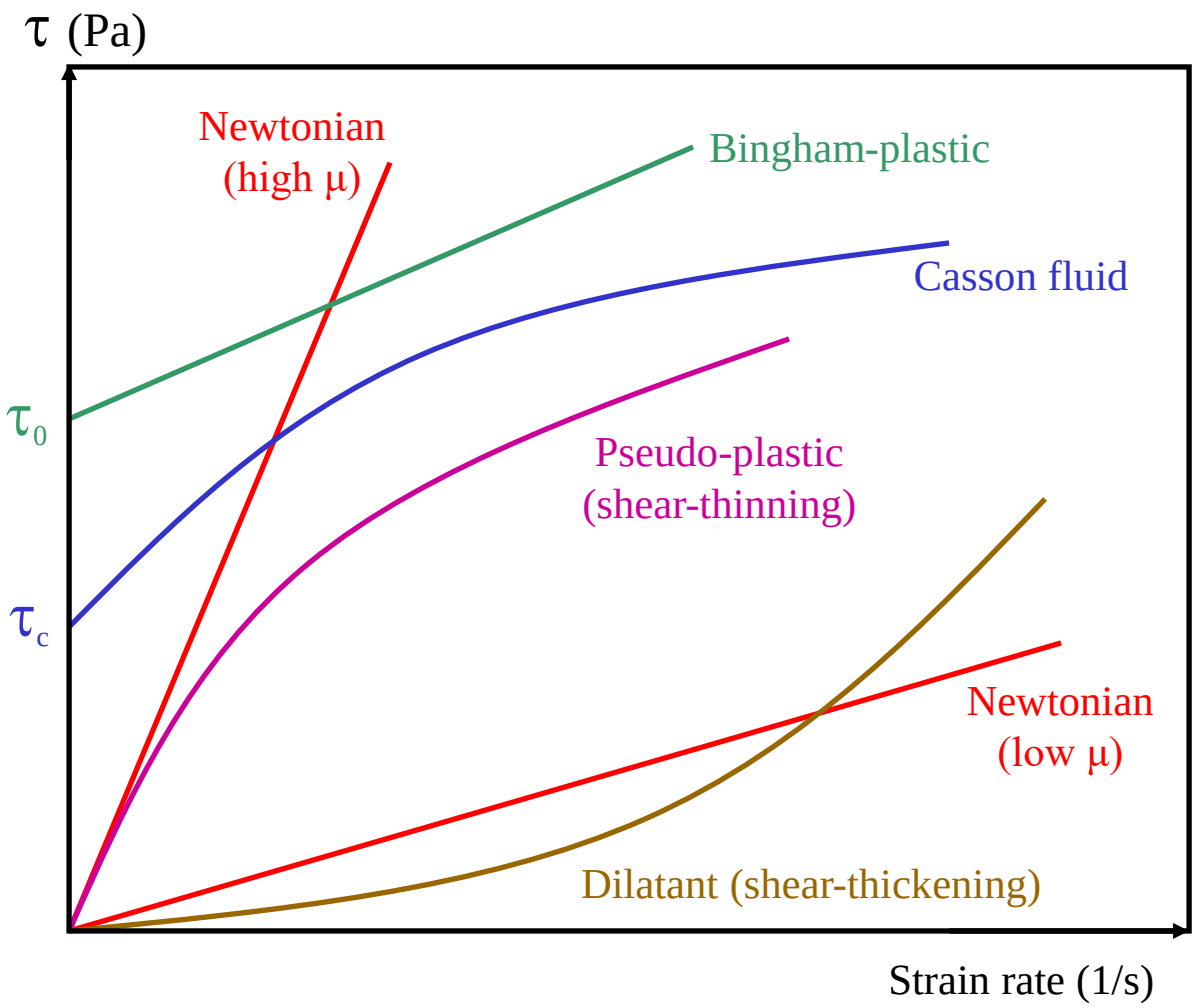
Images: Homsy et al. [2]

Flow classifications

- Laminar vs. turbulent flow.
  - Laminar flow: fluid particles move in smooth, layered fashion (no substantial mixing of fluid occurs).
  - Turbulent flow: fluid particles move in a chaotic, “tangled” fashion (significant mixing of fluid occurs).
- Steady vs. unsteady flow.
  - Steady flow: flow properties at any given point in space are constant in time, e.g., $p = p(x,y,z)$.
  - Unsteady flow: flow properties at any given point in space change with time, e.g., $p = p(x,y,z,t)$.

Newtonian vs. non-Newtonian

- Newtonian fluids: water, air.
- Pseudoplastic fluids: paint, printing ink.
- Dilatant fluids: dense slurries, wet cement.
- Bingham fluids: toothpaste, clay.
- Casson fluids: blood, yogurt.
- Visco-elastic fluids: polymers (not shown in graph because viscosity is not isotropic).



Flow classifications

- Incompressible vs. compressible flow.
  - Incompressible flow: volume of a given fluid particle does not change.
    - Implies that density is constant everywhere.
    - Essentially valid for all liquid flows.
  - Compressible flow: volume of a given fluid particle can change with position.
    - Implies that density will vary throughout the flow field.
    - Compressible flows are further classified according to the value of the Mach number (M), where.

$$M = \frac{V}{c}$$

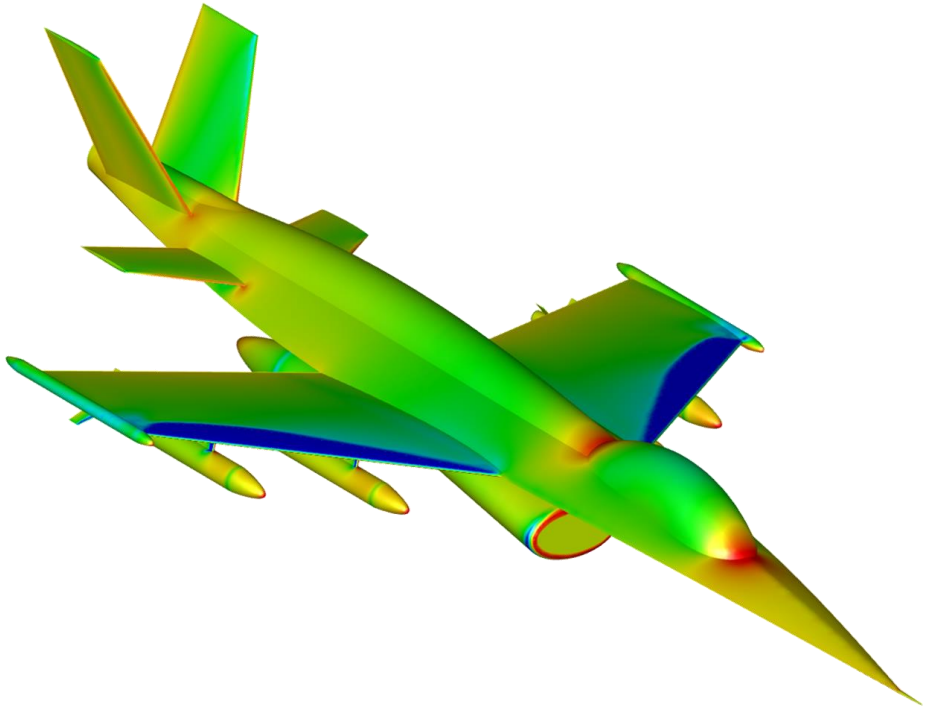
    - M < 1 - Subsonic.
    - M > 1 - Supersonic.

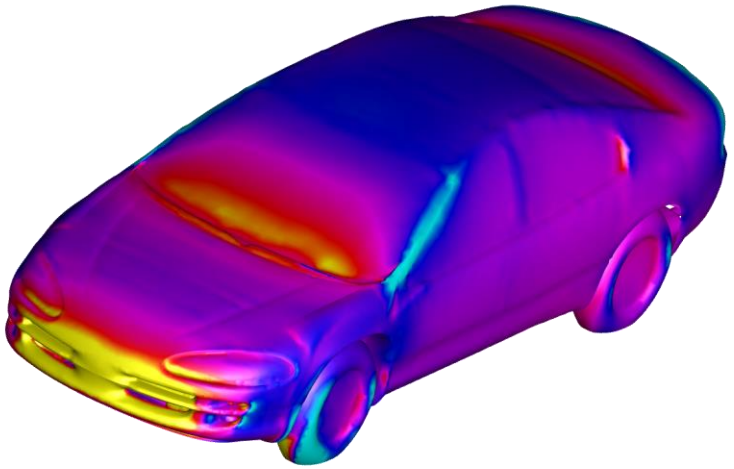
Flow classifications

- Single phase vs. multiphase flow.
  - Single phase flow: fluid flows without phase change (either liquid or gas).
  - Multiphase flow: multiple phases are present in the flow field (e.g., liquid-gas, liquid-solid, gas-solid).
- Homogeneous vs. heterogeneous flow.
  - Homogeneous flow: only one fluid material exists in the flow field.
  - Heterogeneous flow: multiple fluid/solid materials are present in the flow field (multi-species flows).

Flow configurations - external flow

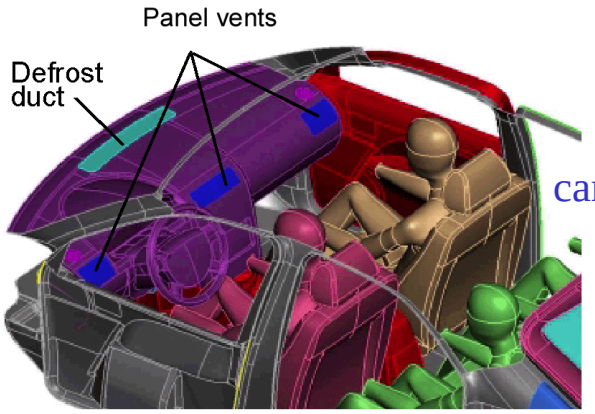
- Fluid flows over an object in an unconfined domain.
- Viscous effects are important only in the vicinity of the object.
- Away from the object, the flow is essentially inviscid.
- Examples: flows over aircraft, projectiles, ground vehicles.



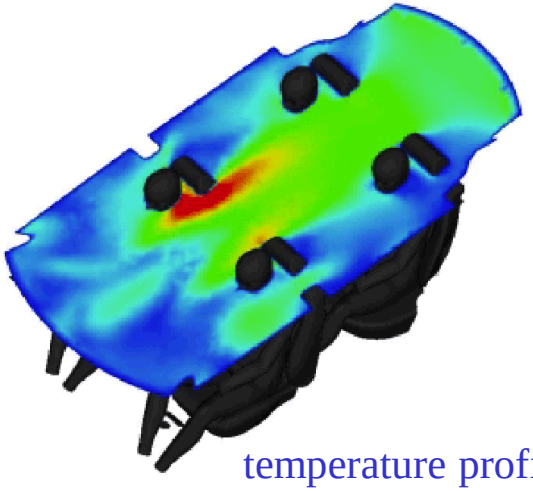


Flow configurations - internal flow

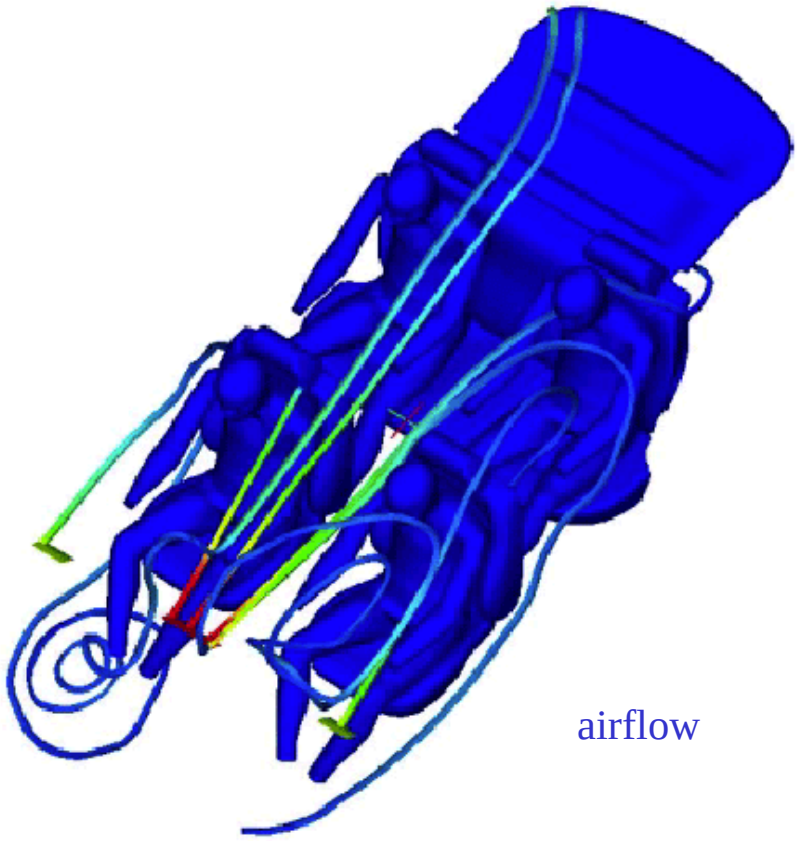
- Fluid flow is confined by walls, partitions, and other boundaries.
- Viscous effects extend across the entire domain.
- Examples: flows in pipes, ducts, diffusers, enclosures, nozzles.



car interior



temperature profile



airflow

Classification of partial differential equations

- A general partial differential equation in coordinates x and y:

$$a\frac{\partial^2\phi}{\partial x^2}+b\frac{\partial^2\phi}{\partial x\partial y}+c\frac{\partial^2\phi}{\partial y^2}+d\frac{\partial\phi}{\partial x}+e\frac{\partial\phi}{\partial y}+f\phi+g=0$$

- Characterization depends on the roots of the higher order (here second order) terms:
  - $(b^2\text{-}4ac) > 0$ then the equation is called hyperbolic.
  - $(b^2\text{-}4ac) = 0$ then the equation is called parabolic.
  - $(b^2\text{-}4ac) < 0$ then the equation is called elliptic.
- Note: if a, b, and c themselves depend on x and y, the equations may be of different type, depending on the location in x-y space. In that case the equations are of *mixed* type.

Origin of the terms

- The origin of the terms “elliptic,” “parabolic,” or “hyperbolic” used to label these equations is simply a direct analogy with the case for conic sections.
- The general equation for a conic section from analytic geometry is:

$$ax^2 + bxy + cy^2 + dx + ey + f = 0$$

where if.

  - $(b^2-4ac) > 0$ the conic is a hyperbola.
  - $(b^2-4ac) = 0$ the conic is a parabola.
  - $(b^2-4ac) < 0$ the conic is an ellipse.

Elliptic problems

- Elliptic equations are characteristic of equilibrium problems, this includes many (but not all) steady state flows.
- Examples are potential flow, the steady state temperature distribution in a rod of solid material, and equilibrium stress distributions in solid objects under applied loads.
- For potential flows the velocity is expressed in terms of a velocity potential: $\mathbf{u}=\nabla\phi$. Because the flow is incompressible, $\nabla.\mathbf{u}=0$, which results in $\nabla^2\phi=0$. This is also known as Laplace's equation:

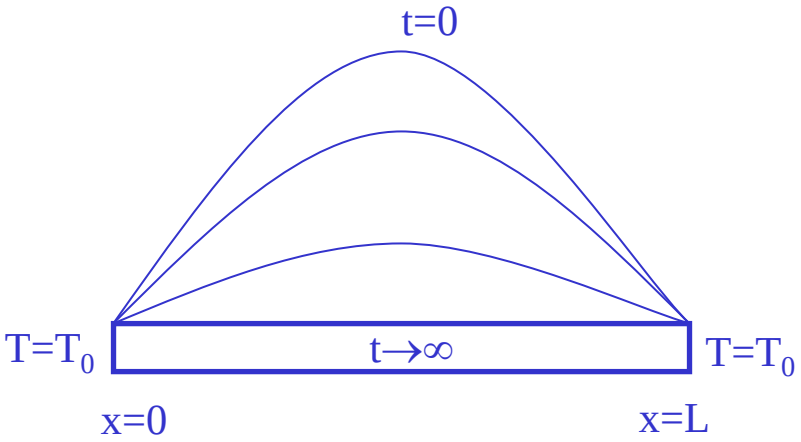
$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$$

- The solution depends solely on the boundary conditions. This is also known as a boundary value problem.
- A disturbance in the interior of the solution affects the solution everywhere else. The disturbance signals travel in all directions.
- As a result, solutions are always smooth, even when boundary conditions are discontinuous. This makes numerical solution easier!

Parabolic problems

- Parabolic equations describe marching problems. This includes time dependent problems which involve significant amounts of dissipation. Examples are unsteady viscous flows and unsteady heat conduction. Steady viscous boundary layer flow is also parabolic (march along streamline, not in time).
- An example is the transient temperature distribution in a cooling down rod:

$$\frac{\partial \phi}{\partial t} = \alpha \frac{\partial^2 \phi}{\partial x^2}$$



- The temperature depends on both the initial and boundary conditions. This is also called an initial-boundary-value problem.
- Disturbances can only affect solutions at a later time.
- Dissipation ensures that the solution is always smooth.

Hyperbolic problems

- Hyperbolic equations are typical of marching problems with negligible dissipation.
- An example is the wave equation: $$\frac{\partial^2 \phi}{\partial t^2} = c^2 \frac{\partial^2 \phi}{\partial x^2}$$
- This describes the transverse displacement of a string during small amplitude vibrations. If y is the displacement, x the coordinate along the string, and a the initial amplitude, the solution is:

$$y(x,t) = a\cos\left(\frac{\pi c t}{L}\right)\sin\left(\frac{\pi x}{L}\right)$$

- Note that the amplitude is independent of time, i.e., there is no dissipation.
- Hyperbolic problems can have discontinuous solutions.
- Disturbances may affect only a limited region in space. This is called the *zone of influence*. Disturbances propagate at the wave speed c.
- Local solutions may only depend on initial conditions in the *domain of dependence*.
- Examples of flows governed by hyperbolic equations are shockwaves in transonic and supersonic flows.

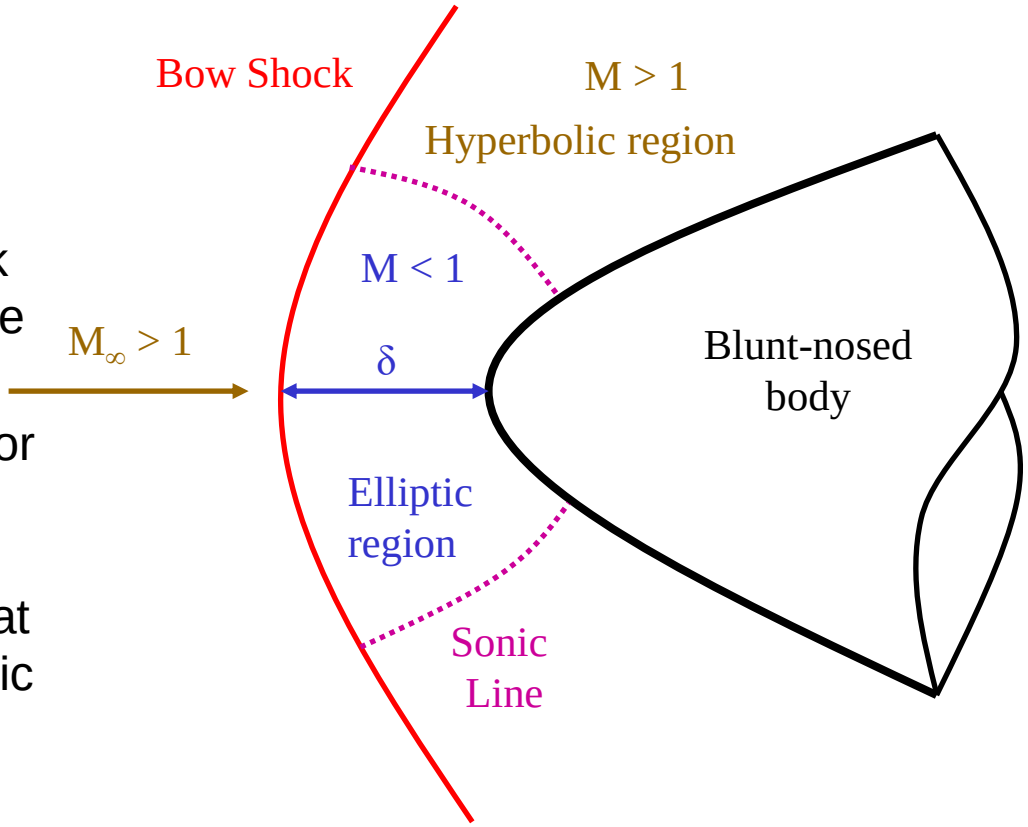
Classification of fluid flow equations

	Steady Flow	**Unsteady Flow**
Viscous flow	Elliptic	Parabolic
Inviscid flow	M < 1 (subsonic) Elliptic	Hyperbolic
	M> 1 (supersonic) Hyperbolic	Hyperbolic
Thin shear layers	Parabolic	Parabolic

- For inviscid flows at M<1, pressure disturbances travel faster than the flow speed (M is Mach number). If M>1, pressure disturbances cannot travel upstream. Limited zone of influence is a characteristic of hyperbolic problems.
- In thin shear layer flows, velocity derivatives in flow direction are much smaller than those in the cross-flow direction. Equations then effectively contain only one (second order) term and become parabolic. Also, the case for other strongly directional flows such as fully developed duct flow and jets.

Example: the blunt-nosed body

- Blunt-nosed body designs are used for supersonic and hypersonic speeds (e.g., Apollo capsules and space shuttle) because they are less susceptible to aerodynamic heating than sharp nosed bodies.
- There is a strong, curved bow shock wave, detached from the nose by the shock detachment distance δ.
- Calculating this flow field was a major challenge during the 1950s and 1960s because of the difficulties involved in solving for a flow field that is elliptic in one region and hyperbolic in others.
- Today's CFD solvers can routinely handle such problems, provided that the flow is calculated as being transient.



Initial and boundary conditions

- Initial conditions for unsteady flows:
  - Everywhere in the solution region ρ, **u** and T must be given at time t=0.
- Typical boundary conditions for unsteady and steady flows:
  - On solid walls:
    - $\mathbf{u} = \mathbf{u}_{wall}$ (no-slip condition).
    - $T=T_{wall}$ (fixed temperature) or $k\partial T/\partial n=-q_{wall}$ (fixed heat flux).
  - On fluid boundaries.
    - For most flows, inlet: ρ, **u**, and T must be known as a function of position. For external flows (flows around objects) and inviscid subsonic flows, inlet boundary conditions may be different.
    - For most flows, outlet: $-p+\mu\ \partial u_n/\partial n=F_n$ and $\mu\ \partial u_t/\partial n=F_n$ (stress continuity). F is the given surface stress. For fully developed flow $F_n=-p$ ($\partial u_n/\partial n =0$) and $F_t=0$. For inviscid supersonic flows, outlet conditions may be different.
- A more detailed discussion of boundary conditions will follow.

Summary

- Fluid flows can be classified in a variety of ways:
  - Internal vs. external.
  - Laminar vs. turbulent.
  - Compressible vs. incompressible.
  - Steady vs. unsteady.
  - Supersonic vs. transonic vs. subsonic.
  - Single-phase vs. multiphase.
  - Elliptic vs. parabolic vs. hyperbolic.

Lecture 5 - Solution Methods

Applied Computational Fluid Dynamics

André Bakker

Solution methods

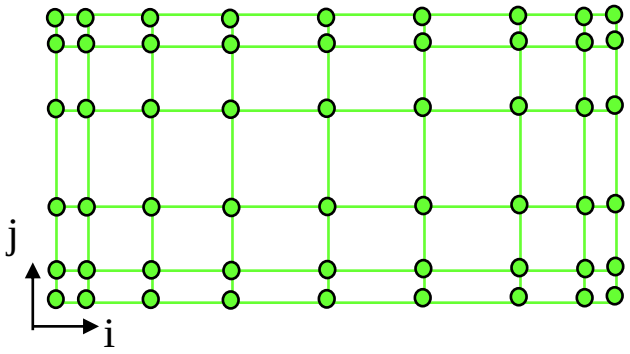
- Focus on finite volume method.
- Background of finite volume method.
- Discretization example.
- General solution method.
- Convergence.
- Accuracy and numerical diffusion.
- Pressure velocity coupling.
- Segregated versus coupled solver methods.
- Multigrid solver.
- Summary.

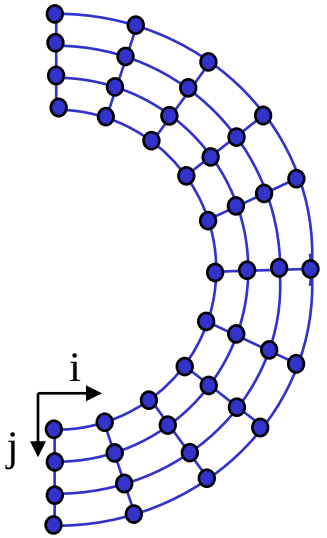
Overview of numerical methods

- Many CFD techniques exist.
- The most common in commercially available CFD programs are:
  - The finite volume method has the broadest applicability (~80%).
  - Finite element (~15%).
- Here we will focus on the finite volume method.
- There are certainly many other approaches (5%), including:
  - Finite difference.
  - Finite element.
  - Spectral methods.
  - Boundary element.
  - Vorticity based methods.
  - Lattice gas/lattice Boltzmann.
  - And more!

Finite difference: basic methodology

- The domain is discretized into a series of grid points.
- A “structured” (ijk) mesh is required.

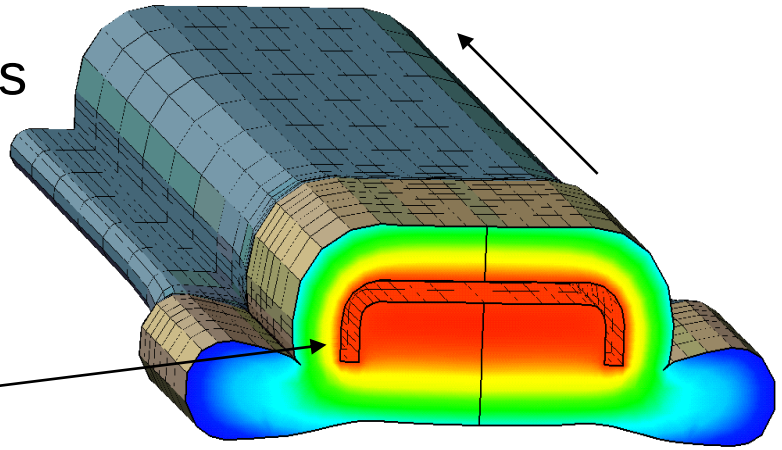




- The governing equations (in differential form) are discretized (converted to algebraic form).
- First and second derivatives are approximated by truncated Taylor series expansions.
- The resulting set of linear algebraic equations is solved either iteratively or simultaneously.

Finite element method (FEM)

- Earliest use was by Courant (1943) for solving a torsion problem.
- Clough (1960) gave the method its name.
- Method was refined greatly in the 60's and 70's, mostly for analyzing structural mechanics problem.
- FEM analysis of fluid flow was developed in the mid- to late 70's.
- Advantages: highest accuracy on coarse grids. Excellent for diffusion dominated problems (viscous flow) and viscous, free surface problems.
- Disadvantages: slow for large problems and not well suited for turbulent flow.



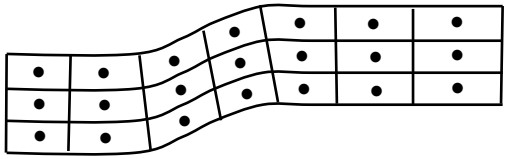
contours of velocity magnitude

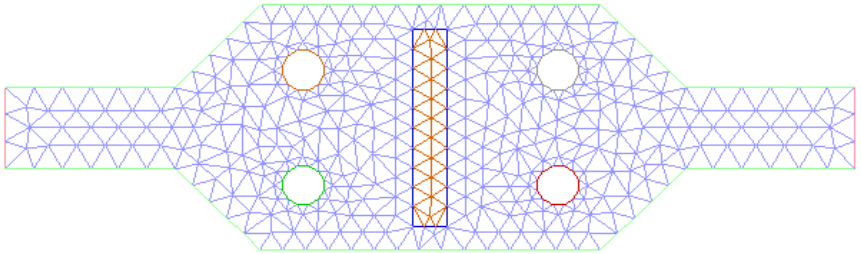
Finite volume method (FVM)

- First well-documented use was by Evans and Harlow (1957) at Los Alamos and Gentry, Martin and Daley (1966).
- Was attractive because while variables may not be continuously differentiable across shocks and other discontinuities mass, momentum and energy are always conserved.
- FVM enjoys an advantage in memory use and speed for very large problems, higher speed flows, turbulent flows, and source term dominated flows (like combustion).
- Late 70’s, early 80’s saw development of body-fitted grids. By early 90’s, unstructured grid methods had appeared.
- Advantages: basic FV control volume balance does not limit cell shape; mass, momentum, energy conserved even on coarse grids; efficient, iterative solvers well developed.
- Disadvantages: false diffusion when simple numerics are used.

Finite volume: basic methodology

- Divide the domain into control volumes.

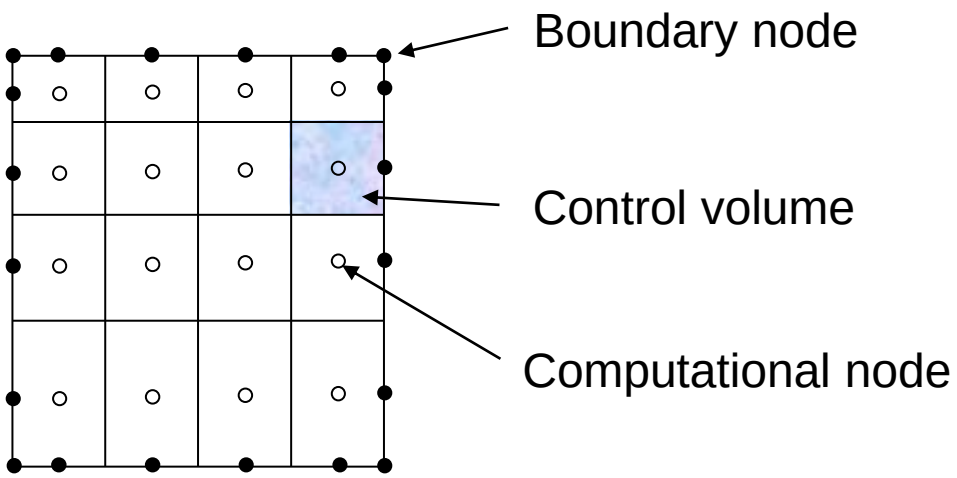




- Integrate the differential equation over the control volume and apply the divergence theorem.
- To evaluate derivative terms, values at the control volume faces are needed: have to make an assumption about how the value varies.
- Result is a set of linear algebraic equations: one for each control volume.
- Solve iteratively or simultaneously.

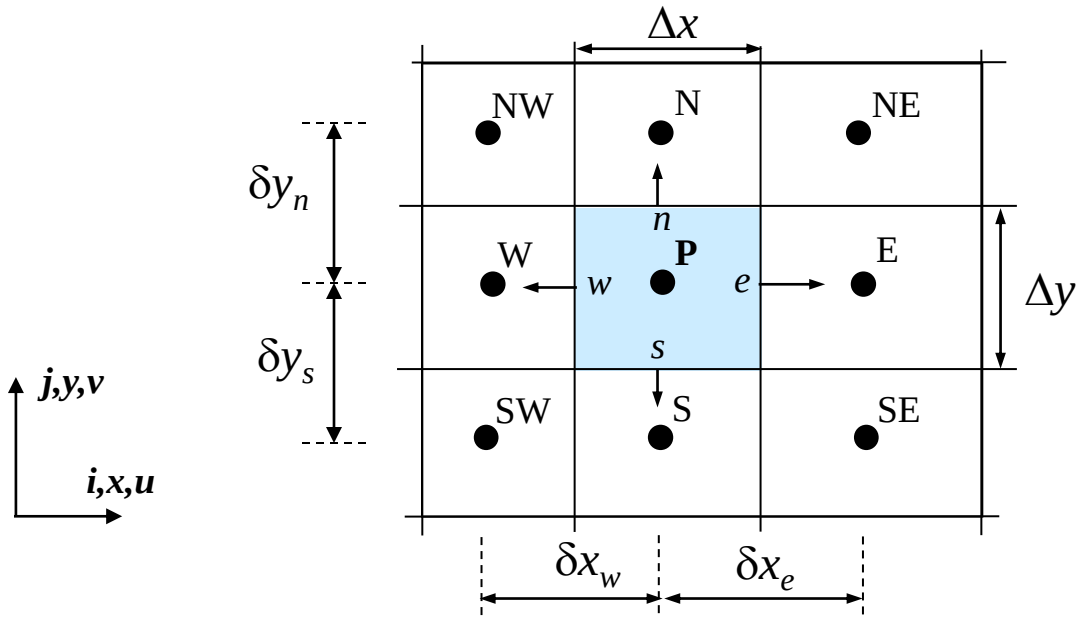
Cells and nodes

- Using finite volume method, the solution domain is subdivided into a finite number of small control volumes (cells) by a grid.
- The grid defines the boundaries of the control volumes while the computational node lies at the center of the control volume.
- The advantage of FVM is that the integral conservation is satisfied exactly over the control volume.



Typical control volume

- The net flux through the control volume boundary is the sum of integrals over the four control volume faces (six in 3D). The control volumes do not overlap.
- The value of the integrand is not available at the control volume faces and is determined by interpolation.

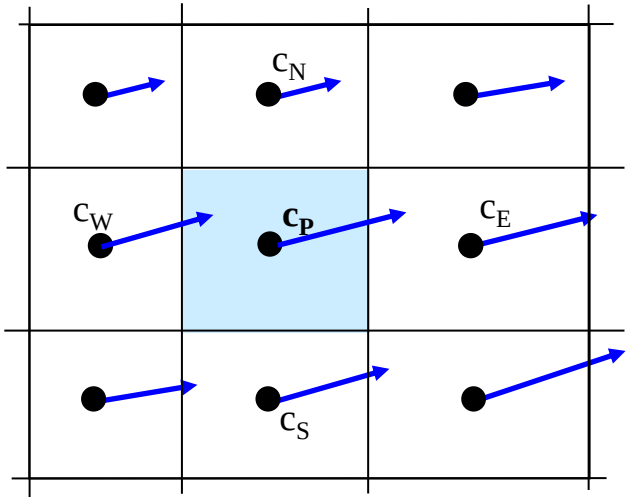


Discretization example

- To illustrate how the conservation equations used in CFD can be discretized we will look at an example involving the transport of a chemical species in a flow field.
- The species transport equation (constant density, incompressible flow) is given by:

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_i}(u_i c) = \frac{\partial}{\partial x_i}\left(\mathbf{D}\frac{\partial c}{\partial x_i}\right) + S$$

- Here c is the concentration of the chemical species and $\mathbf{D}$ is the diffusion coefficient. S is a source term.
- We will discretize this equation (convert it to a solvable algebraic form) for the simple flow field shown on the right, assuming steady state conditions.



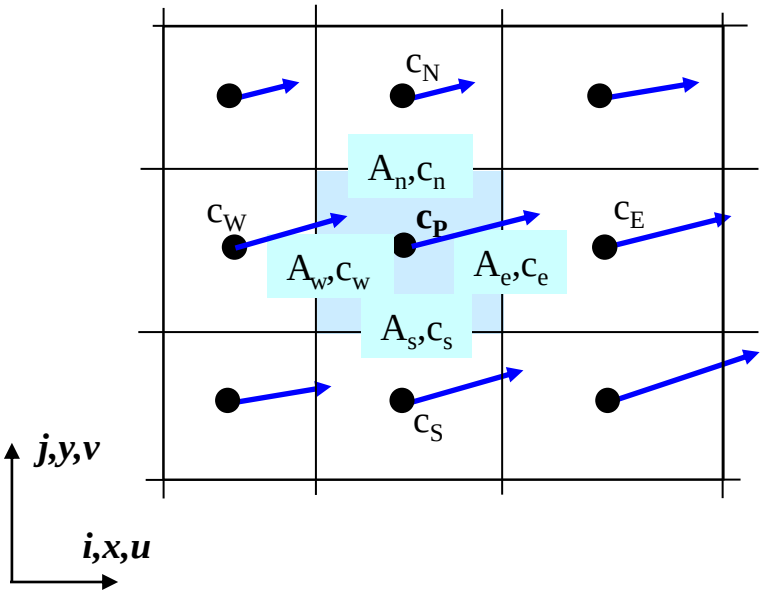
Discretization example - continued

- The balance over the control volume is given by:

$$A_e u_e c_e - A_w u_w c_w + A_n v_n c_n - A_s v_s c_s =$$

$$\mathbf{D}A_e \left.\frac{dc}{dx}\right|_e - \mathbf{D}A_w \left.\frac{dc}{dx}\right|_w + \mathbf{D}A_n \left.\frac{dc}{dy}\right|_n - \mathbf{D}A_s \left.\frac{dc}{dy}\right|_s + S_p$$

- This contains values at the faces, which need to be determined from interpolation from the values at the cell centers.



Notation

A_w, A_n, A_e, A_s : areas of the faces

c_w, c_n, c_e, c_s : concentrations at the faces

c_W, c_N, c_E, c_S : concentrations at the cell centers

$u_w, u_n, u_e, u_s, v_w, v_n, v_e, v_s$: velocities at the faces

$u_W, u_N, u_E, u_S, v_W, v_N, v_E, v_S$: velocities at the cell centers

S_P: source in cell P

D: diffusion coefficient

Discretization example - continued

- The simplest way to determine the values at the faces is by using first order upwind differencing. Here, let's assume that the value at the face is equal to the value in the center of the cell upstream of the face. Using that method results in:

$$A_e u_P c_P - A_w u_W c_W + A_n v_P c_P - A_s v_S c_S = \mathbf{D} A_e (c_E - c_P)/\delta x_e$$
$$-\mathbf{D} A_w (c_P - c_W)/\delta x_w + \mathbf{D} A_n (c_N - c_P)/\delta y_n - \mathbf{D} A_s (c_P - c_S)/\delta y_s + S_P$$

- This equation can then be rearranged to provide an expression for the concentration at the center of cell P as a function of the concentrations in the surrounding cells, the flow field, and the grid.

Discretization example - continued

- Rearranging the previous equation results in:

$$c_P(A_n v_P + A_e u_P + \mathbf{D}A_w/\delta x_w + \mathbf{D}A_n/\delta y_p + \mathbf{D}A_e/\delta x_e + \mathbf{D}A_s/\delta y_s) = c_W(A_w u_W + \mathbf{D}A_w/\delta x_w) + c_N(\mathbf{D}A_n/\delta y_n) + c_E(\mathbf{D}A_e/\delta x_e) + c_S(A_s v_S + \mathbf{D}A_s/\delta y_s) + S_P$$

- This equation can now be simplified to:

$$a_P c_P = a_W c_W + a_N c_N + a_E c_E + a_S c_S + b$$

$$= \sum_{nb} a_{nb} c_{nb} + b$$

- Here nb refers to the neighboring cells. The coefficients a_{nb} and b will be different for every cell in the domain at every iteration. The species concentration field can be calculated by recalculating c_P from this equation iteratively for all cells in the domain.

General approach

- In the previous example we saw how the species transport equation could be discretized as a linear equation that can be solved iteratively for all cells in the domain.
- This is the general approach to solving partial differential equations used in CFD. It is done for all conserved variables (momentum, species, energy, etc.).
- For the conservation equation for variable ϕ, the following steps are taken:
  - Integration of conservation equation in each cell.
  - Calculation of face values in terms of cell-centered values.
  - Collection of like terms.
- The result is the following discretization equation (with nb denoting cell neighbors of cell P):

$$a_P \phi_P = \sum_{nb} a_{nb} \phi_{nb} + b$$

General approach - relaxation

- At each iteration, at each cell, a new value for variable ϕ in cell P can then be calculated from that equation.
- It is common to apply relaxation as follows:

$$\phi_P^{new,\,used} = \phi_P^{old} + U(\phi_P^{new,\,predicted} - \phi_P^{old})$$

- Here U is the relaxation factor:
  - U < 1 is underrelaxation. This may slow down speed of convergence but increases the stability of the calculation, i.e., it decreases the possibility of divergence or oscillations in the solutions.
  - U = 1 corresponds to no relaxation. One uses the predicted value of the variable.
  - U > 1 is overrelaxation. It can sometimes be used to accelerate convergence but will decrease the stability of the calculation.

Underrelaxation recommendation

- Underrelaxation factors are there to suppress oscillations in the flow solution that result from numerical errors.
- Underrelaxation factors that are too small will significantly slow down convergence, sometimes to the extent that the user thinks the solution is converged when it really is not.
- The recommendation is to always use underrelaxation factors that are as high as possible, without resulting in oscillations or divergence.
- Typically, one should stay with the default factors in the solver.
- When the solution is converged but the pressure residual is still relatively high, the factors for pressure and momentum can be lowered to further refine the solution.

General approach - convergence

- The iterative process is repeated until the change in the variable from one iteration to the next becomes so small that the solution can be considered converged.
- At convergence:
  - All discrete conservation equations (momentum, energy, etc.) are obeyed in all cells to a specified tolerance.
  - The solution no longer changes with additional iterations.
  - Mass, momentum, energy and scalar balances are obtained.
- Residuals measure imbalance (or error) in conservation equations.
- The absolute residual at point P is defined as:

$$R_P = \left| a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b \right|$$

Convergence - continued

- Residuals are usually scaled relative to the local value of the property ϕ in order to obtain a relative error:

$$R_{P,scaled} = \frac{\left| a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b \right|}{\left| a_P \phi_P \right|}$$

- They can also be normalized, by dividing them by the maximum residual that was found at any time during the iterative process.
- An overall measure of the residual in the domain is:

$$R^{\phi} = \frac{\sum_{all\ cells} \left| a_P \phi_P - \sum_{nb} a_{nb} \phi_{nb} - b \right|}{\sum_{all\ cells} \left| a_P \phi_P \right|}$$

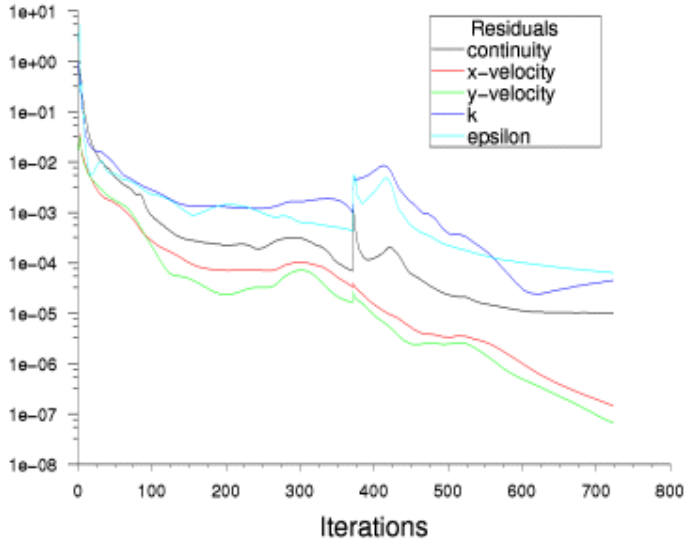
- It is common to require the scaled residuals to be on the order of 1E-3 to 1E-4 or less for convergence.

Notes on convergence

- Always ensure proper convergence before using a solution: unconverged solutions can be misleading!!
- Solutions are converged when the flow field and scalar fields are no longer changing.
- Determining when this is the case can be difficult.
- It is most common to monitor the residuals.

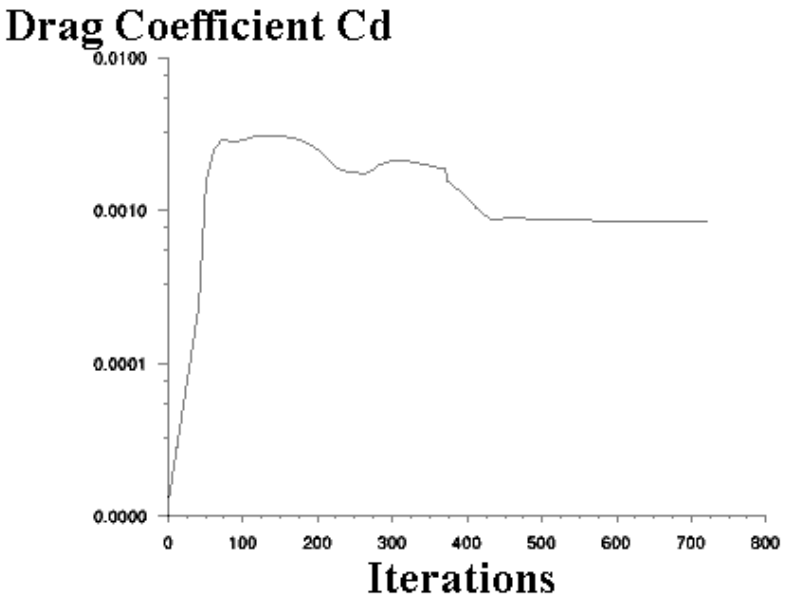
Monitor residuals

- If the residuals have met the specified convergence criterion but are still decreasing, the solution may not yet be converged.
- If the residuals never meet the convergence criterion but are no longer decreasing and other solution monitors do not change either, the solution is converged.
- Residuals are not your solution! Low residuals do not automatically mean a correct solution, and high residuals do not automatically mean a wrong solution.
- Final residuals are often higher with higher order discretization schemes than with first order discretization. That does not mean that the first order solution is better!
- Residuals can be monitored graphically also.



Other convergence monitors

- For models whose purpose is to calculate a force on an object, the predicted force itself should be monitored for convergence.
- E.g., for an airfoil, one should monitor the predicted drag coefficient.



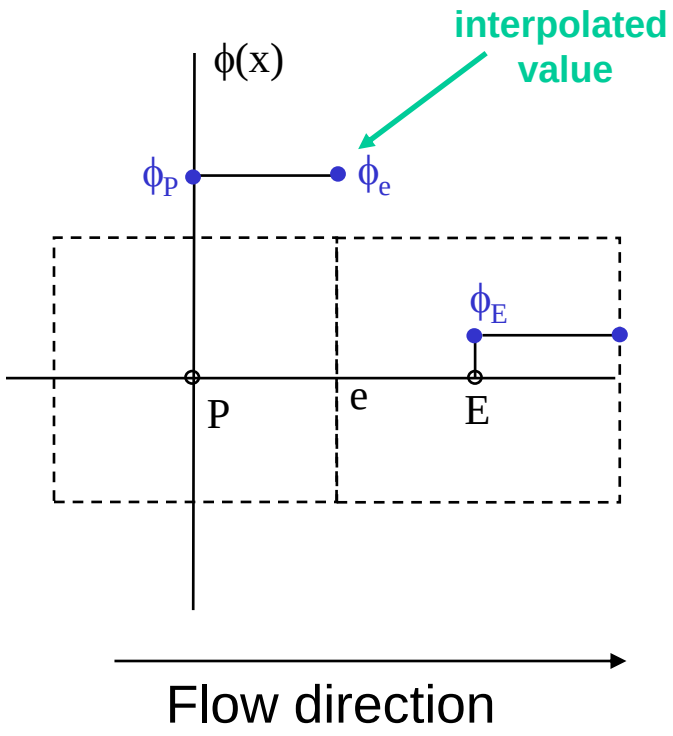
- Overall mass balance should be satisfied.
- When modeling rotating equipment such as turbofans or mixing impellers, the predicted torque should be monitored.
- For heat transfer problems, the temperature at important locations can be monitored.
- One can automatically generate flow field plots every 50 iterations or so to visually review the flow field and ensure that it is no longer changing.

Numerical schemes: finding face values

- Face values of ϕ and $\partial\phi/\partial x$ are found by making assumptions about variation of ϕ between cell centers.
- Number of different schemes can be devised:
  - First-order upwind scheme.
  - Central differencing scheme.
  - Power-law scheme.
  - Second-order upwind scheme.
  - QUICK scheme.
- We will discuss these one by one.

First order upwind scheme

- This is the simplest numerical scheme. It is the method that we used earlier in the discretization example.
- We assume that the value of ϕ at the face is the same as the cell centered value in the cell upstream of the face.
- The main advantages are that it is easy to implement and that it results in very stable calculations, but it also very diffusive. Gradients in the flow field tend to be smeared out, as we will show later.
- This is often the best scheme to start calculations with.

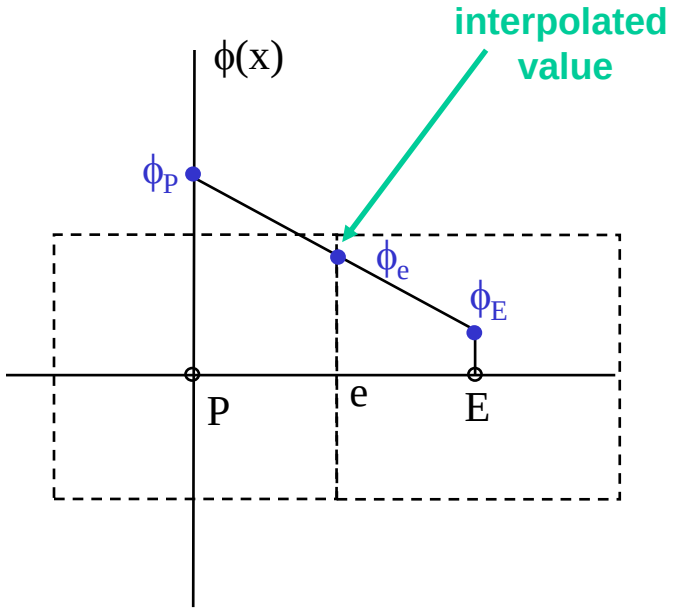


Central differencing scheme

- We determine the value of ϕ at the face by linear interpolation between the cell centered values.
- This is more accurate than the first order upwind scheme, but it leads to oscillations in the solution or divergence if the local Peclet number is larger than 2. The Peclet number is the ratio between convective and diffusive transport:

$$Pe = \frac{\rho u L}{\mathbf{D}}$$

- It is common to then switch to first order upwind in cells where Pe>2. Such an approach is called a hybrid scheme.

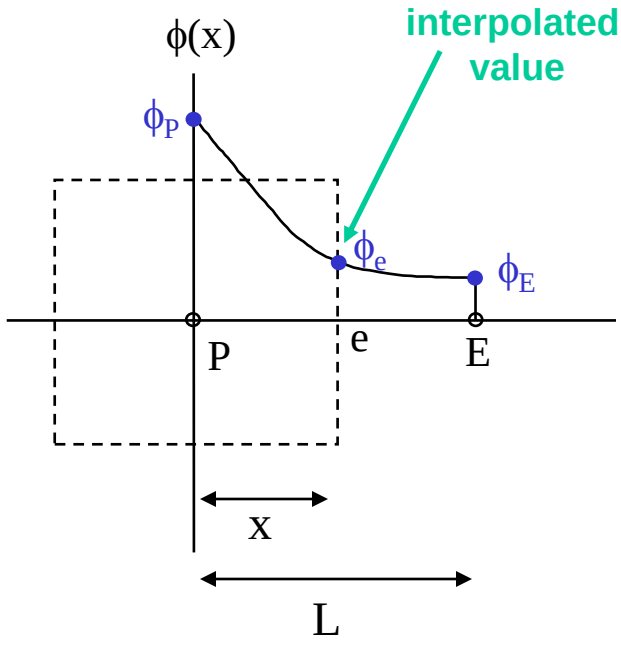


Power law scheme

- This is based on the analytical solution of the one-dimensional convection-diffusion equation.
- The face value is determined from an exponential profile through the cell values. The exponential profile is approximated by the following power law equation:

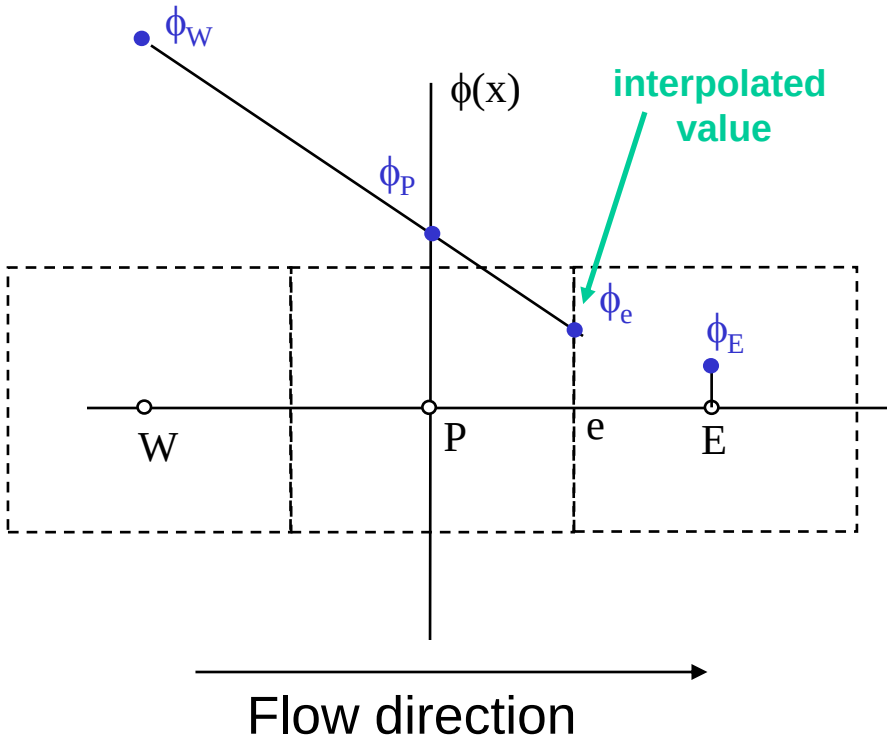
$$\phi_e = \phi_P - \frac{(1-0.1\mathrm{Pe})^5}{\mathrm{Pe}}(\phi_E - \phi_P)$$

- Pe is again the Peclet number.
- For Pe>10, diffusion is ignored and first order upwind is used.



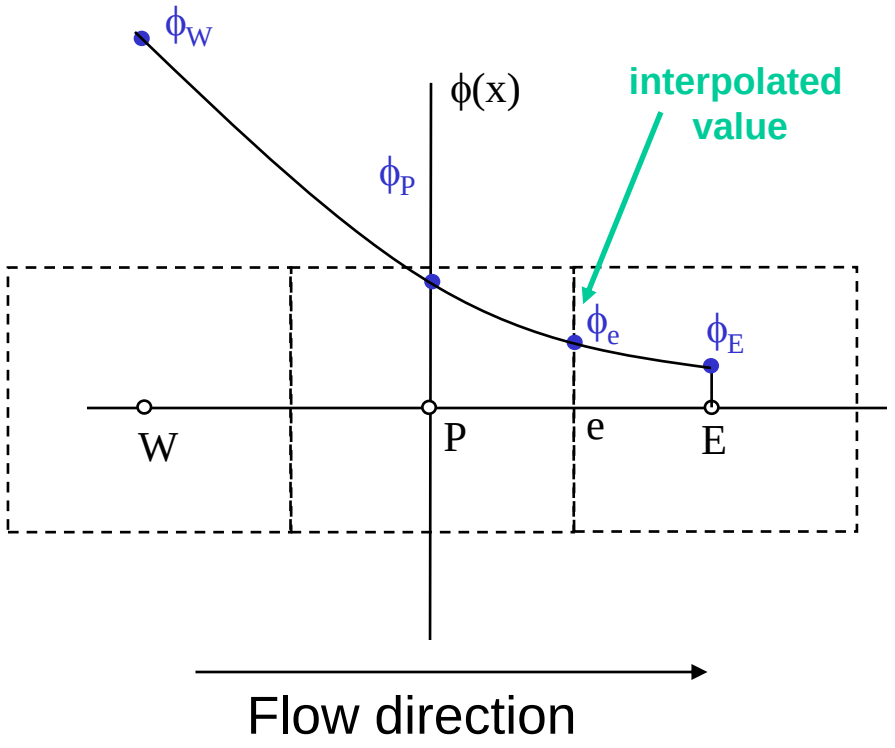
Second-order upwind scheme

- We determine the value of ϕ from the cell values in the two cells upstream of the face.
- This is more accurate than the first order upwind scheme, but in regions with strong gradients it can result in face values that are outside of the range of cell values. It is then necessary to apply limiters to the predicted face values.
- There are many different ways to implement this, but second-order upwind with limiters is one of the more popular numerical schemes because of its combination of accuracy and stability.



QUICK scheme

- QUICK stands for Quadratic Upwind Interpolation for Convective Kinetics.
- A quadratic curve is fitted through two upstream nodes and one downstream node.
- This is a very accurate scheme, but in regions with strong gradients, overshoots and undershoots can occur. This can lead to stability problems in the calculation.



Accuracy of numerical schemes

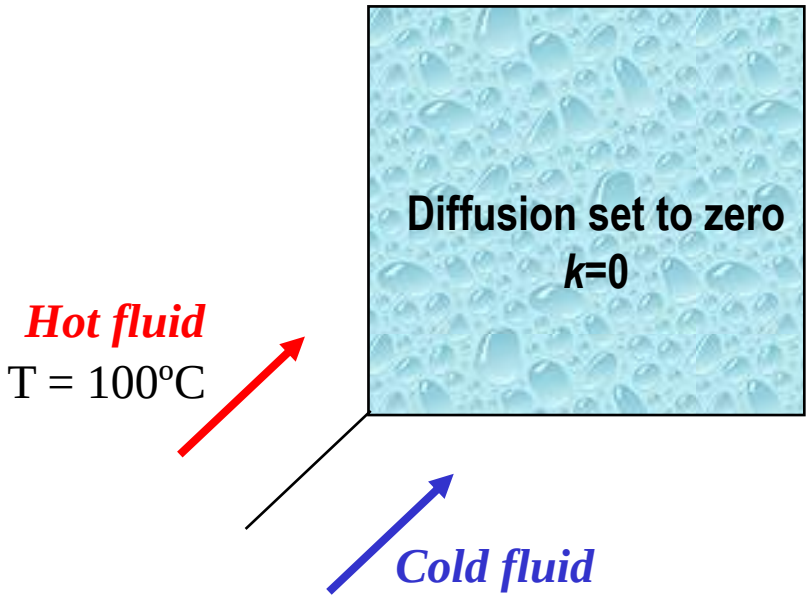
- Each of the previously discussed numerical schemes assumes some shape of the function ϕ. These functions can be approximated by Taylor series polynomials:

$$\phi(x_e) = \phi(x_P) + \frac{\phi'(x_P)}{1!}(x_e - x_P) + \frac{\phi''(x_P)}{2!}(x_e - x_P)^2 + ... + \frac{\phi^n(x_P)}{n!}(x_e - x_P)^n + ...$$

- The first order upwind scheme only uses the constant and ignores the first derivative and consecutive terms. This scheme is therefore considered first order accurate.
- For high Peclet numbers the power law scheme reduces to the first order upwind scheme, so it is also considered first order accurate.
- The central differencing scheme and second order upwind scheme do include the first order derivative but ignore the second order derivative. These schemes are therefore considered second order accurate. QUICK does take the second order derivative into account but ignores the third order derivative. This is then considered third order accurate.

Accuracy and false diffusion (1)

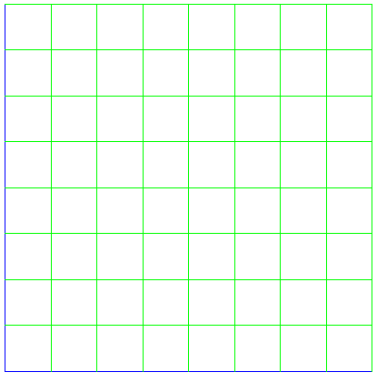
- False diffusion is numerically introduced diffusion and arises in convection dominated flows, i.e., high Pe number flows.
- Consider the problem below. If there is no false diffusion, the temperature will be exactly 100 ºC everywhere above the diagonal and exactly 0 ºC everywhere below the diagonal.
- False diffusion will occur due to the oblique flow direction and non-zero gradient of temperature in the direction normal to the flow.
- Grid refinement coupled with a higher-order interpolation scheme will minimize the false diffusion as shown on the next slide.

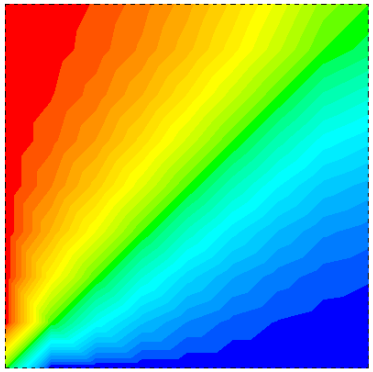


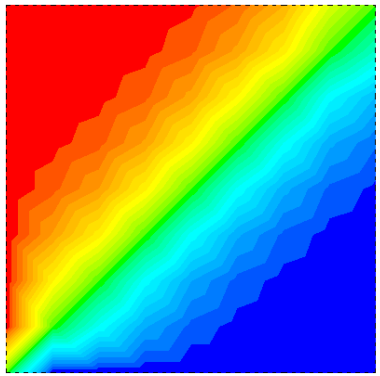
Accuracy and false diffusion (2)

First-order Upwind *Second-order Upwind*

8 x 8







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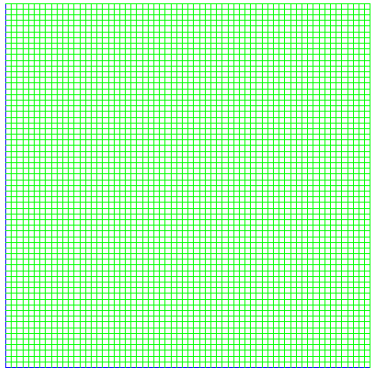
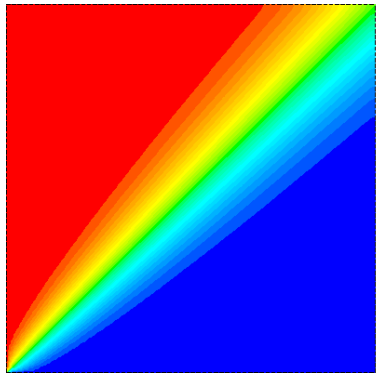
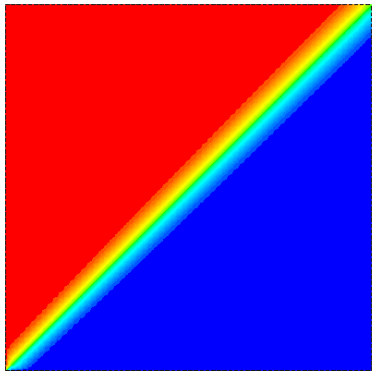






Properties of numerical schemes

- All numerical schemes must have the following properties:
  - Conservativeness: global conservation of the fluid property ϕ must be ensured.
  - Boundedness: values predicted by the scheme should be within realistic bounds. For linear problems without sources, those would be the maximum and minimum boundary values. Fluid flow is non-linear and values in the domain may be outside the range of boundary values.
  - Transportiveness: diffusion works in all directions but convection only in the flow direction. The numerical scheme should recognize the direction of the flow as it affects the strength of convection versus diffusion.
- The central differencing scheme does not have the transportiveness property. The other schemes that were discussed have all three of these properties.

Solution accuracy

- Higher order schemes will be more accurate. They will also be less stable and will increase computational time.
- It is recommended to always start calculations with first order upwind and after 100 iterations or so to switch over to second order upwind.
- This provides a good combination of stability and accuracy.
- The central differencing scheme should only be used for transient calculations involving the large eddy simulation (LES) turbulence models in combination with grids that are fine enough that the Peclet number is always less than one.
- It is recommended to only use the power law or QUICK schemes if it is known that those are somehow especially suitable for the particular problem being studied.

Pressure

- We saw how convection-diffusion equations can be solved. Such equations are available for all variables, except for the pressure.
- Gradients in the pressure appear in the momentum equations, thus the pressure field needs to be calculated in order to be able to solve these equations.
- If the flow is compressible:
  - The continuity equation can be used to compute density.
  - Temperature follows from the enthalpy equation.
  - Pressure can then be calculated from the equation of state $p=p(\rho,T)$.
- However, if the flow is incompressible the density is constant and not linked to pressure.
- The solution of the Navier-Stokes equations is then complicated by the lack of an independent equation for pressure.

Pressure - velocity coupling

- Pressure appears in all three momentum equations. The velocity field also has to satisfy the continuity equation. So even though there is no explicit equation for pressure, we do have four equations for four variables, and the set of equations is closed.
- So-called pressure-velocity coupling algorithms are used to derive equations for the pressure from the momentum equations and the continuity equation.
- A commonly used algorithm is the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations). An algebraic equation for the pressure correction p' is derived, in a form similar to the equations derived for the convection-diffusion equations:

$$a_P p' = \sum_{nb} a_{nb} p' + b'$$

- Each iteration, the pressure field is updated by applying the pressure correction. The source term b' is the continuity imbalance. The other coefficients depend on the mesh and the flow field.

Principle behind SIMPLE

- The principle behind SIMPLE is quite simple!
- It is based on the premise that fluid flows from regions with high pressure to low pressure.
  - Start with an initial pressure field.
  - Look at a cell.
  - If continuity is not satisfied because there is more mass flowing into that cell than out of the cell, the pressure in that cell compared to the neighboring cells must be too low.
  - Thus, the pressure in that cell must be increased relative to the neighboring cells.
  - The reverse is true for cells where more mass flows out than in.
  - Repeat this process iteratively for all cells.
- The trick is in finding a good equation for the pressure correction as a function of mass imbalance. These equations will not be discussed here but can be readily found in the literature.

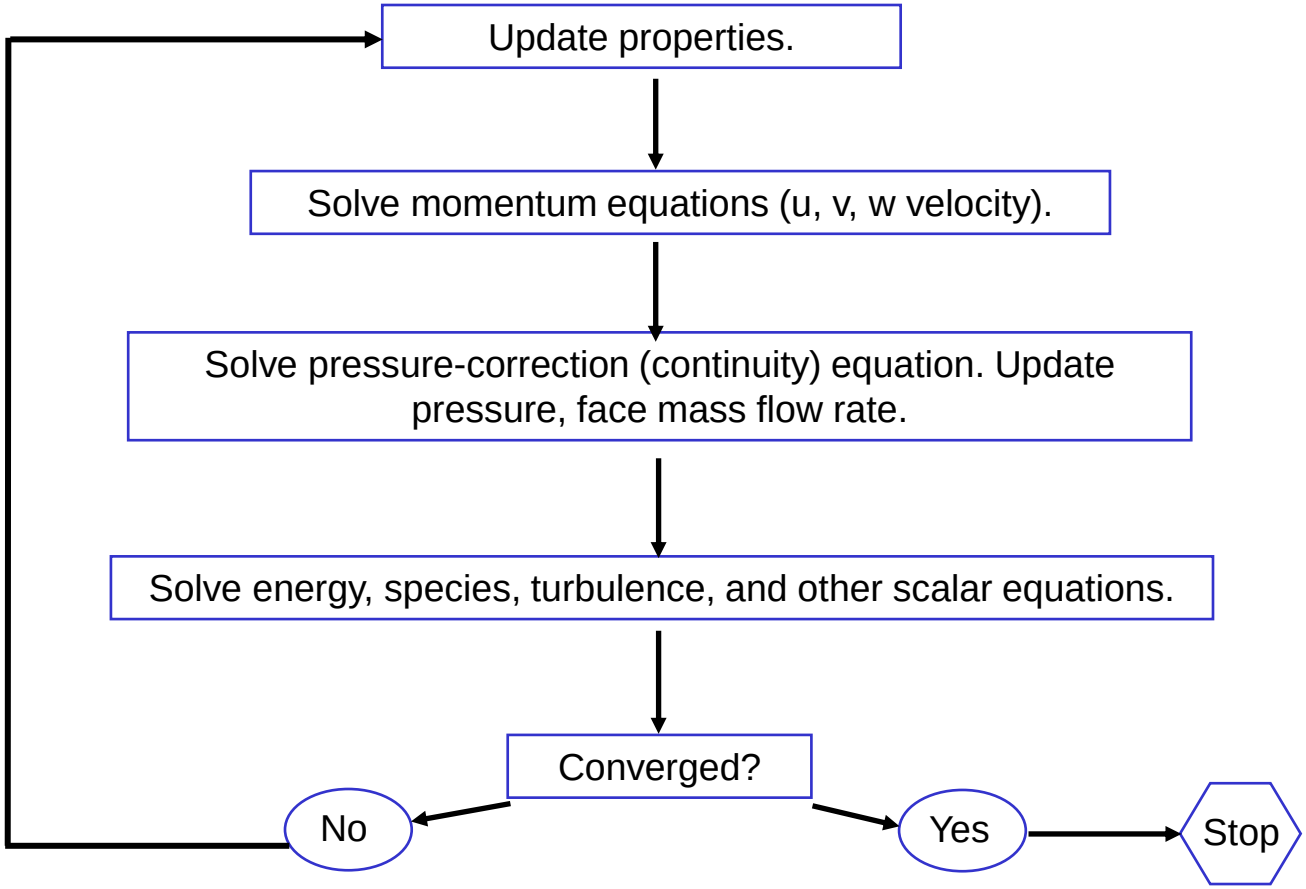
Improvements on SIMPLE

- SIMPLE is the default algorithm in most commercial finite volume codes.
- Improved versions are:
  - SIMPLER (SIMPLE Revised).
  - SIMPLEC (SIMPLE Consistent).
  - PISO (Pressure Implicit with Splitting of Operators).
- All these algorithms can speed up convergence because they allow for the use of larger underrelaxation factors than SIMPLE.
- All of these will eventually converge to the same solution. The differences are in speed and stability.
- Which algorithm is fastest depends on the flow and there is no single algorithm that is always faster than the other ones.

Finite volume solution methods

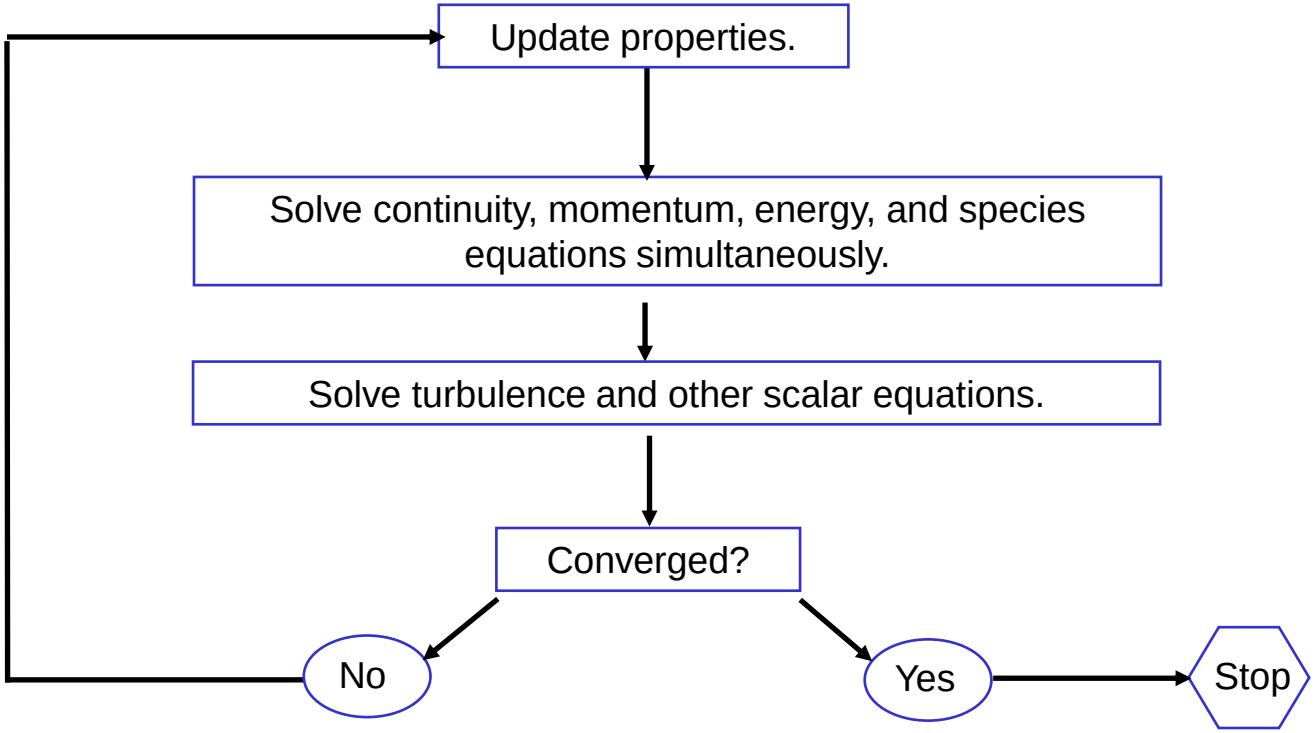
- The finite volume solution method can either use a “segregated” or a “coupled” solution procedure.
- With segregated methods an equation for a certain variable is solved for all cells, then the equation for the next variable is solved for all cells, etc.
- With coupled methods, for a given cell equations for all variables are solved, and that process is then repeated for all cells.
- The segregated solution method is the default method in most commercial finite volume codes. It is best suited for incompressible flows or compressible flows at low Mach number.
- Compressible flows at high Mach number, especially when they involve shock waves, are best solved with the coupled solver.

Segregated solution procedure



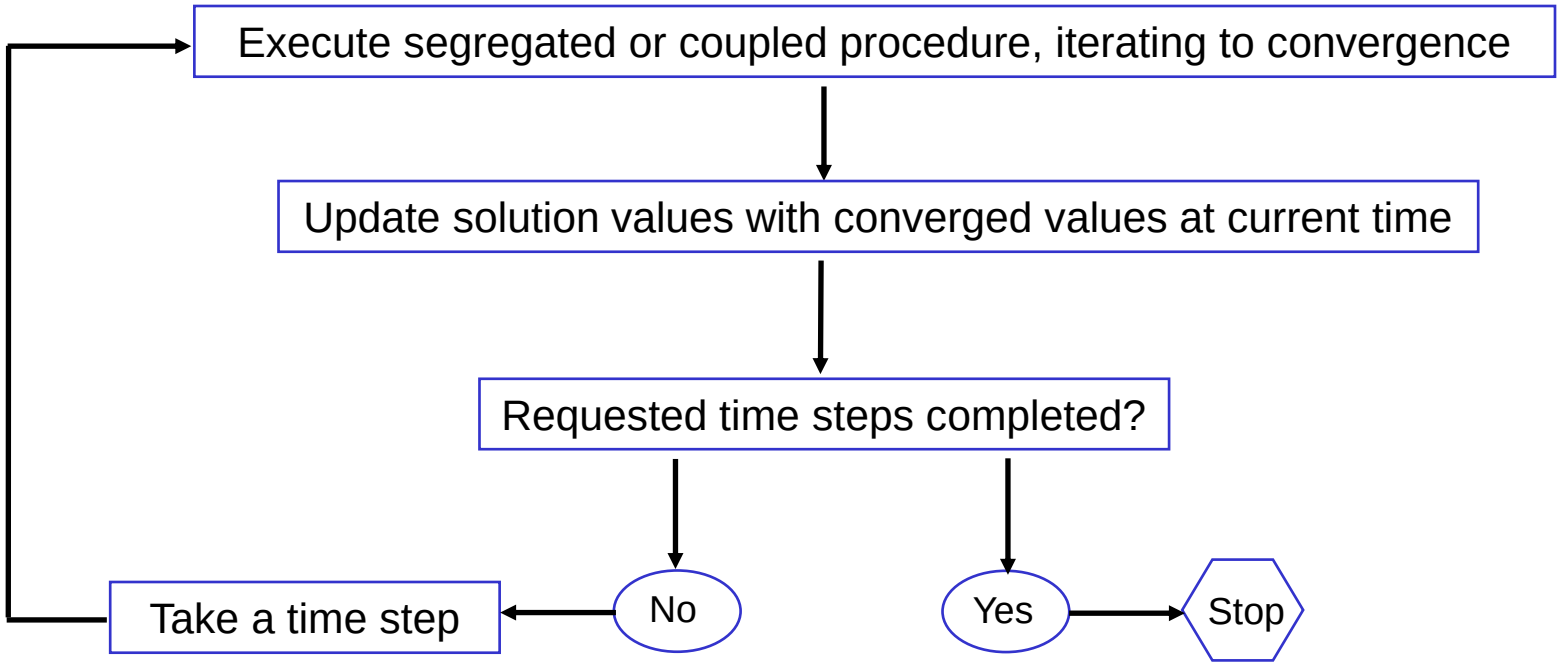
Coupled solution procedure

- When the coupled solver is used for steady state calculations it essentially employs a modified time dependent solution algorithm, using a time step $\Delta t = CFL/(u/L)$ with CFL being the user specified Courant-Friedrich-Levy number, L being a measure of the size of the cell, and u being a measure of the local velocities.



Unsteady solution procedure

- Same procedure for segregated and coupled solvers.
- The user has to specify a time step that matches the time variation in the flow.
- If a time accurate solution is required, the solution should be converged at every time step. Otherwise, convergence at every time step may not be necessary.

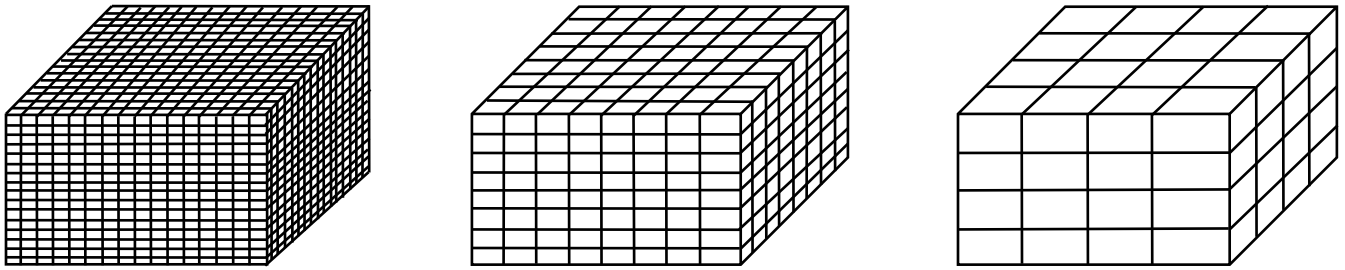


The multigrid solver

- The algebraic equation $a_P \phi_P = \sum_{nb} a_{nb} \phi_{nb} + b$ can be solved by sweeping through the domain cell-by-cell in an iterative manner.
- This method reduces local errors quickly but can be slow in reducing long-wavelength errors.
- On large grids, it can take a long time to see the effect of faraway grid points and boundaries.
- Multigrid acceleration is a method to speed up convergence for:
  - Large number of cells.
  - Large cell aspect ratios (e.g., $\Delta x/\Delta y > 20$).
  - Large differences in thermal conductivity such as in conjugate heat transfer problems.

The multigrid solver

- The multigrid solver uses a sequence of grids going from fine to coarse.
- The influence of boundaries and far-away points is more easily transmitted to the interior on coarse meshes than on fine meshes.
- In coarse meshes, grid points are closer together in the computational space and have fewer computational cells between any two spatial locations.
- Fine meshes give more accurate solutions.



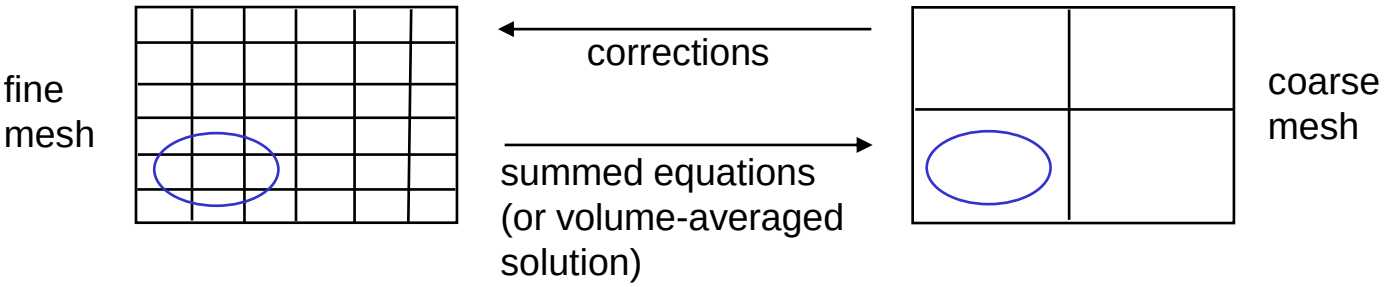
original grid

coarse grid
level 1

coarse grid
level 2

The multigrid solver

- The solution on the coarser meshes is used as a starting point for solutions on the finer meshes.
- The coarse-mesh solution contains the influence of boundaries and far neighbors. These effects are felt more easily on coarse meshes.
- This accelerates convergence on the fine mesh.
- The final solution is obtained for the original (fine) mesh.
- Coarse mesh calculations only accelerate convergence and do not change the final answer.



Finite volume method - summary

- The FVM uses the integral conservation equation applied to control volumes which subdivide the solution domain, and to the entire solution domain.
- The variable values at the faces of the control volume are determined by interpolation. False diffusion can arise depending on the choice of interpolation scheme.
- The grid must be refined to reduce “smearing” of the solution as shown in the last example.
- Advantages of FVM: integral conservation is exactly satisfied, and the method is not limited to grid type (structured or unstructured, Cartesian or body-fitted).
- Always ensure proper convergence.

Lecture 6 - Boundary Conditions

Applied Computational Fluid Dynamics

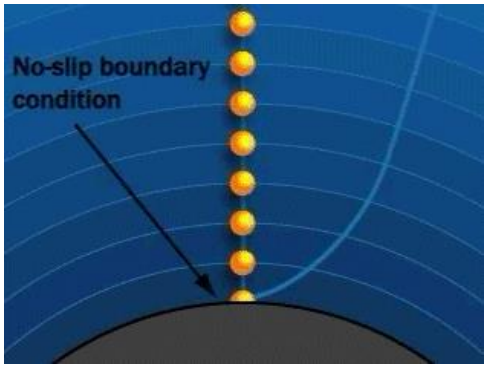
André Bakker

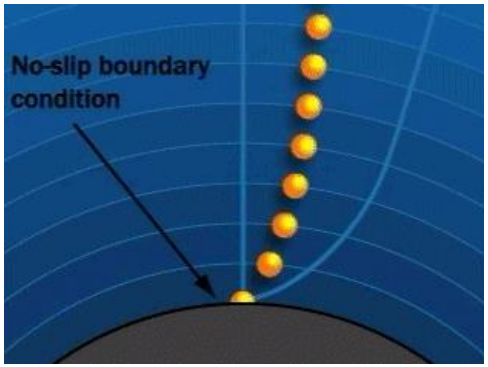
Outline

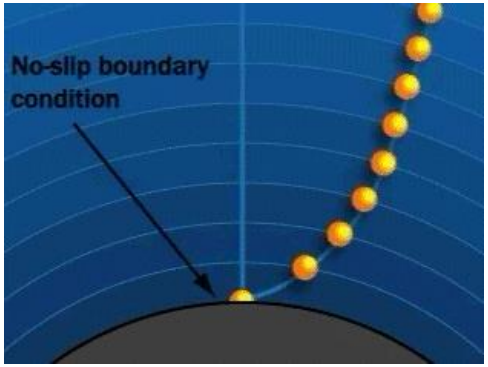
- Overview.
- Inlet and outlet boundaries.
  - Velocity.
  - Pressure boundaries and others.
- Wall, symmetry, periodic and axis boundaries.
- Internal cell zones.
  - Fluid, porous media, moving cell zones.
  - Solid.
- Internal face boundaries.
- Material properties.
- Proper specification.

Boundary conditions

- When solving the Navier-Stokes equation and continuity equation, appropriate initial conditions and boundary conditions need to be applied.
- In the example here, a no-slip boundary condition is applied at the solid wall.
- Boundary conditions will be treated in more detail in this lecture.



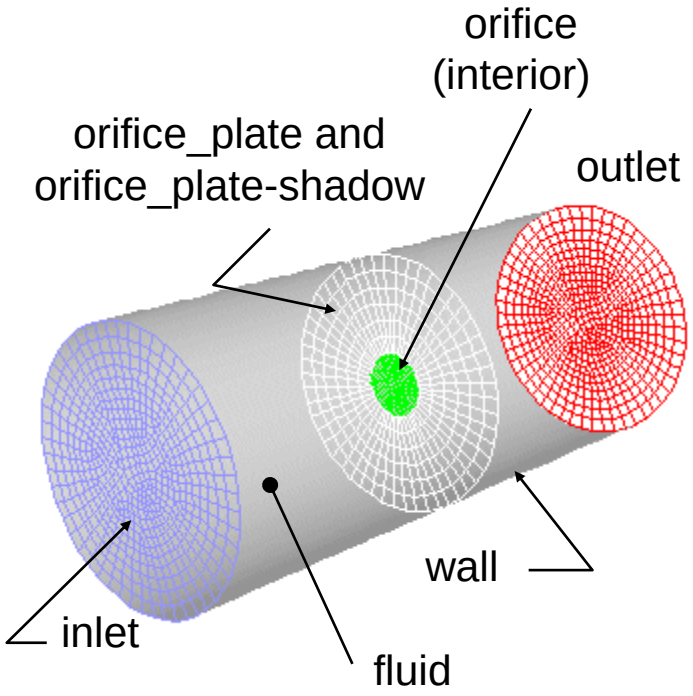




Images: Homsy et al. [2]

Overview

- Boundary conditions are a required component of the mathematical model.
- Boundaries direct motion of flow.
- Specify fluxes into the computational domain, e.g., mass, momentum, and energy.
- Fluid and solid regions are represented by cell zones.
- Material and source terms are assigned to cell zones.
- Boundaries and internal surfaces are represented by face zones.
- Boundary data are assigned to face zones.



Example: face and cell zones associated with pipe flow through orifice plate

Neumann and Dirichlet boundary conditions

- When using a Dirichlet boundary condition, one prescribes the value of a variable at the boundary, e.g., $u(x) = constant$.
- When using a Neumann boundary condition, one prescribes the gradient normal to the boundary of a variable at the boundary, e.g., $\partial_n u(x) = constant$.
- When using a mixed boundary condition, a function of the form $au(x)+b\partial_n u(x) = constant$ is applied.
- Note that at a given boundary, different types of boundary conditions can be used for different variables.

Flow inlets and outlets

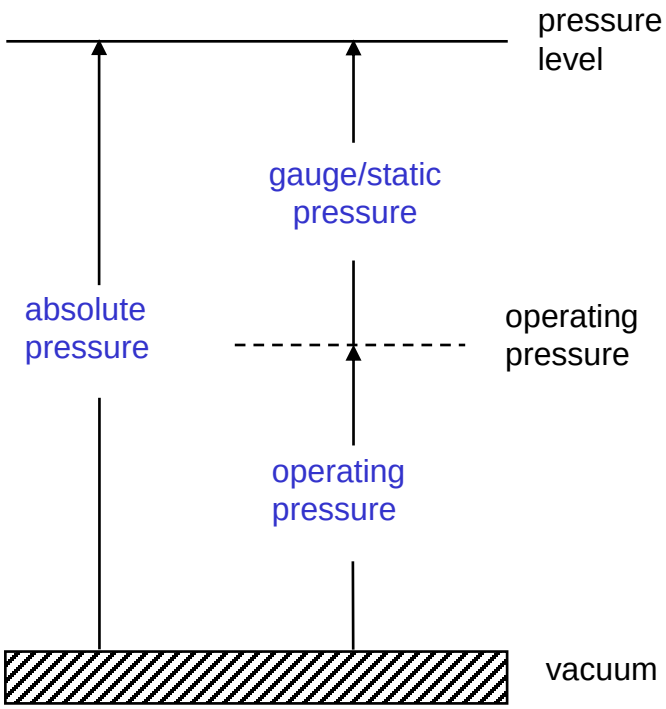
- A wide range of boundary conditions types permit the flow to enter and exit the solution domain:
  - General: pressure inlet, pressure outlet.
  - Incompressible flow: velocity inlet, outflow.
  - Compressible flows: mass flow inlet, pressure far-field.
  - Special: inlet vent, outlet vent, intake fan, exhaust fan.
- Boundary data required depends on physical models selected.
- General guidelines:
  - Select boundary location and shape such that flow either goes in or out. Not mandatory but will typically result in better convergence.
  - Should not observe large gradients in direction normal to boundary near inlets and outlets. This indicates an incorrect problem specification.
  - Minimize grid skewness near boundary.

Pressure boundary conditions

- Pressure boundary conditions require static gauge pressure inputs:

$$p_{absolute} = p_{static} + p_{operating}$$

- The operating pressure input is set separately.
- Useful when:
  - Neither the flow rate nor the velocity are known (e.g., buoyancy-driven flows).
  - A “free” boundary in an external or unconfined flow needs to be defined.



Pressure inlet boundary (1)

- One defines the total gauge pressure, temperature, and other scalar quantities at flow inlets:

$$p_{total} = p_{static} + \frac{1}{2}\rho v^2 \qquad \text{incompressible flows}$$

$$p_{total} = p_{static}\left(1 + \frac{k-1}{2} M^2\right)^{k/(k-1)} \qquad \text{compressible flows}$$

- Here k is the ratio of specific heats (c_p/c_v) and M is the Mach number. If the inlet flow is supersonic you should also specify the static pressure.
- Suitable for compressible and incompressible flows. Mass flux through boundary varies depending on interior solution and specified flow direction.
- The flow direction must be defined, and one can get non-physical results if no reasonable direction is specified.
- Outflow can occur at pressure inlet boundaries. In that case the flow direction is taken from the interior solution.

Pressure inlet boundary (2)

- For non-isothermal incompressible flows, one specifies the inlet temperature.
- For compressible flows, one specifies the total temperature T_0, which is defined as the temperature that the flow would have if it were brought to a standstill under isentropic conditions:

$$T_0 = T_S \left[1 + \frac{k-1}{2} M^2 \right]$$

- Here k is the ratio of specific heats (c_p/c_v), M is the Mach number, and T_s is the static temperature.

Pressure outlet boundary

- Here one defines the static/gauge pressure at the outlet boundary. This is interpreted as the static pressure of the environment into which the flow exhausts.
- Usually, the static pressure is assumed to be constant over the outlet. A radial equilibrium pressure distribution option is available for cases where that is not appropriate, e.g., for strongly swirling flows.
- Backflow can occur at pressure outlet boundaries:
  - During solution process or as part of solution.
  - Backflow is assumed to be normal to the boundary.
  - Convergence difficulties minimized by realistic values for backflow quantities.
  - Value specified for static pressure used as total pressure wherever backflow occurs.
- Pressure outlet must always be used when model is set up with a pressure inlet.

Velocity inlets

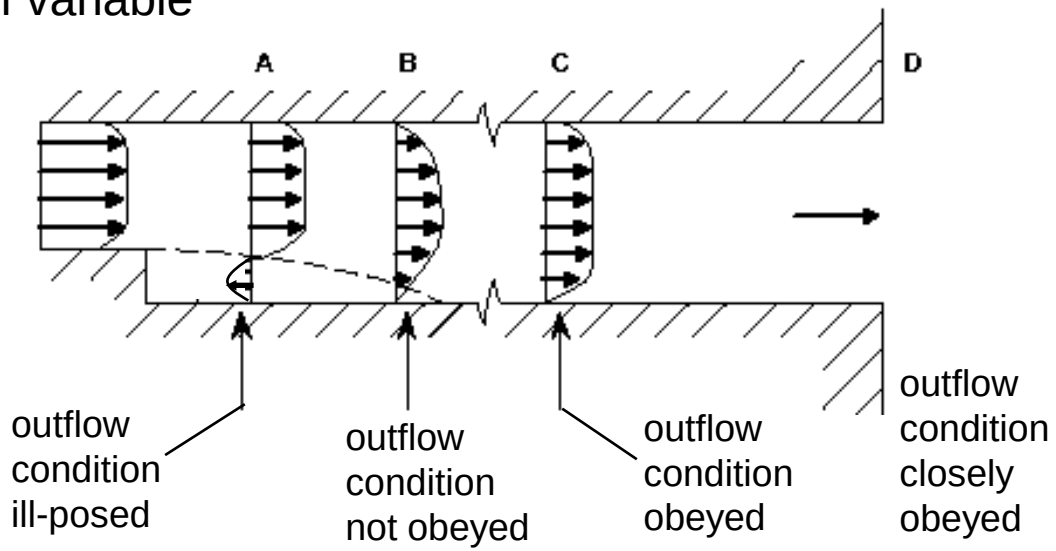
- Defines velocity vector and scalar properties of flow at inlet boundaries.
- Useful when velocity profile is known at inlet. Uniform profile is default but other profiles can be implemented too.
- Intended for incompressible flows. The total (stagnation) properties of flow are not fixed. Stagnation properties vary to accommodate prescribed velocity distribution. Using in compressible flows can lead to non-physical results.
- Avoid placing a velocity inlet too close to a solid obstruction. This can force the solution to be non-physical.

Outflow boundary

- Outflow boundary conditions are used to model flow exits where the details of the flow velocity and pressure are not known prior to solution of the flow problem.
- Appropriate where the exit flow is close to a fully developed condition, as the outflow boundary condition assumes a zero normal gradient for all flow variables except pressure. The solver extrapolates the required information from interior.
- Furthermore, an overall mass balance correction is applied.

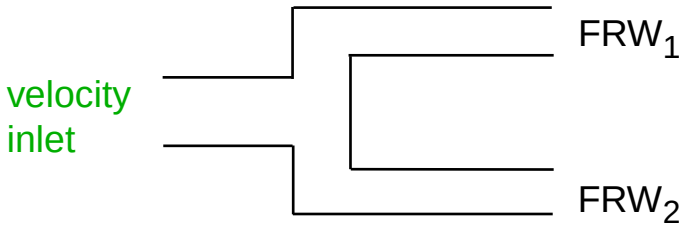
Restrictions on outflow boundaries

- Outflow boundaries cannot be used:
  - With compressible flows.
  - With the pressure inlet boundary condition (use velocity inlet instead) because the combination does not uniquely set a pressure gradient over the whole domain.
  - In unsteady flows with variable density.
- Do not use outflow boundaries where:
  - Flow enters domain or when backflow occurs (in that case use pressure b.c.).
  - Gradients in flow direction are significant.
  - Conditions downstream of exit plane impact flow in domain.

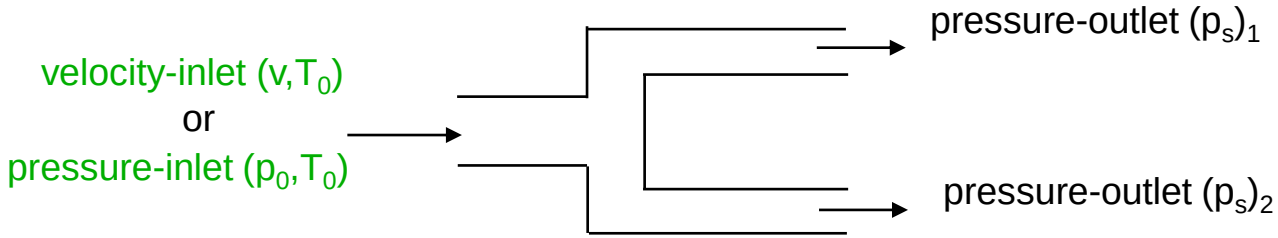


Modeling multiple exits

- Using outflow boundary condition:
  - Mass flow divided equally among all outflow boundaries by default.
  - Flow rate weighting (FRW) set to one by default.
  - For uneven flow distribution one can specify the flow rate weighting for each outflow boundary: $m_i = FRW_i / \Sigma FRW_i$. The static pressure then varies among the exits to accommodate this flow distribution.



- Can also use pressure outlet boundaries to define exits.



Other inlet and outlet boundary conditions

- Mass flow inlet.
  - Used in compressible flows to prescribe mass flow rate at inlet.
  - Not required for incompressible flows.
- Pressure far field.
  - Available when density is calculated from the ideal gas law.
  - Used to model free-stream compressible flow at infinity, with free-stream Mach number and static conditions specified.
- Exhaust fan/outlet vent.
  - Model external exhaust fan/outlet vent with specified pressure jump/loss coefficient and ambient (discharge) pressure and temperature.
- Inlet vent/intake fan.
  - Model inlet vent/external intake fan with specified loss coefficient/ pressure jump, flow direction, and ambient (inlet) pressure and temperature.

Determining turbulence parameters

- When turbulent flow enters domain at inlet, outlet, or at a far-field boundary, boundary values are required for:
  - Turbulent kinetic energy *k.*
  - Turbulence dissipation rate ε.
- Four methods available for specifying turbulence parameters:
  - Set *k* and ε explicitly.
  - Set turbulence intensity and turbulence length scale.
  - Set turbulence intensity and turbulent viscosity ratio.
  - Set turbulence intensity and hydraulic diameter.

Turbulence intensity

- The turbulence intensity I is defined as:

$$I = \frac{\sqrt{\frac{2}{3}k}}{u}$$

- Here *k* is the turbulent kinetic energy and u is the local velocity magnitude.
- Intensity and length scale depend on conditions upstream:
  - Exhaust of a turbine.

    Intensity = 20%. Length scale = 1 - 10 % of blade span.
  - Downstream of perforated plate or screen.

    Intensity = 10%. Length scale = screen/hole size.
  - Fully-developed flow in a duct or pipe.

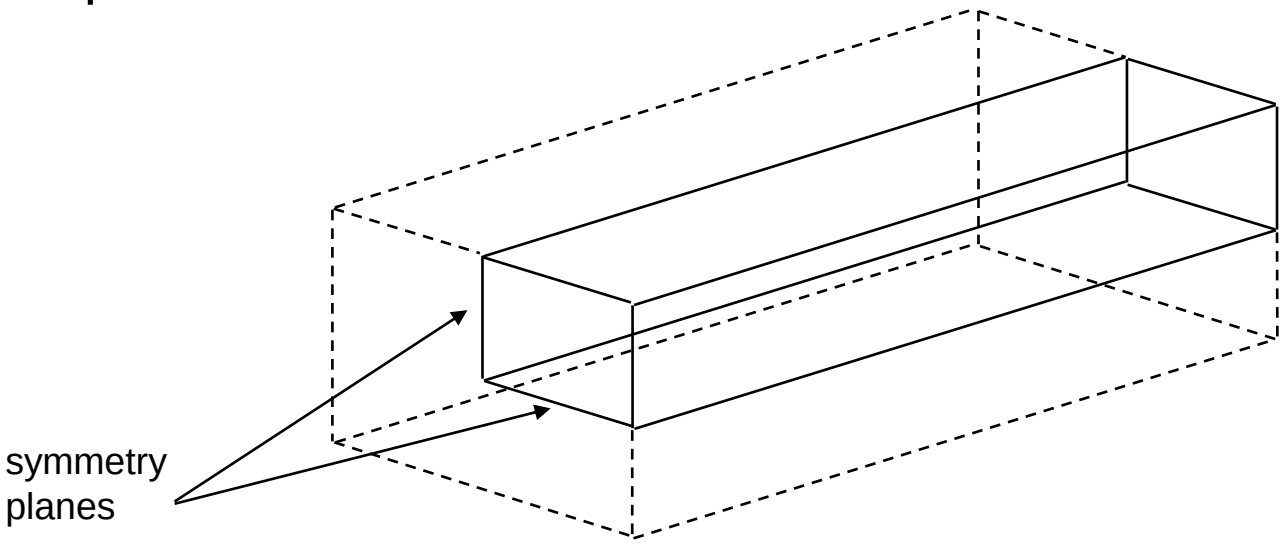
    Intensity = 5%. Length scale = hydraulic diameter.

Wall boundaries

- Used to bound fluid and solid regions.
- In viscous flows, no-slip condition enforced at walls.
  - Tangential fluid velocity equal to wall velocity.
  - Normal velocity component is set to be zero.
- Alternatively, one can specify the shear stress.
- Thermal boundary condition.
  - Several types available.
  - Wall material and thickness can be defined for 1-D or in-plane thin plate heat transfer calculations.
- Wall roughness can be defined for turbulent flows.
  - Wall shear stress and heat transfer based on local flow field.
- Translational or rotational velocity can be assigned to wall.

Symmetry boundaries

- Used to reduce computational effort in problem.
- Flow field and geometry must be symmetric:
  - Zero normal velocity at symmetry plane.
  - Zero normal gradients of all variables at symmetry plane.
- No inputs required.
  - Must take care to correctly define symmetry boundary locations.
- Also used to model slip walls in viscous flow.

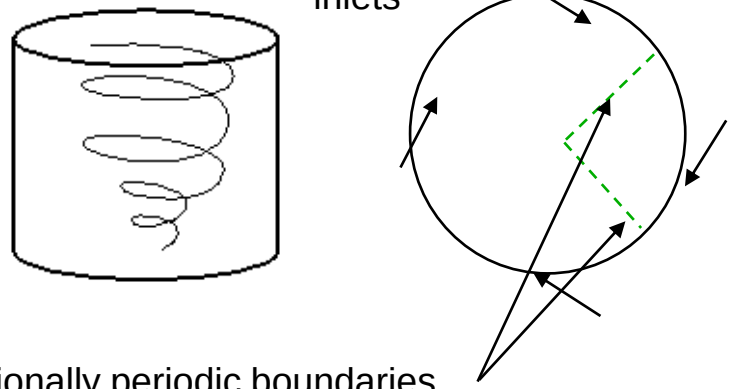


Periodic boundaries

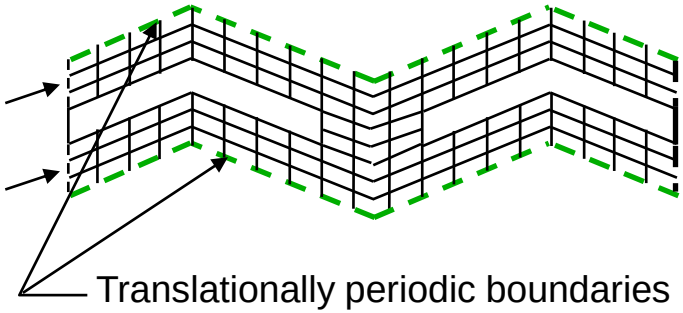
- Used when physical geometry of interest and expected flow pattern and the thermal solution are of a periodically repeating nature.
  - Reduces computational effort in problem.
- Two types available:
  - $\Delta p = 0$ across periodic planes.
    - Rotationally or translationally periodic.
    - Rotationally periodic boundaries require axis of rotation be defined in fluid zone.
  - Δp is finite across periodic planes.
    - Translationally periodic only.
    - Models fully developed conditions.
    - Specify either mean Δp per period or net mass flow rate.

Periodic boundaries: examples

- **$\Delta p = 0$:**

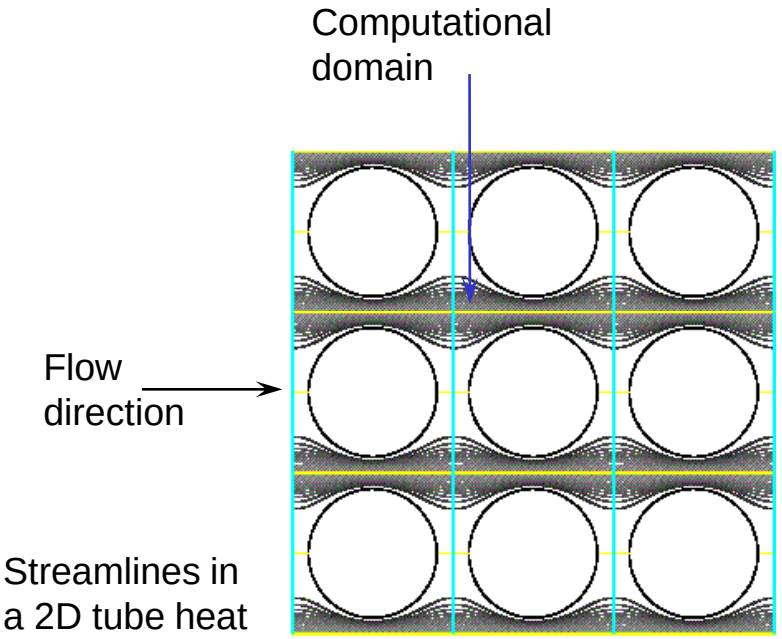


Rotationally periodic boundaries



Translationally periodic boundaries

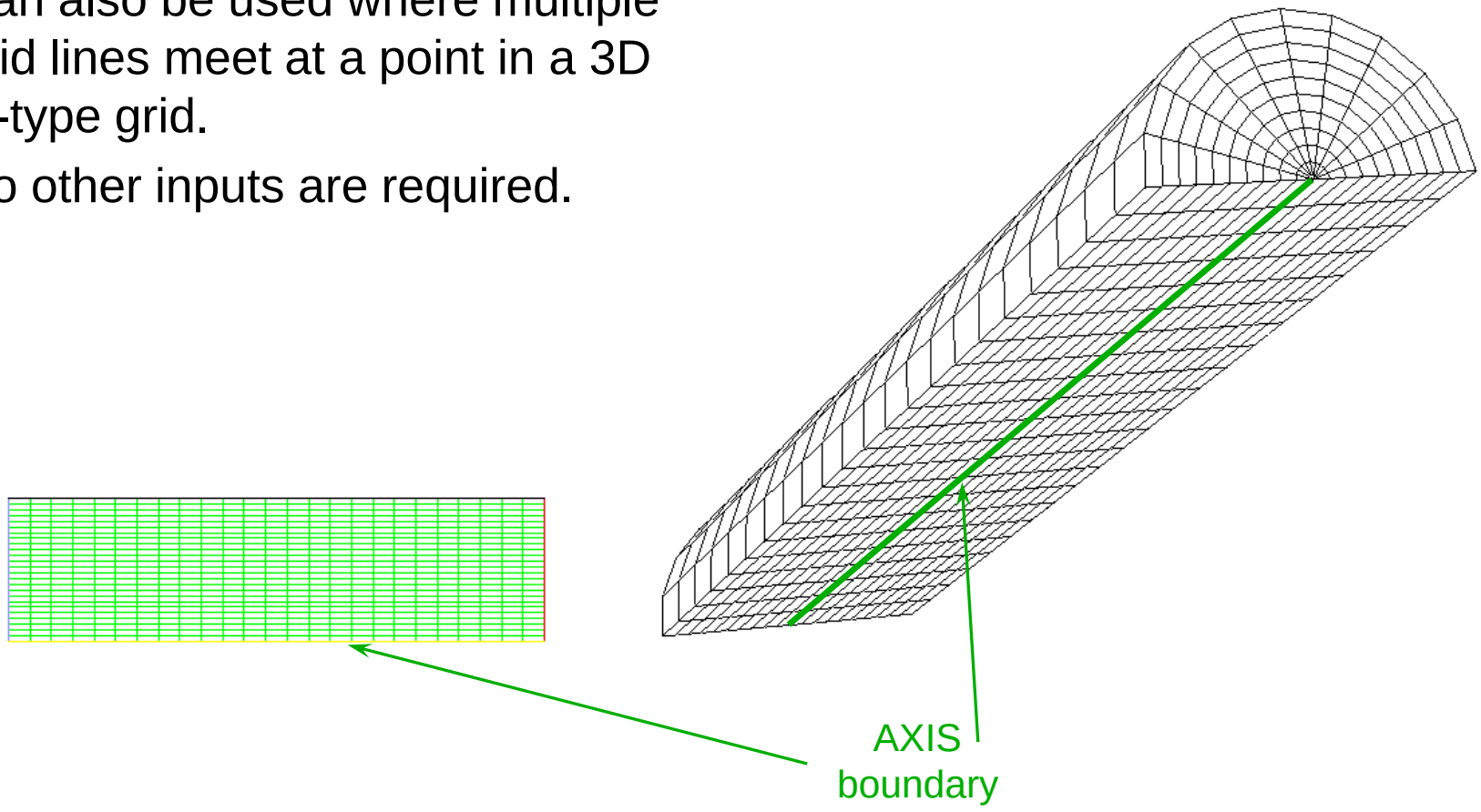
- **$\Delta p > 0$:**



Streamlines in
a 2D tube heat
exchanger

Axis boundaries

- Used at the centerline (y=0) of a 2-D axisymmetric grid.
- Can also be used where multiple grid lines meet at a point in a 3D O-type grid.
- No other inputs are required.

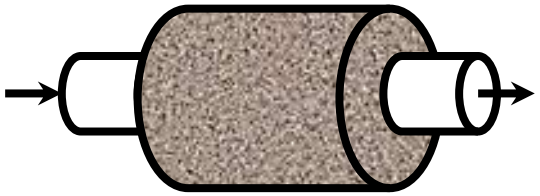


Cell zones: fluid

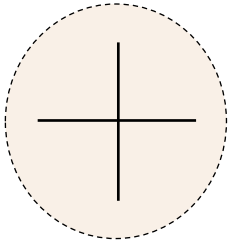
- A fluid zone is the group of cells for which all active equations are solved.
- Fluid material input required.
  - Single species, phase.
- Optional inputs allow setting of source terms:
  - Mass, momentum, energy, etc.
- Define fluid zone as laminar flow region if modeling transitional flow.
- Can define zone as porous media.
- Define axis of rotation for rotationally periodic flows.
- Can define motion for fluid zone.

Porous media conditions

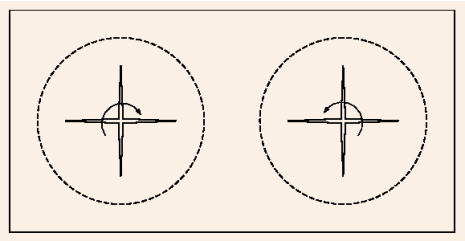
- Porous zone modeled as special type of fluid zone.
  - Enable the porous zone option in the fluid boundary conditions panel.
  - Pressure loss in flow determined via user inputs of resistance coefficients to lumped parameter model.
- Used to model flow through porous media and other “distributed” resistances, e.g.:
  - Packed beds.
  - Filter papers.
  - Perforated plates.
  - Flow distributors.
  - Tube banks.



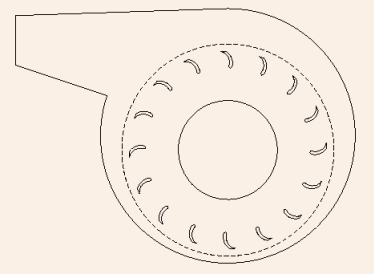
Moving zones



- For single zone problems use the rotating reference frame model. Define the whole zone as moving reference frame. This has limited applicability.
- For multiple zone problems each zone can be specified as having a moving reference frame:
  - Multiple reference frame model. Least accurate, least demanding on CPU.
  - Mixing plane model. Field data are averaged at the outlet of one zone and used as inlet boundary data to adjacent zone.



- Or each zone can be defined as moving mesh using the sliding mesh model. Must then also define interface. Mesh positions are calculated as a function of time. Relative motion must be tangential (no normal translation).



Cell zones: solid

- A solid zone is a group of cells for which only heat conduction is solved, and no flow equations are solved.
- The material being treated as solid may actually be fluid, but it is assumed that no convection takes place.
- The only required input is material type so that appropriate material properties are being used.
- Optional inputs allow you to set a volumetric heat generation rate (heat source).
- Need to specify rotation axis if rotationally periodic boundaries adjacent to solid zone.
- Can define motion for solid zone.

Internal face boundaries

- Defined on cell faces.
  - Do not have finite thickness.
  - Provide means of introducing step change in flow properties.
- Used to implement physical models representing:
  - Fans.
  - Radiators.
  - Porous jumps.
  - Interior walls. In that case also called “thin walls.”

Material properties

- For each zone, a material needs to be specified.
- For the material, relevant properties need to be specified:
  - Density.
  - Viscosity, may be non-Newtonian.
  - Heat capacity.
  - Molecular weight.
  - Thermal conductivity.
  - Diffusion coefficients.
- Which properties need to be specified depends on the model. Not all properties are always required.
- For mixtures, properties may have to be specified as a function of the mixture composition.

Fluid density

- For constant density, incompressible flow: ρ = constant.
- For compressible flow: $\rho = p_{absolute}/RT$.
- Density can also be defined as a function of temperature (polynomial, piece-wise polynomial, or the Boussinesq model where ρ is considered constant except for the buoyancy term in the momentum equations) or be defined with user specified functions.
- For incompressible flows where density is a function of temperature one can also use the so-called incompressible-ideal-gas law: $\rho = p_{operating}/RT$.
- Generally speaking, one should set $p_{operating}$ close to the mean pressure in the domain to avoid round-off errors.
- However, for high Mach number flows using the coupled solver, set $p_{operating}$ to zero.

When is a problem properly specified?

- Proper specification of boundary conditions is very important.
- Incorrect boundary conditions will lead to incorrect results.
- Boundary conditions may be overspecified or underspecified.
- Overspecification occurs when more boundary conditions are specified than appropriate and not all conditions can hold at the same time.
- Underspecification occurs when the problem is incompletely specified, e.g., there are boundaries for which no condition is specified.
- Commercially available CFD codes will usually perform a number of checks on the boundary condition set-up to prevent obvious errors from occurring.

Summary

- Zones are used to assign boundary conditions.
- Wide range of boundary conditions permit flow to enter and exit solution domain.
- Wall boundary conditions used to bound fluid and solid regions.
- Repeating boundaries used to reduce computational effort.
- Internal cell zones used to specify fluid, solid, and porous regions.
- Internal face boundaries provide way to introduce step change in flow properties.

Lecture 7 - Meshing

Applied Computational Fluid Dynamics

André Bakker

Outline

- Why is a grid needed?
- Element types.
- Grid types.
- Grid design guidelines.
- Geometry.
- Solution adaption.
- Grid import.

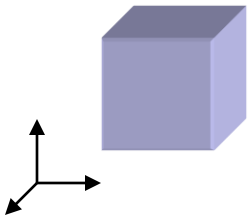
Why is a grid needed?

- The grid:
  - Designates the cells or elements on which the flow is solved.
  - Is a discrete representation of the geometry of the problem.
  - Has cells grouped into boundary zones where b.c.’s are applied.
- The grid has a significant impact on:
  - Rate of convergence (or even lack of convergence).
  - Solution accuracy.
  - CPU time required.
- Importance of mesh quality for good solutions.
  - Grid density.
  - Adjacent cell length/volume ratios.
  - Skewness.
  - Tet vs. hex.
  - Boundary layer mesh.
  - Mesh refinement through adaption.

Geometry

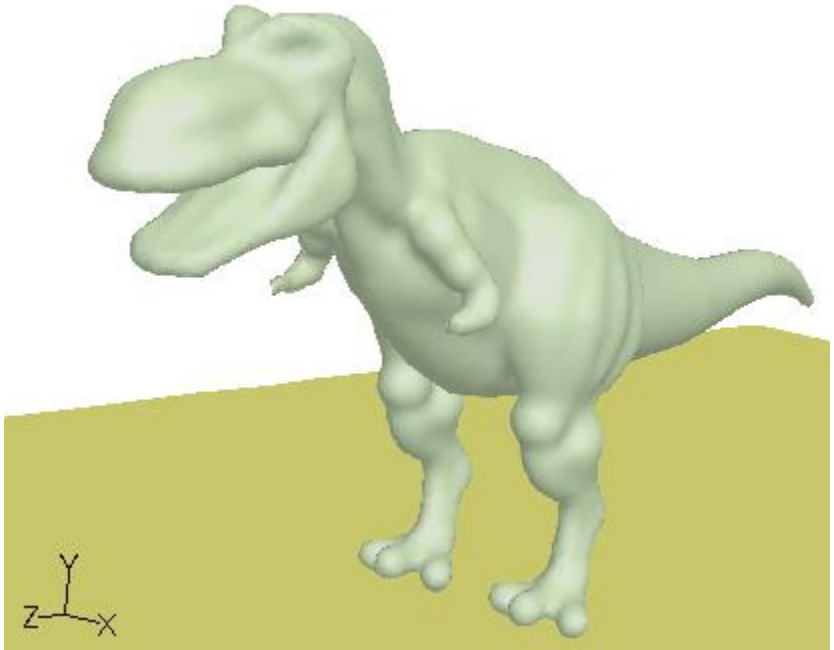
- The starting point for all problems is a “geometry.”
- The geometry describes the shape of the problem to be analyzed.
- Can consist of volumes, faces (surfaces), edges (curves) and vertices (points).

Geometry can be very simple...



geometry
for a “cube”

… or more complex

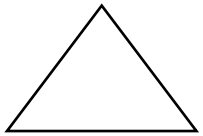


Geometry creation

- Geometries can be created top-down or bottom-up.
- Top-down refers to an approach where the computational domain is created by performing logical operations on primitive shapes such as cylinders, bricks, and spheres.
- Bottom-up refers to an approach where one first creates vertices (points), connects those to form edges (lines), connects the edges to create faces, and combines the faces to create volumes.
- Geometries can be created using the same pre-processor software that is used to create the grid, or created using other programs (e.g., CAD, graphics).

Typical cell shapes

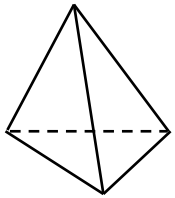
- Many different cell/element and grid types are available. Choice depends on the problem and the solver capabilities.
- Cell or element types:
  - 2D:



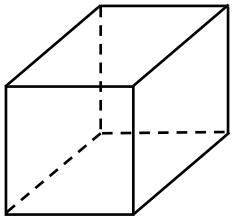
triangle (**"tri"**)

2D prism (**quadrilateral** or **"quad"**)

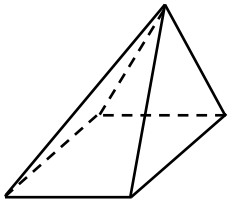
  - 3D:



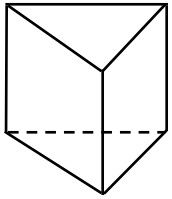
tetrahedron (**"tet"**)



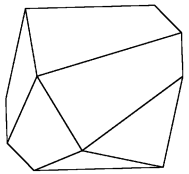
prism with quadrilateral base (**hexahedron** or **"hex"**)



pyramid



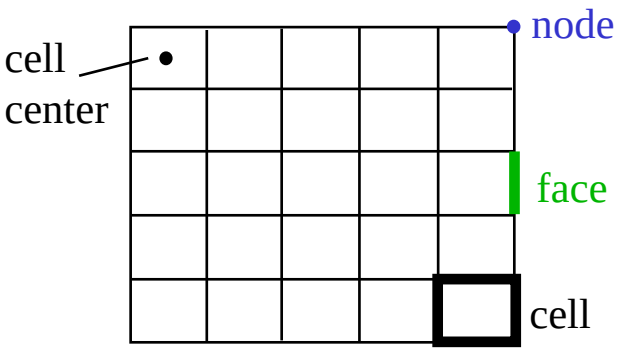
prism with triangular base (**wedge**)



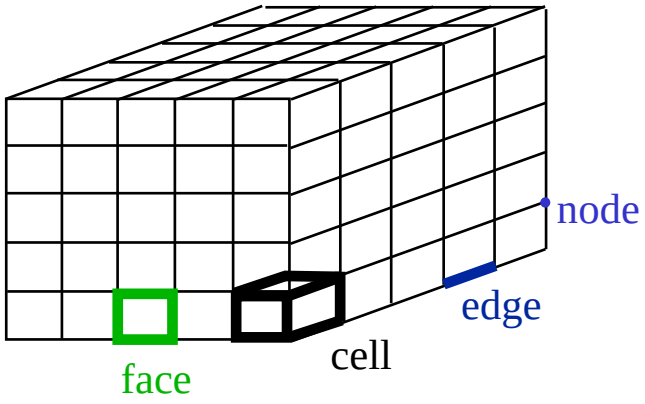
arbitrary polyhedron

Terminology

- Cell = control volume into which domain is broken up.
- Node = grid point.
- Cell center = center of a cell.
- Edge = boundary of a face.
- Face = boundary of a cell.
- Zone = grouping of nodes, faces, and cells:
  - Wall boundary zone.
  - Fluid cell zone.
- Domain = group of node, face and cell zones.



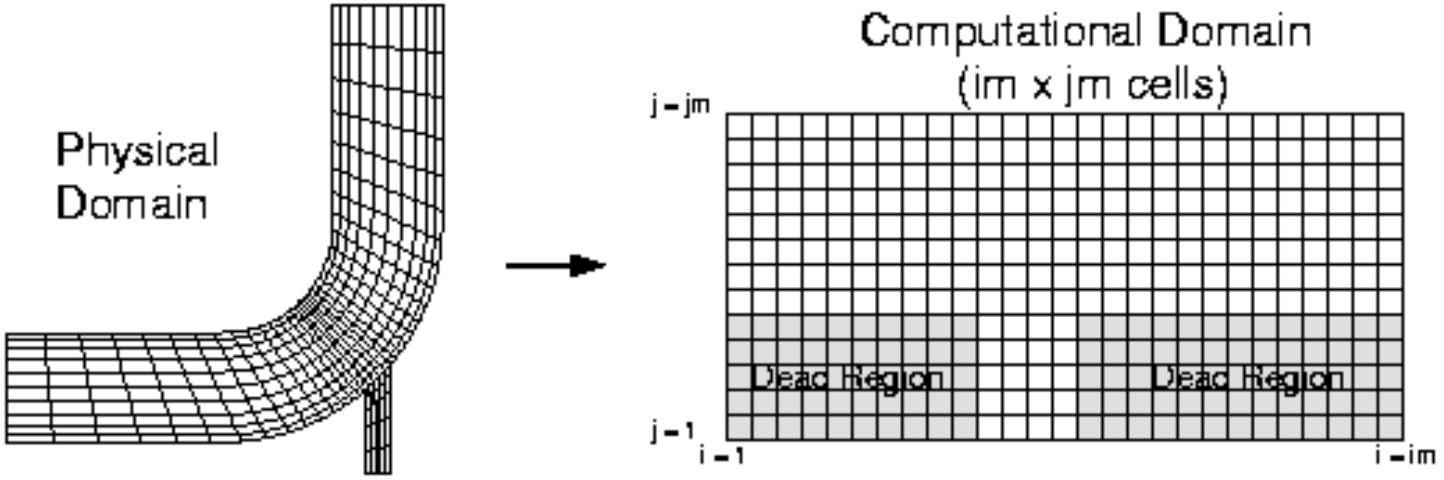
2D computational grid



3D computational grid

Grid types: structured grid

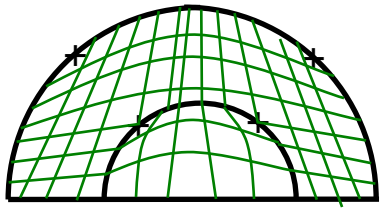
- Single-block, structured grid.
  - i,j,k indexing to locate neighboring cells.
  - Grid lines must pass all through domain.
- Obviously can't be used for very complicated geometries.



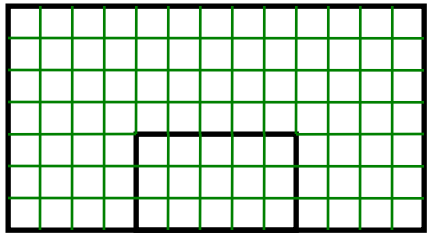
Face meshing: structured grids

- Different types of hexahedral grids.
- Single-block.
  - The mesh has to be represented in a single block.
  - Connectivity information (identifying cell neighbors) for entire mesh is accessed by three index variables: i, j, k.

Single-block geometry



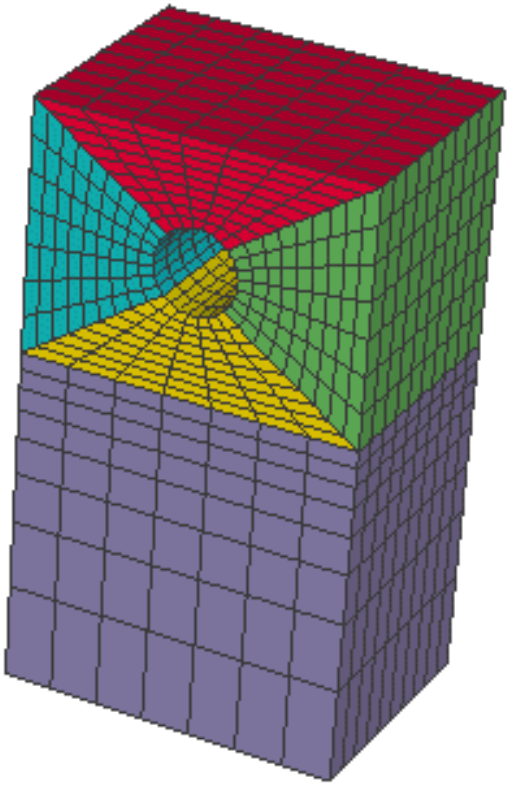
Logical representation.



- Single-block meshes may include 180-degree corners.

Grid types: multiblock

- Multi-block, structured grid.
  - Uses i,j,k indexing within each mesh block.
  - The grid can be made up of (somewhat) arbitrarily-connected blocks.
- More flexible than single block, but still limited.



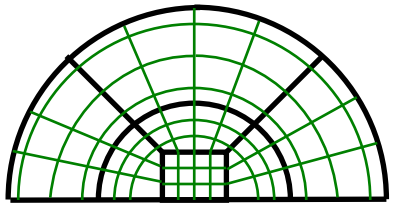
An example of a structured multiblock mesh using point to point connections.

Source: www.cfdreview.com

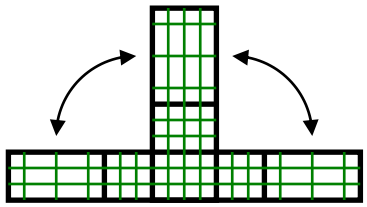
Face meshing: multiblock

- Different types of hexahedral grids.
  - Multi-block.
  - The mesh can be represented in multiple blocks.

Multi-block geometry



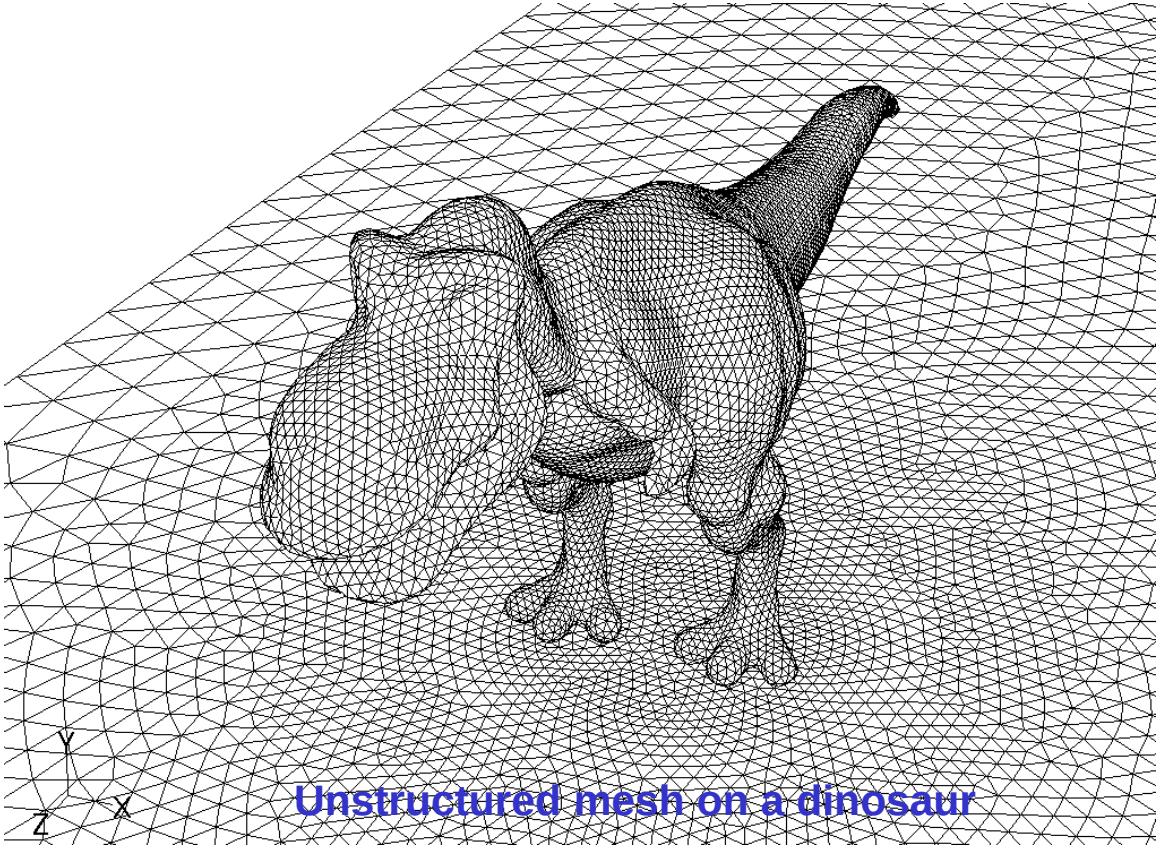
Logical representation.



  - This structure gives full control of the mesh grading, using edge meshing, with high-quality elements.
  - Manual creation of multi-block structures is usually more time-consuming compared to unstructured meshes.

Grid types: unstructured

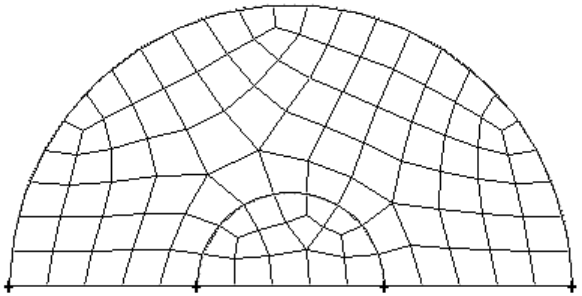
- Unstructured grid.
  - The cells are arranged in an arbitrary fashion.
  - No i,j,k grid index, no constraints on cell layout.
- There is some memory and CPU overhead for unstructured referencing.



Unstructured mesh on a dinosaur

Face meshing: unstructured grids

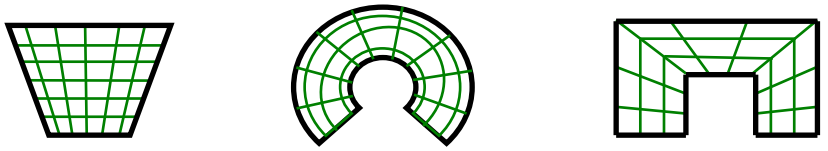
- Different types of hexahedral grids.
  - Unstructured.
  - The mesh has no logical representation.



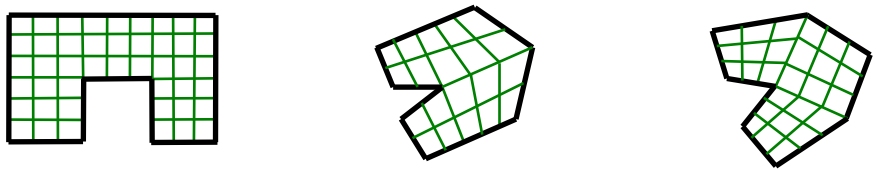
Unstructured Grid

Face meshing: quad examples

- Quad: Map.

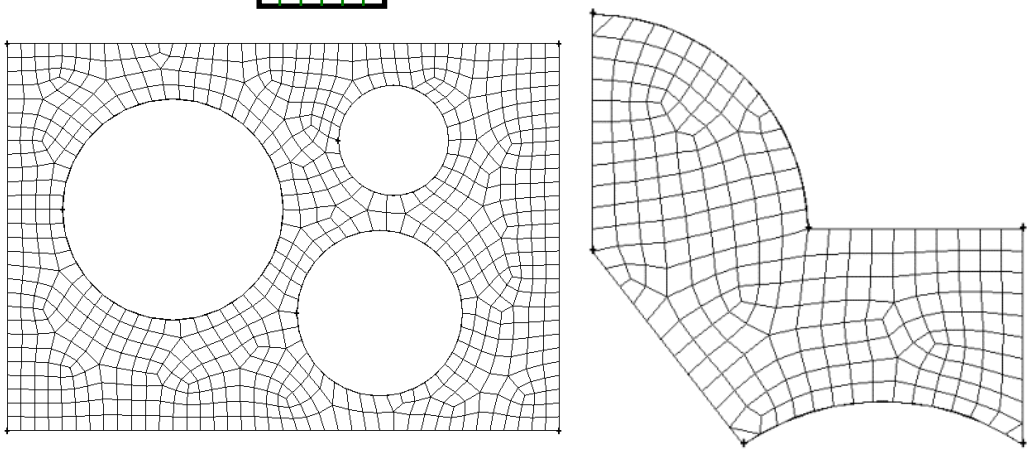


- Quad: Submap.



- Quad: Tri-Primitive.

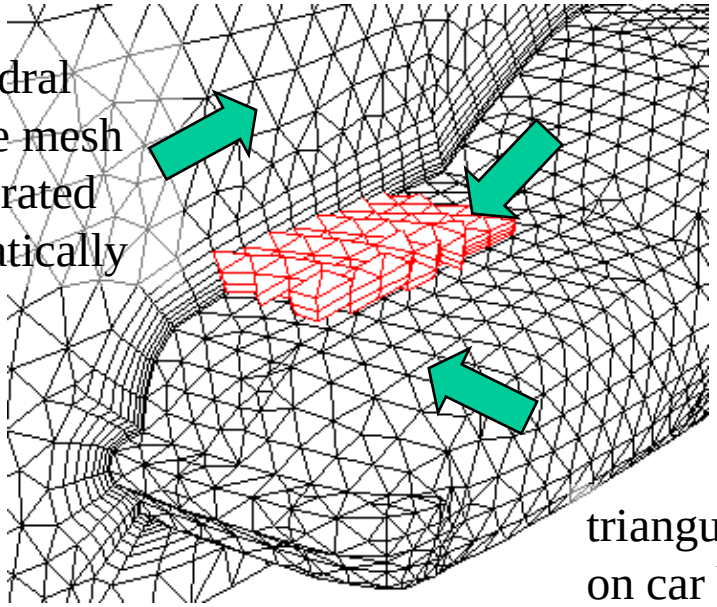
- Quad: Pave and Tri-Pave.



Grid types: hybrid

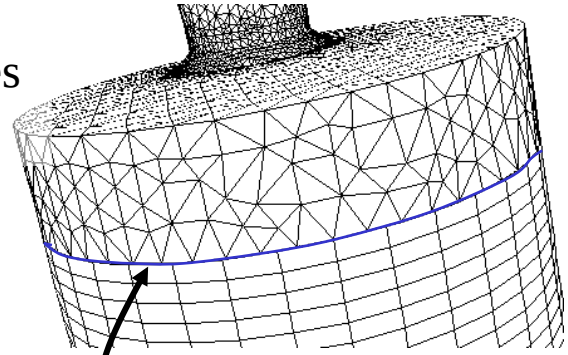
- Hybrid grid.
  - Use the most appropriate cell type in any combination.
    - Triangles and quadrilaterals in 2D.
    - Tetrahedra, prisms and pyramids in 3D.
  - Can be non-conformal: grids lines don't need to match at block boundaries.

tetrahedral volume mesh is generated automatically



triangular surface mesh on car body is quick and easy to create

prism layer efficiently resolves boundary layer

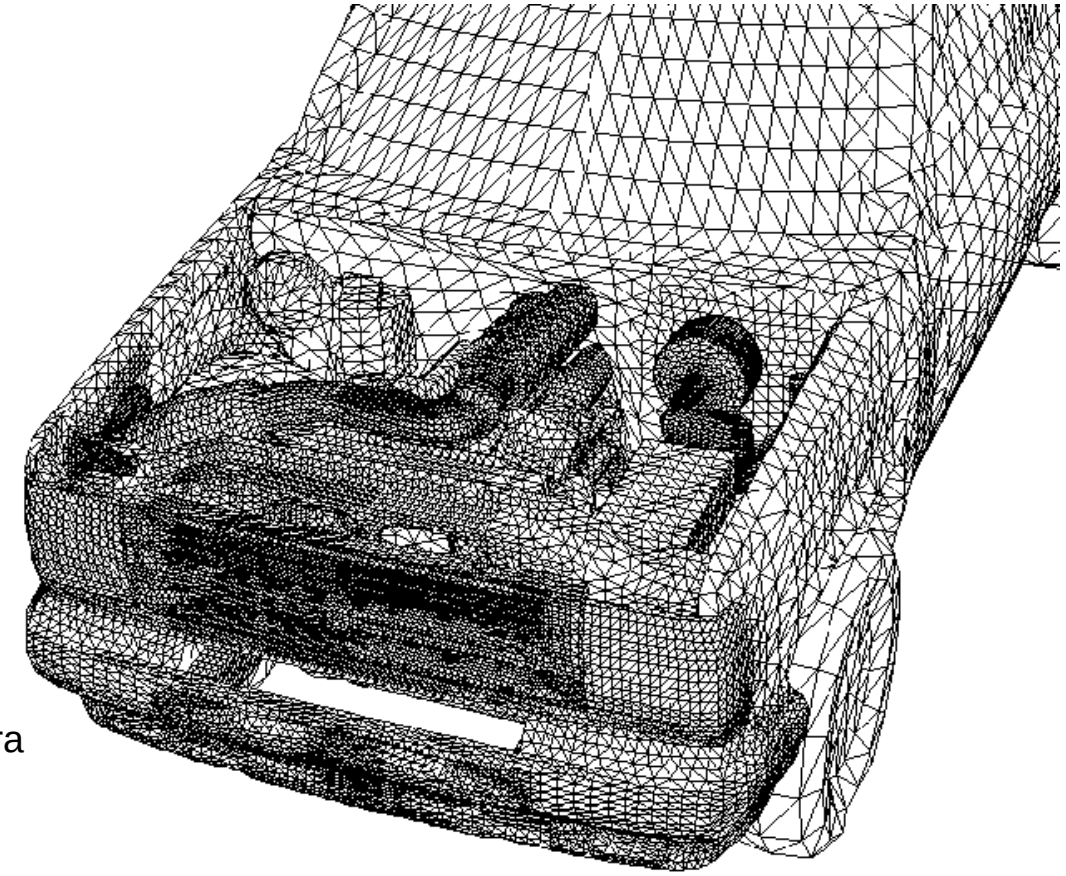


non-conformal interface

Tetrahedral mesh

- Start from 3D boundary mesh containing only triangular faces.
- Generate mesh consisting of tetrahedra.

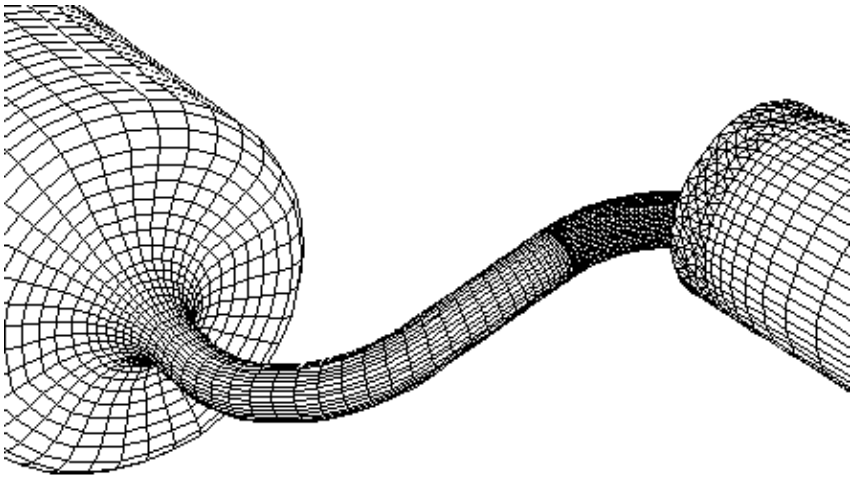
Complex Geometries



Surface mesh for a grid containing only tetrahedra

Zonal hybrid mesh

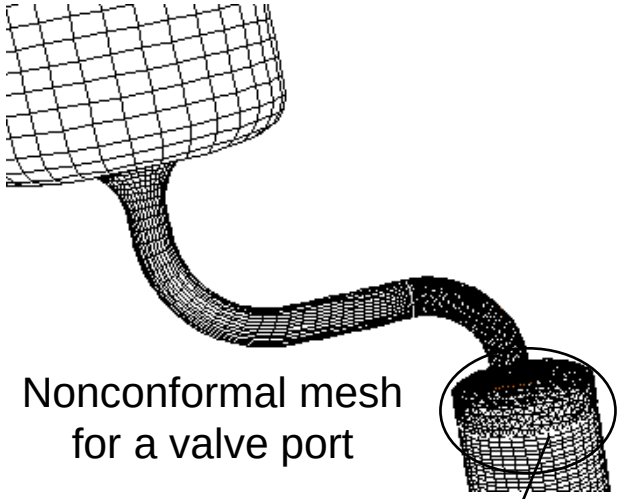
- Flow alignment well defined in specific regions.
- Start from 3D boundary and volume mesh:
  - Triangular and quadrilateral faces.
  - Hexahedral cells.
- Generate zonal hybrid mesh, using:
  - Tetrahedra.
  - Existing hexahedra.
  - Transition elements: pyramids.



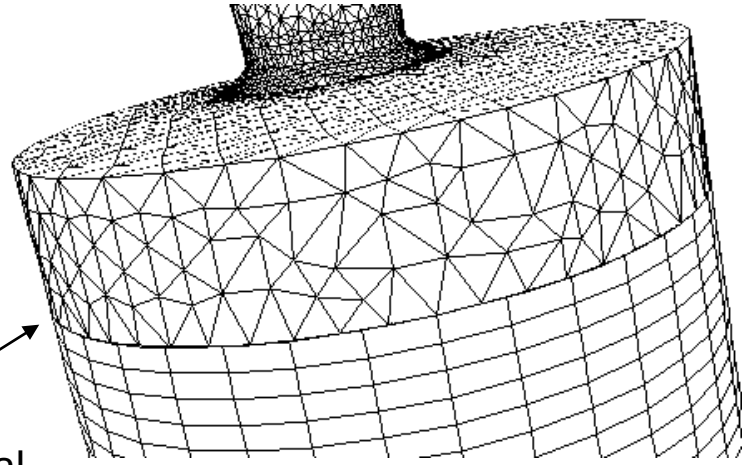
Surface mesh for a grid containing hexahedra, pyramids, and tetrahedra (and prisms)

Nonconformal mesh

- Parametric study of complex geometries.
- Nonconformal capability allows you to replace portion of mesh being changed.
- Start from 3D boundary mesh or volume mesh.
- Add or replace certain parts of mesh.
- Remesh volume if necessary.



Nonconformal mesh for a valve port



Nonconformal interface

Mesh naming conventions - topology

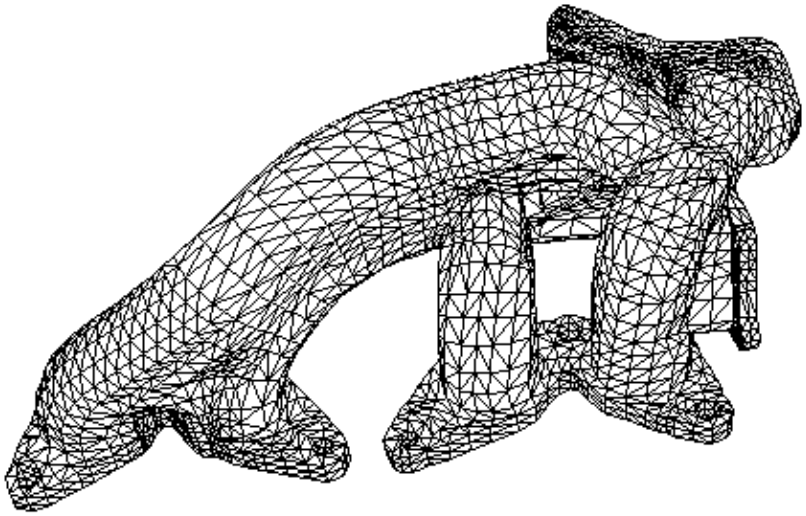
- Structured mesh: the mesh follows a structured i,j,k convention.
- Unstructured mesh: no regularity to the mesh.
- Multiblock: the mesh consists of multiple blocks, each of which can be either structured or unstructured.

Mesh naming conventions – cell type

- Tri mesh: mesh consisting entirely of triangular elements.
- Quad mesh: consists entirely of quadrilateral elements.
- Hex mesh: consists entirely of hexahedral elements.
- Tet mesh: mesh with only tetrahedral elements.
- Hybrid mesh: mesh with one of the following:
    - Triangles and quadrilaterals in 2D.
    - Any combination of tetrahedra, prisms, pyramids in 3D.
    - Boundary layer mesh: prisms at walls and tetrahedra everywhere else.
    - Hexcore: hexahedra in center and other cell types at walls.
- Polyhedral mesh: consists of arbitrary polyhedra.
- Nonconformal mesh: mesh in which grid nodes do not match up along an interface.

Mesh generation process

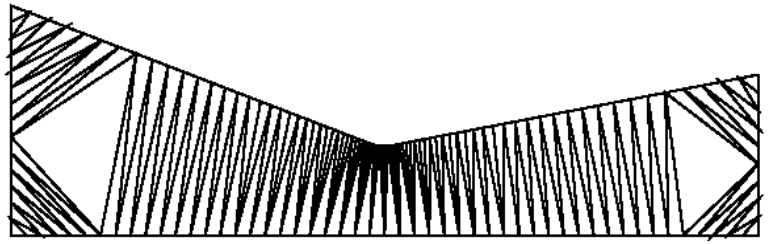
1. Create, read (or import) boundary mesh(es).
2. Check quality of boundary mesh.
3. Improve and repair boundary mesh.
4. Generate volume mesh.
5. Perform further refinement if required.
6. Inspect quality of volume mesh.
7. Remove sliver and degenerate cells.
8. Save volume mesh.



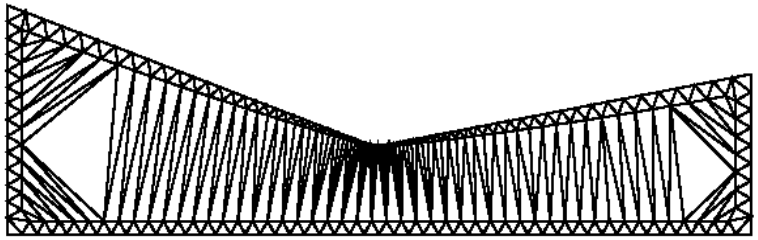
Surface mesh for a grid containing only tetrahedra

Tri/tet grid generation process

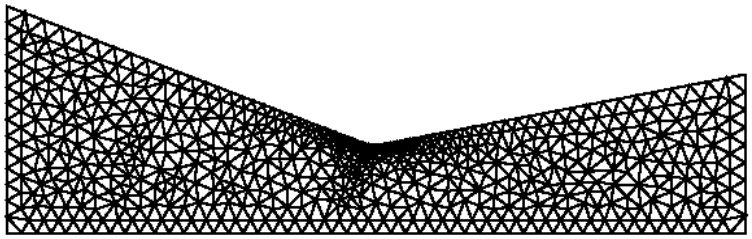
- Two phases:
  - **Initial mesh generation**:
    Triangulate boundary mesh.
  - **Refinement on initial mesh**:
    Insert new nodes.



Initial mesh



Boundary refinement



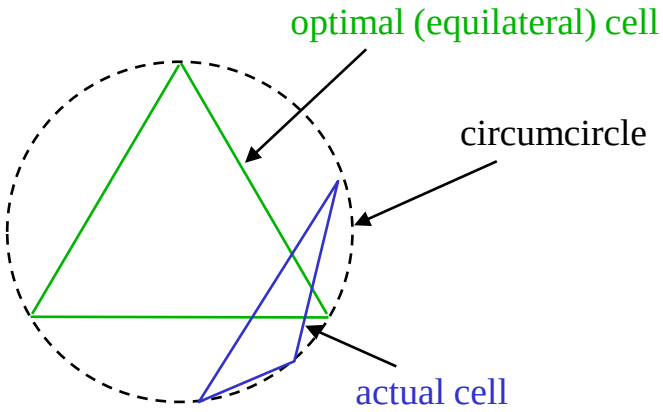
Cell zone refinement

Mesh quality

- For the same cell count, hexahedral meshes will give more accurate solutions, especially if the grid lines are aligned with the flow.
- The mesh density should be high enough to capture all relevant flow features.
- The mesh adjacent to the wall should be fine enough to resolve the boundary layer flow. In boundary layers, quad, hex, and prism/wedge cells are preferred over tri's, tets, or pyramids.
- Three measures of quality:
  - Skewness.
  - Smoothness (change in size).
  - Aspect ratio.

Mesh quality: skewness

- Two common methods for determining skewness:
  1. Based on the equilateral volume:
     - Skewness = $\dfrac{\text{optimal cell size} - \text{cell size}}{\text{optimal cell size}}$
     - Applies only to triangles and tetrahedra.
     - Default method for tris and tets.



  2. Based on the deviation from a normalized equilateral angle:
     - Skewness (for a quad) = $\max\left[\dfrac{\theta_{\max} - 90}{90}, \dfrac{90 - \theta_{\min}}{90}\right]$
     - Applies to all cell and face shapes.
     - Always used for prisms and pyramids.

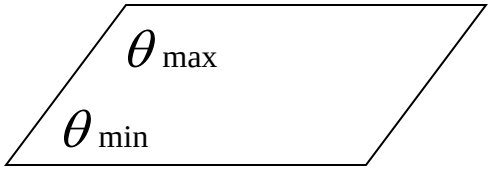
Equiangle skewness

- Common measure of quality is based on equiangle skew.
- Definition of equiangle skew:

$$\max\left[\frac{\theta_{\max}-\theta_e}{180-\theta_e}, \frac{\theta_e-\theta_{\min}}{\theta_e}\right]$$

where:

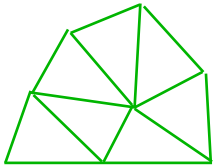
  - θ_{max} = largest angle in face or cell.
  - θ_{min} = smallest angle in face or cell.
  - θ_e = angle for equiangular face or cell.
    - e.g., 60 for triangle, 90 for square.



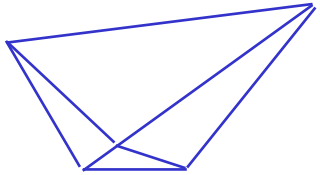
- Range of skewness:

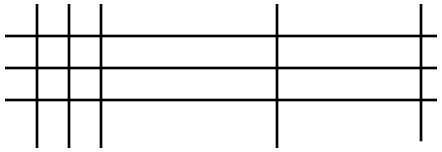
Grid design guidelines: smoothness

- Change in cell/element size should be gradual (smooth).



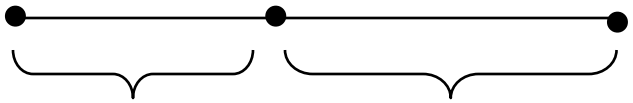
smooth change
in cell size





sudden change
in cell size — AVOID!

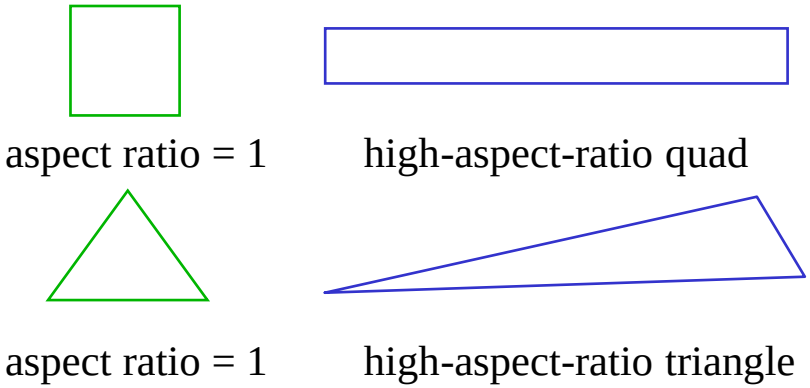
- Ideally, the maximum change in grid spacing should be <20%:



$$\frac{\Delta x_{i+1}}{\Delta x_i} \leq 1.2$$

Mesh quality: aspect ratio

- Aspect ratio is ratio of longest edge length to shortest edge length. Equal to 1 (ideal) for an equilateral triangle or a square.



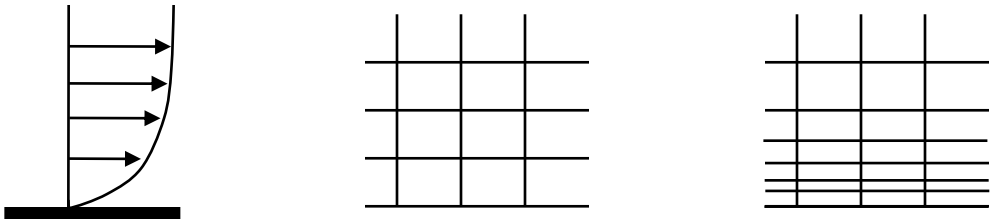
Striving for quality

- A poor-quality grid will cause inaccurate solutions and/or slow convergence.
- Minimize equiangle skew:
  - Hex and quad cells: skewness should not exceed 0.85.
  - Tri's: skewness should not exceed 0.85.
  - Tets: skewness should not exceed 0.9.
- Minimize local variations in cell size:
  - e.g., adjacent cells should not have 'size ratio' greater than 20%.
- If such violations exist: delete mesh, perform necessary decomposition and/or pre-mesh edges and faces, and remesh.

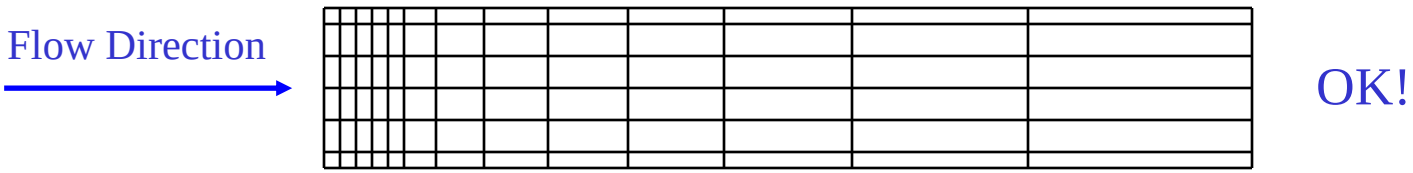
Value of Skewness	0-0.25	0.25-0.50	0.50-0.80	0.80-0.95	0.95-0.99	0.99-1.00
Cell Quality	excellent	good	acceptable	poor	sliver	degenerate

Grid design guidelines: resolution

- Pertinent flow features should be adequately resolved.



- Cell aspect ratio (width/height) should be near one where flow is multi-dimensional.
- Quad/hex cells can be stretched where flow is fully-developed and essentially one-dimensional.

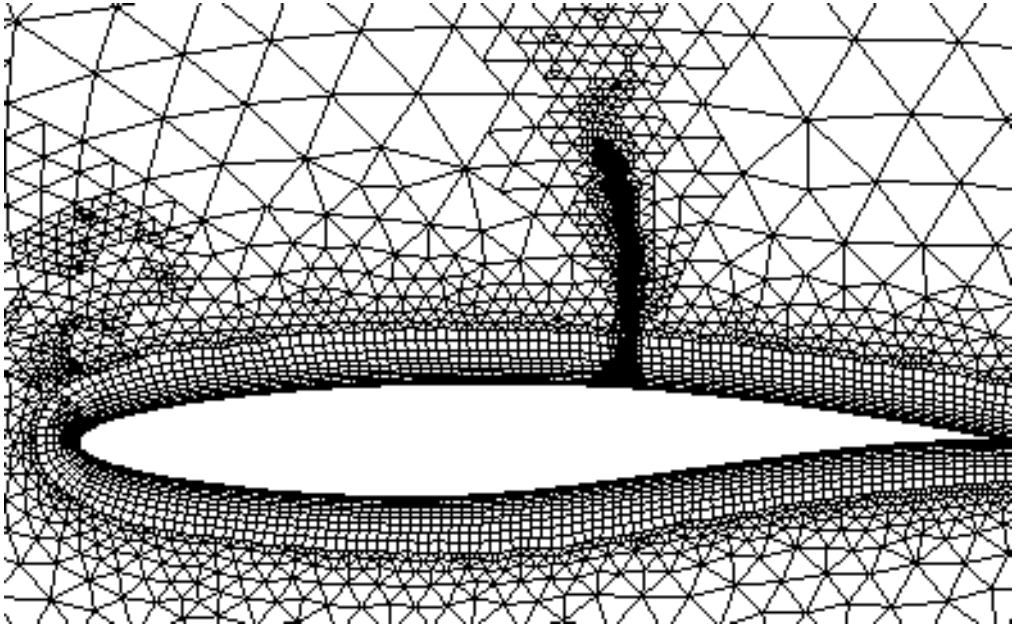


Grid design guidelines: total cell count

- More cells *can* give higher accuracy. The downside is increased memory and CPU time.
- To keep cell-count down:
  - Use a non-uniform grid to cluster cells only where they are needed.
  - Use solution adaption to further refine only selected areas.
- Cell counts of the order:
  - 1E4 are relatively small problems.
  - 1E5 are intermediate size problems.
  - 1E6 are large. Such problems can be efficiently run using multiple CPUs, but mesh generation and post-processing may become slow.
  - 1E7 are huge and should be avoided if possible. However, they are common in aerospace and automotive applications.
  - 1E8 and more are department of defense style applications.

Solution adaption

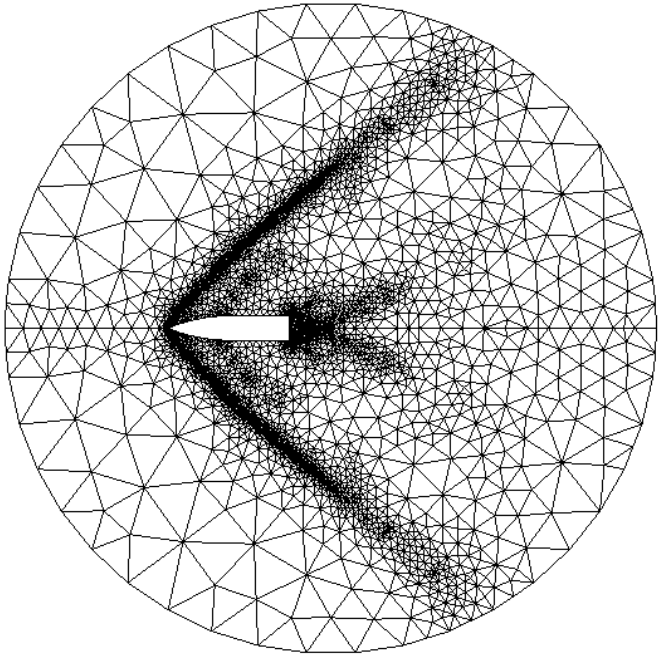
- How do you ensure adequate grid resolution, when you don't necessarily know the flow features? Solution-based grid adaption!
- The grid can be refined or coarsened by the solver based on the developing flow:
  - Solution values.
  - Gradients.
  - Along a boundary.
  - Inside a certain region.



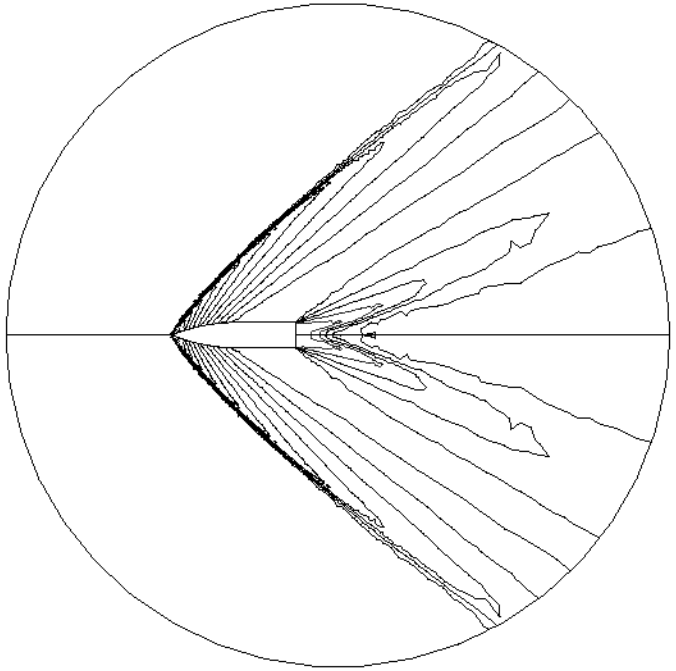
Grid adaption

- Grid adaption adds more cells where needed to resolve the flow field.
- Fluent adapts on cells listed in register. Registers can be defined based on:
  - Gradients of flow or user-defined variables.
  - Isovalues of flow or user-defined variables.
  - All cells on a boundary.
  - All cells in a region.
  - Cell volumes or volume changes.
  - y^+ in cells adjacent to walls.
- To assist adaption process, you can:
  - Combine adaption registers.
  - Draw contours of adaption function.
  - Display cells marked for adaption.
  - Limit adaption based on cell size and number of cells.

Adaption example: final grid and solution



2D planar shell - final grid



2D planar shell - contours of pressure final grid

Main sources of errors

- Mesh too coarse.
- High skewness.
- Large jumps in volume between adjacent cells.
- Large aspect ratios.
- Interpolation errors at non-conformal interfaces.
- Inappropriate boundary layer mesh.

Summary

- Design and construction of a quality grid is crucial to the success of the CFD analysis.
- Appropriate choice of grid type depends on:
  - Geometric complexity.
  - Flow field.
  - Cell and element types supported by solver.
- Hybrid meshing offers the greatest flexibility.
- Take advantage of solution adaption.

Lecture 8 - Turbulence

Applied Computational Fluid Dynamics

André Bakker

Turbulence

- What is turbulence?
- Effect of turbulence on Navier-Stokes equations.
- Reynolds averaging.
- Reynolds stresses.

Sketch by Leonardo DaVinci

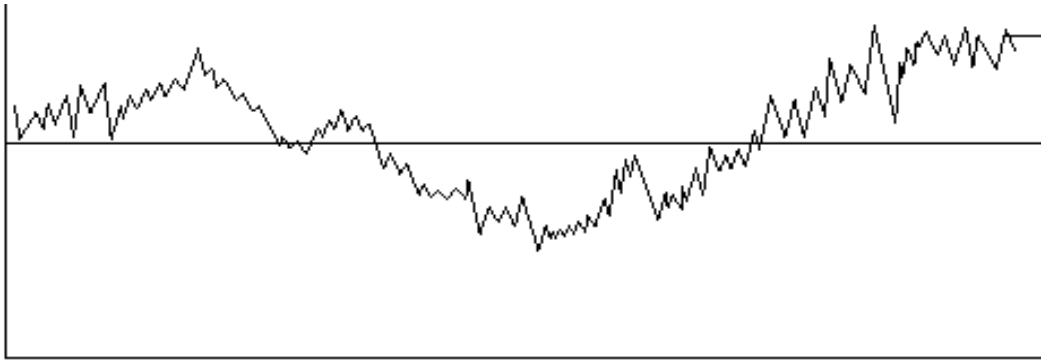
Instability

- All flows become unstable above a certain Reynolds number.
- At low Reynolds numbers flows are laminar.
- For high Reynolds numbers flows are turbulent.
- The transition occurs anywhere between 2000 and 1E6, depending on the flow.
- For laminar flow problems, flows can be solved using the conservation equations developed previously.
- For turbulent flows, the computational effort involved in solving those for all time and length scales is prohibitive.
- An engineering approach to calculate time-averaged flow fields for turbulent flows will be developed.

What is turbulence?

- Unsteady, aperiodic motion in which all three velocity components fluctuate, mixing matter, momentum, and energy.
- Decompose velocity into mean and fluctuating parts:

$$U_i(t) \equiv U_i + u_i(t).$$

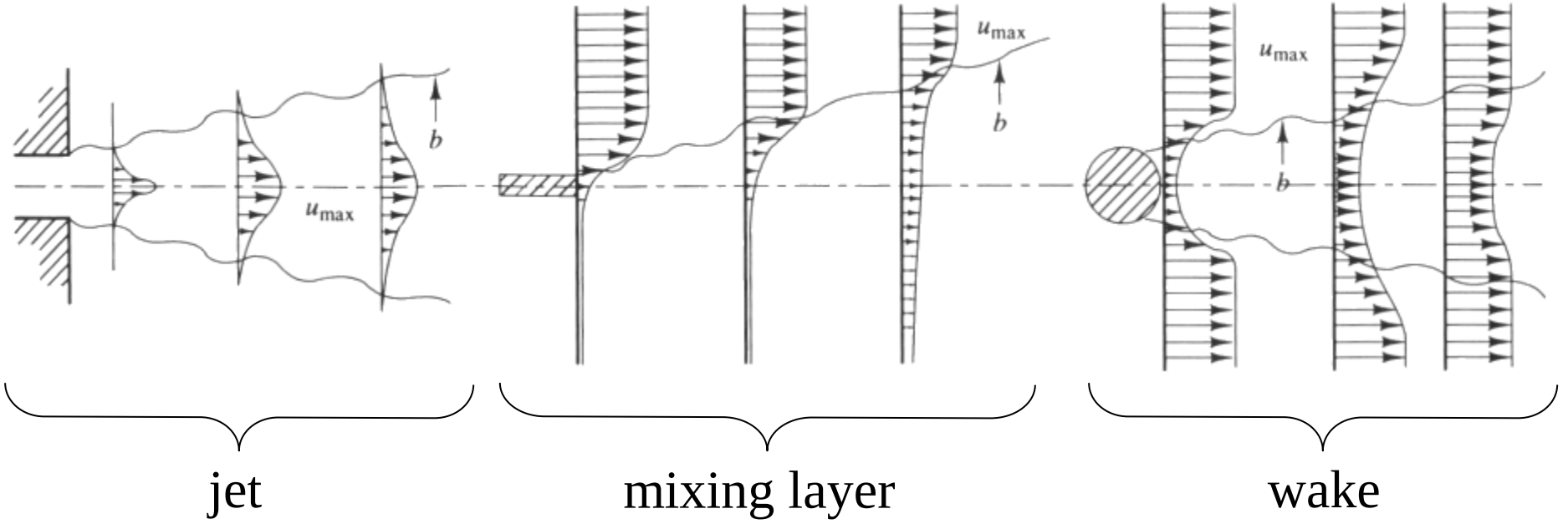


Time

- Similar fluctuations for pressure, temperature, and species concentration values.

Examples of simple turbulent flows

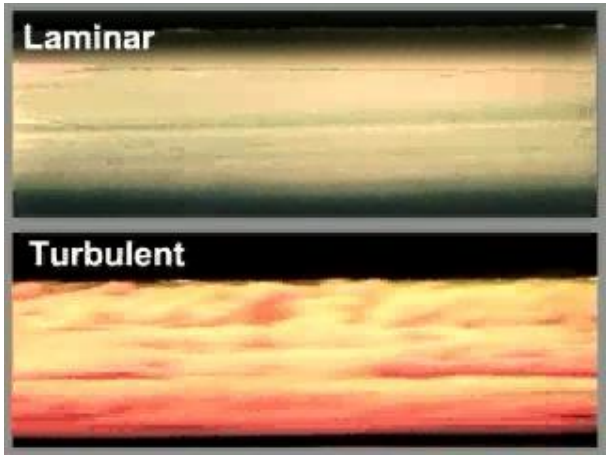
- Some examples of simple turbulent flows are a jet entering a domain with stagnant fluid, a mixing layer, and the wake behind objects such as cylinders.
- Such flows are often used as test cases to validate the ability of computational fluid dynamics software to accurately predict fluid flows.

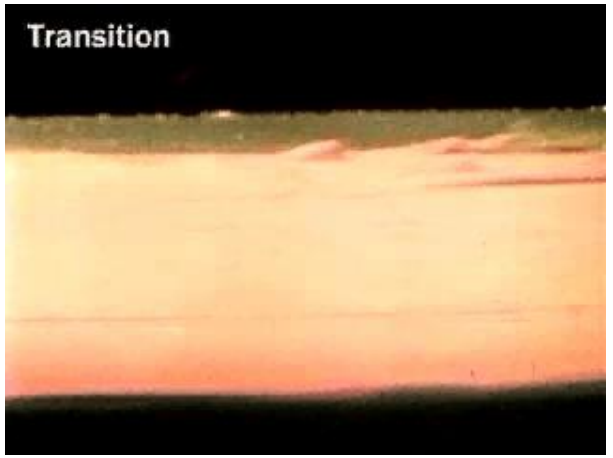


Images: Versteeg and Malalasekera [10, page 53]

Transition

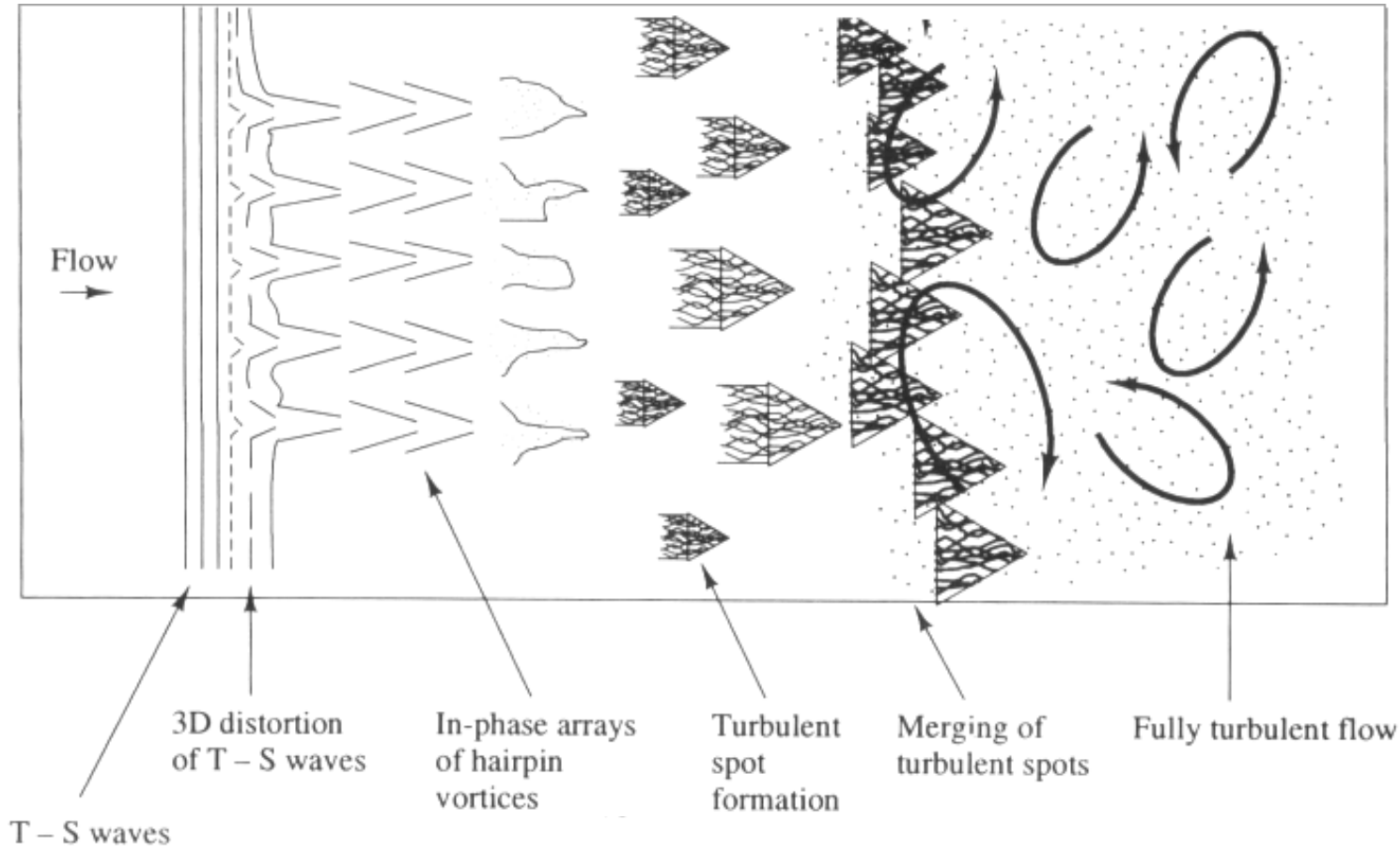
- The photographs show the flow in a boundary layer.
- Below Re_{crit} the flow is laminar and adjacent fluid layers slide past each other in an orderly fashion.
- The flow is stable. Viscous effects lead to small disturbances being dissipated.
- Above the transition point Re_{crit} small disturbances in the flow start to grow.
- A complicated series of events takes place that eventually leads to the flow becoming fully turbulent.

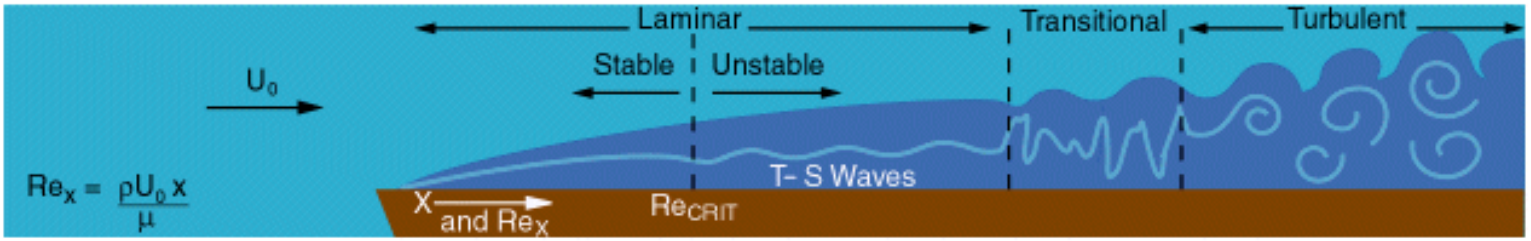




Images: Homsy et al. [2]

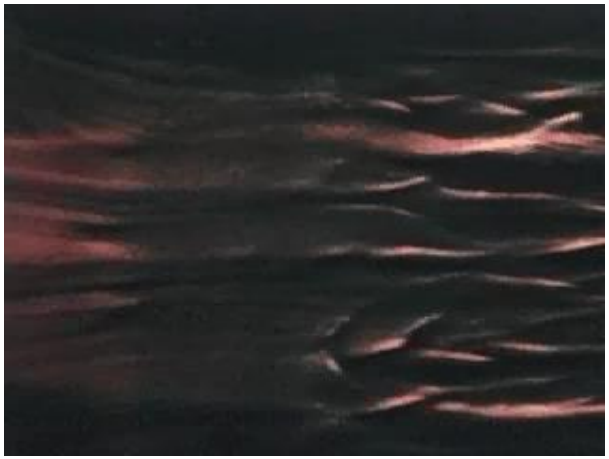
Transition in boundary layer flow over flat plate





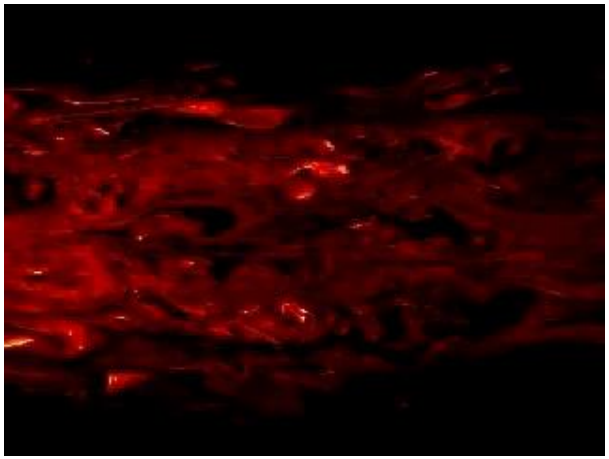
Images: Versteeg and Malalasekera [10, page 47] and Homsy et al. [2]

Transition in boundary layer flow over flat plate



Tollmien-Schlichting (T-S) Waves

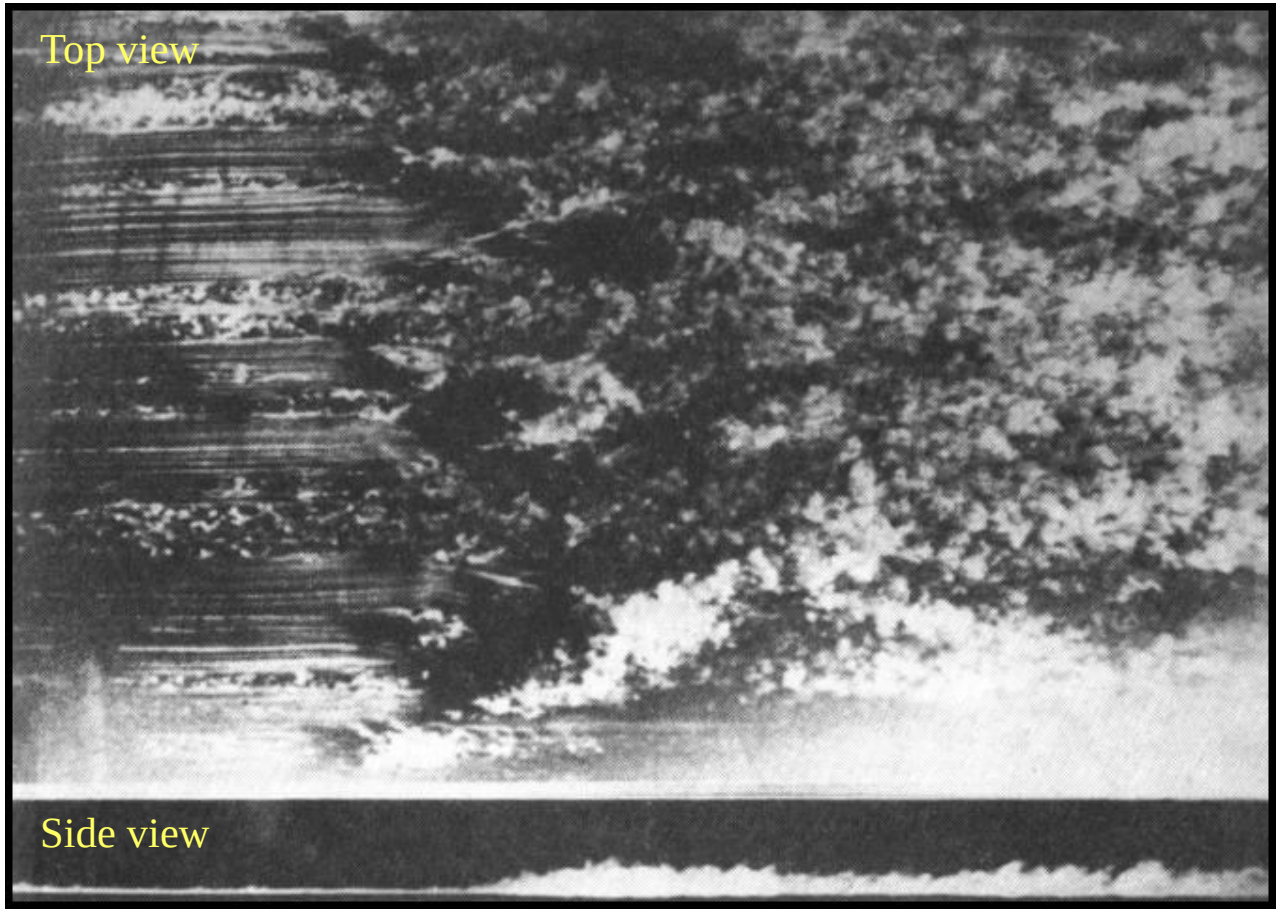
Turbulent spots



Fully turbulent flow

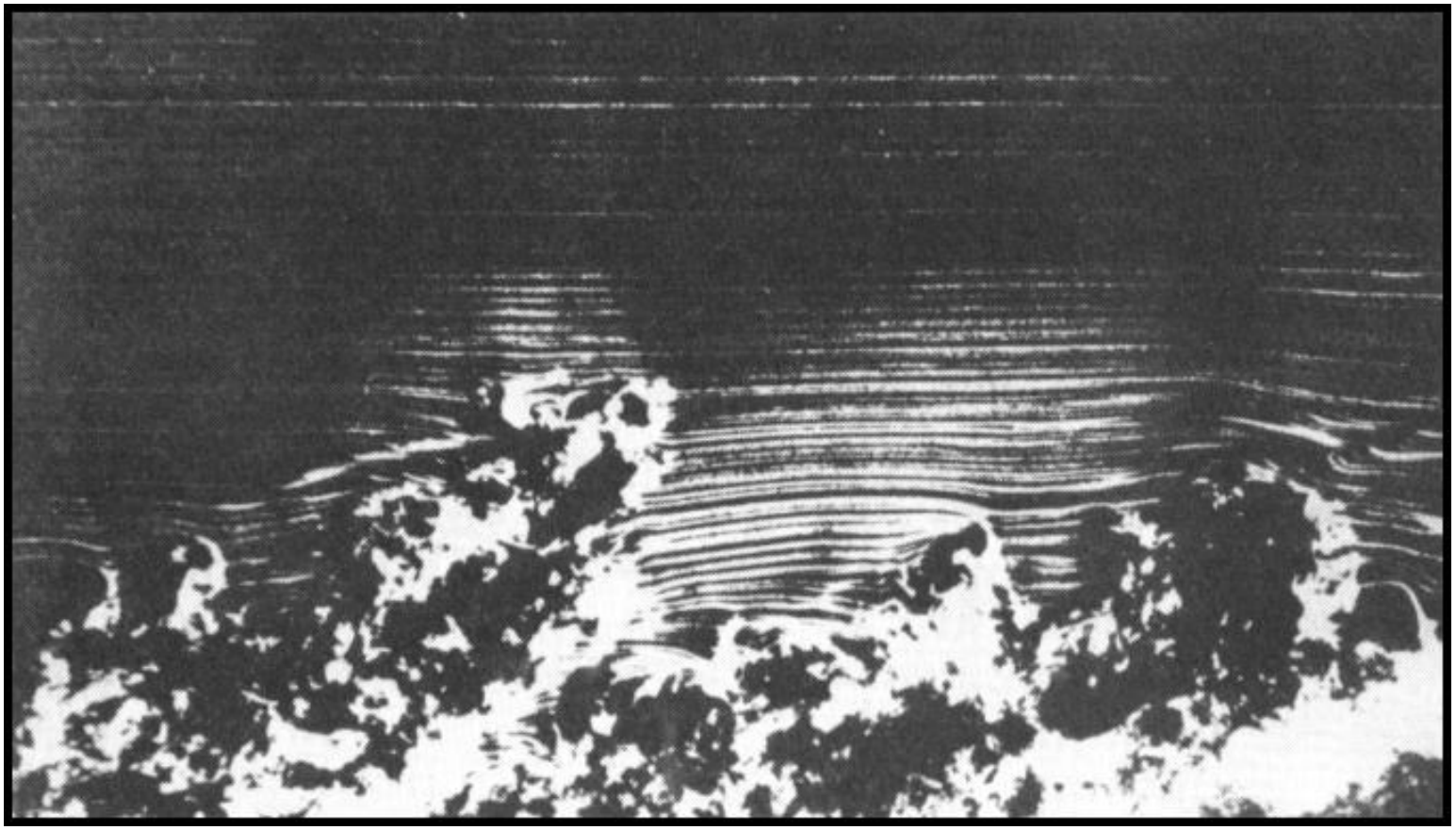
Images: Homsy et al. [2]

Turbulent boundary layer



Merging of turbulent spots and transition to turbulence
in a natural flat plate boundary layer.
Image: Van Dyke [8]

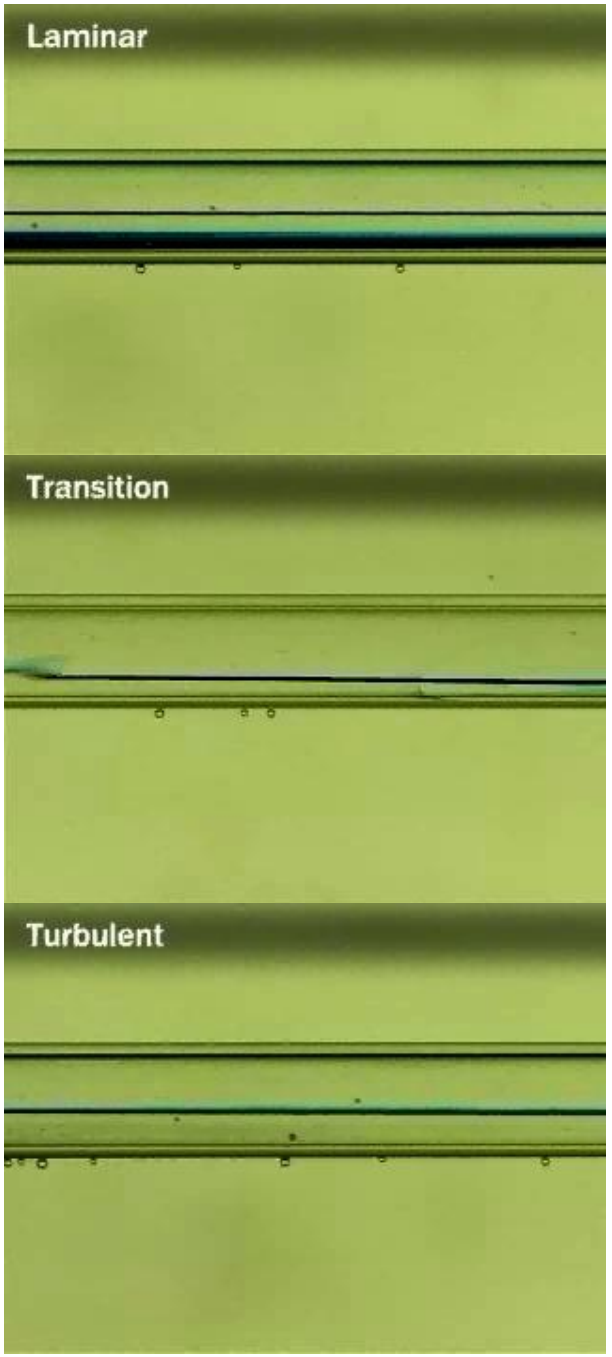
Turbulent boundary layer



Close-up view of the turbulent boundary layer.
Image: Van Dyke [8]

Transition in a channel flow

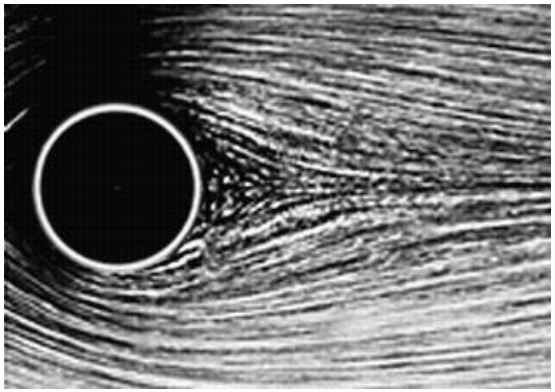
- Instability and turbulence is also seen in internal flows such as channels and ducts.
- The Reynolds number is constant throughout the pipe and is a function of flow rate, fluid properties and diameter.
- Three flow regimes are shown:
  - Re < 2200 with laminar flow.
  - Re = 2200 with a flow that alternates between turbulent and laminar. This is called transitional flow.
  - Re > 2200 with fully turbulent flow.



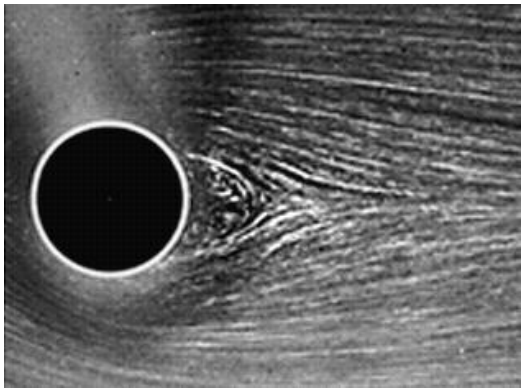
Images: Homsy et al. [2]

Flow transitions around a cylinder

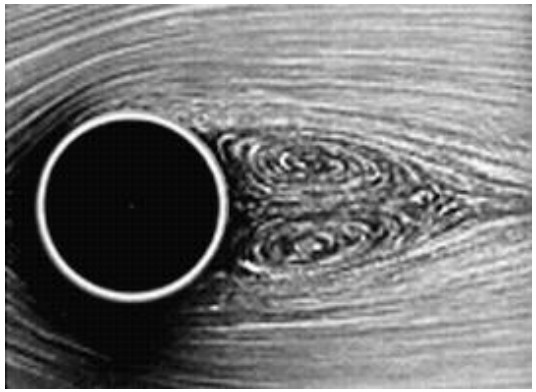
- For flow around a cylinder, the flow starts separating at Re = 5. For Re below 30, the flow is stable. Oscillations appear for higher Re.
- The separation point moves upstream, increasing drag up to Re = 2000.



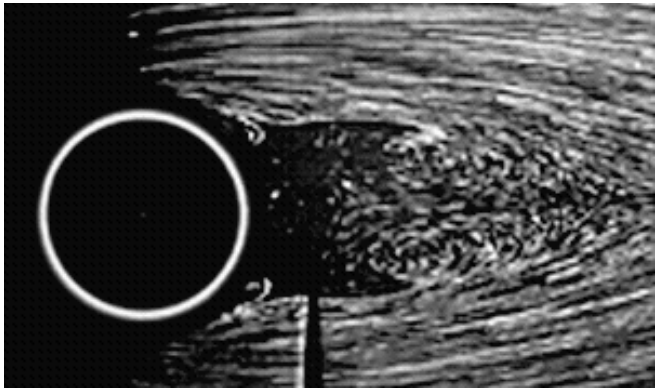
Re = 9.6



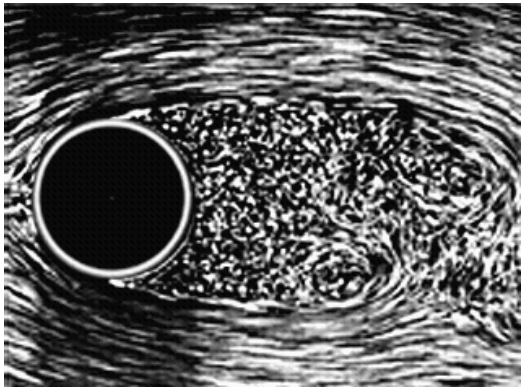
Re = 13.1



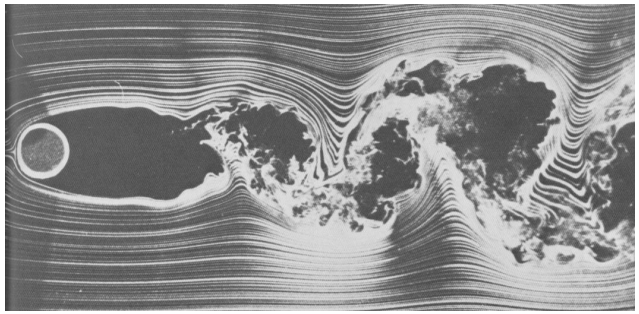
Re = 26



Re = 30.2

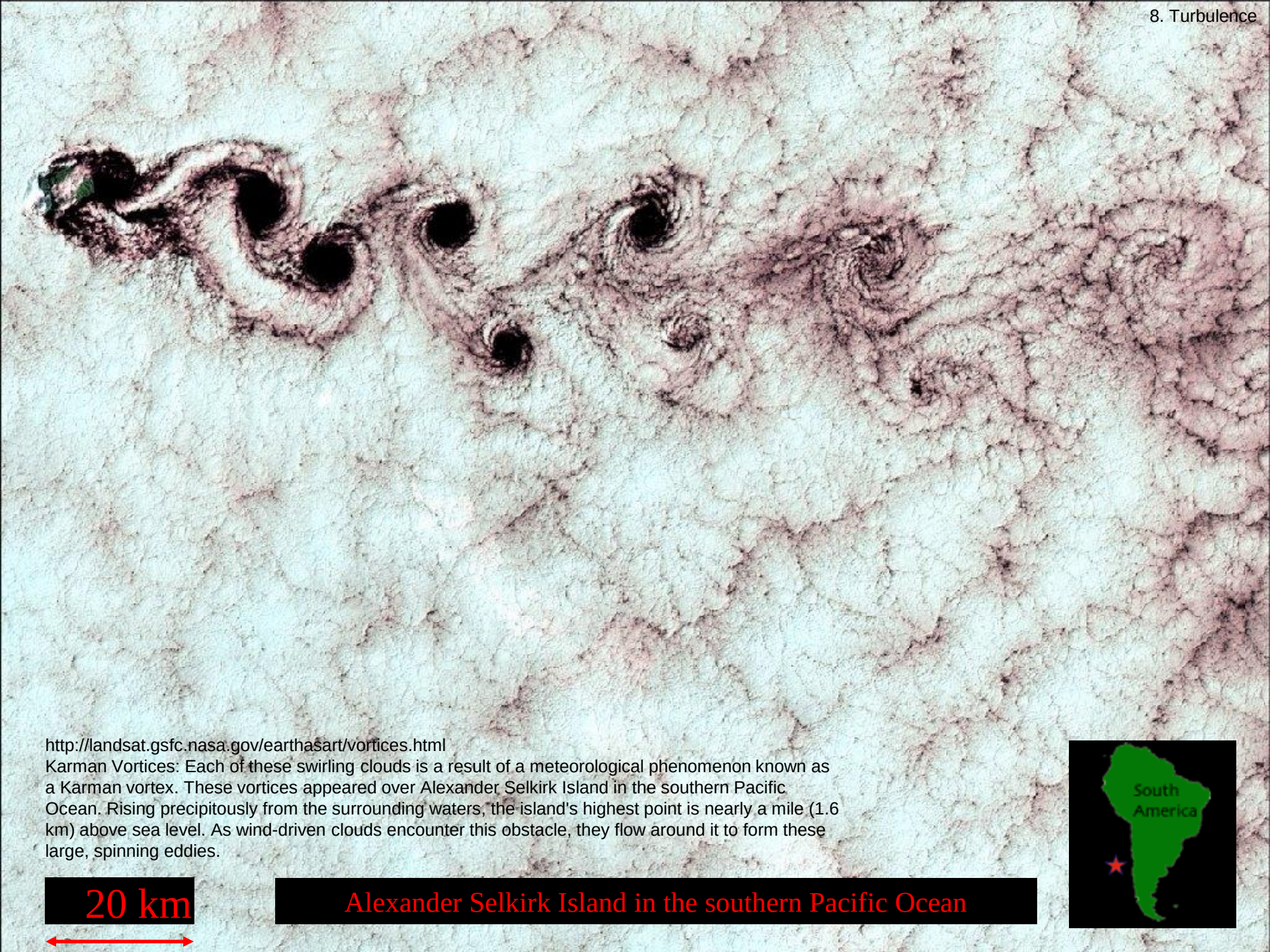


Re = 2000



Re = 10,000

Images: Van Dyke [8].



http://landsat.gsfc.nasa.gov/earthasart/vortices.html
Karman Vortices: Each of these swirling clouds is a result of a meteorological phenomenon known as a Karman vortex. These vortices appeared over Alexander Selkirk Island in the southern Pacific Ocean. Rising precipitously from the surrounding waters, the island's highest point is nearly a mile (1.6 km) above sea level. As wind-driven clouds encounter this obstacle, they flow around it to form these large, spinning eddies.

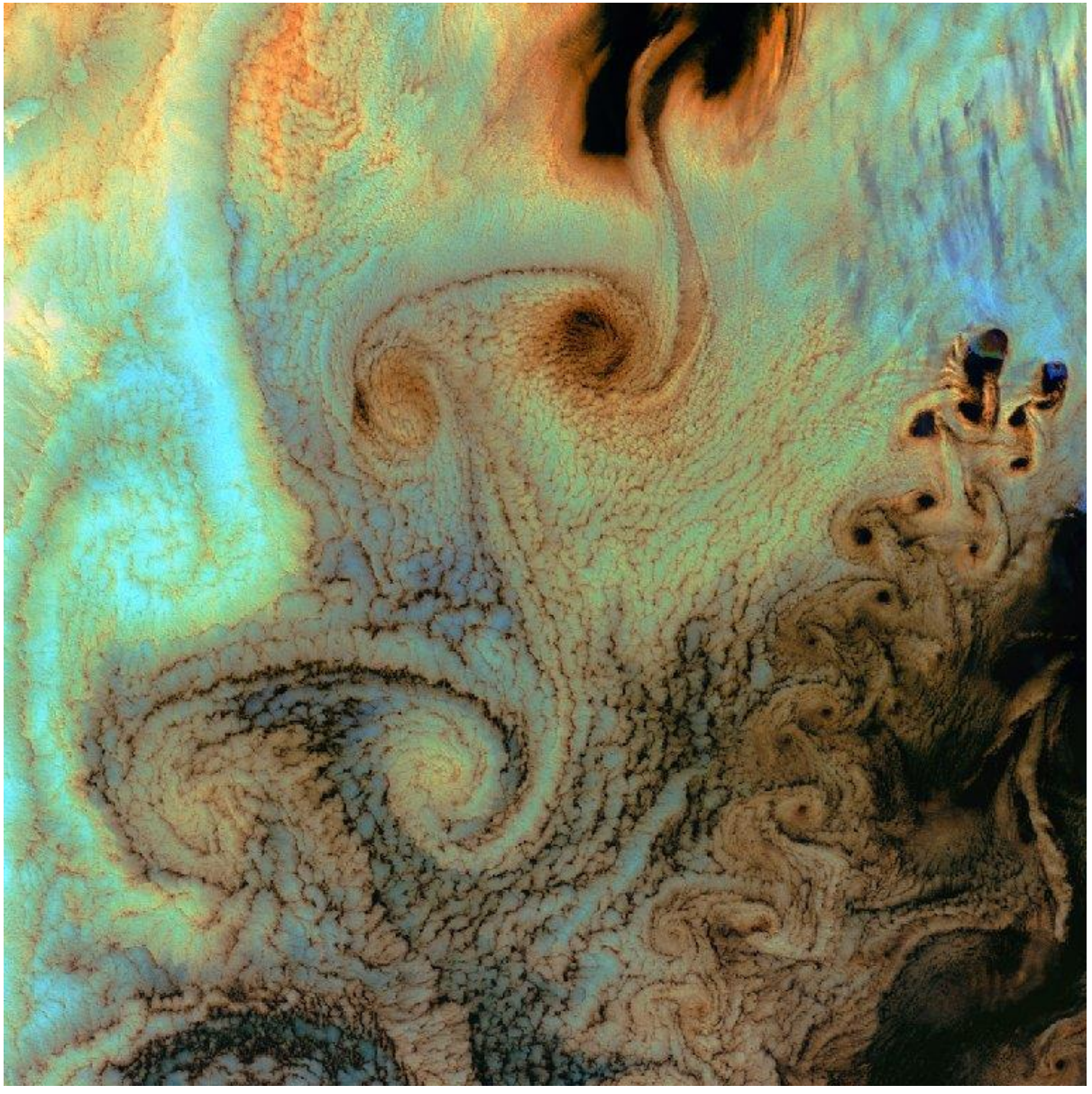
20 km

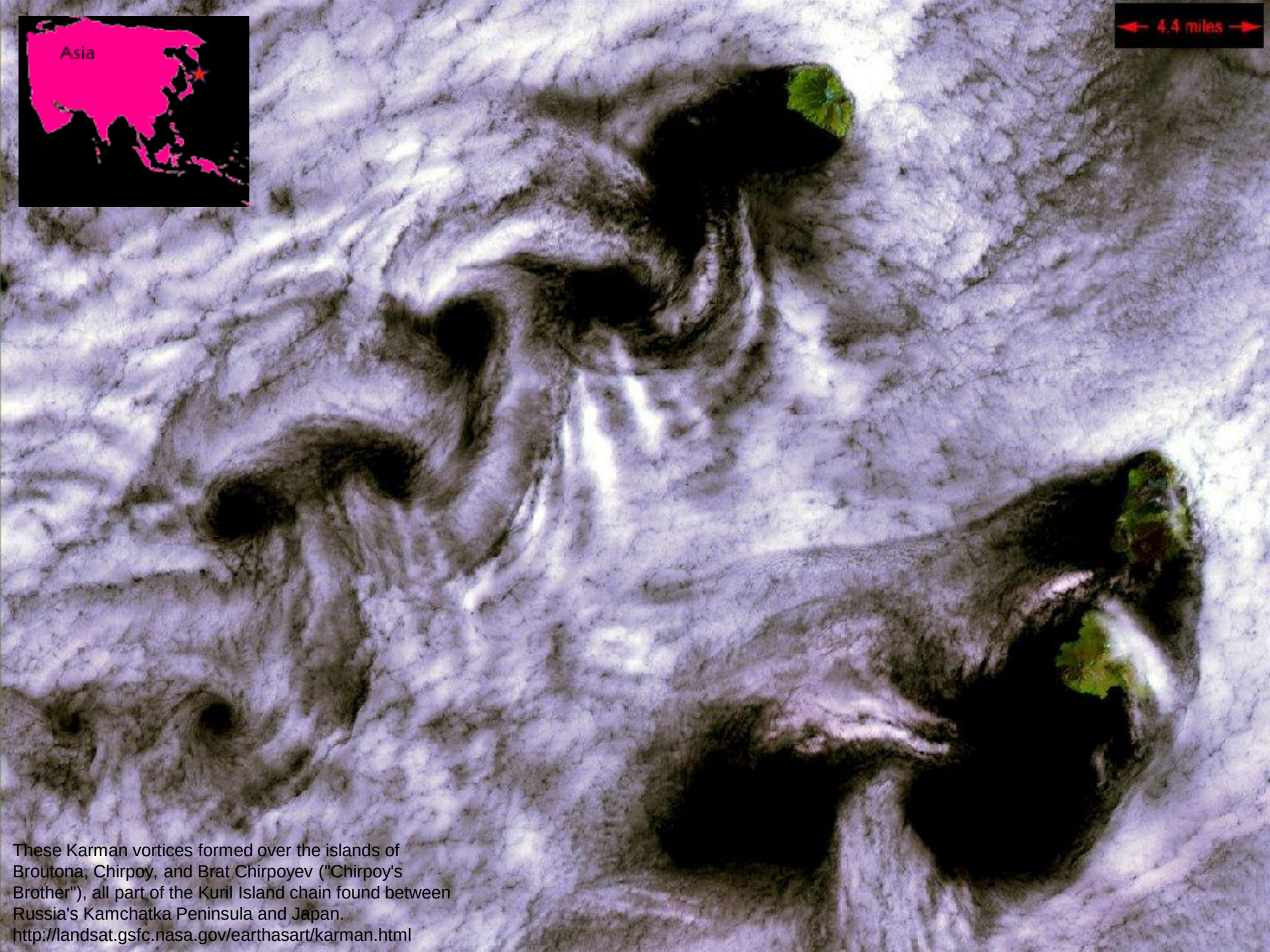
Alexander Selkirk Island in the southern Pacific Ocean

Alaska's Aleutian Islands

- As air flows over and around objects in its path, spiraling eddies, known as Von Karman vortices, may form.
- The vortices in this image were created when prevailing winds sweeping east across the northern Pacific Ocean encountered Alaska's Aleutian Islands

http://landsat.gsfc.nasa.gov/earthasart/vonkar.html





These Karman vortices formed over the islands of Broutona, Chirpoy, and Brat Chirpoyev ("Chirpoy's Brother"), all part of the Kuril Island chain found between Russia's Kamchatka Peninsula and Japan.
http://landsat.gsfc.nasa.gov/earthasart/karman.html

Transition in a jet flow

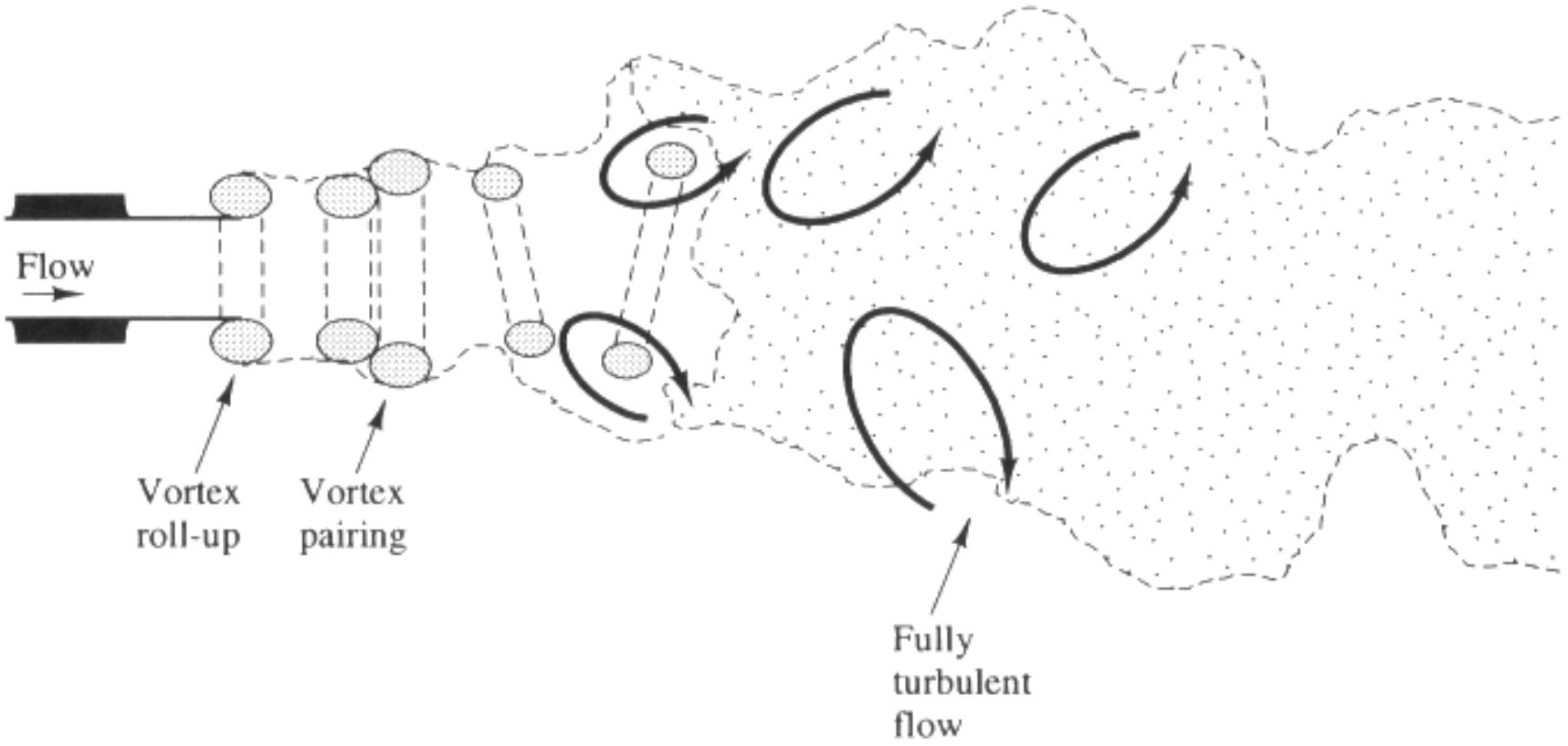


Image: Versteeg and Malalasekera [10, page 46]

Large-scale vs. small-scale structure

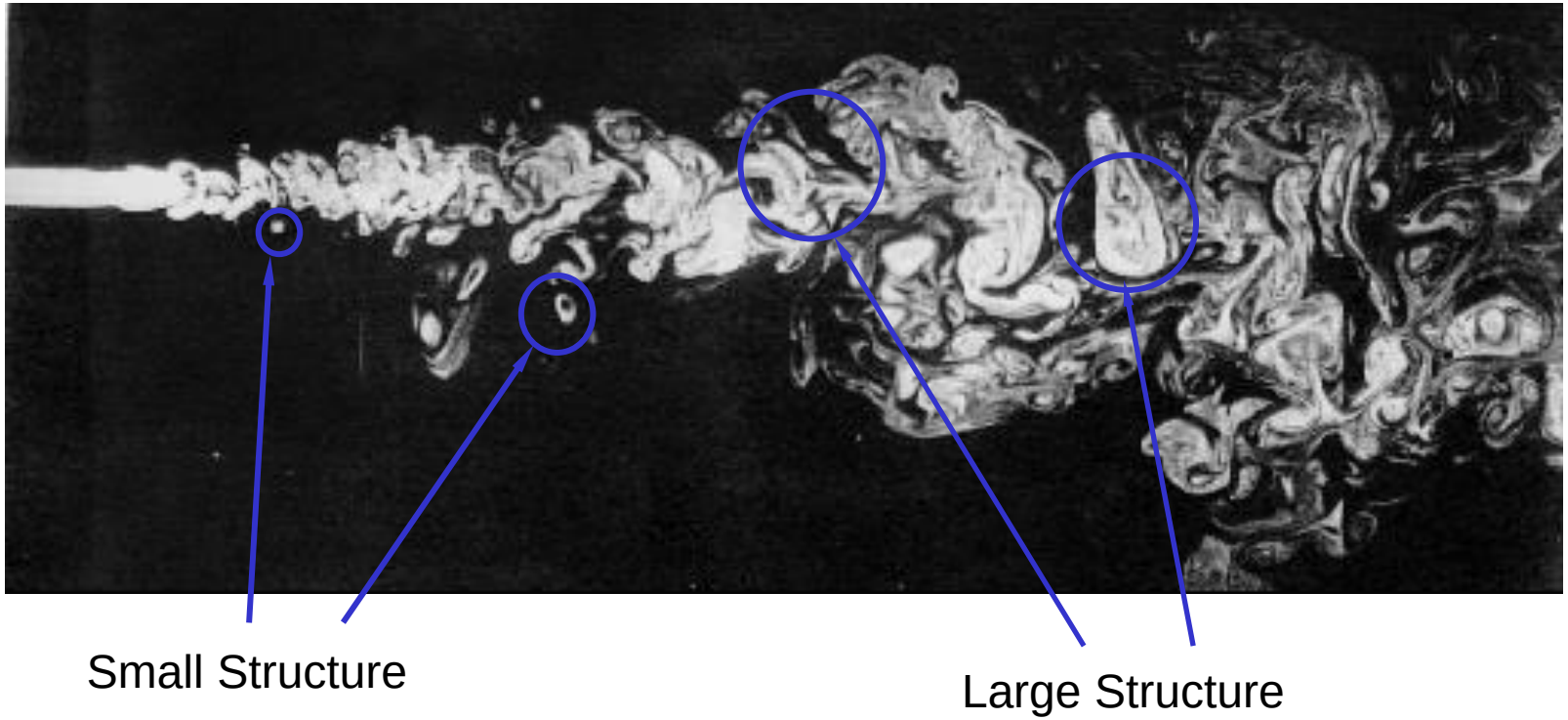
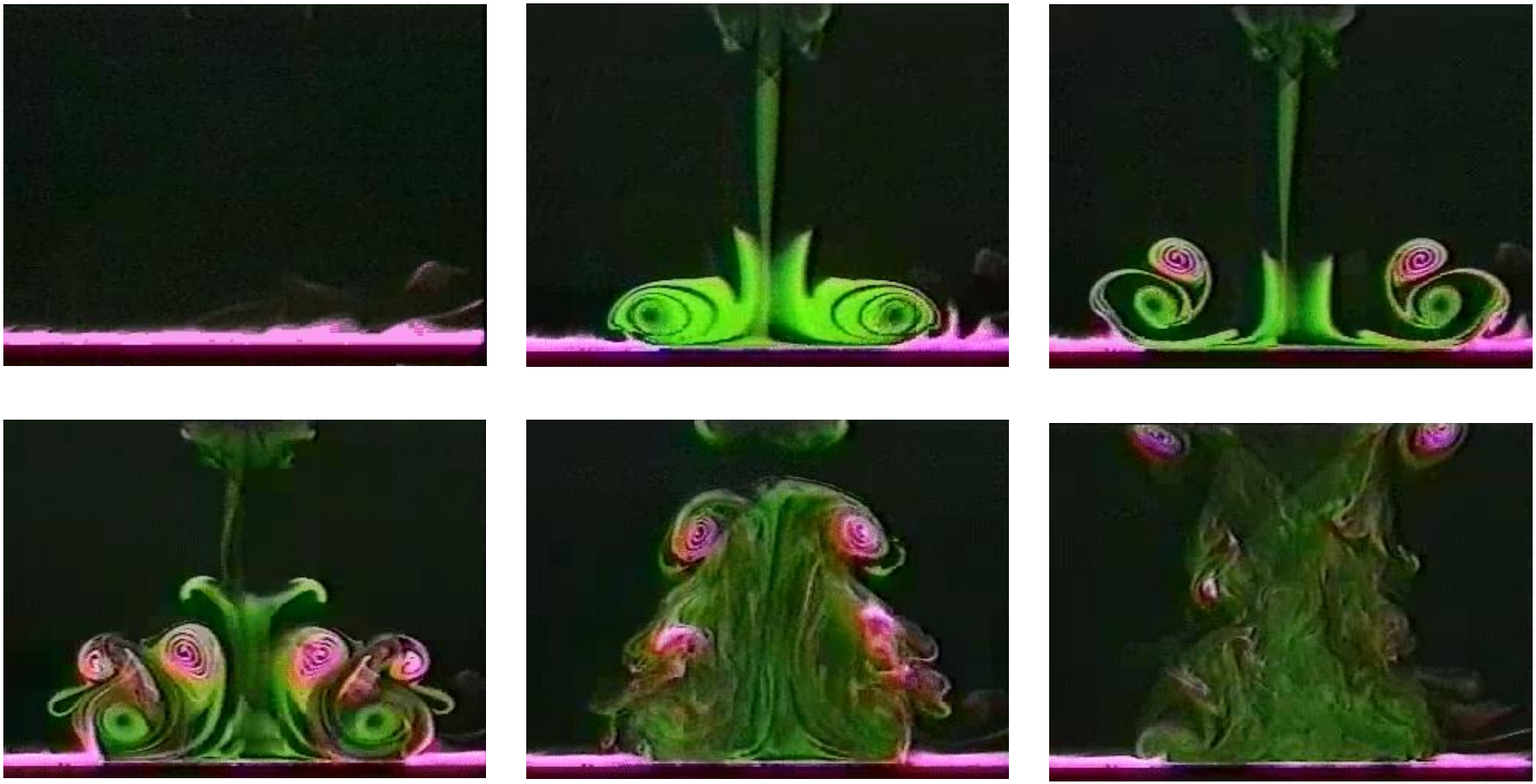


Image: Van Dyke [8]

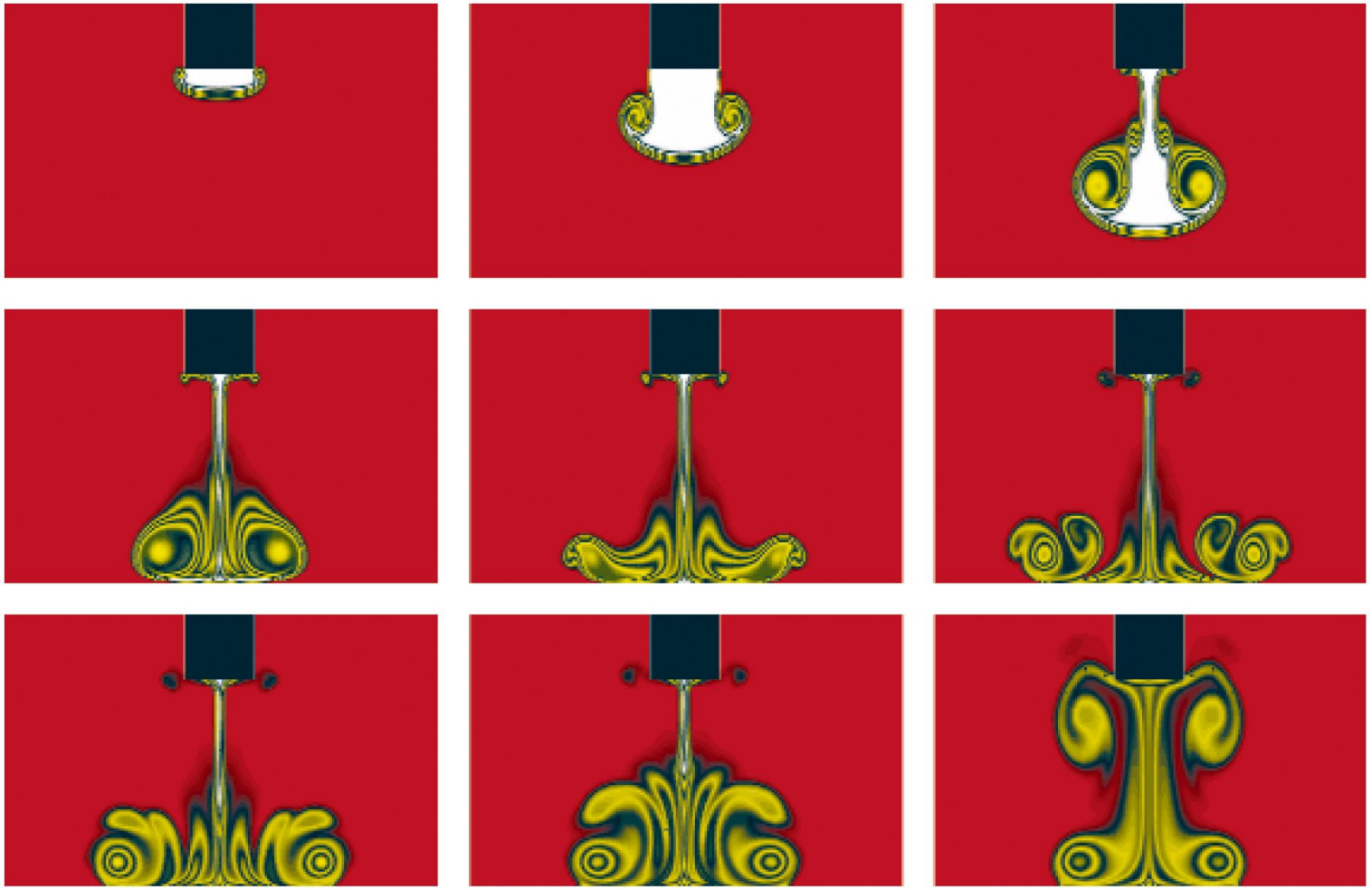
Smoke ring



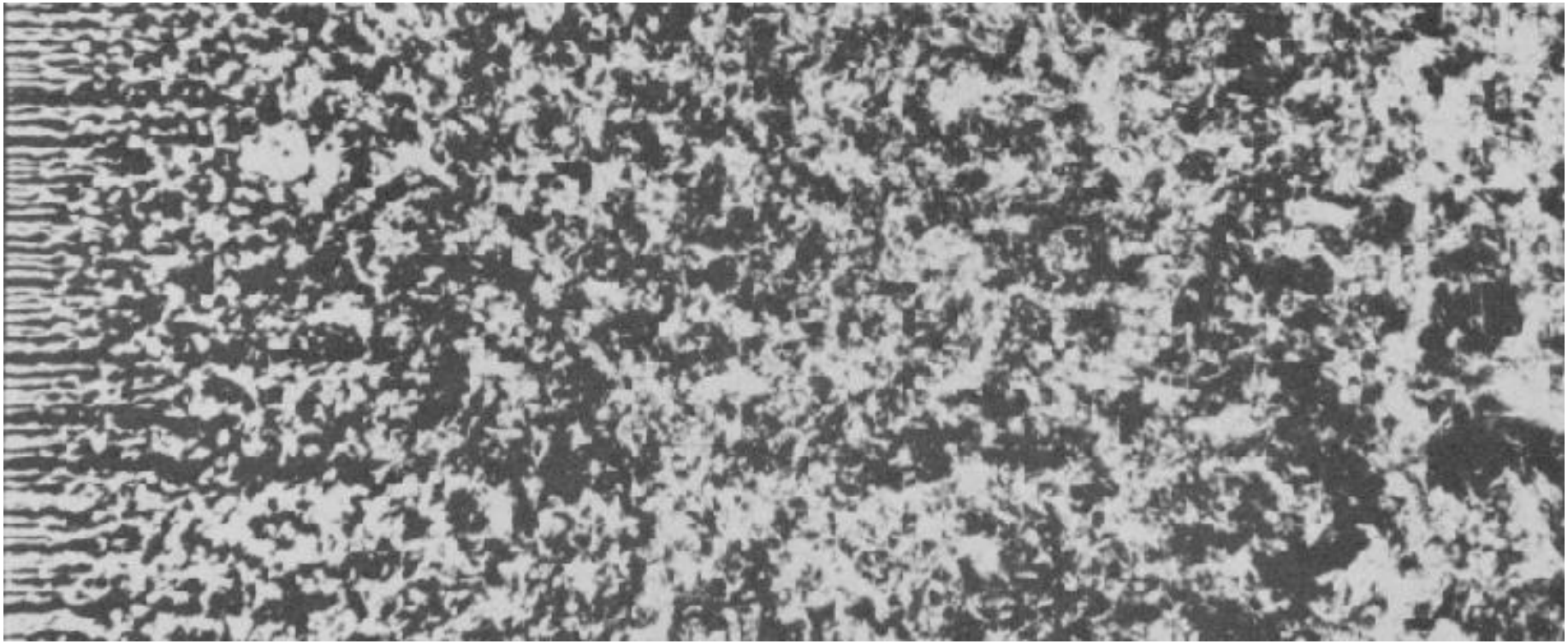
A smoke ring (green) impinges on a plate where it interacts with the slow moving smoke in the boundary layer (pink). The vortex ring stretches and new rings form. The size of the vortex structures decreases over time.

Images: Homsy et al. [2]

Simulation – species mixing

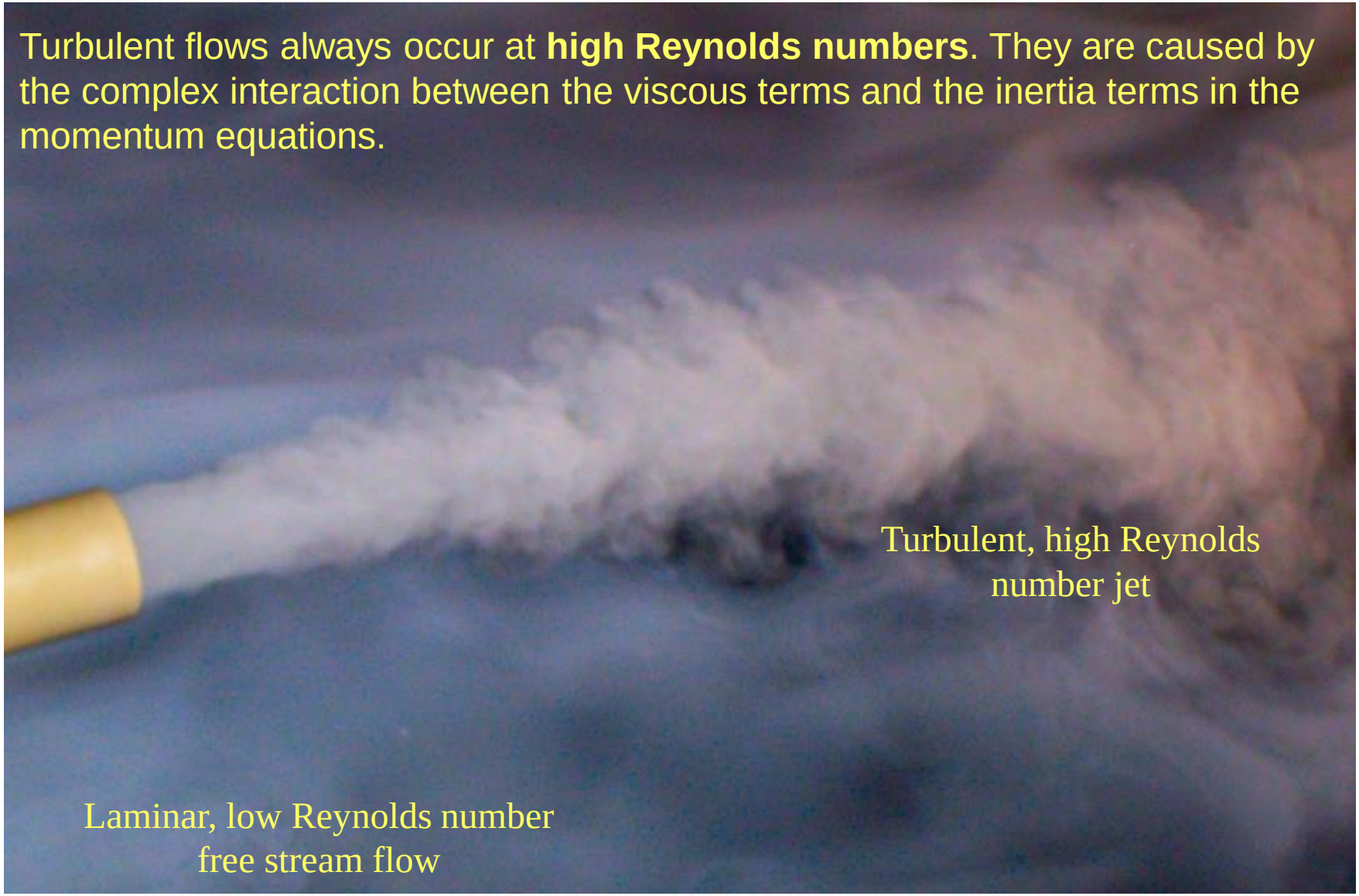


Homogeneous, decaying, grid-generated turbulence

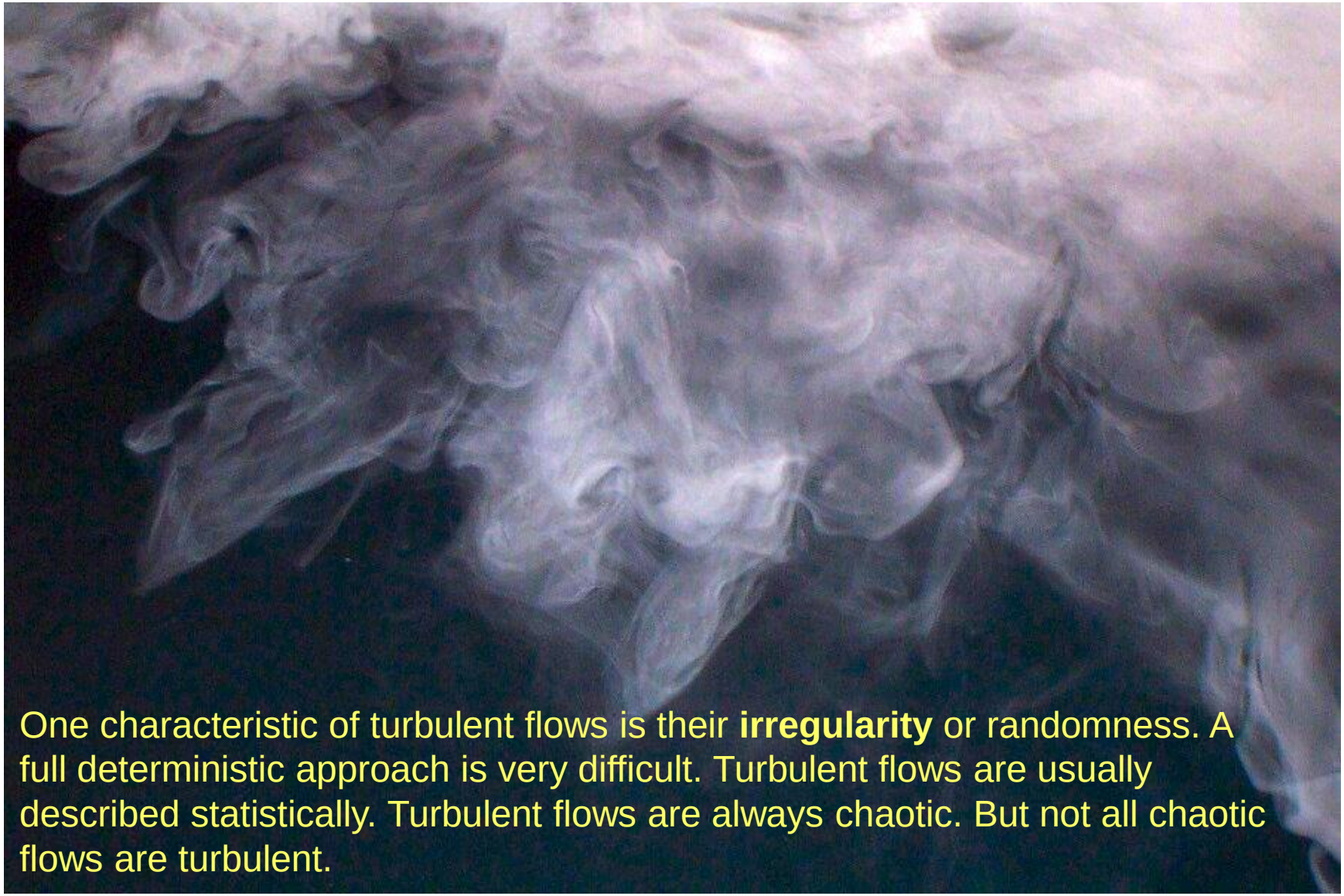


Turbulence is generated at the grid as a result of high stresses in the immediate vicinity of the grid. The turbulence is made visible by injecting smoke into the flow at the grid. The eddies are visible because they contain the smoke. Beyond this point, there is no source of turbulence as the flow is uniform. The flow is dominated by convection and dissipation. For homogeneous decaying turbulence, the turbulent kinetic energy decreases with distance from grid as x^{-1} and the turbulent eddies grows in size as $x^{1/2}$. Image: Van Dyke [8]

Turbulence: high Reynolds numbers

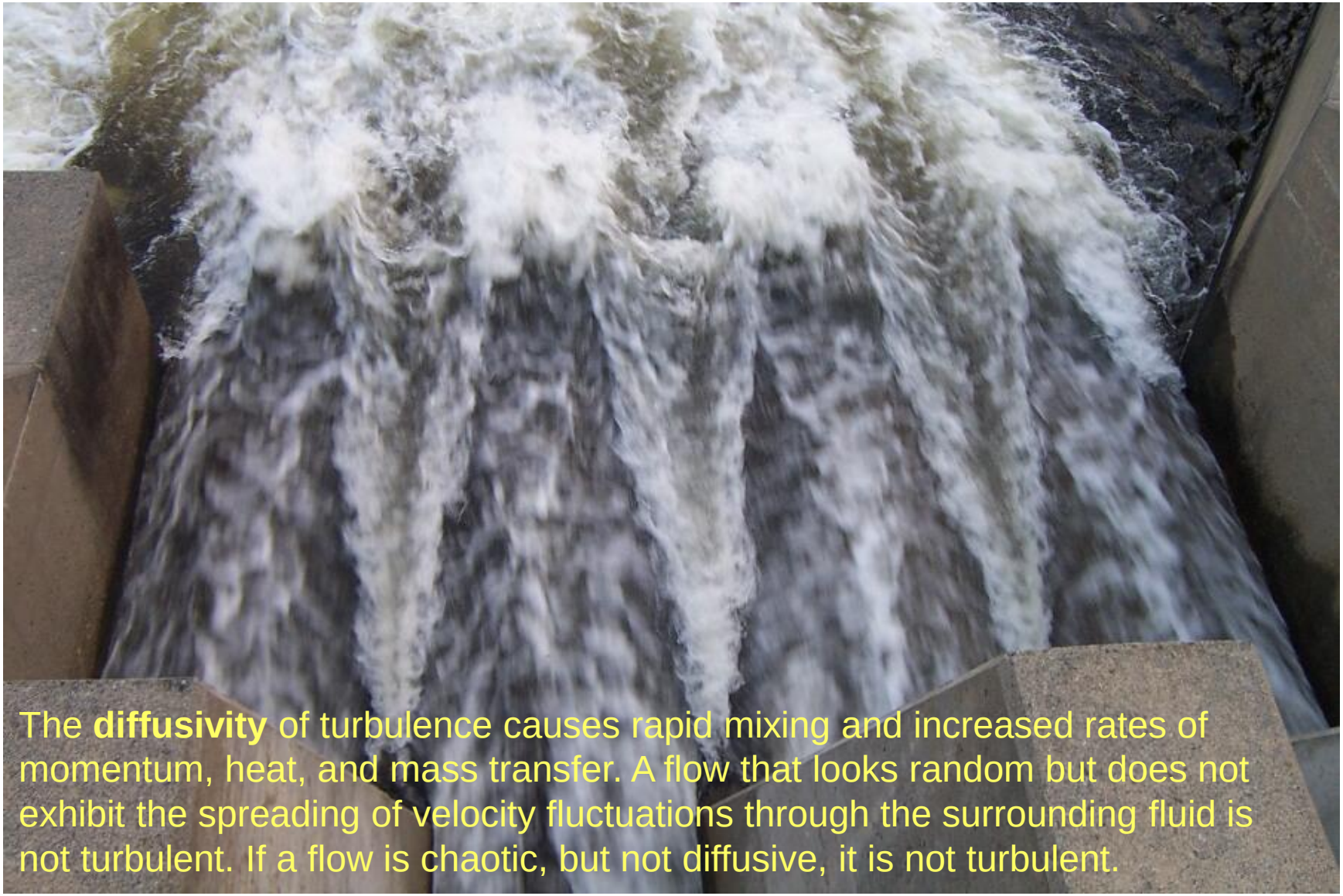


Turbulent flows are chaotic



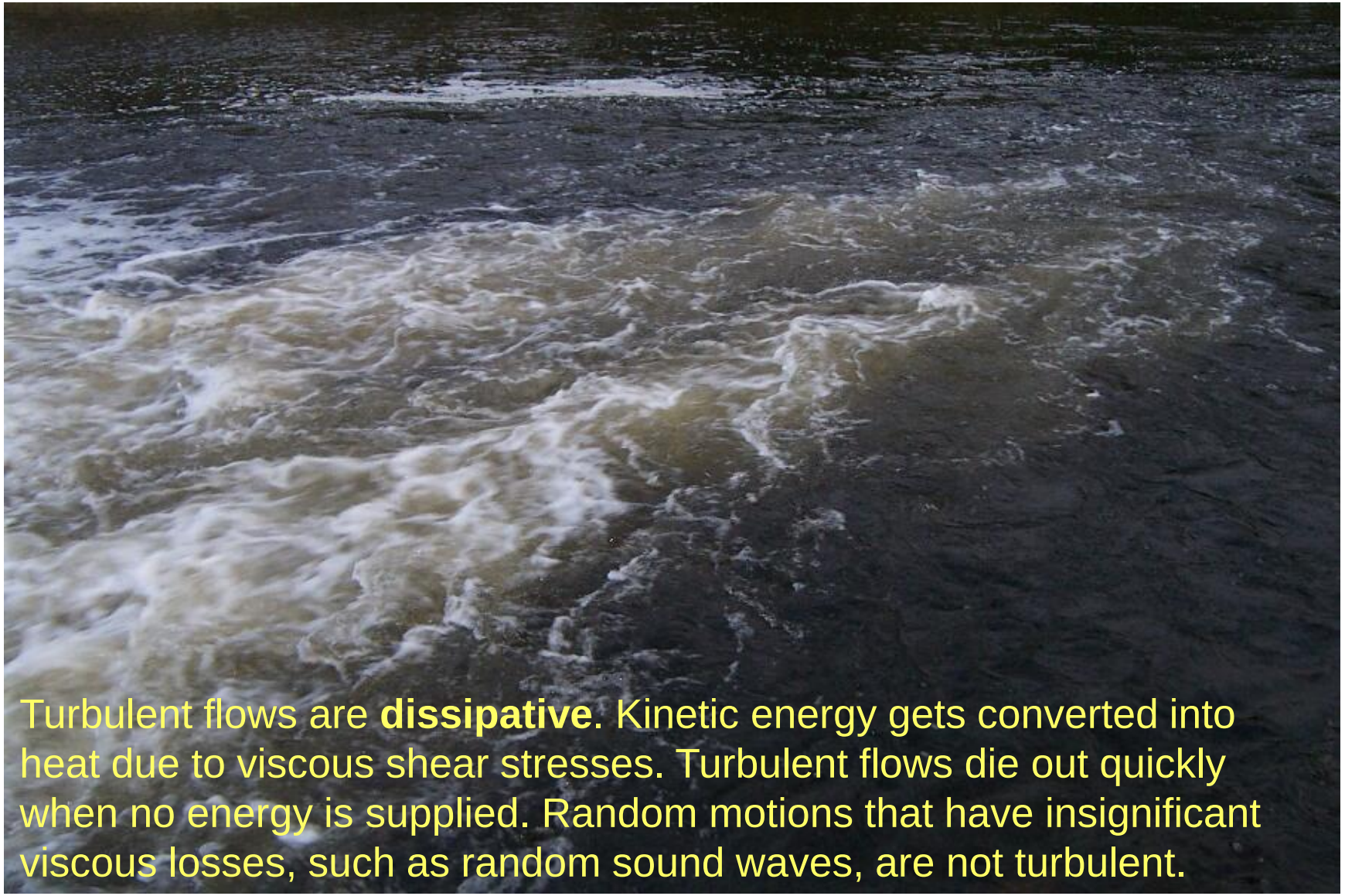
One characteristic of turbulent flows is their **irregularity** or randomness. A full deterministic approach is very difficult. Turbulent flows are usually described statistically. Turbulent flows are always chaotic. But not all chaotic flows are turbulent.

Turbulence: diffusivity



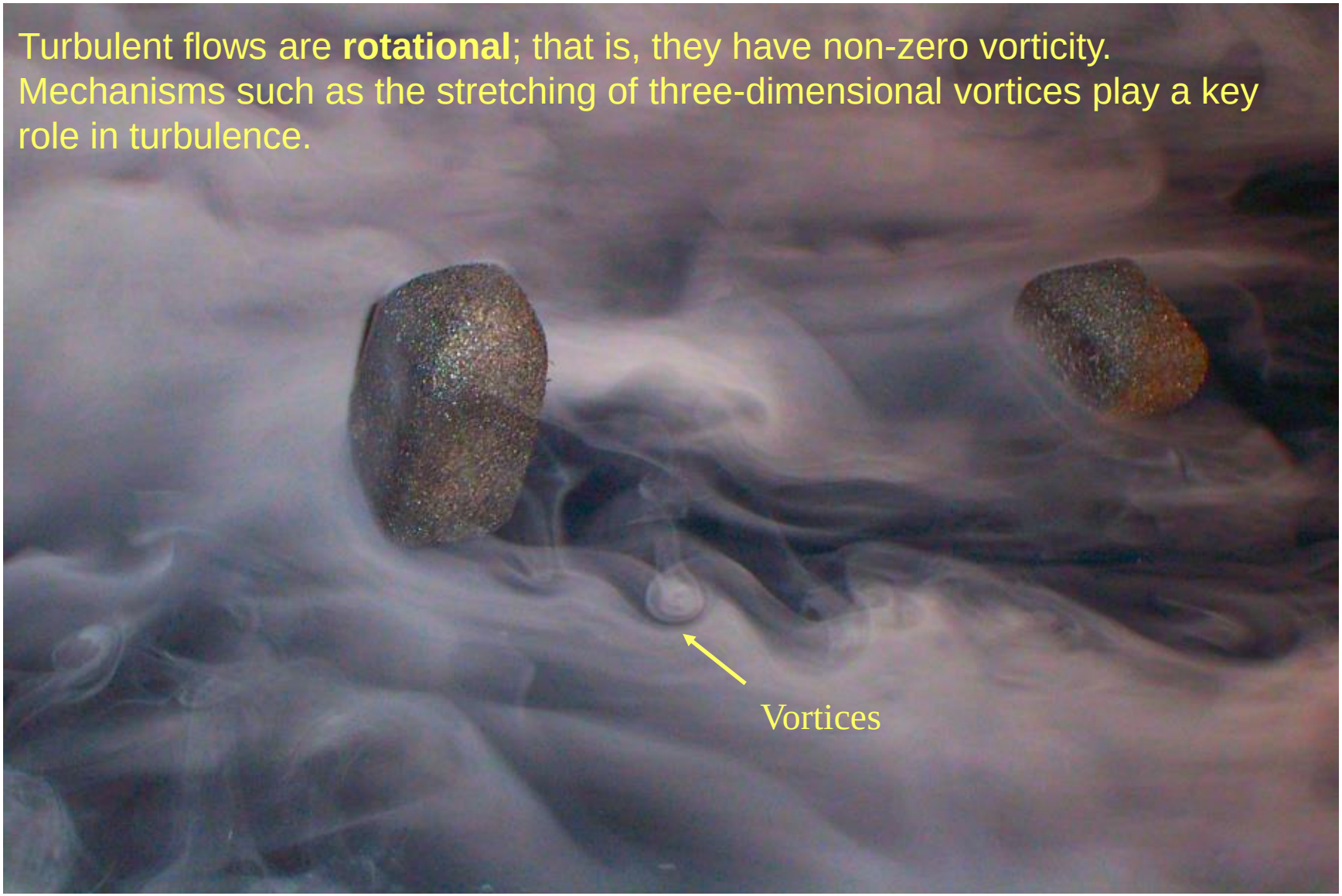
The **diffusivity** of turbulence causes rapid mixing and increased rates of momentum, heat, and mass transfer. A flow that looks random but does not exhibit the spreading of velocity fluctuations through the surrounding fluid is not turbulent. If a flow is chaotic, but not diffusive, it is not turbulent.

Turbulence: dissipation



Turbulent flows are **dissipative**. Kinetic energy gets converted into heat due to viscous shear stresses. Turbulent flows die out quickly when no energy is supplied. Random motions that have insignificant viscous losses, such as random sound waves, are not turbulent.

Turbulence: rotation and vorticity



What is turbulence?

- Turbulent flows have the following characteristics*:
  - One characteristic of turbulent flows is their **irregularity** or randomness. A full deterministic approach is very difficult. Turbulent flows are usually described statistically. Turbulent flows are always **chaotic**. But not all chaotic flows are turbulent. Waves in the ocean, for example, can be chaotic but are not necessarily turbulent.
  - The **diffusivity** of turbulence causes rapid mixing and increased rates of momentum, heat, and mass transfer. A flow that looks random but does not exhibit the spreading of velocity fluctuations through the surrounding fluid is not turbulent. If a flow is chaotic, but not diffusive, it is not turbulent. The trail left behind a jet plane that seems chaotic but does not diffuse for miles is then not turbulent.
  - Turbulent flows always occur at **high Reynolds numbers**. They are caused by the complex interaction between the viscous terms and the inertia terms in the momentum equations.
  - Turbulent flows are **rotational**; that is, they have non-zero vorticity. Mechanisms such as the stretching of three-dimensional vortices play a key role in turbulence.

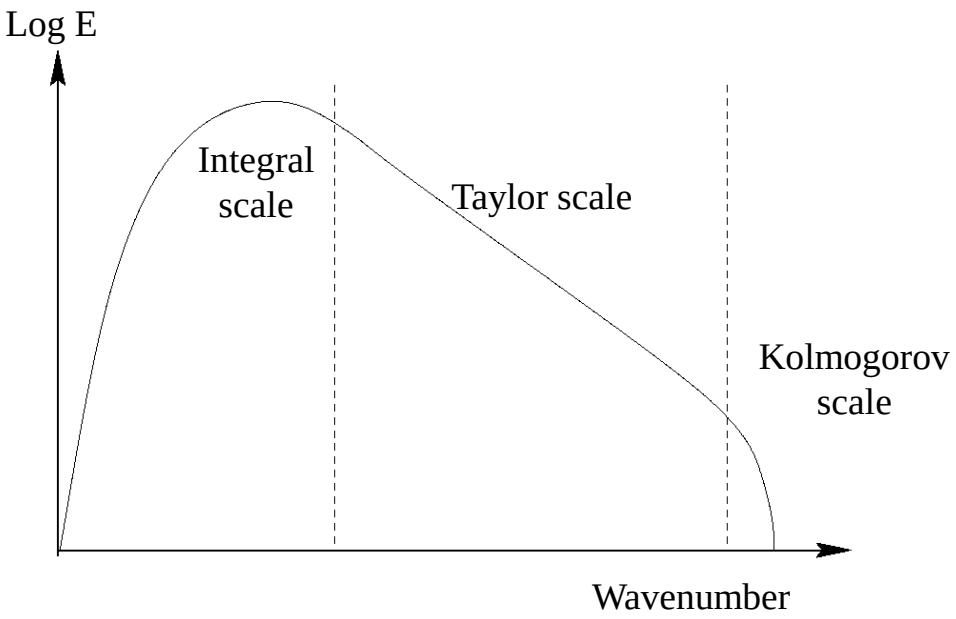
* Tennekes and Lumley [7]

What is turbulence? - Continued

- Turbulent flows are **dissipative**. Kinetic energy gets converted into heat due to viscous shear stresses. Turbulent flows die out quickly when no energy is supplied. Random motions that have insignificant viscous losses, such as random sound waves, are not turbulent.
- Turbulence is a **continuum** phenomenon. Even the smallest eddies are significantly larger than the molecular scales. Turbulence is therefore governed by the equations of fluid mechanics.
- Turbulent flows are flows. Turbulence is a **feature of fluid flow**, not of the fluid. When the Reynolds number is high enough, most of the dynamics of turbulence are the same whether the fluid is an actual fluid or a gas. Most of the dynamics are then independent of the properties of the fluid.

Kolmogorov energy spectrum

- Energy cascade, from large-scale to small-scale.
- E is energy contained in eddies of wavelength λ.
- Length scales:
  - Largest eddies. Integral length scale ($k^{3/2}/\varepsilon$).
  - Length scales at which turbulence is isotropic. Taylor microscale $(15\nu u'^2/\varepsilon)^{1/2}$.
  - Smallest eddies. Kolmogorov length scale $(\nu^3/\varepsilon)^{1/4}$. These eddies have a velocity scale $(\nu.\varepsilon)^{1/4}$ and a time scale $(\nu/\varepsilon)^{1/2}$.



ε is the energy dissipation rate (m^2/s^3)

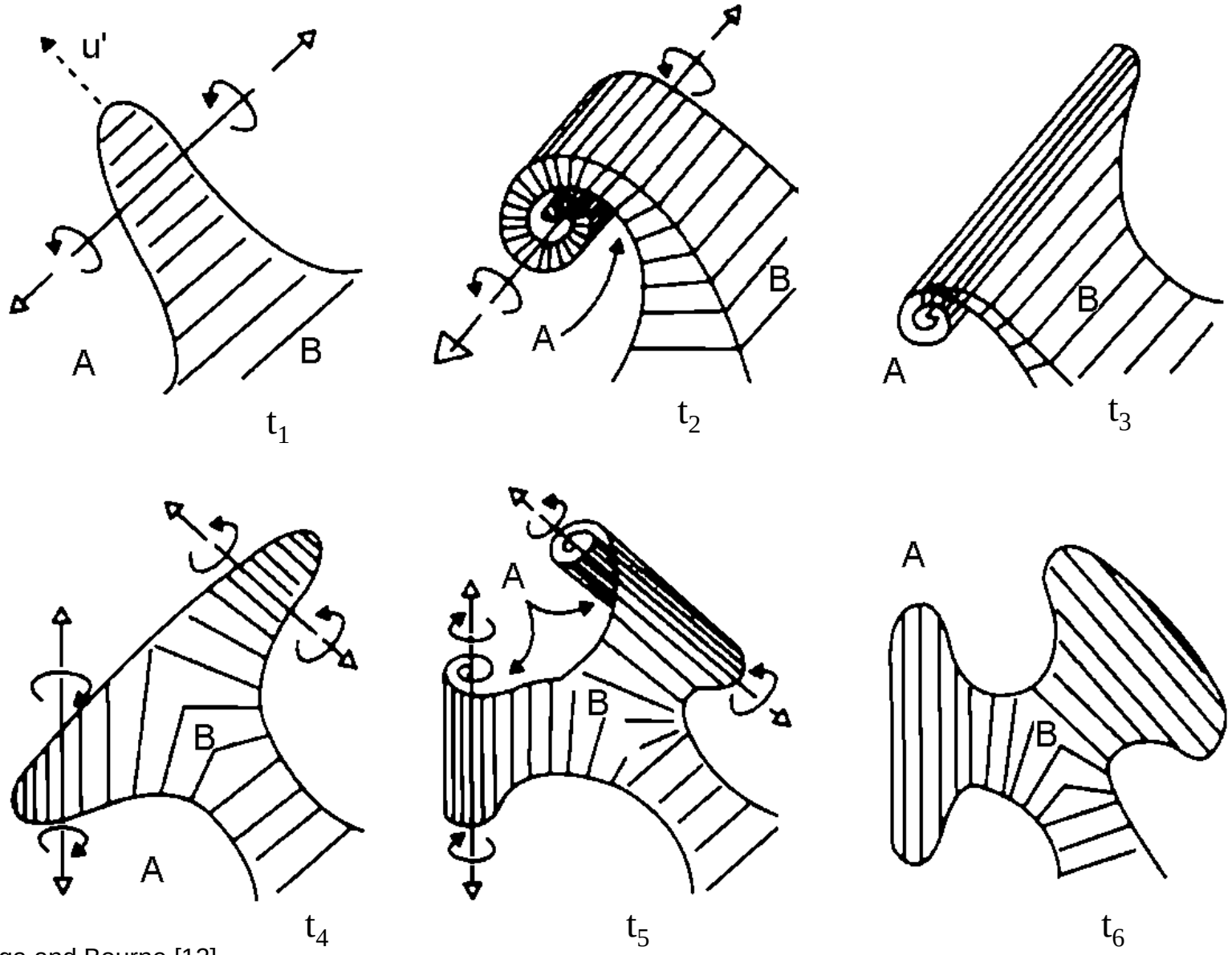
k is the turbulent kinetic energy (m^2/s^2)

ν is the kinematic viscosity (m^2/s)

Vorticity and vortex stretching

- Existence of eddies implies rotation or vorticity.
- Vorticity concentrated along contorted vortex lines or bundles.
- As end points of a vortex line move randomly further apart the vortex line increases in length but decreases in diameter. Vorticity increases because angular momentum is nearly conserved. Kinetic energy increases at rate equivalent to the work done by large-scale motion that stretches the bundle.
- Viscous dissipation in the smallest eddies converts kinetic energy into thermal energy.
- Vortex-stretching cascade process maintains the turbulence and dissipation is approximately equal to the rate of production of turbulent kinetic energy.
- Typically, energy gets transferred from the large eddies to the smaller eddies. However, sometimes smaller eddies can interact with each other and transfer energy to the (i.e., form) larger eddies, a process known as backscatter.

Vortex stretching



Images: Baldyga and Bourne [12]

Is the flow turbulent?

External flows:

$Re_x \geq 5 \times 10^5$ along a surface

$Re_D \geq 20{,}000$ around an obstacle

Internal flows:

$\mathrm{Re}_{D_h} \geq \sim 2{,}200$

where $Re_L \equiv \dfrac{\rho U L}{\mu}$

$L = x$, D, D_h, etc.

Other factors such as free-stream turbulence, surface conditions, and disturbances may cause earlier transition to turbulent flow.

Natural convection:

$Ra \geq 10^8 - 10^{10}$

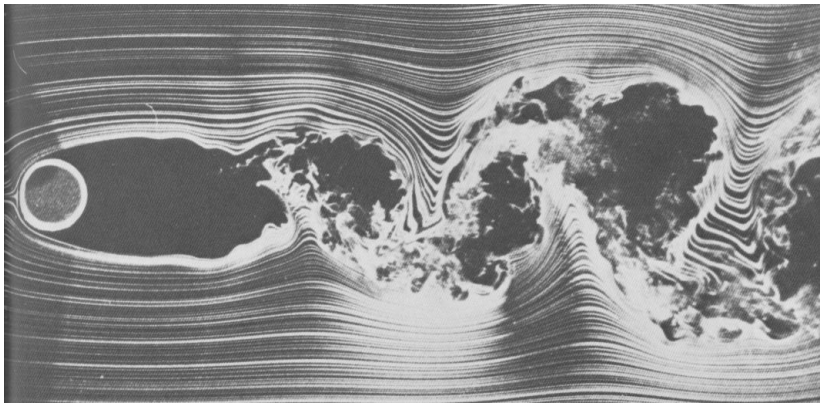
where $Ra \equiv \dfrac{g\beta\Delta T L^3 \rho}{\mu\alpha}$

Turbulence modeling objective

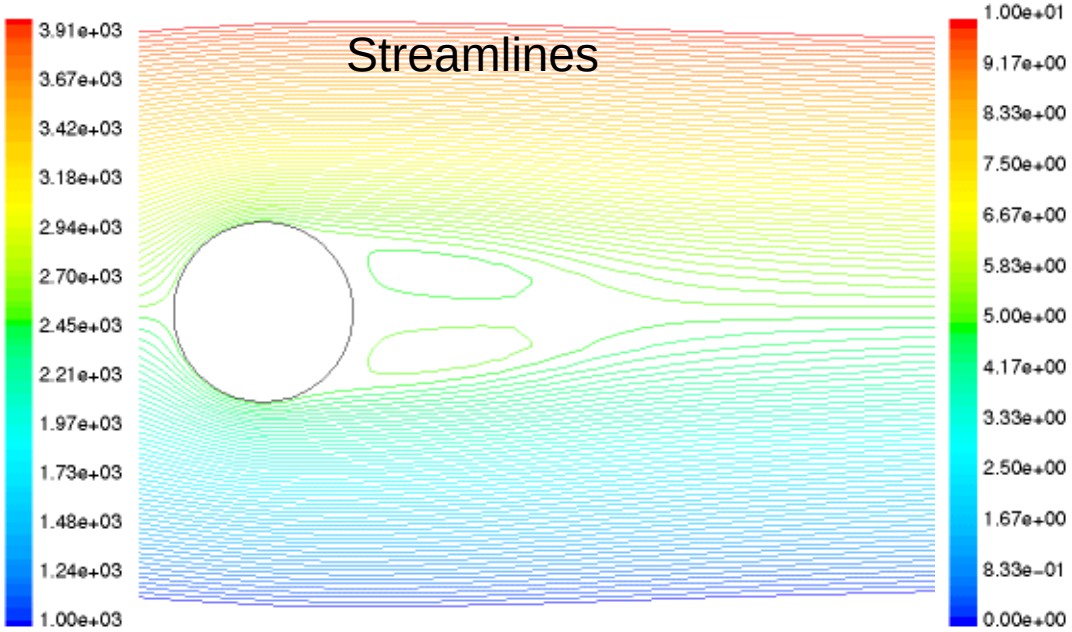
- The objective of turbulence modeling is to develop equations that will predict the time-averaged velocity, pressure, and temperature fields without calculating the complete turbulent flow pattern as a function of time.
  - This saves us a lot of work!
  - Most of the time it is all we need to know.
  - We may also calculate other statistical properties, such as RMS values.
- Important to understand: the time averaged flow pattern is a statistical property of the flow.
  - It is not an existing flow pattern!
  - It does not usually satisfy the steady Navier-Stokes equations!
  - The flow never actually looks that way!!

Example: flow around a cylinder at Re=1E4

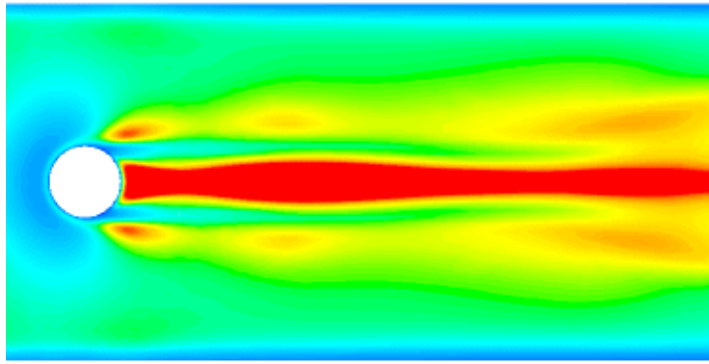
- The figures show:
  - An experimental snapshot.
  - Streamlines for time averaged flow field. Note the difference between the time averaged and the instantaneous flow field.
  - Effective viscosity used to predict time averaged flow field.



Experimental Snapshot (Van Dyke [8])



Effective Viscosity



Decomposition

Flow property φ. The mean Φ is defined as :

$$\Phi = \frac{1}{\Delta t}\int_0^{\Delta t} \varphi(t)\, dt$$

Δt should be larger than the time scale of the slowest turbulent fluctuations.

Time dependence : $\varphi(t) = \Phi + \varphi'(t)$

Write shorthand as : $\varphi = \Phi + \varphi'$

$$\overline{\varphi}' = \frac{1}{\Delta t}\int_0^{\Delta t} \varphi'(t)\, dt = 0 \quad \text{by definition}$$

Information regarding the fluctuating part of the flow can be obtained from the root – mean - square (rms) of the fluctuations :

$$\varphi_{rms} = \sqrt{\overline{(\varphi')^2}} = \left[\frac{1}{\Delta t}\int_0^{\Delta t} (\varphi')^2\, dt\right]^{1/2}$$

Velocity decomposition

- Velocity and pressure decomposition:

$$\text{Velocity}: \ \mathbf{u} = \mathbf{U} + \mathbf{u}'$$

$$\text{Pressure}: \ p = P + p'$$

- Turbulent kinetic energy k (per unit mass) is defined as:

$$k = \frac{1}{2}\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right)$$

$$\text{Turbulence intensity}: \ T_i = \frac{(\frac{2}{3}k)^{1/2}}{U_{ref}}$$

- Continuity equation:

$$div\,\mathbf{u} = 0; \ Time\ average: \overline{div\,\mathbf{u}} = div\,\mathbf{U} = 0$$

$$\Rightarrow \text{continuity equation for the mean flow}: \ div\,\mathbf{U} = 0$$

- Next step, time average the momentum equation. This results in the Reynolds equations.

Turbulent flow - Reynolds equations

$$x-momentum: \quad \frac{\partial(\rho U)}{\partial t} + div(\rho U \mathbf{U}) = -\frac{\partial P}{\partial x} + div(\mu\ grad\ U) + S_{Mx}$$
$$+\left[-\frac{\partial(\rho\overline{u'^2})}{\partial x} - \frac{\partial(\rho\overline{u'v'})}{\partial y} - \frac{\partial(\rho\overline{u'w'})}{\partial z}\right]$$

$$y-momentum: \quad \frac{\partial(\rho V)}{\partial t} + div(\rho V \mathbf{U}) = -\frac{\partial P}{\partial y} + div(\mu\ grad\ V) + S_{My}$$
$$+\left[-\frac{\partial(\rho\overline{u'v'})}{\partial x} - \frac{\partial(\rho\overline{v'^2})}{\partial y} - \frac{\partial(\rho\overline{v'w'})}{\partial z}\right]$$

$$z-momentum: \quad \frac{\partial(\rho W)}{\partial t} + div(\rho W \mathbf{U}) = -\frac{\partial P}{\partial z} + div(\mu\ grad\ W) + S_{Mz}$$
$$+\left[-\frac{\partial(\rho\overline{u'w'})}{\partial x} - \frac{\partial(\rho\overline{v'w'})}{\partial y} - \frac{\partial(\rho\overline{w'^2})}{\partial z}\right]$$

Reynolds stresses

- These equations contain an additional stress tensor. These are called the Reynolds stresses.

$$\boldsymbol{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix} = \begin{pmatrix} -\rho\overline{u'^2} & -\rho\overline{u'v'} & -\rho\overline{u'w'} \\ -\rho\overline{u'v'} & -\rho\overline{v'^2} & -\rho\overline{v'w'} \\ -\rho\overline{u'w'} & -\rho\overline{v'w'} & -\rho\overline{w'^2} \end{pmatrix}$$

- In turbulent flow, the Reynolds stresses are usually large compared to the viscous stresses.
- The normal stresses are always non-zero because they contain squared velocity fluctuations. The shear stresses would be zero if the fluctuations were statistically independent. However, they are correlated (amongst other reasons because of continuity) and the shear stresses are therefore usually also non-zero.

Turbulent flow - continuity and scalars

- Continuity: $$\frac{\partial \rho}{\partial t} + div(\rho\, \mathbf{U}) = 0$$

- Scalar transport equation:

$$\frac{\partial(\rho\Phi)}{\partial t} + div(\rho\Phi\mathbf{U}) = div(\Gamma_\Phi\ grad\ \Phi) + S_\Phi$$

$$+\left[-\frac{\partial(\rho\overline{u'\varphi'})}{\partial x} - \frac{\partial(\rho\overline{v'\varphi'})}{\partial y} - \frac{\partial(\rho\overline{w'\varphi'})}{\partial z}\right]$$

- Notes on density:
  - Here ρ is the mean density.
  - This form of the equations is suitable for flows where changes in the mean density are important, but the effect of density fluctuations on the mean flow is negligible.
  - For flows with T_i<5% this is up to Mach 5 and with T_i<20% this is valid up to around Mach 1.

Closure modeling

- The time averaged equations now contain six additional unknowns in the momentum equations.
- Additional unknowns have also been introduced in the scalar equation.
- Turbulent flows are usually quite complex, and there are no simple formulae for these additional terms.
- The main task of turbulence modeling is to develop computational procedures of sufficient accuracy and generality for engineers to be able to accurately predict the Reynolds stresses and the scalar transport terms.
- This will then allow for the computation of the time averaged flow and scalar fields without having to calculate the actual flow fields over long time periods.

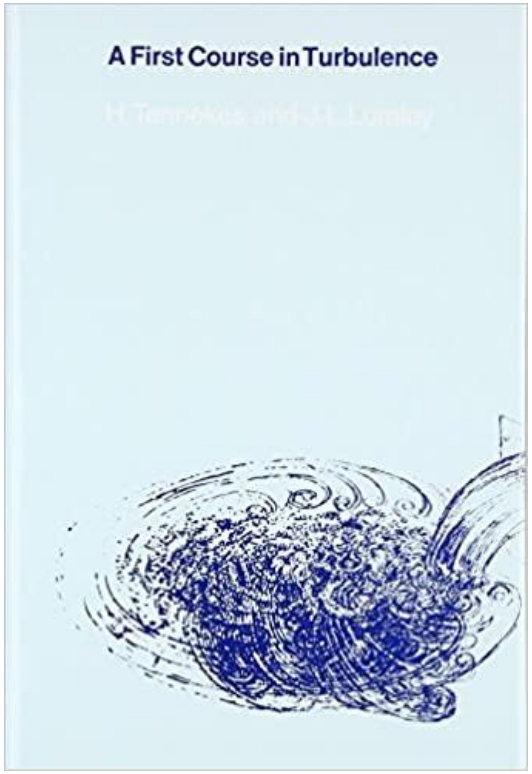
Lecture 9 - Kolmogorov's Theory

Applied Computational Fluid Dynamics

André Bakker

Eddy size

- Kolmogorov's theory describes how energy is transferred from larger to smaller eddies; how much energy is contained by eddies of a given size; and how much energy is dissipated by eddies of each size.
- We will derive three main turbulent length scales: the integral scale, the Taylor scale, and the Kolmogorov scale; and corresponding Reynolds numbers.
- We will also discuss the concept of energy and dissipation spectra.

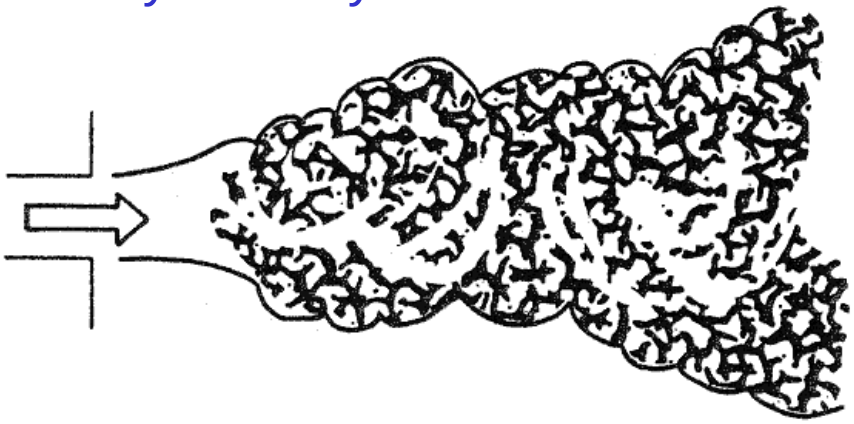


The book by Tennekes and Lumley features a sketch by Leonardo DaVinci on its cover.

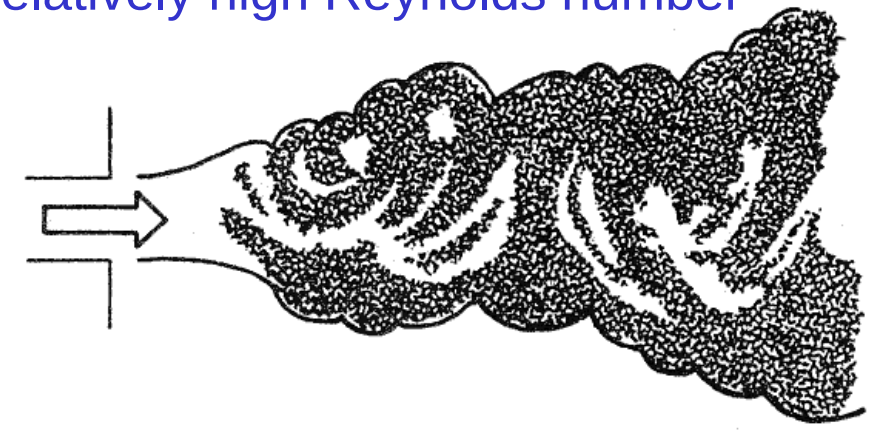
This lecture closely follows Pope [4] and Tennekes and Lumley [7]

Jets at two different Reynolds numbers

Relatively low Reynolds number



Relatively high Reynolds number



Images: Tennekes & Lumley. [12, page 22]

Turbulent eddies

- Consider fully turbulent flow at high Reynolds number Re=UL/ν.
- Turbulence can be considered to consist of eddies of different sizes.
- An ‘eddy’ preludes precise definition, but it is conceived to be a turbulent motion, localized over a region of size l, that is at least moderately coherent over this region.
- The region occupied by a larger eddy can also contain smaller eddies.
- Eddies of size l have a characteristic velocity $u(l)$ and timescale $\tau(l) \equiv l/u(l)$.
- Eddies in the largest size range are characterized by the lengthscale l_0 which is comparable to the flow length scale L.
- Their characteristic velocity $u_0 \equiv u(l_0)$ is on the order of the r.m.s. turbulence intensity $u' \equiv (2k/3)^{1/2}$ which is comparable to U.
- Here the turbulent kinetic energy is defined as: $k = \frac{1}{2} < u_i u_i > = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$
- The Reynolds number of these eddies $\mathrm{Re}_0 \equiv u_0 l_0/\nu$ is therefore large (comparable to Re) and the direct effects of viscosity on these eddies are negligibly small.

Integral scale

- We can derive an estimate of the lengthscale l_0 of the larger eddies based on the following:
  - Eddies of size l_0 have a characteristic velocity u_0 and timescale $\tau_0 \equiv l_0/u_0$
  - Their characteristic velocity $u_0 \equiv u(l_0)$ is on the order of the r.m.s. turbulence intensity $u' \equiv (2k/3)^{1/2}$
  - Assume that energy of eddy with velocity scale u_0 is dissipated in time τ_0
- We can then derive the following equation for this length scale:

$$l_0 \propto \frac{k^{3/2}}{\varepsilon}$$

- Here, ε(m^2/s^3) is the energy dissipation rate. The proportionality constant is of the order one. This lengthscale is usually referred to as the ***integral scale*** of turbulence.
- The Reynolds number associated with these large eddies is referred to as the turbulence Reynolds number Re_L, which is defined as:

$$\mathrm{Re}_L = \frac{k^{1/2} l_0}{\nu} = \frac{k^2}{\varepsilon \nu}$$

Energy transfer

- The large eddies are unstable and break up, transferring their energy to somewhat smaller eddies.
- These smaller eddies undergo a similar break-up process and transfer their energy to yet smaller eddies.
- This *energy cascade* – in which energy is transferred to successively smaller and smaller eddies – continues until the Reynolds number $\mathrm{Re}(l) \equiv u(l)l/\nu$ is sufficiently small that the eddy motion is stable, and molecular viscosity is effective in dissipating the kinetic energy.
- At these small-scales, the kinetic energy of turbulence is converted into heat.

Richardson

- L.F. Richardson ("Weather Prediction by Numerical Process." Cambridge University Press, 1922, [6]) summarized this in the following often cited verse:

Big whirls have little whirls
Which feed on their velocity;
And little whirls have lesser whirls,
And so on to viscosity
in the molecular sense.

Based on a poem by Augustus de Morgan (1872)
"Great fleas have little fleas …"

Dissipation

- Note that dissipation takes place at the end of the sequence of processes.
- The rate of dissipation ε is determined, therefore by the first process in the sequence, which is the transfer of energy from the largest eddies.
- These eddies have energy of order u_0^2 and timescale $\tau_0 = l_0/u_0$ so the rate of transfer of energy can be supposed to scale as

  $u_0^2/\tau_0 = u_0^3/l_0$
- Consequently, consistent with experimental observations in free shear flows, this picture of the energy cascade indicates that ε is proportional to u_0^3/l_0 independent of ν (at high Reynolds numbers).

Kolmogorov's theory

- Many questions remain unanswered.
  - What is the size of the smallest eddies that are responsible for dissipating the energy?
  - As l decreases, do the characteristic velocity and timescales $\mathrm{u}(l)$ and $\tau(l)$ increase, decrease, or stay the same? The assumed decrease of the Reynolds number $u_0 l_0/\nu$ by itself is not sufficient to determine these trends.
- These and others are answered by Kolmogorov's theory of turbulence (1941, see Pope (2000)).
- Kolmogorov's theory was first published in 1941 ("K41 theory") with later papers in 1962.
- Kolmogorov's theory is based on three important hypotheses combined with dimensional arguments and experimental observations.

Kolmogorov's hypothesis of local isotropy

- For homogenous turbulence, the turbulent kinetic energy k is the same everywhere. For isotropic turbulence the eddies also behave the same in all directions: $\overline{u'^2} = \overline{v'^2} = \overline{w'^2}$
- Kolmogorov argued that the directional biases of the large-scales are lost in the chaotic scale-reduction process as energy is transferred to successively smaller eddies.
- Hence Kolmogorov's hypothesis of local isotropy states that *at sufficiently high Reynolds numbers, the small-scale turbulent motions ($l << l_0$) are statistically isotropic.*
- Here, the term local isotropy means isotropy at small-scales. large-scale turbulence may still be anisotropic.
- l_{EI} is the length scale that forms the demarcation between the large-scale anisotropic eddies ($l>l_{EI}$) and the small-scale isotropic eddies ($l<l_{EI}$). For many high Reynolds number flows l_{EI} can be estimated as $l_{EI} \approx l_0/6$.

Kolmogorov's first similarity hypothesis

- Kolmogorov also argued that not only does the directional information get lost as the energy passes down the cascade, but that all information about the geometry of the eddies gets lost also.
- As a result, the statistics of the small-scale motions are universal: they are *similar* in every high Reynolds number turbulent flow, independent of the mean flow field and the boundary conditions.
- These small-scale eddies depend on the rate T_{EI} at which they receive energy from the larger scales (which is approximately equal to the dissipation rate ε) and the viscous dissipation, which is related to the kinematic viscosity ν.
- Kolmogorov's first similarity hypothesis states *that in every turbulent flow at sufficiently high Reynolds number, the statistics of the small-scale motions ($l<l_{EI}$) have a universal form that is uniquely determined by ε and ν.*

Universal equilibrium range

- The size range ($l<l_{EI}$) is referred to as the universal equilibrium range.
- In this range, the timescales $l/u(l)$ are small compared to l_0/u_0 so that the small eddies can adapt quickly to maintain dynamic equilibrium with the energy transfer rate T_{EI} imposed by the large eddies.
- On these scales all high Reynolds number flow fields are statistically identical if the flow fields are scaled by the Kolmogorov scales.

Kolmogorov scales

- Given the two parameters ε and ν we can form the following unique length, velocity, and time scales:

$$length\ scale: \quad \eta = (\nu^3 / \varepsilon)^{1/4}$$

$$velocity\ scale: \quad u_\eta = (\varepsilon\nu)^{1/4}$$

$$time\ scale: \quad \tau_\eta = (\nu / \varepsilon)^{1/2}$$

$$(u_\eta / \eta) = 1/\tau_\eta$$

$$\mathrm{Re}_\eta = \eta u_\eta / \nu = 1$$

- These scales are indicative of the smallest eddies present in the flow, the scale at which the energy is dissipated.
- Note that the fact that the Kolmogorov Reynolds number Re_η of the small eddies is 1, is consistent with the notion that the cascade proceeds to smaller and smaller scales until the Reynolds number is small enough for dissipation to be effective.

Kolmogorov scales - derivation

$$\tau_\eta = \eta / u_\eta \quad [1]$$

$$\mathrm{Re}_\eta = \frac{\eta\, u_\eta}{\nu} = 1 \quad \Rightarrow \quad u_\eta = \frac{\nu}{\eta} \quad [2]$$

$$\varepsilon = \frac{u_\eta^2}{\tau_\eta} \sim \frac{u_\eta^2 . u_\eta}{\eta} \sim \frac{u_\eta^3}{\eta} \Rightarrow u_\eta \sim (\varepsilon\, \eta)^{1/3} \quad [3]$$

$$[2] \wedge [3] \Rightarrow \eta = \frac{\nu}{\varepsilon^{1/3}\, \eta^{1/3}} \Rightarrow \eta^{4/3} = \frac{\nu}{\varepsilon^{1/3}} \Rightarrow$$

$$\Rightarrow \textit{length scale} \quad \eta = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4} \quad [4]$$

$$\varepsilon \sim \frac{u_\eta^3}{\eta} \wedge \eta = \left(\frac{\nu^3}{\varepsilon} \right)^{1/4} \Rightarrow \textit{velocity scale}: \quad u_\eta = (\varepsilon\nu)^{1/4} \quad [5]$$

$$[1] \wedge [4] \wedge [5] \Rightarrow \textit{time scale}: \quad \tau_\eta = (\nu / \varepsilon)^{1/2} \quad [6]$$

Ratio between large and small-scales

- When we use the relationship $l_0 \sim k^{3/2}/\varepsilon$ and substitute it in the equations for the Kolmogorov scales, we can calculate the ratios between the small-scale and large-scale eddies.

$$\eta / l_0 \sim \mathrm{Re}_L^{-3/4}$$

$$u_\eta / u_0 \sim \mathrm{Re}_L^{-1/4}$$

$$\tau_\eta / \tau_0 \sim \mathrm{Re}_L^{-1/2}$$

- As expected, at high Reynolds numbers, the velocity and timescales of the smallest eddies are small compared to those of the largest eddies.
- Since η/l_0 decreases with increasing Reynolds number, at high Reynolds number there will be a range of intermediate scales l which is small compared to l_0 and large compared with η.

Kolmogorov's second similarity hypothesis

- Because the Reynolds number of the intermediate scales l is relatively large, they will not be affected by the viscosity ν.
- Based on that, Kolmogorov's second similarity hypothesis states that *in every turbulent flow at sufficiently high Reynolds number, the statistics of the motions of scale l in the range $l_0 >> l >> \eta$ have a universal form that is uniquely determined by ε independent of ν.*
- We introduce a new length scale l_{DI}, (with $l_{DI} \approx 60\eta$ for many turbulent high Reynolds number flows) so that this range can be written as $l_{EI} > l > l_{DI}$
- This length scale splits the universal equilibrium range into two subranges:
  - The inertial subrange ($l_{EI} > l > l_{DI}$) where motions are determined by inertial effects and viscous effects are negligible.
  - The dissipation range ($l < l_{DI}$) where motions experience viscous effects.

Eddy sizes in the inertial subrange

- For eddies in the inertial subrange of size l, using:

$$\varepsilon = u_\eta^3 / \eta = \eta^2 / \tau_\eta^3$$

and the previously shown relationships between the turbulent Reynolds number and various scales, velocity scales and timescales can be formed from ε and l:

$$u(l) = (\varepsilon l)^{1/3} = u_\eta (l/\eta)^{1/3} \sim u_0 (l/l_0)^{1/3}$$

$$\tau(l) = (l^2/\varepsilon)^{1/3} = \tau_\eta (l/\eta)^{2/3} \sim \tau_0 (l/l_0)^{2/3}$$

- A consequence, then, of the second similarity hypothesis is that in the inertial subrange the velocity scales and timescales $u(l)$ and $\tau(l)$ decrease as l decreases.

Taylor microscale

- The energy dissipation rate ε is given by the following equation, which comes from the analytically derived conservation equation for turbulent kinetic energy:

$$\overline{s_{ij}s_{ij}} >> S_{ij}S_{ij}; \qquad \varepsilon = 2\nu\overline{s_{ij}s_{ij}}; \qquad s_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- The lower case indicates the fluctuating components. The dissipation rate depends on the viscosity and velocity gradients ("shear") in the turbulent eddies.
- Working out this equation further for isotropic turbulence (mainly bookkeeping for all the terms) results in:

$$\varepsilon = 15\nu \ \overline{(\partial u_1 / \partial x_1)^2}$$

- We can now define the Taylor microscale λ as follows:

$$\overline{(\partial u_1 / \partial x_1)^2} \equiv \overline{u_1^2} / \lambda^2 = u'^2 / \lambda^2$$

Taylor microscale - continued

- This then results in the following relationship for the Taylor microscale λ:

$$\varepsilon = 15\nu u'^2 / \lambda^2$$

- From $k = (1/2)(u'^2+v'^2+w'^2)$ we can derive $k = (2/3)u'^2$, and:

$$\lambda \approx (10\nu k / \varepsilon)^{1/2}$$

- The Taylor microscale falls in between the large-scale eddies and the small-scale eddies, which can be seen by calculating the ratios between λ and l_0 and η:

$$\lambda / l_0 = \sqrt{10}\,\mathrm{Re}_L^{-1/2}$$

$$\eta / l_0 = \mathrm{Re}_L^{-3/4}$$

$$\lambda / \eta = \sqrt{10}\,\mathrm{Re}_L^{1/4}$$

$$\lambda = \sqrt{10}\,\eta^{2/3} l_0^{1/3}$$

Taylor-scale Reynolds number

- A commonly used quantity in the characterization of turbulence is the Taylor-scale Reynolds number R_λ.
- This is based on the length scale λ and the corresponding velocity scale:

$$R_\lambda = u'\lambda / \nu$$

- R_λ can be related to the turbulence Reynolds number as follows:

$$R_\lambda = \left(\frac{20}{3} \mathrm{Re}_L \right)^{1/2}$$

- We can also relate the timescale of the eddies of length scale λ to the Kolmogorov timescale:

$$\lambda / u' = (15\nu / \varepsilon)^{1/2} = \sqrt{15}\,\tau_\eta$$

Taylor scales

- The eddy size in the inertial subrange is given by the Taylor microscale λ:

$$\lambda \approx (10\nu k/\varepsilon)^{1/2}$$

- A commonly used quantity in the characterization of turbulence is the Taylor-scale Reynolds number R_λ.
- This is based on the length scale λ and the corresponding velocity scale:

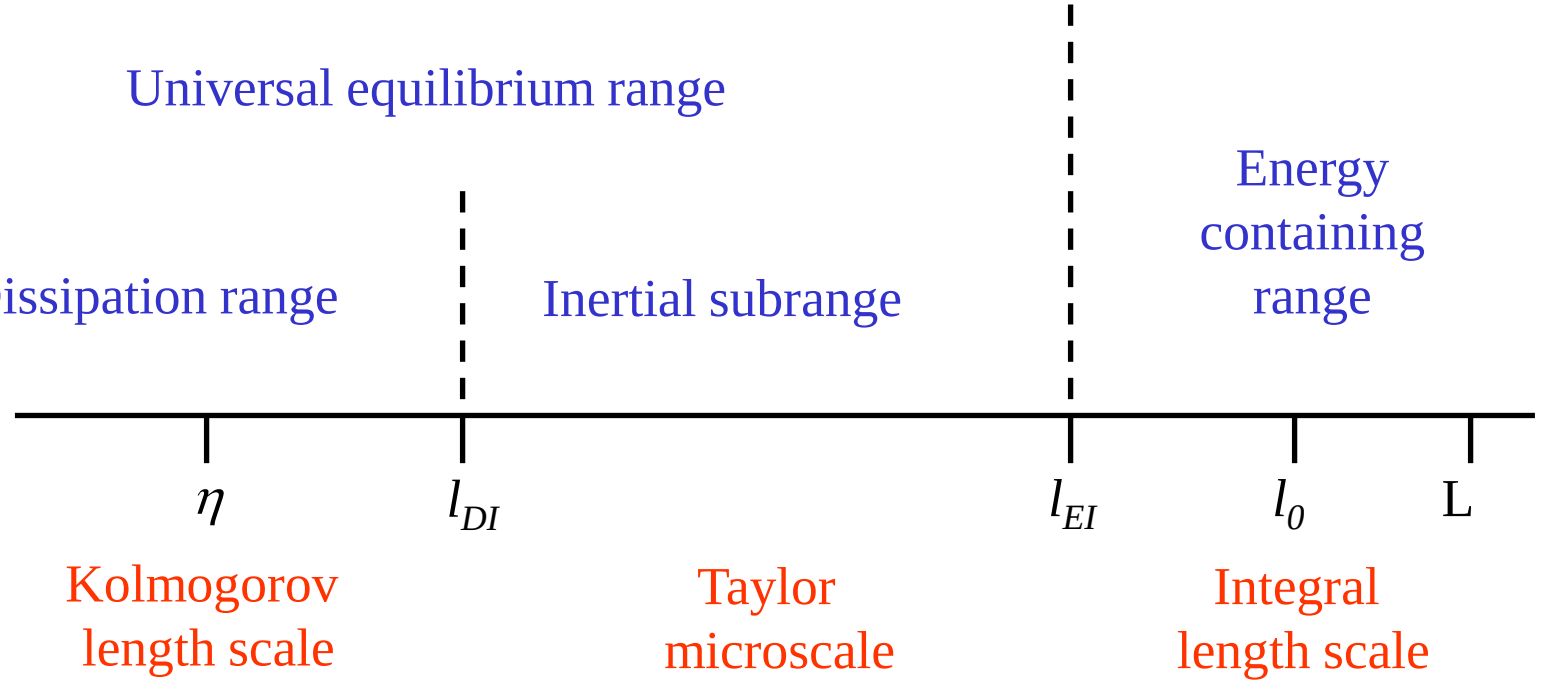
$$R_\lambda = u'\lambda/\nu$$

- R_λ can be related to the turbulence Reynolds number as follows:

$$R_\lambda = \left(\frac{20}{3}\mathrm{Re}_L\right)^{1/2}$$

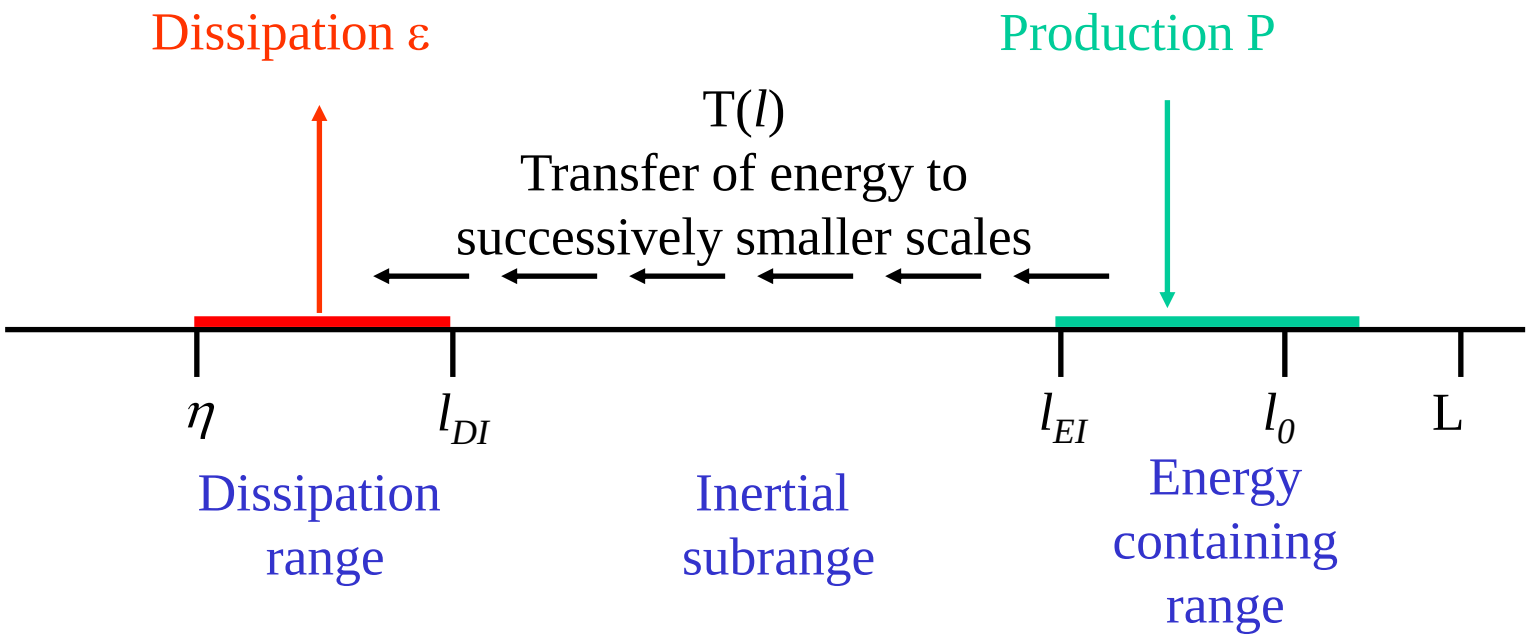
Eddy sizes

- The bulk of the energy is contained in the larger eddies in the size range $l_{EI} = l_0/6 < l < 6l_0$, which is therefore called the energy-containing range.
- The suffixes EI and DI indicate that l_{EI} is the demarcation line between energy (E) and inertial (I) ranges, as l_{DI} is that between the dissipation (D) and inertial (I) ranges.



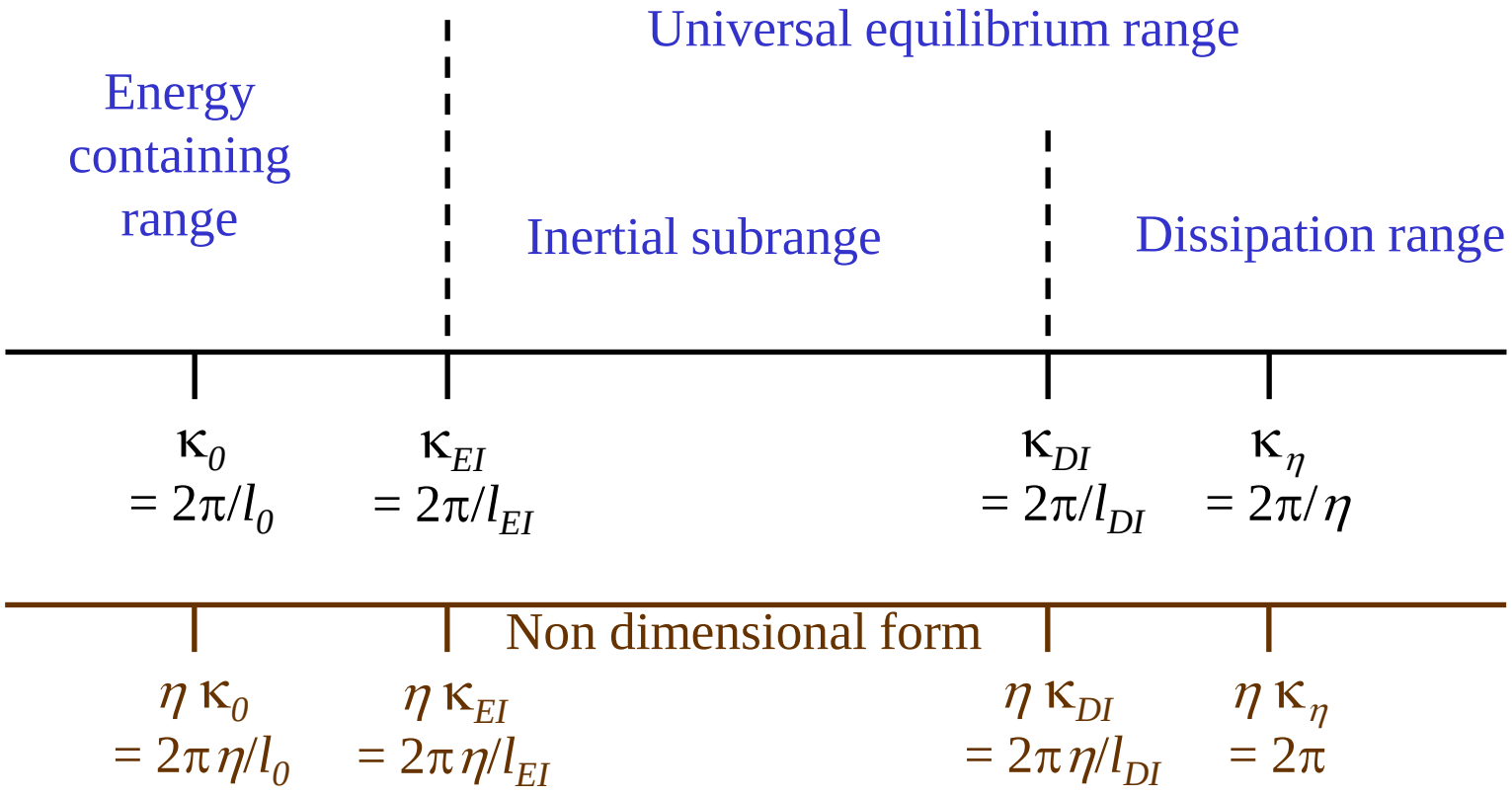
Energy transfer rate

- The rate at which energy is transferred from the larger scales to the smaller scales is T(l).
- Under the equilibrium conditions in the inertial subrange this is equal to the dissipation rate ε and is proportional to $u(l)^2/\tau$.



Wavenumbers

- The wavenumber κ is defined as $\kappa = 2\pi/l$.
- The different ranges can be shown as a function of wavenumber.
- The wavenumber can also be made non-dimensional by multiplying it with the Kolmogorov length scale η to result in the commonly used dimensionless group ($\eta\ \kappa$).



Energy spectrum

- The turbulent kinetic energy *k* is given by: $k = \frac{1}{2} < u_i u_i > = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$
- It remains to be determined how the turbulent kinetic energy is distributed among the eddies of different sizes.
- This is usually done by considering the energy spectrum E(κ).
- Here E(κ) is the energy contained in eddies of size *l* and wavenumber κ, defined as $\kappa = 2\pi/l$.
- By definition *k* is the integral of E(κ) over all wavenumbers:

$$k = \int_0^\infty E(\kappa) d\kappa$$

- The energy contained in eddies with wavenumbers between κ_A and κ_B is then:

$$k_{(\kappa_A, \kappa_B)} = \int_{\kappa_A}^{\kappa_B} E(\kappa) d\kappa$$

E(κ) in inertial subrange

- We will develop an equation for E(κ) in the inertial subrange.
- According to the second similarity hypothesis E(κ) will solely depend on κ and ε.
- We can then perform the following dimensional analysis:

$$[k] = m^2 s^{-2} \; ; \quad [\varepsilon] = m^2 s^{-3} \; ; \quad [\kappa] = m^{-1} \; ;$$

$$[E(\kappa)] = [k]/[\kappa] = m^3 s^{-2}$$

$$\textit{Dimensional analysis}: \quad [\varepsilon^{2/3} \kappa^{-5/3}] = m^3 s^{-2}$$

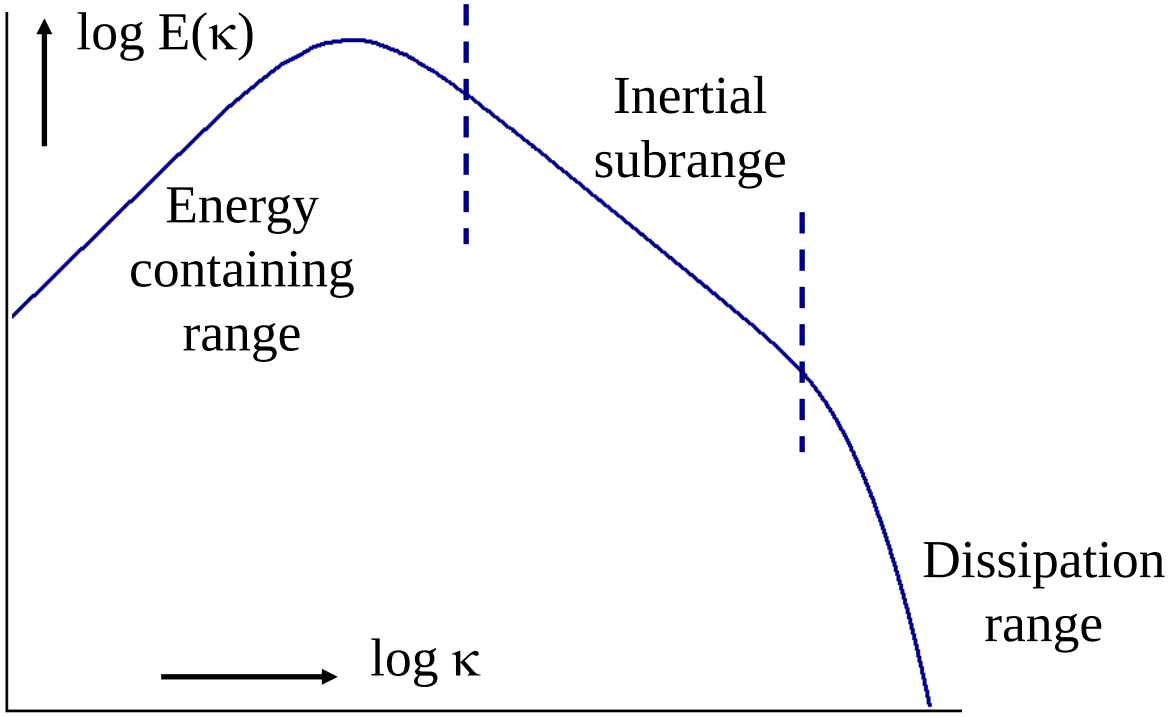
$$\Rightarrow \; E(\kappa) \; \propto \; \varepsilon^{2/3} \kappa^{-5/3}$$

$$\Rightarrow \; E(\kappa) \; = \; C \, \varepsilon^{2/3} \kappa^{-5/3}$$

- The last equation describes the famous Kolmogorov –5/3 spectrum. C is the universal Kolmogorov constant, which experimentally was determined to be C = 1.5.

Full spectrum E(κ)

- Model equations for E(κ) in the production range and dissipation range have been developed. We will not discuss the theory behind them here.
- The full spectrum is given by: $E(\kappa) = C\varepsilon^{2/3}\kappa^{-5/3} f_L f_\eta$
- Will not discuss f_L and f_η here.



Full spectrum E(κ)

- Model equations for E(κ) in the production range and dissipation range have been developed. We will not discuss the theory behind them here.
- The full spectrum is given by: $E(\kappa) = C\varepsilon^{2/3}\kappa^{-5/3} f_L\ f_\eta$
- The production range is governed by f_L (which goes to unity for large ($\kappa\, l_0$):

$$f_L = \left(\frac{\kappa l_0}{\left[(\kappa l_0)^2 + c_L \right]^{1/2}} \right)^{p_0+5/3}$$

- The dissipation range is governed by f_η (which goes to unity for small ($\kappa\, \eta$):

$$f_\eta = \exp\{-\beta\{[(\kappa\eta)^4 + c_\eta^4]^{1/4} - c_\eta\}\}$$

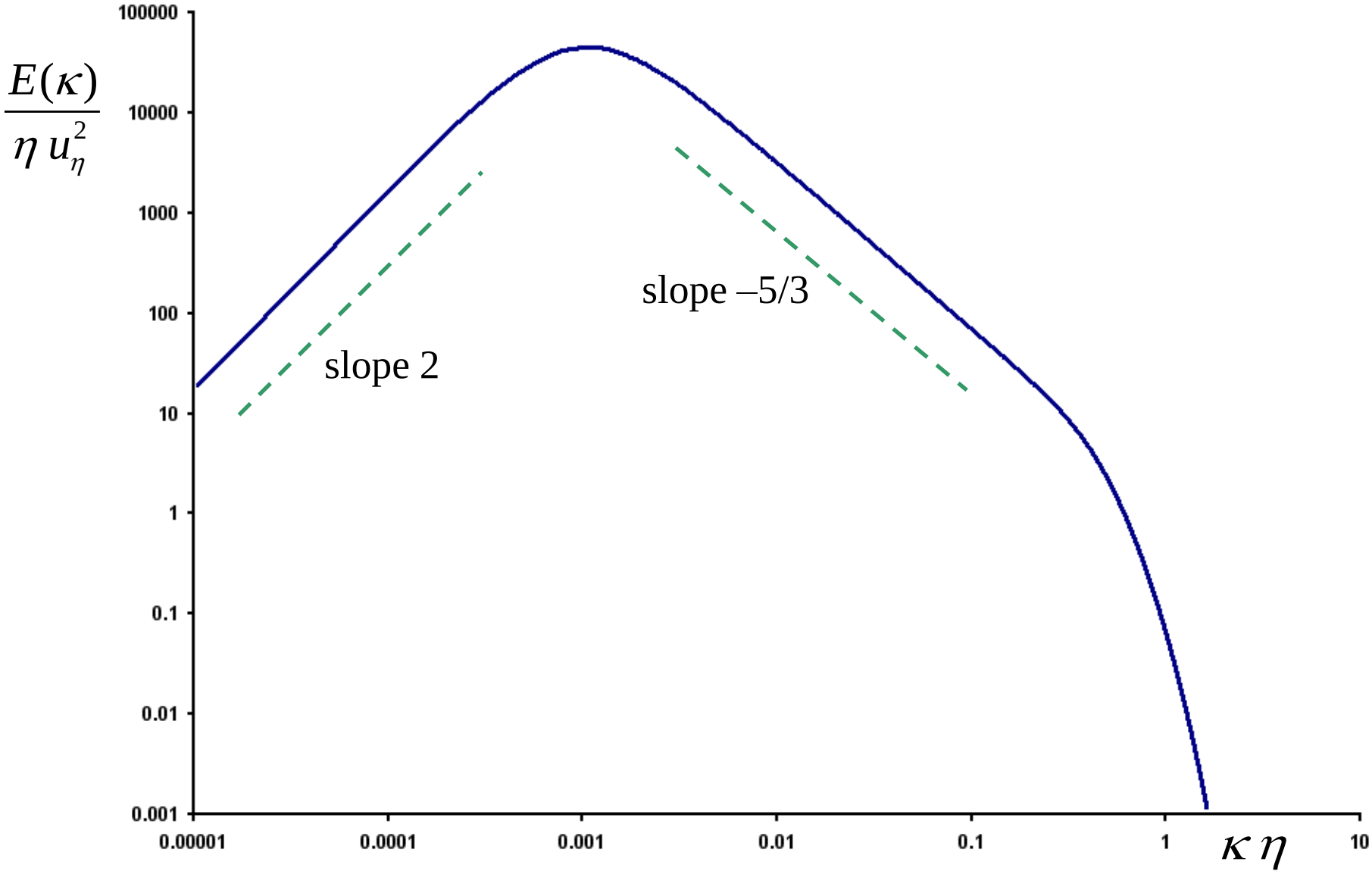
- The model constants were determined experimentally and based on the constraint that E(κ) integrate to *k*. Their values are:

$$c_L \approx 6.78; \quad c_\eta \approx 0.40; \quad C = 1.5; \quad p_0 = 2; \quad \beta = 5.2.$$

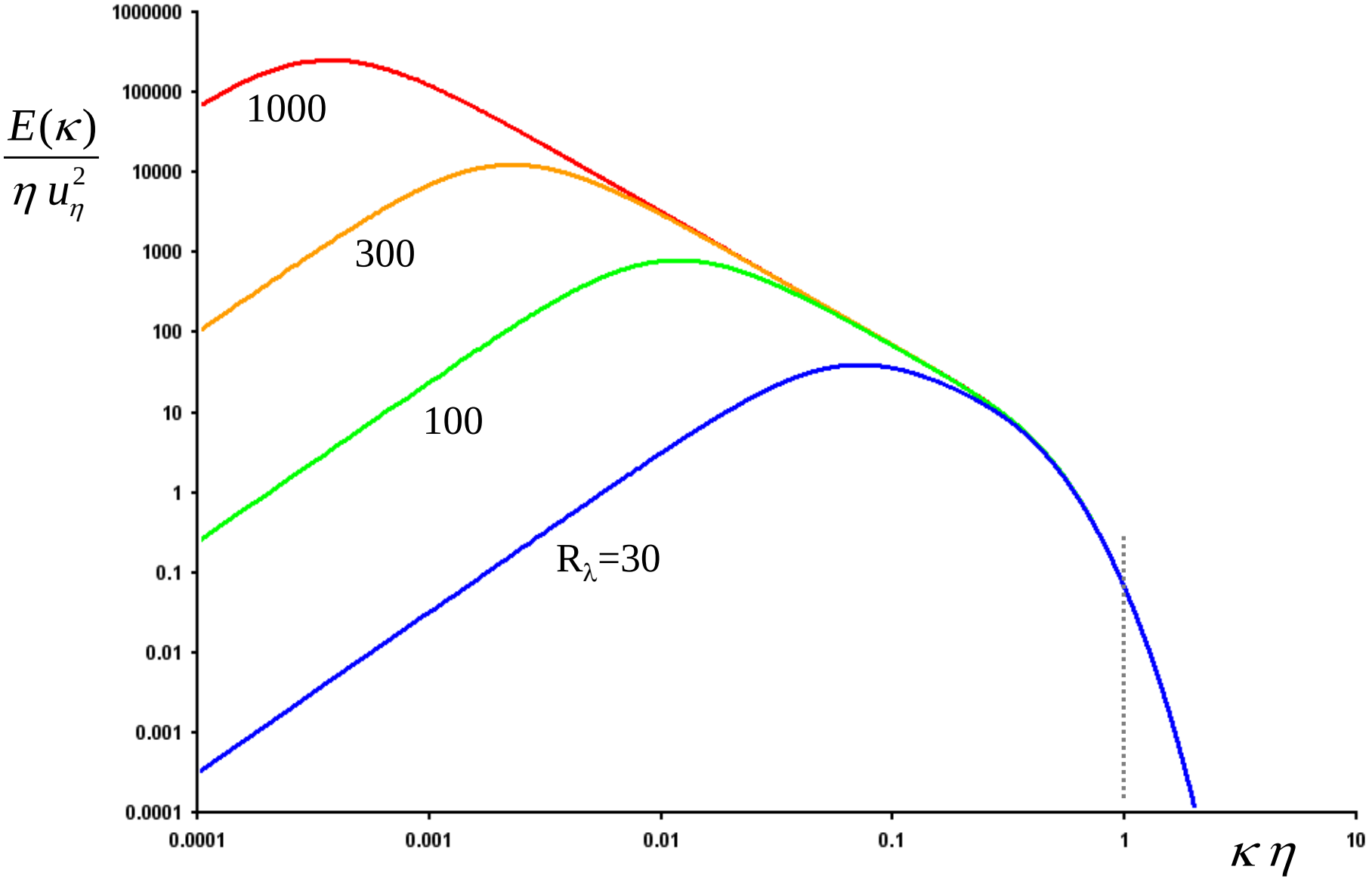
Normalized spectrum

- For given values of ε, ν, and k the full spectrum can now be calculated based on these equations.
- It is, however, common to normalize the spectrum in one of two ways: based on the Kolmogorov scales or based on the integral length scale.
- Based on Kolmogorov scale:
  - Measure of length scale becomes ($\eta\ \kappa$).
  - E(κ) is made dimensionless as E(κ)/($\eta\ u_\eta^2$)
- Based on integral scale:
  - Measure of length scale becomes ($l_0\ \kappa$).
  - E(κ) is made dimensionless as E(κ)/($k\ l_0$)
- Instead of having three adjustable parameters (ε,ν,k), the normalized spectrum then has only one adjustable parameter: R_λ.

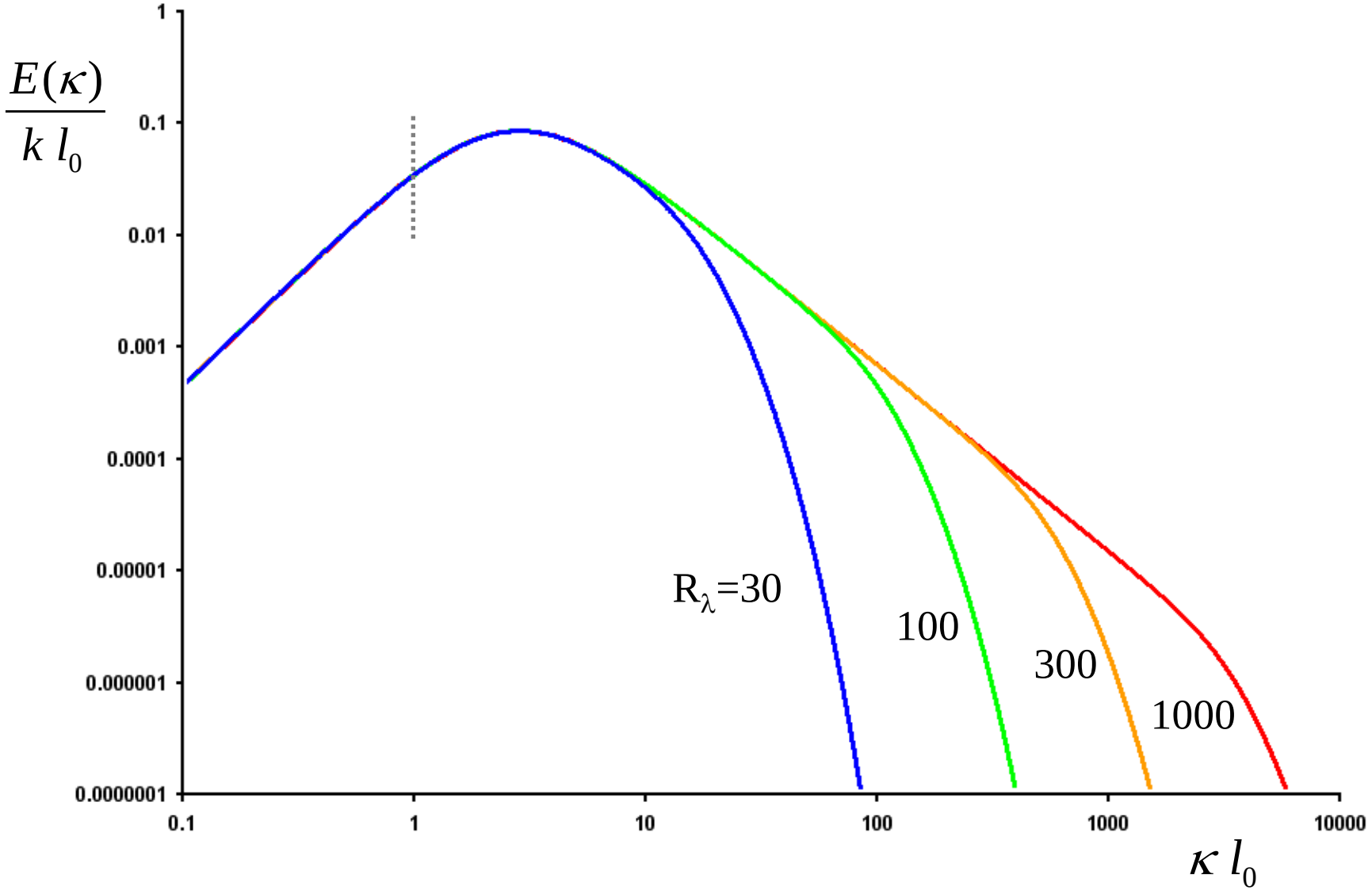
The normalized energy spectrum for $R_\lambda = 500$



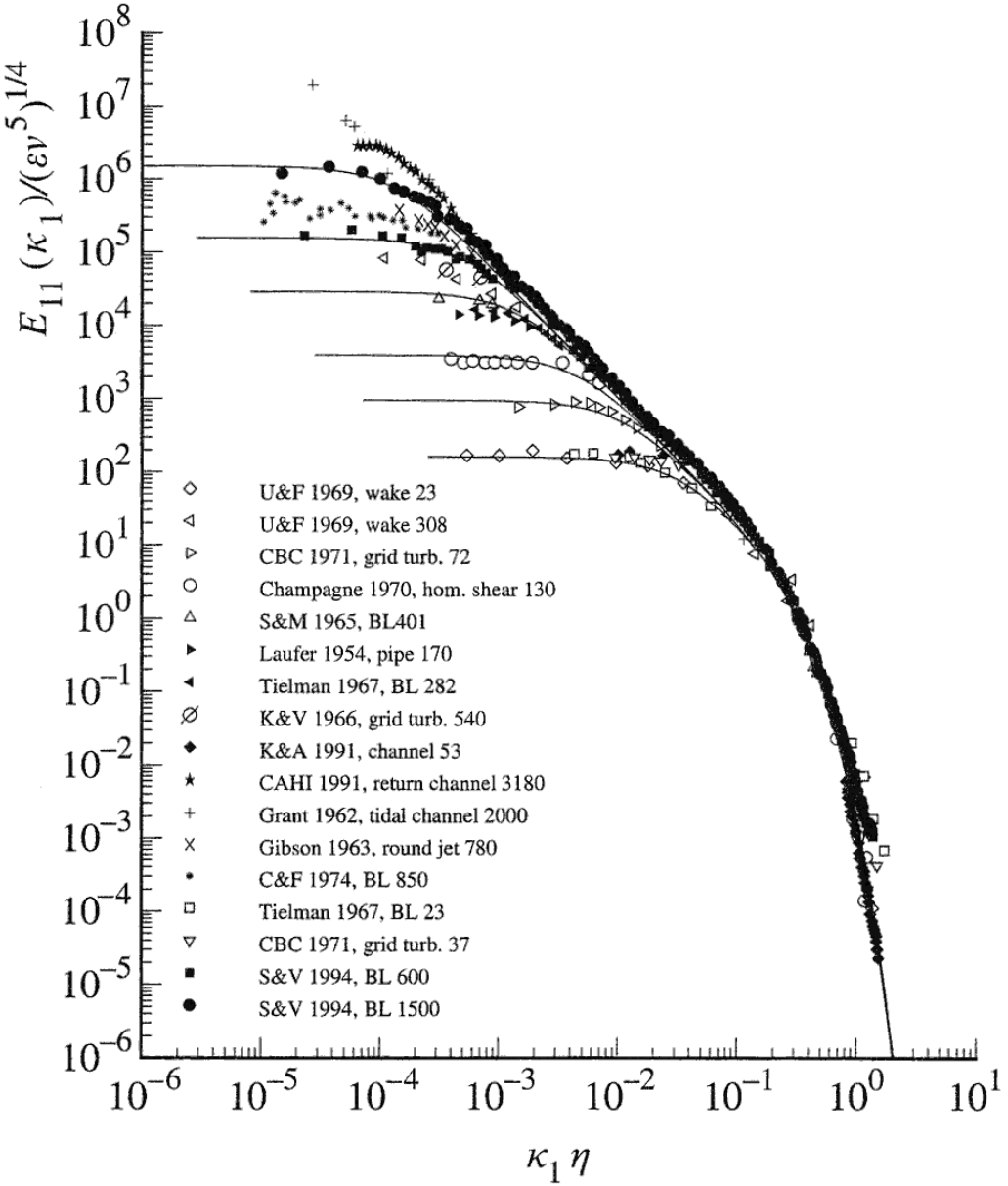
The energy spectrum as a function of R_λ



The energy spectrum as a function of R_λ



Measurements of spectra



The figure shows experimentally measured one dimensional spectra (one velocity component was measured only, as indicated by the "1" and "11" subscripts). The number at the end of the reference denotes the value of R_λ for which the measurements were done. Source: Pope, page 235.

Determination of the spectrum requires simultaneous measurements of all velocity components at multiple points, which is usually not possible. It is common to measure one velocity component at one point over a certain period of time and convert the time signal to a spatial signal using x = Ut with U being the time averaged velocity. This is commonly referred to as Taylor's hypothesis of frozen turbulence. It is only valid for u'/U << 1, which is not always the case. Spectrum measurements remain a challenging field of research.

Energy containing range

- From the energy spectrum, we can derive which length scales contain most of the turbulent kinetic energy in the flow.
- The derivation will not be reproduced here.
- The conclusion is that most of the energy (~80%) is contained in eddies of length scale $l_{EI} = l_0/6 < l < 6l_0$.

The dissipation rate spectrum

- We now know which eddies contain most of the energy. The question remains, which eddies exactly dissipate the energy.
- This question can be answered by constructing a dissipation rate spectrum D(κ). The integral of D(κ) over the full wavelength range is by definition the energy dissipation rate ε:

$$\varepsilon = \int_0^\infty D(\kappa) d\kappa$$

- Furthermore, with ε being defined as the multiple of the kinematic viscosity and squared velocity gradients (of order $\nu(du/dx)^2 \sim \nu k/l^2 \sim \nu k\kappa^2 \sim \nu\kappa^2 E(\kappa)$) we can then deduce:

$$D(\kappa) = 2\nu\kappa^2 E(\kappa)$$

Dissipation rate spectrum - continued

- This then leads to the following:

$$\varepsilon = \int_0^\infty D(\kappa)d\kappa = \int_0^\infty 2\nu\kappa^2 E(\kappa)d\kappa$$

$$\varepsilon(0,\kappa) = \int_0^\kappa D(\kappa)d\kappa$$

- Here $\varepsilon(0,\kappa)$ is the cumulative dissipation; the energy dissipated by eddies with a wavelength between 0 and κ.
- The unit of $D(\kappa)$ is m^3/s^3 and it can thus be normalized with a velocity scale cubed, typically the Kolmogorov velocity scale.
- Just as the normalized $E(\kappa)$ only depended on R_λ, so does the normalized $D(\kappa)$ depend only on R_λ.

The dissipation rate spectrum

- We now know which eddies contain most of the energy. The question remains, which eddies exactly dissipate the energy.
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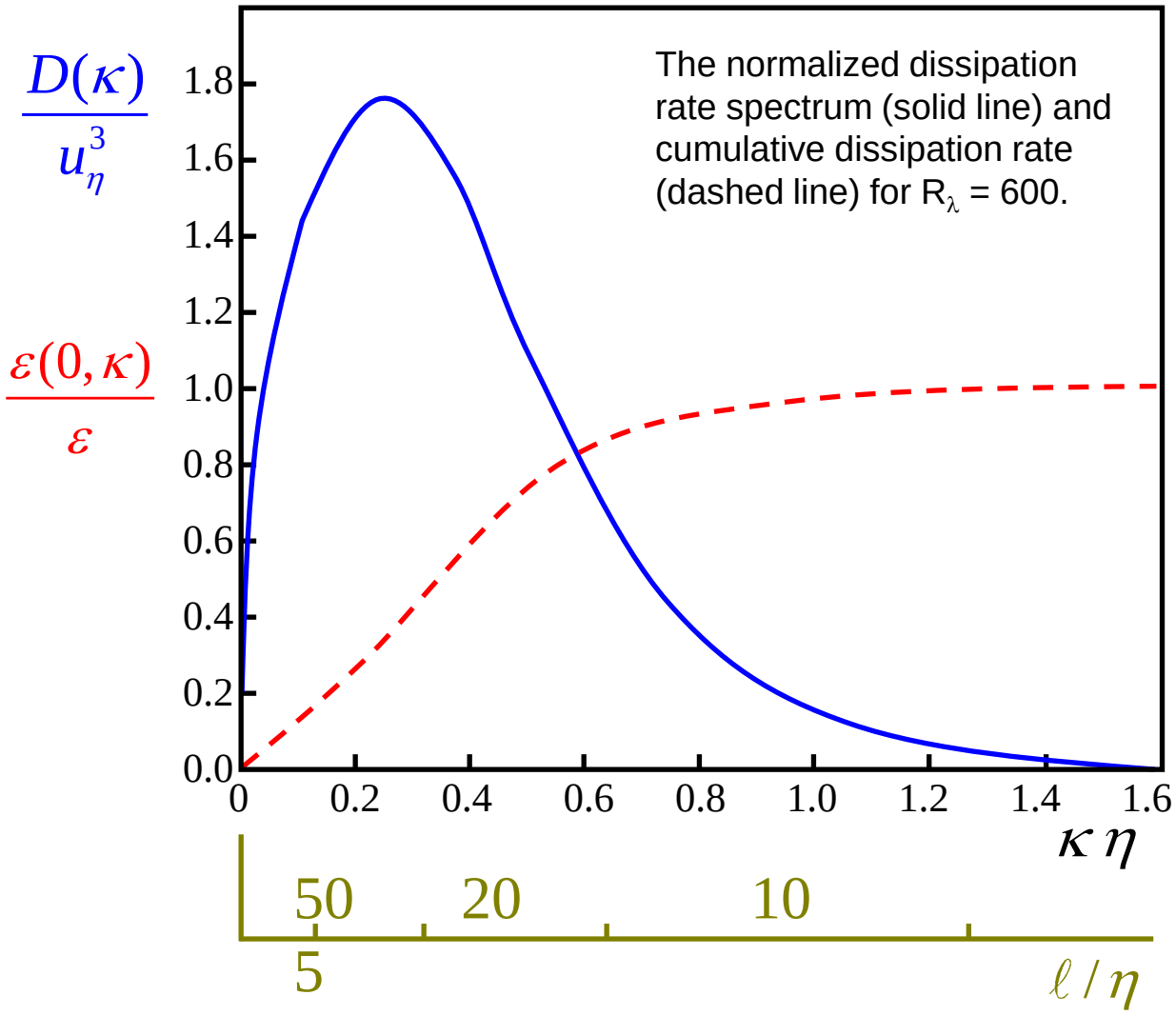
Dissipation rate spectrum



Dissipation range

- The dissipation rate spectrum can be integrated to show that most of the dissipation (~90%) occurs in eddies of length scales $l_{DI}/\eta = 60 > l/\eta > 8$.
- This means that most of the dissipation occurs at scales that are larger than the Kolmogorov scale η. The Kolmogorov scale should be interpreted as a measure of the smallest eddies that are present in a turbulent flow at high Reynolds numbers.
- How long does it take for a large-scale eddy to break up and be dissipated? The spectra can be further analyzed to show that eddies spend about 90% of their total lifetime $\tau=k/\varepsilon$ in the production range, and that once eddies enter the inertial subrange it takes only about $\tau/10$ before the energy is being dissipated. This time $\tau/10$ is also referred to as the cascade timescale.

Intermittency

- Neither *k* nor ε are constant in time or space.
- Within a turbulent flow field, *k* and ε may vary widely in space, sometimes by orders of magnitude.
- Also, at a given point in space the instantaneous values of ε may vary in time. This is called intermittency. The peak values of ε relative to the mean tend to increase with Reynolds number. Peak values may be of the order of 15 times the average ε in laboratory scale flows and 50 times the average in atmospheric flows.

Summary – Reynolds numbers

- The following Reynolds numbers have been defined:
  - Flow Reynolds number: $\mathrm{Re} = UL/\nu$
  - Turbulence Reynolds number: $\mathrm{Re}_L = k^2/\varepsilon\nu$
  - Taylor Reynolds number: $R_\lambda = u'\lambda/\nu$
  - Kolmogorov Reynolds number: $\mathrm{Re}_\eta = \eta u_\eta/\nu = 1$

- The flow Reynolds number is on the order of one to ten times the turbulence Reynolds number.
- The turbulence and Taylor Reynolds numbers can be related as follows: $R_\lambda = \left(\frac{20}{3}\mathrm{Re}_L\right)^{1/2}$

Summary – length scales

- The integral length scale is a measure of the large-scale eddies in the production range: $l_0 \propto k^{3/2} / \varepsilon$

  The proportionality constant is of the order one.
- The Taylor microscale is a measure of the size of the eddies in the inertial subrange: $\lambda \approx (10 \nu k / \varepsilon)^{1/2}$
- The Kolmogorov microscale is the size of the smallest eddies present in the flow: $\eta = (\nu^3 / \varepsilon)^{1/4}$
- The length scales can be related as follows:

$$\lambda / l_0 = \sqrt{10}\, \mathrm{Re}_L^{-1/2}$$

$$\eta / l_0 = \mathrm{Re}_L^{-3/4}$$

$$\lambda / \eta = \sqrt{10}\, \mathrm{Re}_L^{1/4}$$

$$\lambda = \sqrt{10}\, \eta^{2/3} l_0^{1/3}$$

Validity of Kolmogorov's theory

- Kolmogorov's theory is an asymptotic theory: it has been shown to work well in the limit of very high Reynolds numbers.
- The exact shape of the normalized spectra may deviate from Kolmogorov's model spectra for intermediate Reynolds numbers. e.g., for many laboratory scale flows which have Reynolds numbers on the order of 10,000 with $R_\lambda \sim 250$, the exponent of $E(\kappa) \sim \kappa^{-p}$ in the inertial subrange is often measured to be $p \sim 1.5$ instead of 5/3 (~1.67).
- Kolmogorov's theory assumes that the energy cascade is one way: from large eddies to small eddies. Experimental studies have shown that energy is also transferred from smaller scales to larger scales (a process called backscatter), albeit at a much lower rate and the dominant energy transfer is indeed from large to small.
- The theory assumes that turbulence at high Reynolds numbers is completely random. In practice, large-scale coherent structures may form.
- Research into the fundamental aspects of turbulence continues, both experimentally and by means of large computer simulations using DNS (direct numerical simulation); and the theory continues to be refined.

Lecture 10 - Turbulence Models

Applied Computational Fluid Dynamics

André Bakker

Turbulence modeling objective

- The objective of turbulence modeling is to develop equations that will predict the time-averaged velocity, pressure, and temperature fields without calculating the complete turbulent flow pattern as a function of time.
  - This saves us a lot of work!
  - Most of the time it is all we need to know.
  - We may also calculate other statistical properties, such as RMS values.
- The time averaged equations now contain six additional unknowns in the momentum equations: the Reynolds stresses. Additional unknowns have also been introduced in the scalar equation.

Turbulence models

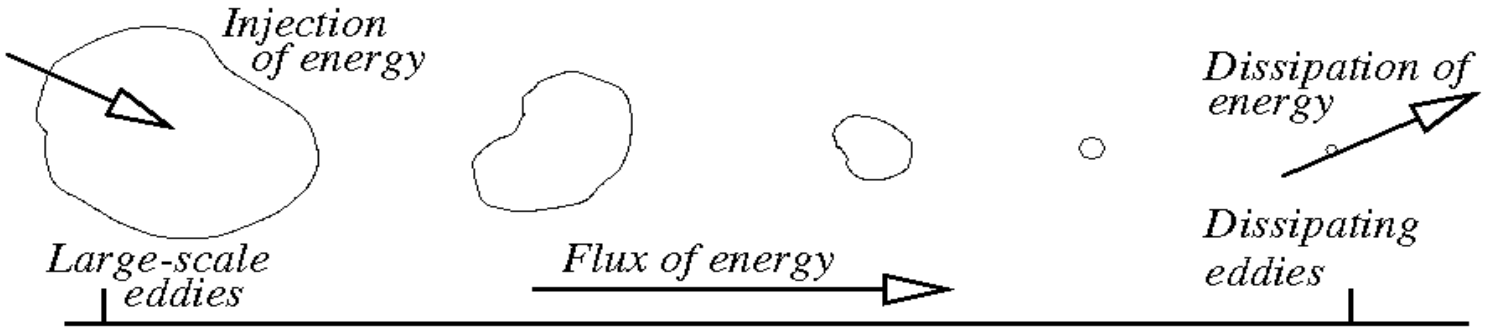
- A turbulence model is a computational procedure to close the system of *mean flow* equations.
- For most engineering applications it is unnecessary to resolve the details of the turbulent fluctuations.
- Turbulence models allow the calculation of the mean flow without first calculating the full time-dependent flow field.
- We only need to know how turbulence affected the mean flow.
- In particular we need expressions for the Reynolds stresses.
- For a turbulence model to be useful it:
  - must have wide applicability,
  - be accurate,
  - simple,
  - and economical to run.

Common turbulence models

- Classical models. Based on Reynolds Averaged Navier-Stokes (RANS) equations (time averaged):
  - 1. Zero-equation* model: mixing length model.
  - 2. One-equation model: Spalart-Almaras.
  - 3. Two-equation models: k-ε style models (standard, RNG, realizable), k-ω model, and ASM.
  - 4. Seven-equation model: Reynolds stress model.
- The number of equations denotes the number of additional PDEs that are being solved.
- Large eddy simulation. Based on space-filtered equations. Time dependent calculations are performed. Large eddies are explicitly calculated. For small eddies, their effect on the flow pattern is taken into account with a “subgrid model” of which many styles are available.

* Really, we only count PDEs, not algebraic equations.

Prediction Methods



Resolved

Direct numerical simulation (**DNS**)

Δ_{DNS}

Resolved *Modeled*

Large eddy simulation (**LES**) Δ_{LES}

Resolved *Modeled*

Δ_{RANS} Reynolds averaged Navier-Stokes equations (**RANS**)

Boussinesq hypothesis

- Many turbulence models are based upon the Boussinesq hypothesis.
  - It was experimentally observed that turbulence decays unless there is shear in isothermal incompressible flows.
  - Turbulence was found to increase as the mean rate of deformation increases.
  - Boussinesq proposed in 1877 that the Reynolds stresses could be linked to the mean rate of deformation.
- Using the suffix notation where i, j, and k denote the x-, y-, and z-directions respectively, viscous stresses are given by:

$$\tau_{ij} = \mu\, e_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- Similarly, link Reynolds stresses to the mean rate of deformation:

$$\tau_{ij} = -\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)$$

Turbulent viscosity

- A new quantity appears: the turbulent viscosity μ_t.

$$\tau_{ij} = -\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)$$

- Its unit is the same as that of the molecular viscosity: Pa.s.
- It is also called the eddy viscosity.
- We can also define a kinematic turbulent viscosity: $\nu_t = \mu_t/\rho$. Its unit is m^2/s.
- The turbulent viscosity is not homogeneous, i.e., it varies in space.
- It is, however, assumed to be isotropic. It is the same in all directions. This assumption is valid for many flows, but not for all (e.g., flows with strong separation or swirl).

Turbulent Schmidt number

- The turbulent viscosity is used to close the momentum equations.
- We can use a similar assumption for the turbulent fluctuation terms that appear in the scalar transport equations.
- For a scalar property $\phi(t) = \Phi + \varphi'(t)$:

$$-\overline{\rho u_i' \varphi'} = \Gamma_t \frac{\partial \Phi}{\partial x_i}$$

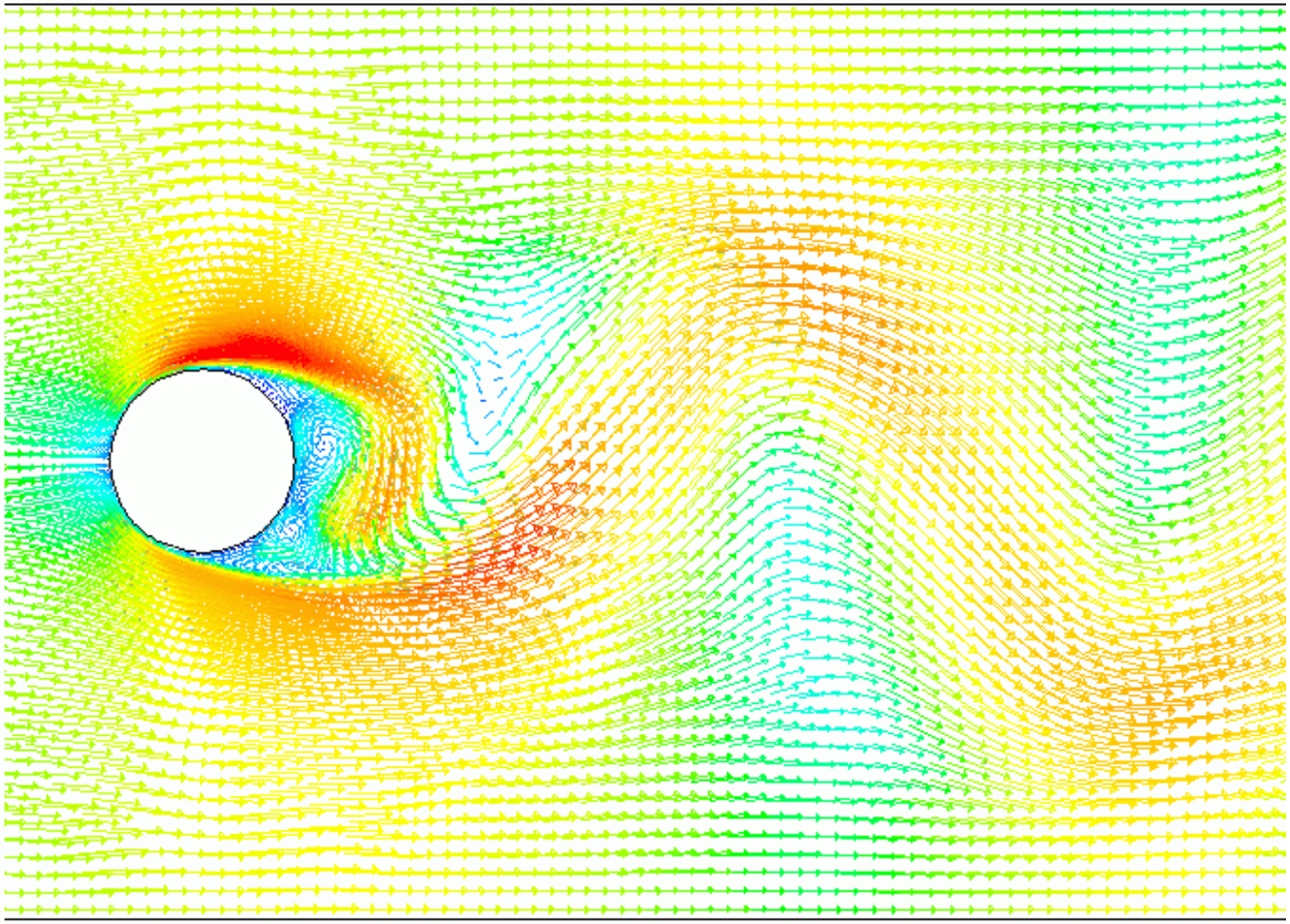
- Here Γ_t is the turbulent diffusivity.
- The turbulent diffusivity is calculated from the turbulent viscosity, using a model constant called the turbulent Schmidt number (AKA Prandtl number) σ_t:

$$\sigma_t = \frac{\mu_t}{\Gamma_t}$$

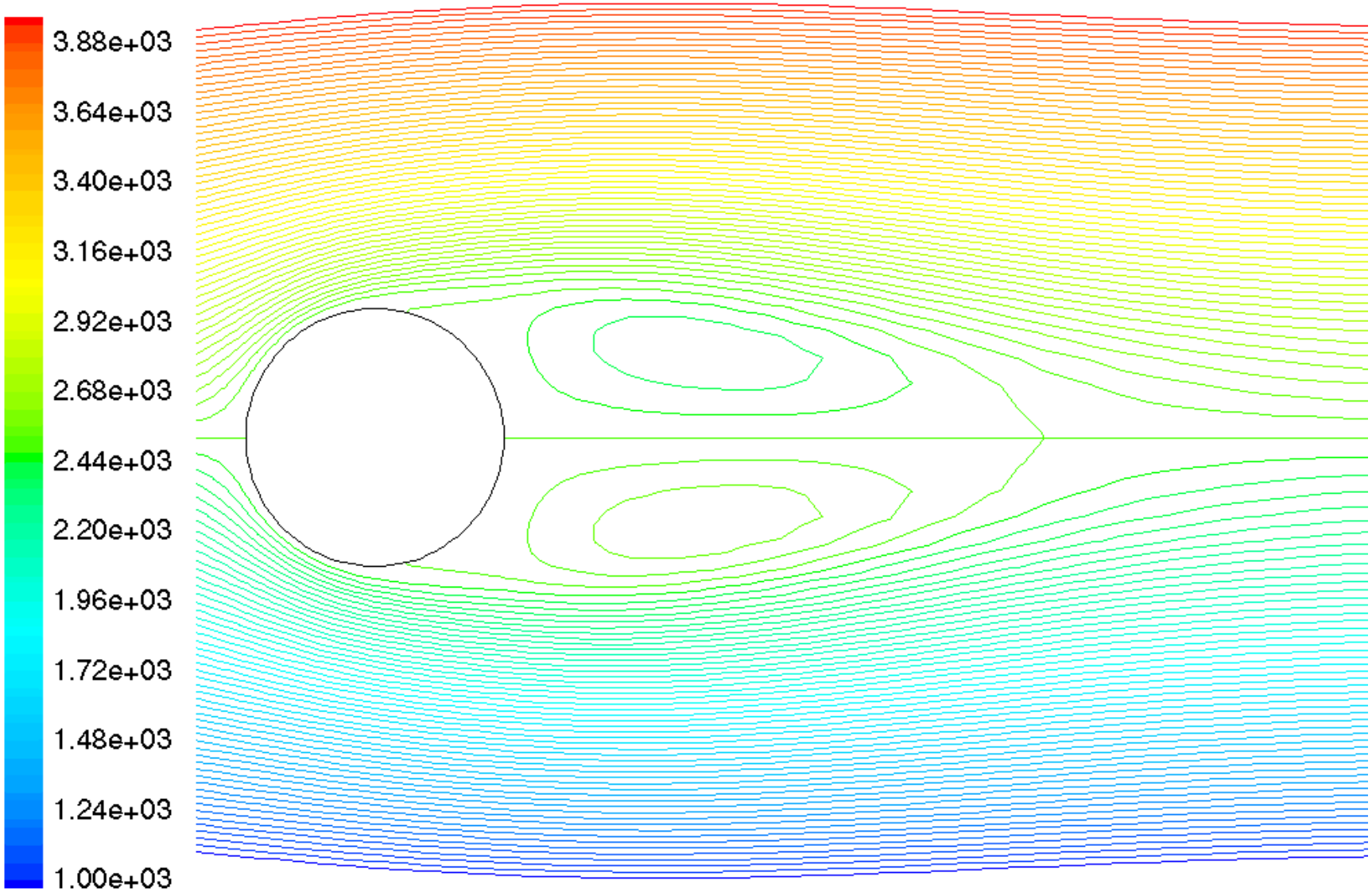
- Experiments have shown that the turbulent Schmidt number is nearly constant with typical values between 0.7 and 1.

Flow around a cylinder

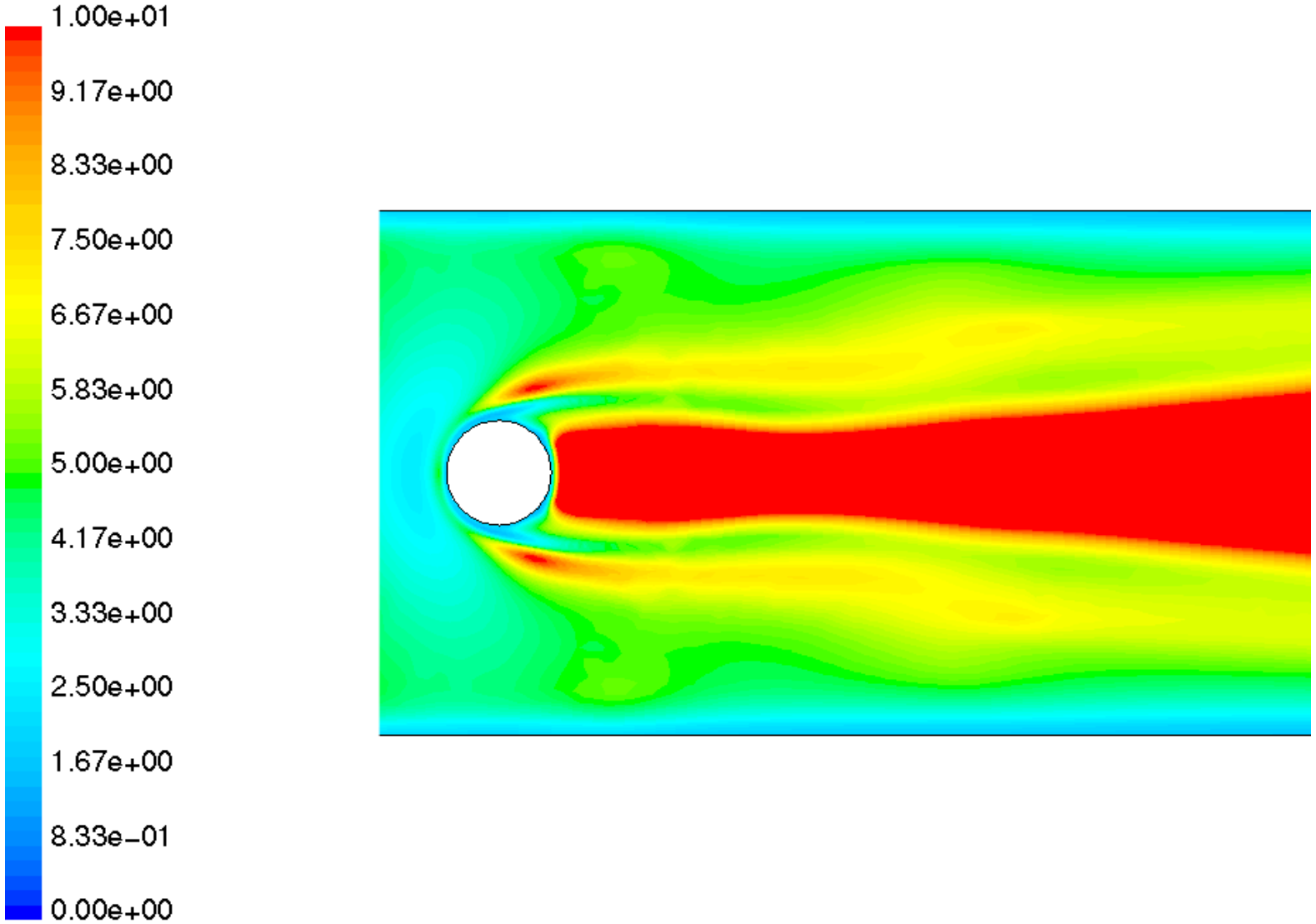
- The flow is stable for Reynolds numbers below ~40.
- For higher Reynolds numbers the flow is unstable.
- This figure shows an instantaneous flow pattern at Re = 1000.



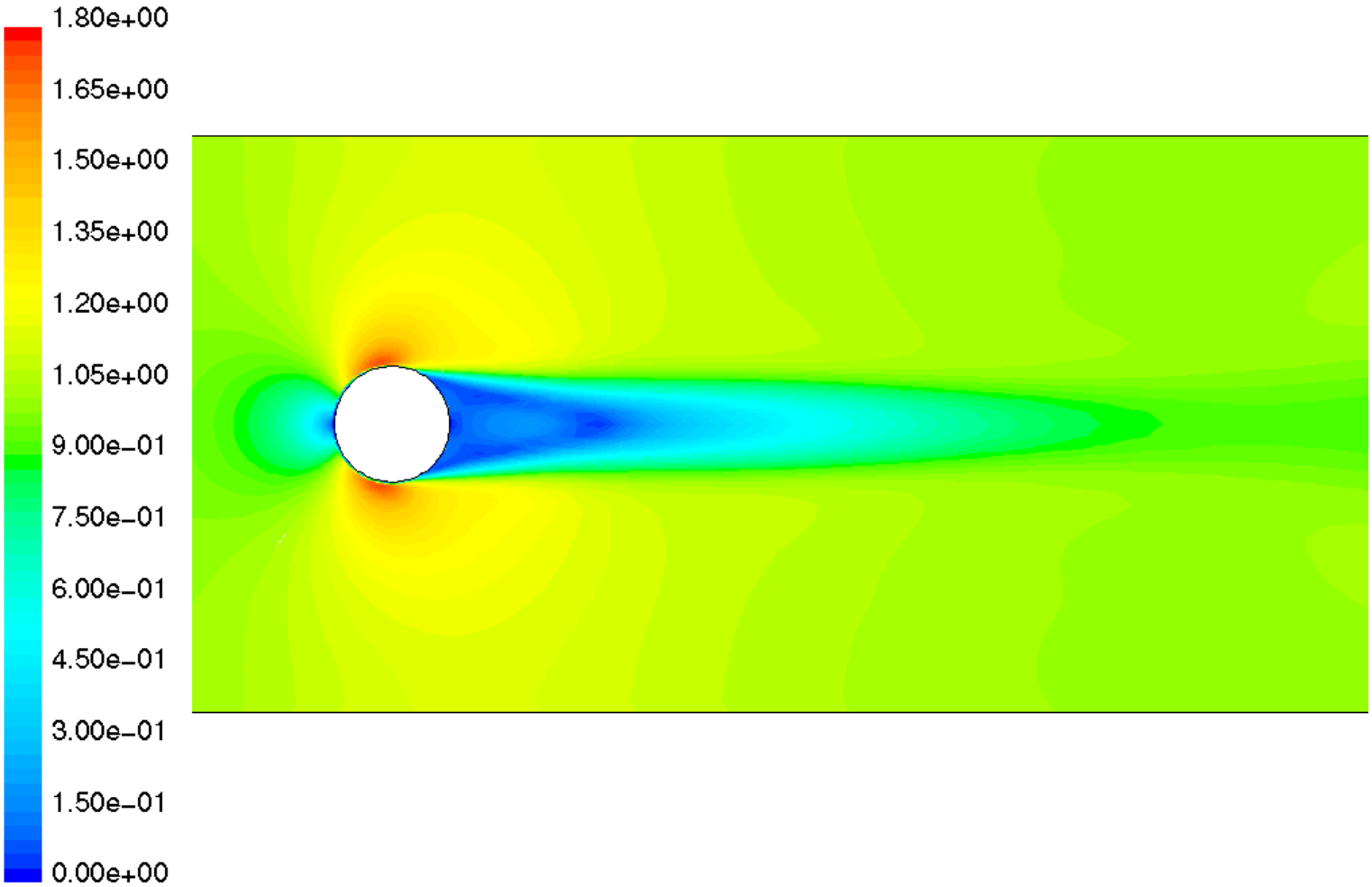
Time average streamlines (kg/s) - Re = 1000



Effective viscosity (kg/m-s) - Re =1000

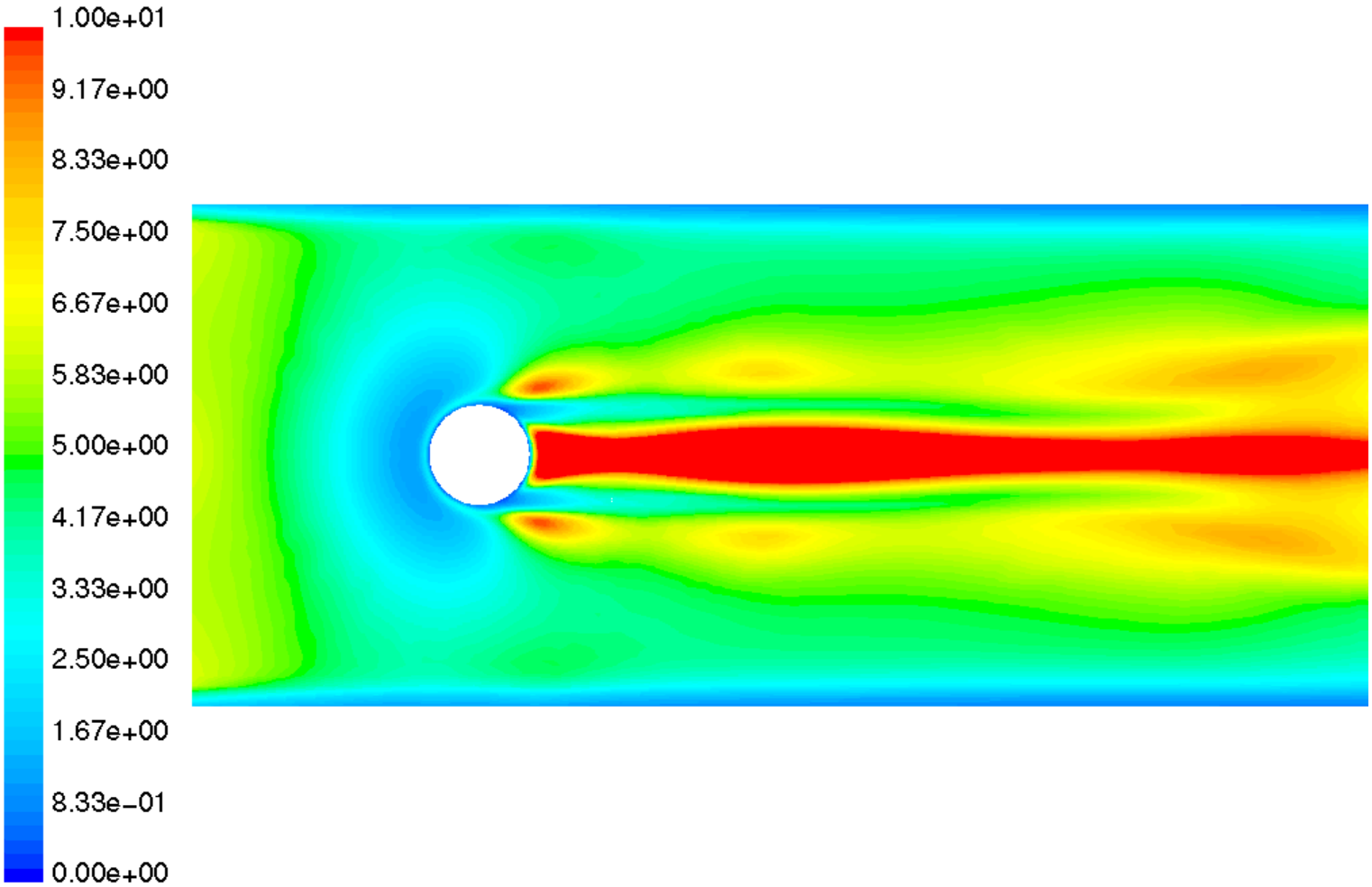


Time averaged velocity – Re = 1E4



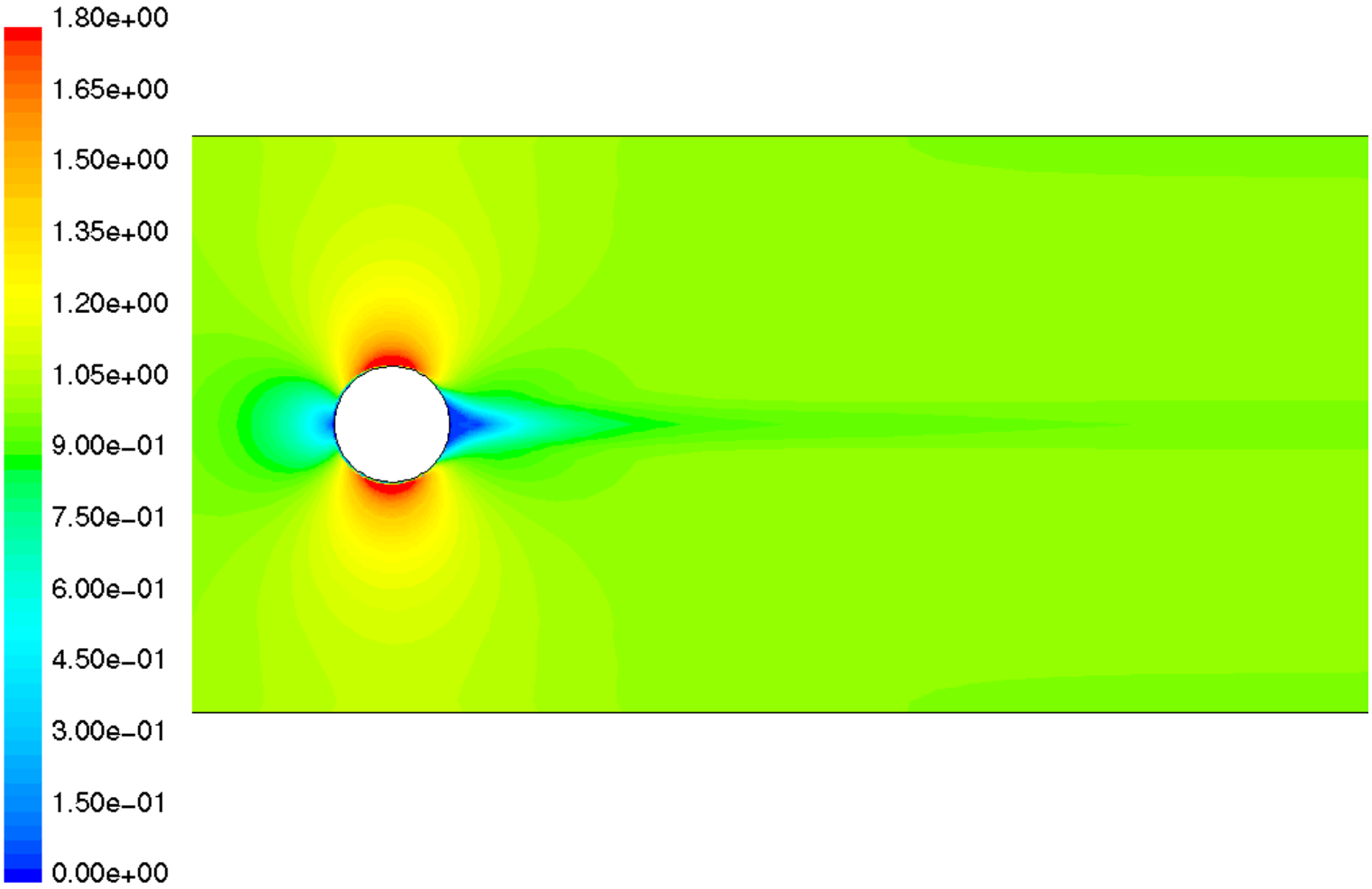
Re=10,000
Contours of Velocity Magnitude (m/s)
max = 1.73 m/s

Effective viscosity – Re = 1E4



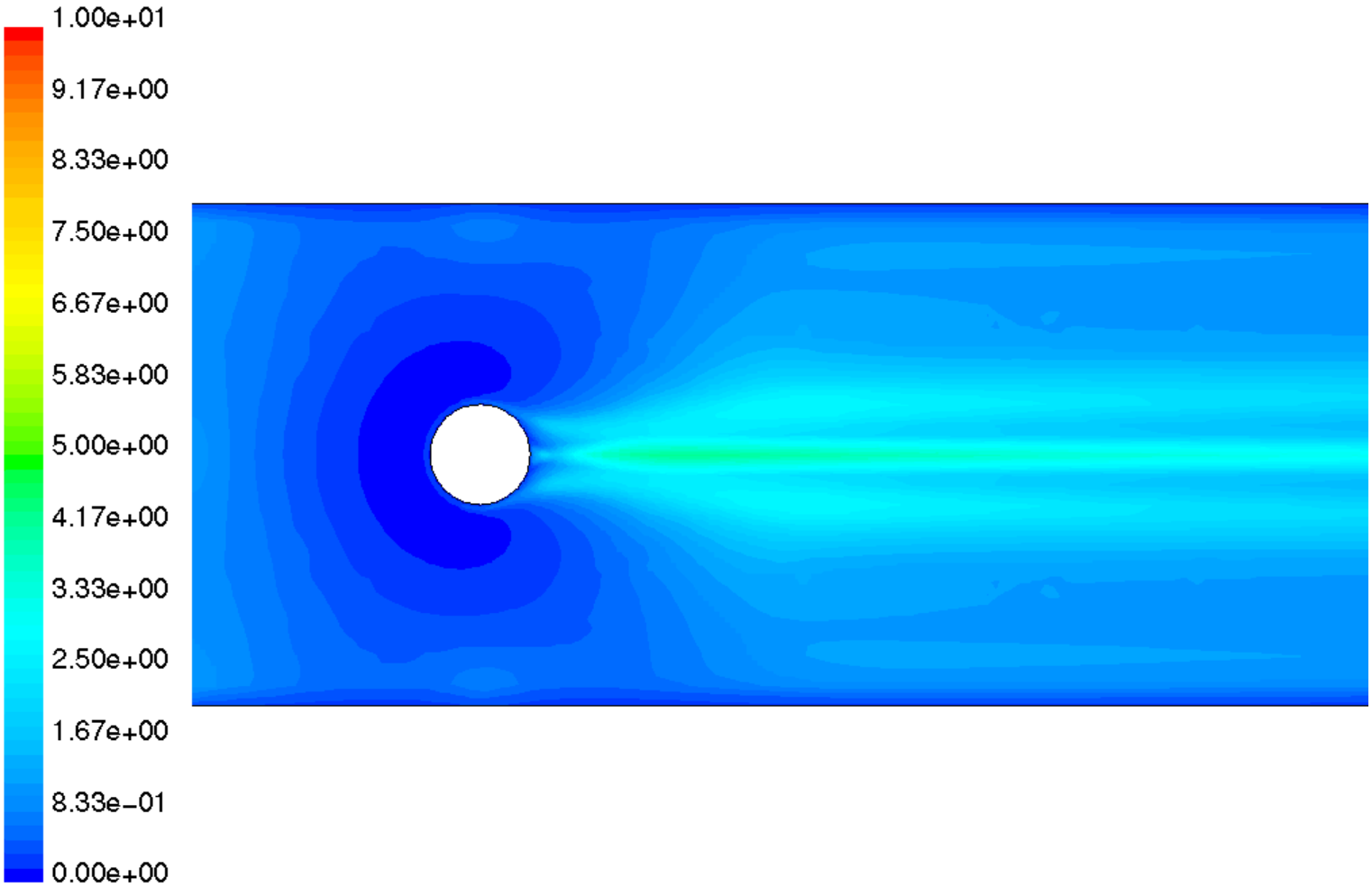
Re = 1E4
Contours of Effective Viscosity (kg/m-s)
<effective viscosity ratio> = 5.3

Time averaged velocity – Re = 1E7



Re=10,000,000
Contours of Velocity Magnitude (m/s)
max = 1.99 m/s

Effective viscosity – Re = 1E7



Re = 1E7
Contours of Effective Viscosity (kg/m-s)
<effect i ve viscosity ratio> = 1.16

Predicting the turbulent viscosity

- The following models can be used to predict the turbulent viscosity:
  - Mixing length model.
  - Spalart-Allmaras model.
  - Standard k-ε model.
  - k-ε RNG model.
  - Realizable k-ε model.
  - k-ω model.
- We will discuss these one by one.

Mixing length model

- On dimensional grounds one can express the kinematic turbulent viscosity as the product of a velocity scale and a length scale:

$$\nu_t\,(m^2/s) \;\propto\; \vartheta(m/s)\,\ell(m)$$

- If we then assume that the velocity scale is proportional to the length scale and the gradients in the velocity (shear rate, which has dimension 1/s):

$$\vartheta \;\propto\; \ell \left|\frac{\partial U}{\partial y}\right|$$

  we can derive Prandtl's (1925) mixing length model:

$$\nu_t \;=\; \ell_m^2 \left|\frac{\partial U}{\partial y}\right|$$

- Algebraic expressions exist for the mixing length for simple 2-D flows, such as pipe and channel flow.

Mixing length model discussion

- Advantages:
  - Easy to implement.
  - Fast calculation times.
  - Good predictions for simple flows where experimental correlations for the mixing length exist.
- Disadvantages:
  - Completely incapable of describing flows where the turbulent length scale varies, i.e., anything with separation or circulation.
  - Only calculates mean flow properties and turbulent shear stress.
- Use:
  - Sometimes used for simple external aero flows.
  - Pretty much completely ignored in commercial CFD programs today.
- Much better models are available.

Spalart-Allmaras one-equation model

- Solves a single conservation equation (PDE) for the turbulent viscosity:
  - This conservation equation contains convective and diffusive transport terms, as well as expressions for the production and dissipation of ν_t.
  - Developed for use in unstructured codes in the aerospace industry.
- Economical and accurate for:
  - Attached wall-bounded flows.
  - Flows with mild separation and recirculation.
- Weak for:
  - Massively separated flows.
  - Free shear flows.
  - Decaying turbulence.
- Because of its relatively narrow use we will not discuss this model in detail.

The *k*-ε model

- The *k*-ε model focuses on the mechanisms that affect the turbulent kinetic energy (per unit mass) *k*.
- The instantaneous kinetic energy *k(t)* of a turbulent flow is the sum of mean kinetic energy *K* and turbulent kinetic energy *k*:

$$K = \tfrac{1}{2}\left(U^2 + V^2 + W^2\right)$$

$$k = \tfrac{1}{2}\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right)$$

$$k(t) = K + k$$

- ε is the dissipation rate of *k*.
- If *k* and ε are known, we can model the turbulent viscosity as:

$$\nu_t \propto \vartheta \ell \propto k^{1/2} \frac{k^{3/2}}{\varepsilon} = \frac{k^2}{\varepsilon}$$

- We now need equations for *k* and ε.

Turbulent kinetic energy *k*

- The equation for the turbulent kinetic energy *k* is as follows:

$$\frac{\partial(\rho k)}{\partial t} + div(\rho k \mathbf{U}) = div\left(-\overline{p'\mathbf{u}'} + 2\mu\overline{\mathbf{u}'e_{ij}'} - \rho\tfrac{1}{2}\overline{u_i'.u_i'u_j'}\right) - 2\mu\overline{e_{ij}'.e_{ij}'} + (-\rho\overline{u_i'u_j'}.E_{ij})$$

$$(I) \qquad (II) \qquad (III) \quad (IV) \qquad (V) \qquad (VI) \qquad (VII)$$

- Here e_{ij}' is fluctuating component of rate of deformation tensor.
- This equation can be read as:
  - (I) the rate of change of *k*, plus
  - (II) transport of *k* by convection, equals
  - (III) transport of *k* by pressure, plus
  - (IV) transport of *k* by viscous stresses, plus
  - (V) transport of *k* by Reynolds stresses, minus
  - (VI) rate of dissipation of *k*, plus
  - (VII) turbulence production.

Model equation for *k*

- The equation for *k* contains additional turbulent fluctuation terms, that are unknown. Again, using the Boussinesq assumption, these fluctuation terms can be linked to the mean flow.
- The following (simplified) model equation for *k* is commonly used.

$$\underbrace{\frac{\partial(\rho k)}{\partial t}}_{\text{Rate of increase}} + \underbrace{div(\rho k \mathbf{U})}_{\text{Convective transport}} = \underbrace{div\left[\frac{\mu_t}{\sigma_k} grad\ k\right]}_{\text{Diffusive transport}} + \underbrace{2\mu_t E_{ij}.E_{ij}}_{\text{Rate of production}} - \underbrace{\rho\varepsilon}_{\text{Rate of destruction}}$$

- The Prandtl number σ_k connects the diffusivity of *k* to the eddy viscosity. Typically, a value of 1.0 is used.

Turbulent dissipation

- The equations look quite similar.
- However, the *k* equation mainly contains primed quantities, indicating that changes in *k* are mainly governed by turbulent interactions.
- Furthermore, term (VII) is equal in both equations. But it is actually negative in the K equation (destruction) and positive in the *k* equation: energy transfers from the mean flow to the turbulence.
- The viscous dissipation term (VI) in the *k* equation $-2\mu\overline{e_{ij}'.e_{ij}'}$ describes the dissipation of *k* because of the work done by the smallest eddies against the viscous stresses.
- We can now define the rate of dissipation per unit mass ε as:

$$\varepsilon = 2\nu\overline{e_{ij}'.e_{ij}'}$$

Dissipation rate - analytical equation

- The analytical equation for ε is shown below. Because of the many unknown higher order terms, this equation cannot be solved, and simplified model equations need to be derived.

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = -\frac{\partial}{\partial x_k}\left(\nu \overline{u_k \frac{\partial u_i}{\partial x_l} \frac{\partial u_i}{\partial x_l}} + 2 \frac{\nu}{\rho} \overline{\frac{\partial p}{\partial x_i} \frac{\partial u_k}{\partial x_i}} - \nu \frac{\partial \varepsilon}{\partial x_k} \right)$$

$$- 2 \nu \frac{\partial U_i}{\partial x_k} \left(\overline{\frac{\partial u_i}{\partial x_l} \frac{\partial u_k}{\partial x_l}} + \overline{\frac{\partial u_l}{\partial x_i} \frac{\partial u_l}{\partial x_k}} \right) - 2 \nu \overline{u_k \frac{\partial u_i}{\partial x_l}} \frac{\partial^2 U_i}{\partial x_k \partial x_l}$$

$$- 2 \nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_l} \frac{\partial u_k}{\partial x_l}} - 2 \overline{\left(\nu \frac{\partial^2 u_i}{\partial x_k \partial x_l} \right)^2}$$

Model equation for ε

- A model equation for ε is derived by multiplying the *k* equation by (ε/*k*) and introducing model constants.
- The following (simplified) model equation for ε is commonly used.

$$\underbrace{\frac{\partial(\rho\varepsilon)}{\partial t}}_{\text{Rate of increase}} + \underbrace{div(\rho\varepsilon\mathbf{U})}_{\text{Convective transport}} = \underbrace{div\left[\frac{\mu_t}{\sigma_\varepsilon}\, grad\ \varepsilon\right]}_{\text{Diffusive transport}} + \underbrace{C_{1\varepsilon}\frac{\varepsilon}{k}2\mu_t E_{ij}.E_{ij}}_{\text{Rate of production}} - \underbrace{C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}}_{\text{Rate of destruction}}$$

- The Prandtl number σ_ε connects the diffusivity of ε to the eddy viscosity. Typically, a value of 1.30 is used.
- Typically values for the model constants $C_{1\varepsilon}$ and $C_{2\varepsilon}$ of 1.44 and 1.92 are used.

Calculating the Reynolds stresses from *k* and ε

- The turbulent viscosity is calculated from:

$$\mu_t = C_\mu \frac{k^2}{\varepsilon} \qquad C_\mu = 0.09$$

- The Reynolds stresses are then calculated as follows:

$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{2}{3}\rho k\delta_{ij} = 2\mu_t E_{ij} - \frac{2}{3}\rho k\delta_{ij}$$

$$\delta_{ij} = 1 \quad if \quad i = j \quad and \quad \delta_{ij} = 0 \quad if \quad i \neq j$$

- The $(2/3)\rho k\delta_{ij}$ term ensures that the normal stresses sum to *k*.
- Note that the *k*-ε model leads to all normal stresses being equal, which is usually inaccurate.

k-ε model discussion

- Advantages:
  - Relatively simple to implement.
  - Leads to stable calculations that converge relatively easily.
  - Reasonable predictions for many flows.
- Disadvantages:
  - Poor predictions for:
    - swirling and rotating flows,
    - flows with strong separation,
    - axisymmetric jets,
    - certain unconfined flows, and
    - fully developed flows in non-circular ducts.
  - Valid only for fully turbulent flows.
  - Simplistic ε equation.

More two-equation models

- The *k*-ε model was developed in the early 1970s. Its strengths as well as its shortcomings are well documented.
- Many attempts have been made to develop two-equation models that improve on the standard *k*-ε model.
- We will discuss some here:
  - *k*-ε RNG model.
  - *k*-ε realizable model.
  - *k*-ω model.
  - Algebraic stress model.
  - Non-linear models.

Improvement: RNG *k*- ε

- *k*-ε equations are derived from the application of a rigorous statistical technique (Renormalization Group Method) to the instantaneous Navier-Stokes equations.
- Similar in form to the standard *k*-ε equations but includes:
  - Additional term in ε equation for interaction between turbulence dissipation and mean shear.
  - The effect of swirl on turbulence.
  - Analytical formula for turbulent Prandtl number.
  - Differential formula for effective viscosity.
- Improved predictions for:
  - High streamline curvature and strain rate.
  - Transitional flows.
  - Wall heat and mass transfer.
- But still does not predict the spreading of a round jet correctly.

Improvement: realizable *k*-ε

- Shares the same turbulent kinetic energy equation as the standard *k*-ε model.
- Improved equation for ε.
- Variable C_μ instead of constant.
- Improved performance for flows involving:
  - Planar and round jets (predicts round jet spreading correctly).
  - Boundary layers under strong adverse pressure gradients or separation.
  - Rotation, recirculation.
  - Strong streamline curvature.

k-ω model

- This is another two-equation model. In this model ω is an inverse time scale that is associated with the turbulence.
- This model solves two additional PDEs:
  - A modified version of the *k* equation used in the *k*-ε model.
  - A transport equation for ω.
- The turbulent viscosity is then calculated as follows:

$$\mu_t = \rho \frac{k}{\omega}$$

- Its numerical behavior is similar to that of the *k*-ε models.
- It suffers from some of the same drawbacks, such as the assumption that μ_t is isotropic.

Algebraic stress model

- The same *k* and ε equations are solved as with the standard *k*-ε model.
- However, the Boussinesq assumption is not used.
- The full Reynolds stress equations are first derived, and then some simplifying assumptions are made that allow the derivation of algebraic equations for the Reynolds stresses.
- Thus, fewer PDEs have to be solved than with the full RSM and it is much easier to implement.
- The algebraic equations themselves are not very stable, however, and computer time is significantly more than with the standard *k*-ε model.
- This model was used in the 1980s and early 1990s. Research continues but this model is rarely used in industry anymore now that most commercial CFD codes have full RSM implementations available.

Non-linear models

- The standard *k*-ε model is extended by including second and sometimes third order terms in the equation for the Reynolds stresses.
- One example is the Speziale model:

$$\tau_{ij} = -\rho\overline{u_i' u_j'} = -\frac{2}{3}k\delta_{ij} + \rho C_\mu \frac{k^2}{\varepsilon} 2E_{ij} - 4C_D C_\mu^2 \frac{k^3}{\varepsilon^2} * f(E, \partial E/\partial t, \mathbf{u}, \partial U/\partial x)$$

- Here $f(...)$ is a complex function of the deformation tensor, velocity field and gradients, and the rate of change of the deformation tensor.
- The standard *k*-ε model reduces to a special case of this model for flows with low rates of deformation.
- These models are relatively new and not yet used very widely.

Reynolds stress model

- RSM closes the Reynolds-Averaged Navier-Stokes equations by solving additional transport equations for the six independent Reynolds stresses.
  - Transport equations derived by Reynolds averaging the product of the momentum equations with a fluctuating property.
  - Closure also requires one equation for turbulent dissipation.
  - Isotropic eddy viscosity assumption is avoided.
- Resulting equations contain terms that need to be modeled.
- RSM is good for accurately predicting complex flows.
  - Accounts for streamline curvature, swirl, rotation and high strain rates.
    - Cyclone flows, swirling combustor flows.
    - Rotating flow passages, secondary flows.
    - Flows involving separation.

Reynolds stress transport equation

- The exact equation for the transport of the Reynolds stress R_{ij}:

$$\frac{DR_{ij}}{Dt} = P_{ij} + D_{ij} - \varepsilon_{ij} + \Pi_{ij} + \Omega_{ij}$$

- This equation can be read as:
  - rate of change of $R_{ij} = \overline{u_i' u_j'}$ plus
  - transport of R_{ij} by convection, equals
  - rate of production P_{ij}, plus
  - transport by diffusion D_{ij}, minus
  - rate of dissipation ε_{ij}, plus
  - transport due to turbulent pressure-strain interactions π_{ij}, plus
  - transport due to rotation Ω_{ij}.
- This equation describes six partial differential equations, one for the transport of each of the six independent Reynolds stresses.

Reynolds stress transport equation

- The various terms are modeled as follows:
  - Production P_{ij} is retained in its exact form.
  - Diffusive transport D_{ij} is modeled using a gradient diffusion assumption.
  - The dissipation ε_{ij}, is related to ε as calculated from the standard ε equation, although more advanced ε models are available also.
  - Pressure strain interactions Π_{ij}, are very important. These include pressure fluctuations due to eddies interacting with each other, and due to interactions between eddies and regions of the flow with a different mean velocity. The overall effect is to make the normal stresses more isotropic and to decrease shear stresses. It does not change the total turbulent kinetic energy. This is a difficult to model term, and various models are available. Common is the Launder model [5]. Improved, non-equilibrium models are available also.
  - Transport due to rotation Ω_{ij} is retained in its exact form.

Comparison of RANS turbulence models

Model	Strengths	Weaknesses
Spalart-Allmaras	Economical (1-eq.); good track record for mildly complex B.L. type of flows.	Not very widely tested yet; lack of submodels (e.g. combustion, buoyancy).
STD k-ε	Robust, economical, reasonably accurate; long accumulated performance data.	Mediocre results for complex flows with severe pressure gradients, strong streamline curvature, swirl and rotation. Predicts that round jets spread 15% faster than planar jets whereas in actuality they spread 15% slower.
RNG k-ε	Good for moderately complex behavior like jet impingement, separating flows, swirling flows, and secondary flows.	Subjected to limitations due to isotropic eddy viscosity assumption. Same problem with round jets as standard k-ε.
Realizable k-ε	Offers largely the same benefits as RNG but also resolves the round-jet anomaly.	Subjected to limitations due to isotropic eddy viscosity assumption.
Reynolds Stress Model	Physically most complete model (history, transport, and anisotropy of turbulent stresses are all accounted for).	Requires more cpu effort (2-3x); tightly coupled momentum and turbulence equations.

Recommendation

- Start calculations by performing 100 iterations or so with standard *k*-ε model and first order upwind differencing. For very simple flows (no swirl or separation) converge with second order upwind and *k*-ε model.
- If the flow involves jets, separation, or moderate swirl, converge solution with the realizable *k*-ε model and second order differencing.
- If the flow is dominated by swirl (e.g., a cyclone or unbaffled stirred vessel) converge solution deeply using RSM and a second order differencing scheme. If the solution will not converge, use first order differencing instead.
- Ignore the existence of mixing length models and the algebraic stress model.
- Only use the other models if you know from other sources that somehow these are especially suitable for your particular problem (e.g., Spalart-Allmaras for certain external flows, *k*-ε RNG for certain transitional flows, or *k*-ω).

Setting boundary conditions

- Characterize turbulence at inlets and outlets (potential backflow).
  - k-ε models require k and ε.
  - Reynolds stress model requires R_{ij} and ε.
- Other options:
  - Turbulence intensity and length scale.
    - Length scale is related to size of large eddies that contain most of energy.
    - For boundary layer flows, 0.4 times boundary layer thickness: $l \approx 0.4\delta_{99}$

      δ_{99} is the boundary layer thickness – 99% of the free stream velocity.
    - For flows downstream of grids /perforated plates: $l \approx$ opening size.
  - Turbulence intensity and hydraulic diameter.
    - Ideally suited for duct and pipe flows.
  - Turbulence intensity and turbulent viscosity ratio.
    - For external flows: $1 < \mu_t / \mu < 10$

Lecture 11 – Boundary Layers and Separation

Applied Computational Fluid Dynamics

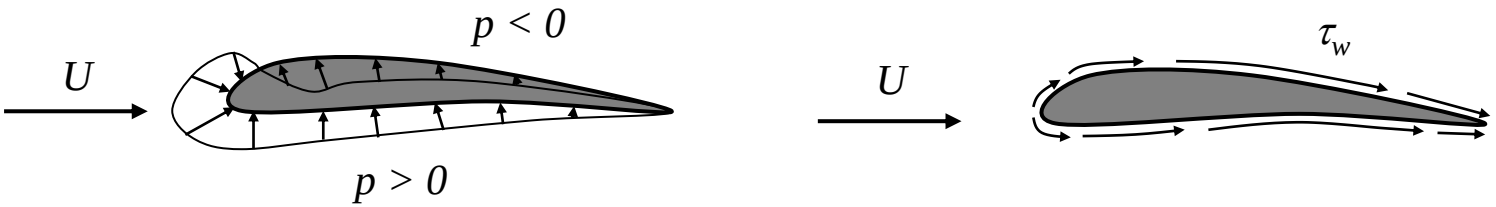
André Bakker

Overview

- Drag.
- The boundary-layer concept.
- Laminar boundary-layers.
- Turbulent boundary-layers.
- Flow separation.

The drag force

- The surrounding fluid exerts pressure forces and viscous forces on an object.



- The components of the resultant force acting on the object immersed in the fluid are the drag force and the lift force.
- The drag force acts in the direction of the motion of the fluid relative to the object.
- The lift force acts normal to the flow direction.
- Both are influenced by the size and shape of the object and the Reynolds number of the flow.

Drag prediction

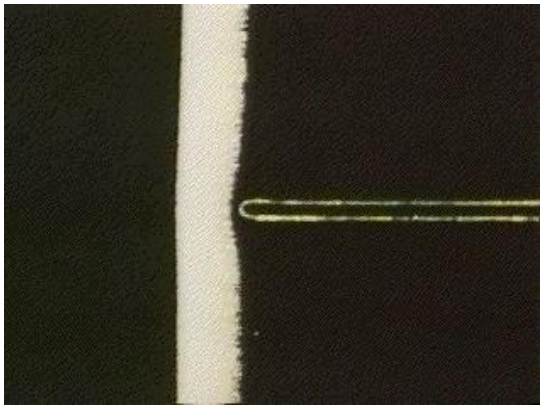
- The drag force is due to the pressure and shear forces acting on the surface of the object.
- The tangential shear stresses acting on the object produce friction drag (or viscous drag). Friction drag is dominant in flow past a flat plate and is given by the surface shear stress times the area:

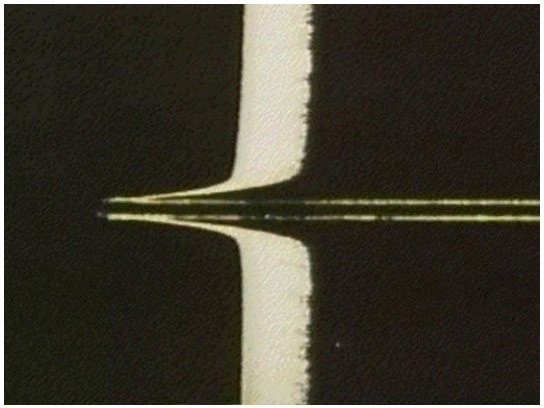
$$F_{d,viscous} = A.\tau_w$$

- Pressure or form drag results from variations in the normal pressure around the object: $F_{d,pressure} = \oint_A p\, da_n$
- In order to predict the drag on an object correctly, we need to correctly predict the pressure field and the surface shear stress.
- This, in turn, requires correct treatment and prediction of boundary layers and flow separation.
- We will discuss both in this lecture.

Viscous boundary layer

- An originally laminar flow is affected by the presence of the walls.
- Flow over flat plate is visualized by introducing bubbles that follow the local fluid velocity.
- Most of the flow is unaffected by the presence of the plate.
- However, in the region closest to the wall, the velocity decreases to zero.
- The flow away from the walls can be treated as inviscid and can sometimes be approximated as potential flow.
- The region near the wall where the viscous forces are of the same order as the inertial forces is termed the boundary layer.
- The distance over which the viscous forces have an effect is termed the boundary layer thickness.
- The thickness is a function of the ratio between the inertial forces and the viscous forces, i.e., the Reynolds number. As Re increases, the thickness decreases.

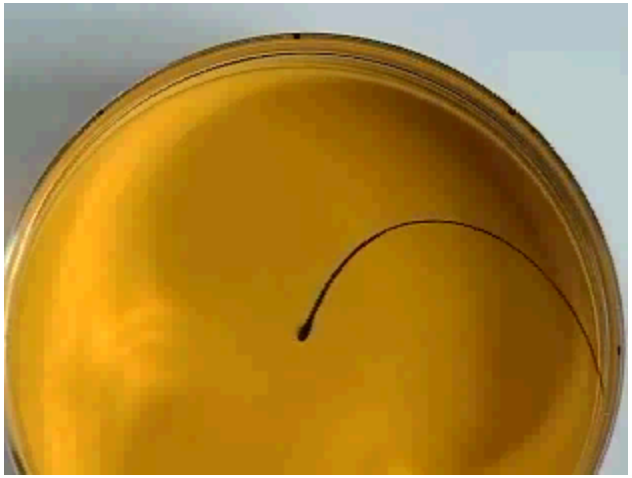




Images: Homsy et al. [2]

Effect of viscosity

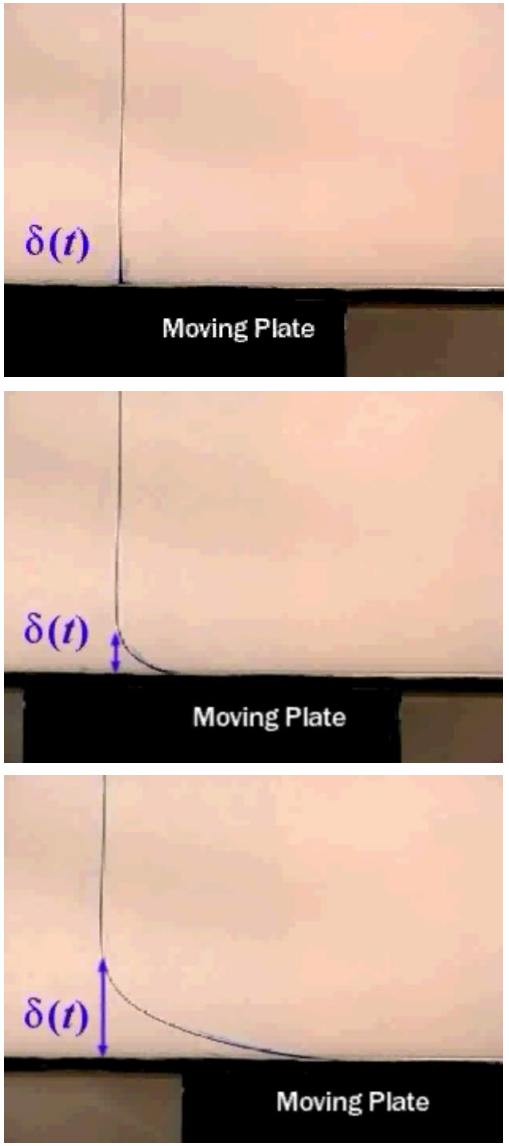
- The layers closer to the wall start moving right away due to the no-slip boundary condition. The layers farther away from the wall start moving later.
- The distance from the wall that is affected by the motion is also called the viscous diffusion length. This distance increases as time goes on.
- The experiment shown on the left is performed with a higher viscosity fluid (100 mPa.s). On the right, a lower viscosity fluid (10 mPa.s) is shown.



Images: Homsy et al. [2]

Moving plate boundary layer

- An impulsively started plate in a stagnant fluid.
- When the wall in contact with the still fluid suddenly starts to move, the layers of fluid close to the wall are dragged along while the layers farther away from the wall move with a lower velocity.
- The viscous layer develops as a result of the no-slip boundary condition at the wall.



Images: Homsy et al. [2]

Viscous boundary layer thickness

- Exact equations for the velocity profile in the viscous boundary layer were derived by Stokes in 1881.
- Start with the Navier-Stokes equation:

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2}$$

- Derive exact solution for the velocity profile:

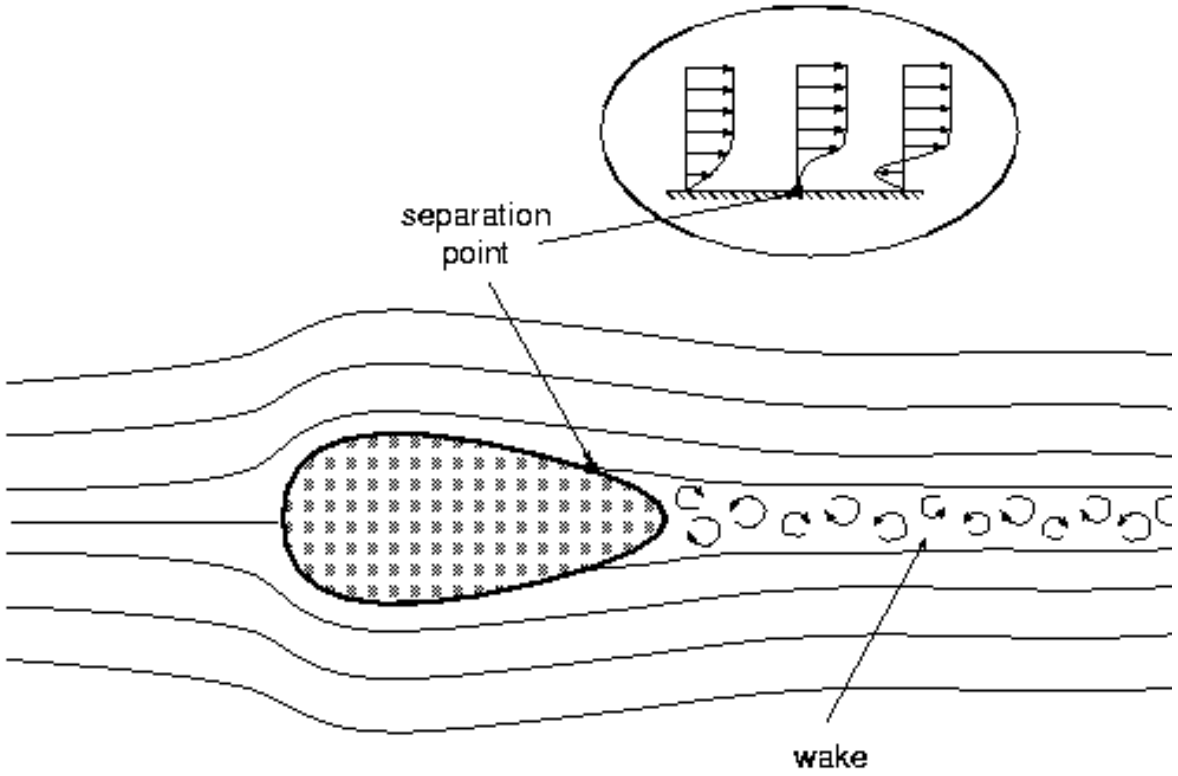
$$U = U_0 \left(1 - erf\left(\frac{y}{2\sqrt{\nu t}} \right) \right)$$

- *erf* is the error function: $erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt$
- The boundary layer thickness can be approximated by:

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2} \Rightarrow \frac{U_0}{t} \approx \nu \frac{U_0}{\delta^2} \Rightarrow \delta \approx \sqrt{\nu t}$$

Flow separation

- Flow separation occurs when:
  - the velocity at the wall is zero or negative and an inflection point exists in the velocity profile,
  - and a positive or adverse pressure gradient occurs in the direction of flow.



Separation at sharp corners

- Corners, sharp turns and high angles of attack all represent sharply decelerating flow situations, leading to separation.
- Here we see how the boundary layer flow is unable to follow the turn in the sharp corner (which would require a very rapid acceleration), causing separation at the edge and recirculation in the aft region of the backward facing step.

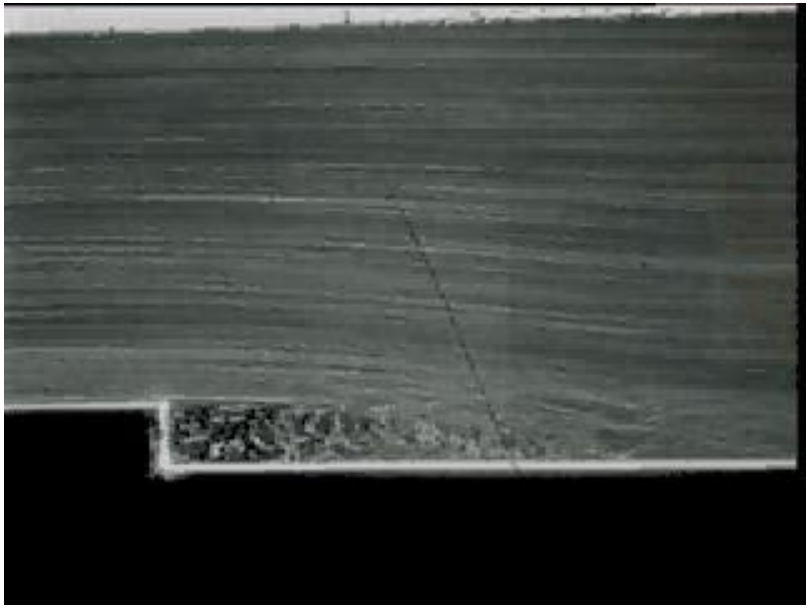


Image: Homsy et al. [2]

Flow around a truck

- Flow over non-streamlined bodies such as trucks leads to considerable drag due to recirculation and separation zones.
- A recirculation zone is clear on the back of the cab, and another one around the edge of the trailer box.
- The addition of air shields to the cab roof ahead of the trailer helps streamline the flow around the trailer and minimize losses, reducing drag by up to 10-15%.

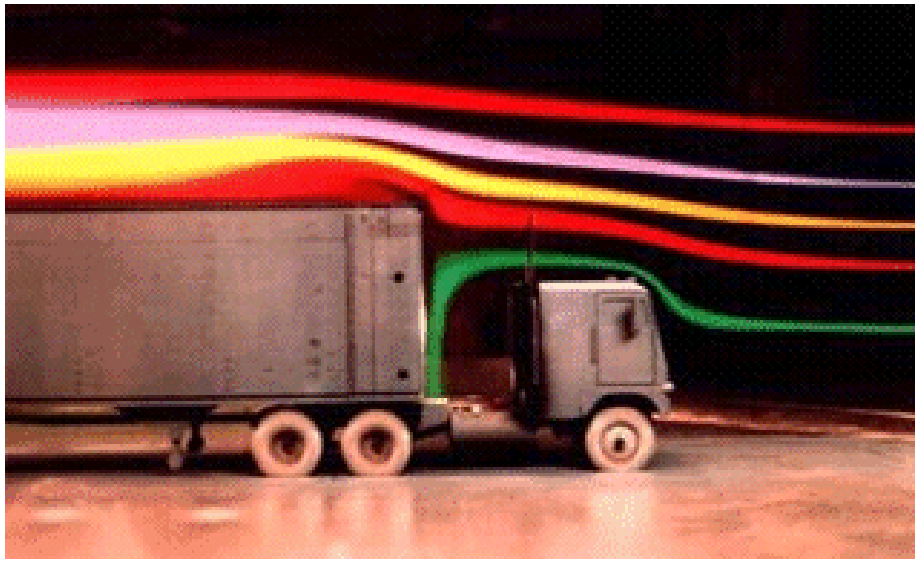


Image: Homsy et al. [2]

Flow separation in a diffuser with a large angle

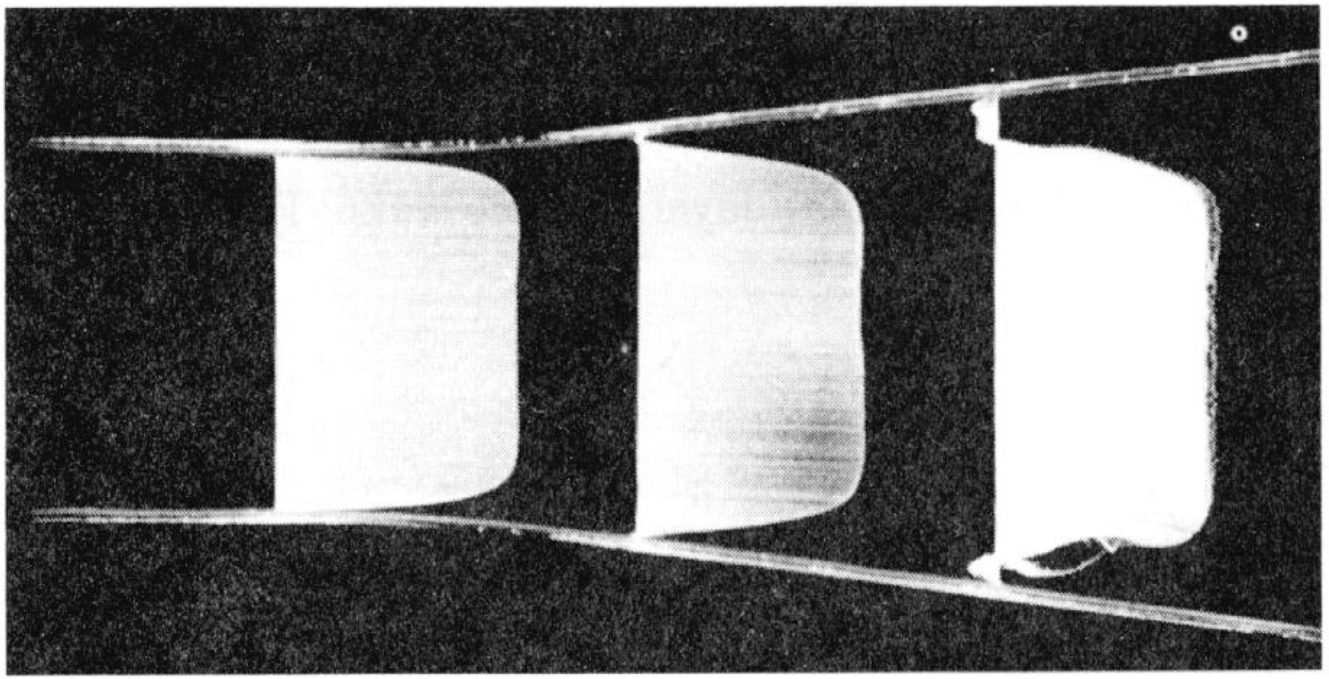
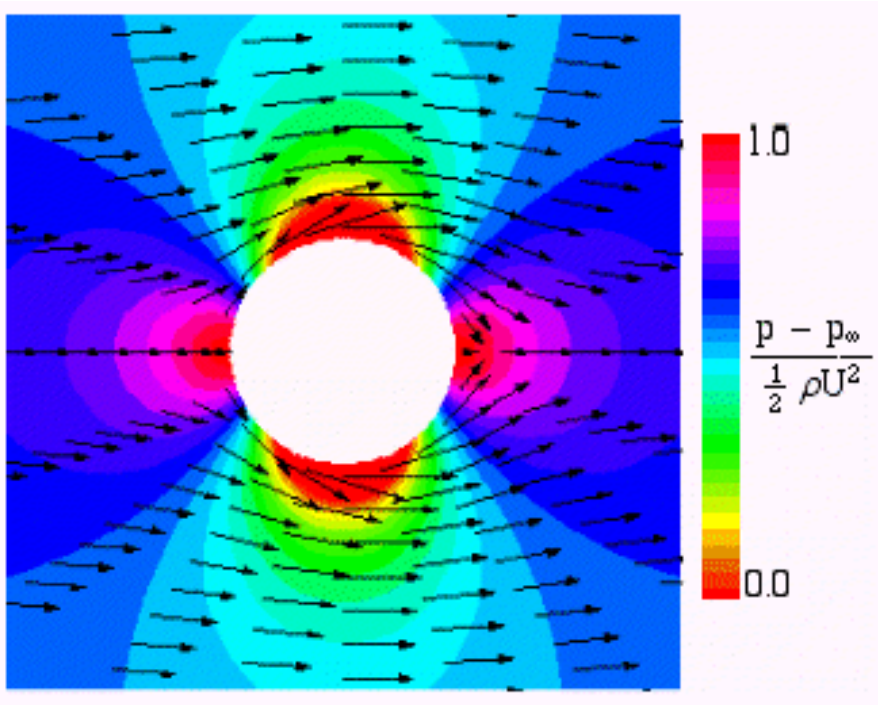


Image: Homsy et al. [2]

Inviscid flow around a cylinder

- The origins of the flow separation from a surface are associated with the pressure gradients impressed on the boundary layer by the external flow.
- The image shows the predictions of inviscid, irrotational flow around a cylinder, with the arrows representing velocity and the color map representing pressure.
- The flow decelerates and stagnates upstream of the cylinder (high pressure zone).
- It then accelerates to the top of the cylinder (lowest pressure).

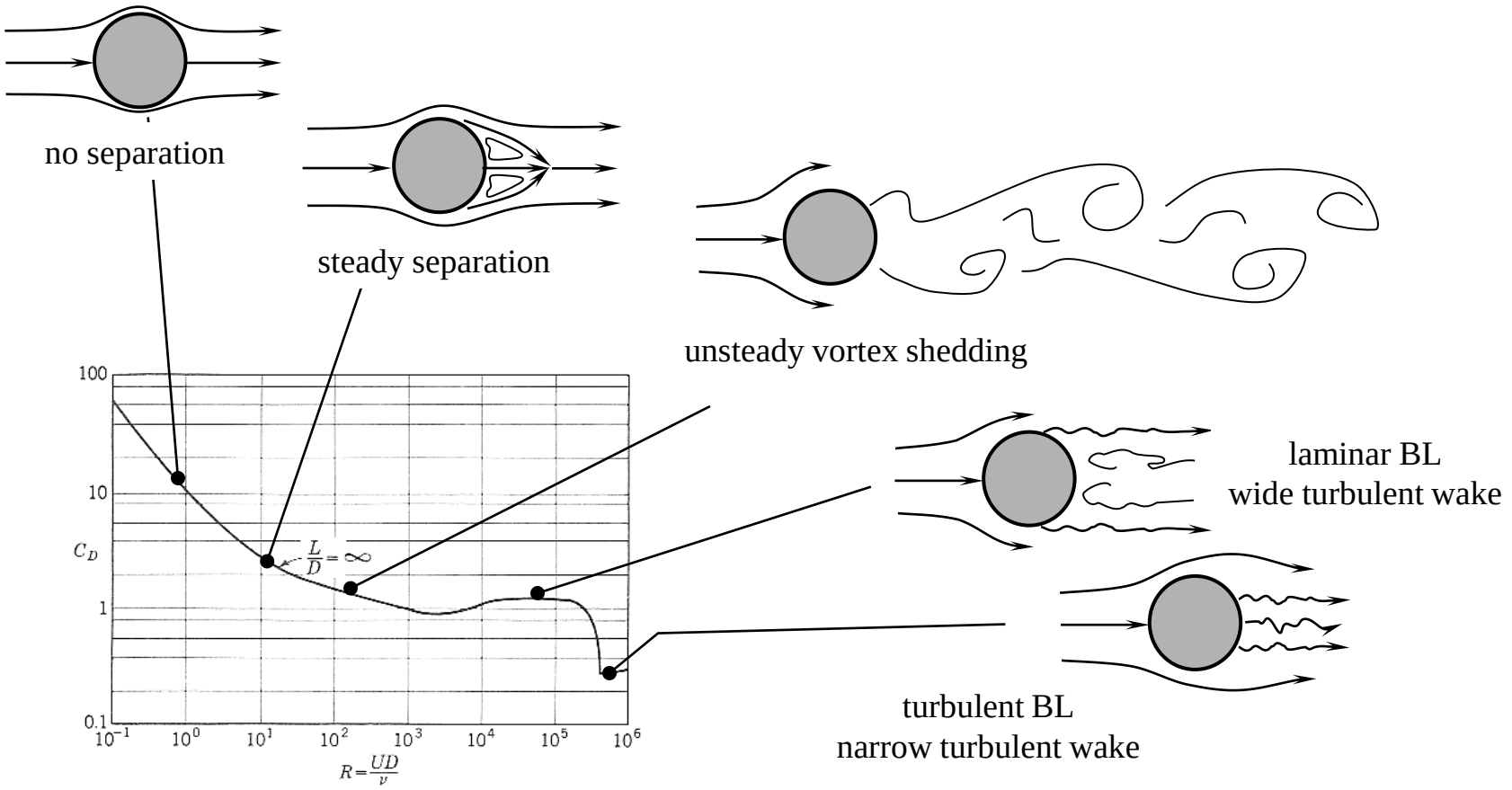


- Next it must decelerate against a high pressure at the rear stagnation point.

Image: Homsy et al. [2]

Drag on a smooth circular cylinder

- The drag coefficient is defined as follows: $F_{drag} = C_D \frac{1}{2} \rho v^2 A_\perp$



Separation - adverse pressure gradients

- Separation of the boundary layers occurs whenever the flow tries to decelerate quickly.
- In the case of the tennis ball, the flow initially decelerates on the upstream side of the ball, while the local pressure increases in accord with Bernoulli's equation.
- Near the top of the ball the local external pressure decreases, and the flow should accelerate as the potential energy of the pressure field is converted to kinetic energy.
- However, because of viscous losses, not all kinetic energy is recovered and the flow reverses around the separation point.

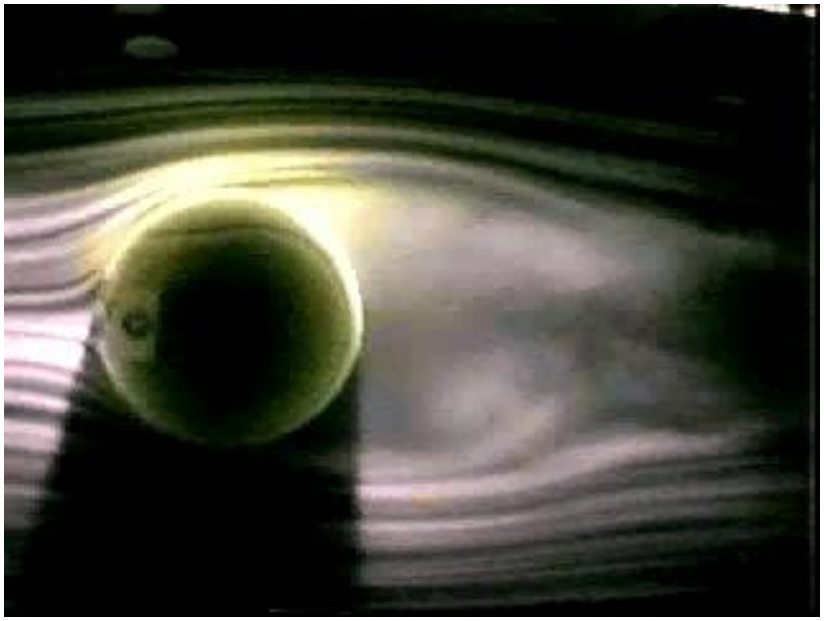
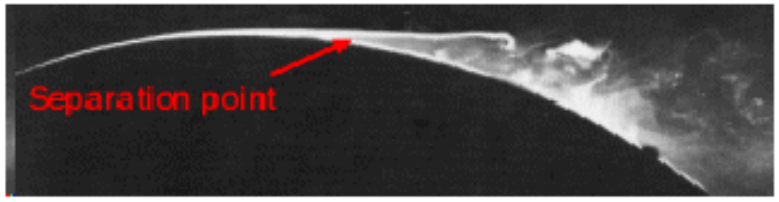


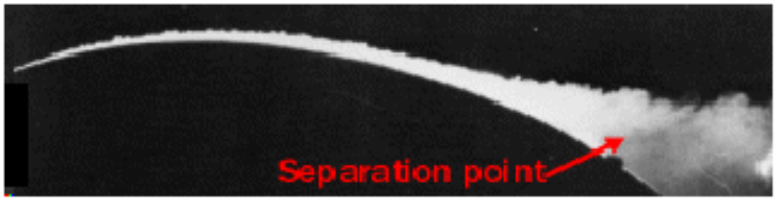
Image: Homsy et al. [2]

Turbulent boundary layer

- Increased momentum transport due to turbulence from the free stream flow to the flow near the wall makes turbulent boundary layers more resistant to flow separation.
- The photographs depict the flow over a strongly curved surface, where there exists a strong adverse (positive) pressure gradient.
- In the case where the boundary layer is laminar, insufficient momentum exchange takes place, the flow is unable to adjust to the increasing pressure and separates from the surface.
- In case where the flow is turbulent, the increased transport of momentum (due to the Reynolds stresses) from the free-stream to the wall increases the streamwise momentum in the boundary layer. This allows the flow to overcome the adverse pressure gradient. It eventually does separate nevertheless, but much further downstream.



Laminar Separation

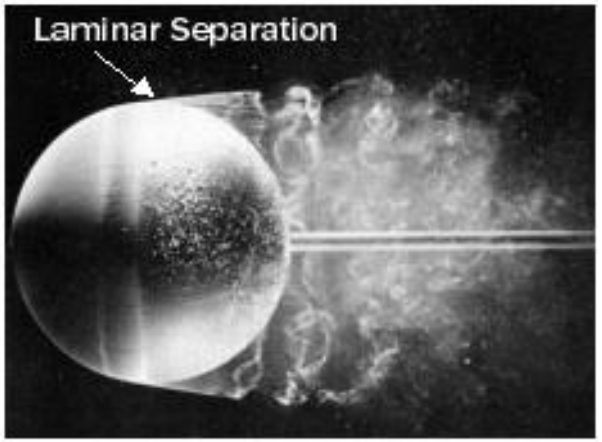


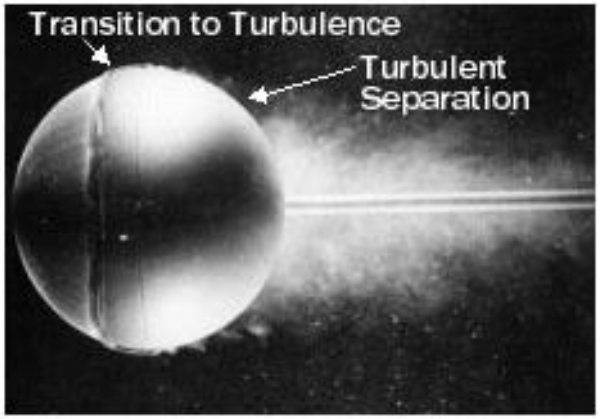
Turbulent Separation

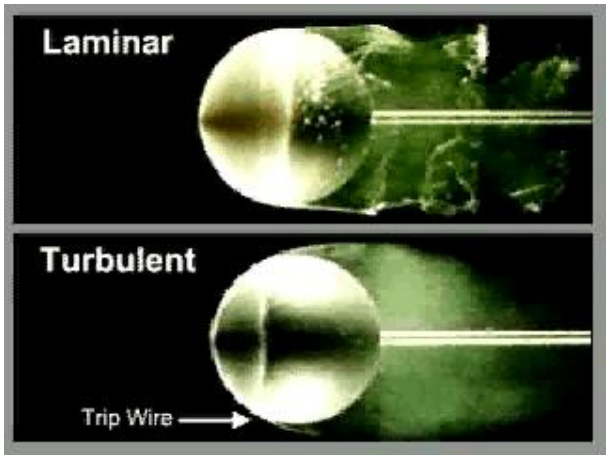
Images: Homsy et al. [2] and Van Dyke [8]

Tripping the boundary layer

- Here we see how the addition of a trip wire to induce transition to turbulence changes the separation line further to the rear of the sphere, reducing the size of the wake and thus drastically diminishing overall drag.
- This well-known fact can be taken advantage of in a number of applications, such as dimples in golf balls and turbulence generation devices on airfoils.



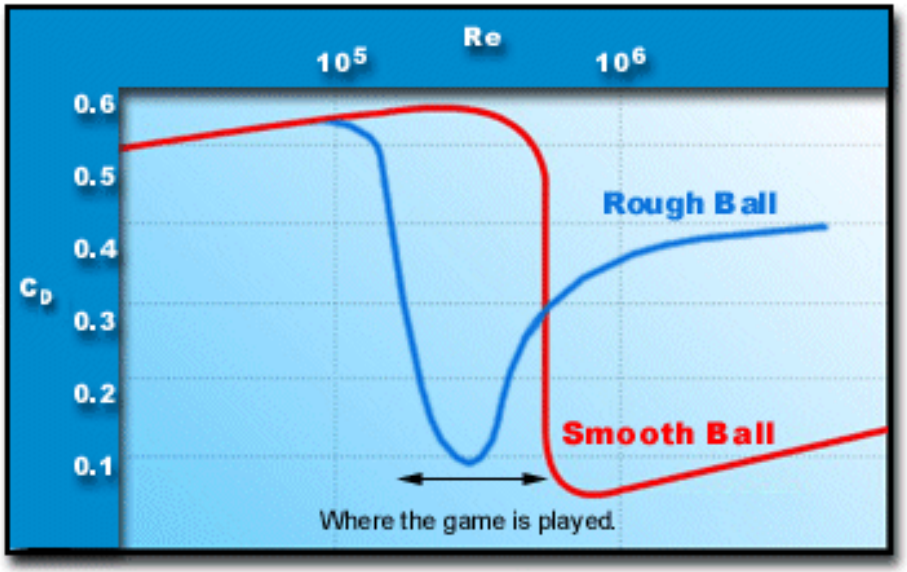




Images: Homsy et al. [2] and Van Dyke [8]

Sports balls

- Many games involve balls designed to use drag reduction brought about by surface roughness.
- Many sports balls have some type of surface roughness, such as the seams on baseballs or cricket balls and the fuzz on tennis balls.
- It is the Reynolds number (not the speed, per se) that determines whether the boundary layer is laminar or turbulent. Thus, the larger the ball, the lower the speed at which a rough surface can be of help in reducing the drag.

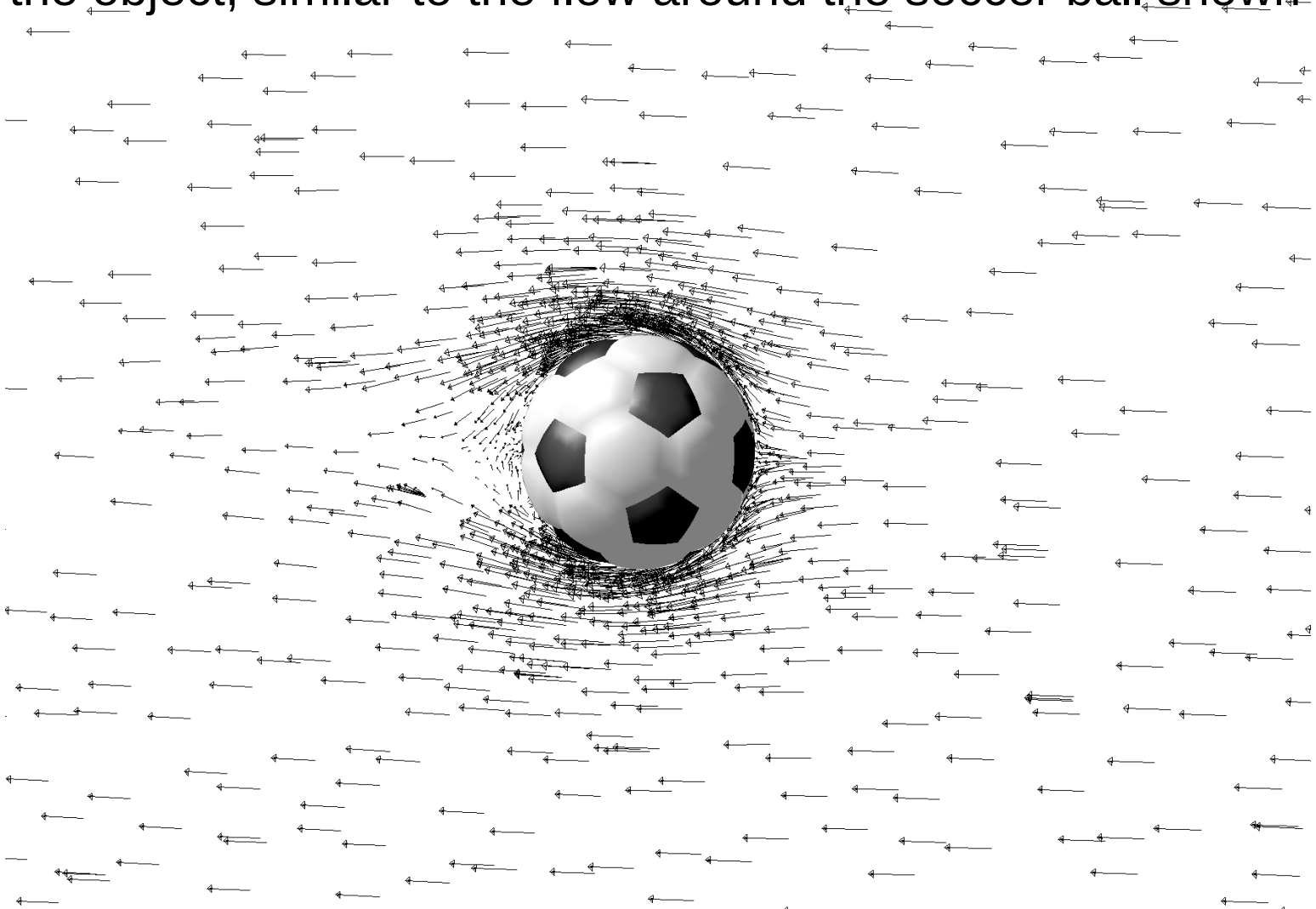


- Typically, sports ball games that use surface roughness to promote an early transition of the boundary layer from a laminar to a turbulent flow are played over a Reynolds number range that is near the “trough” of the Cd versus Re curve, where drag is lowest.

Image: Homsy et al. [2]

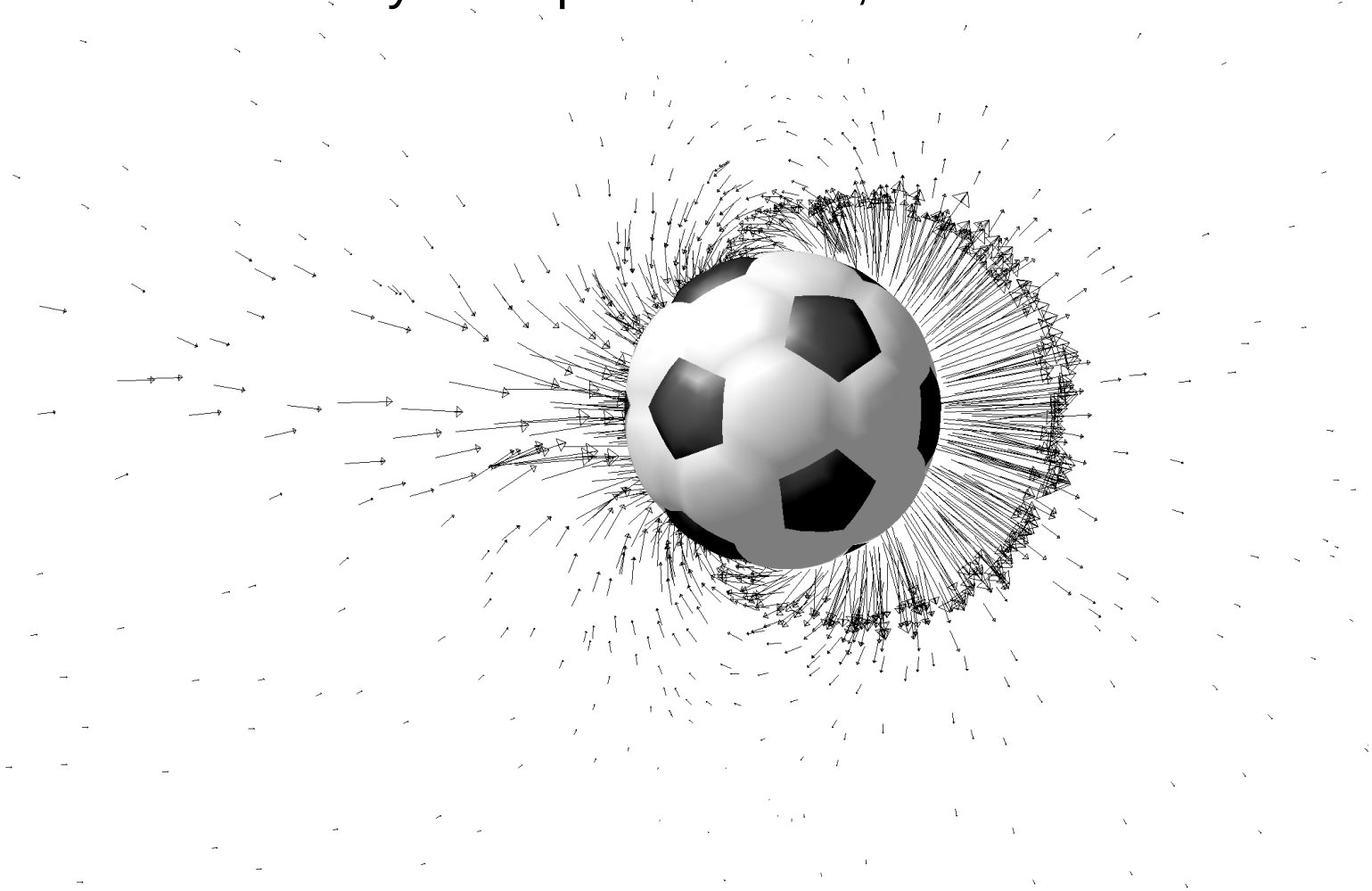
Flow in reference frame relative to the ball

- Note that we have been showing flow fields in the reference frame of the object, similar to the flow around the soccer ball shown here.



Flow in absolute reference frame

- However, one should keep in mind that the flow in the absolute reference frame may look quite different, as shown here.



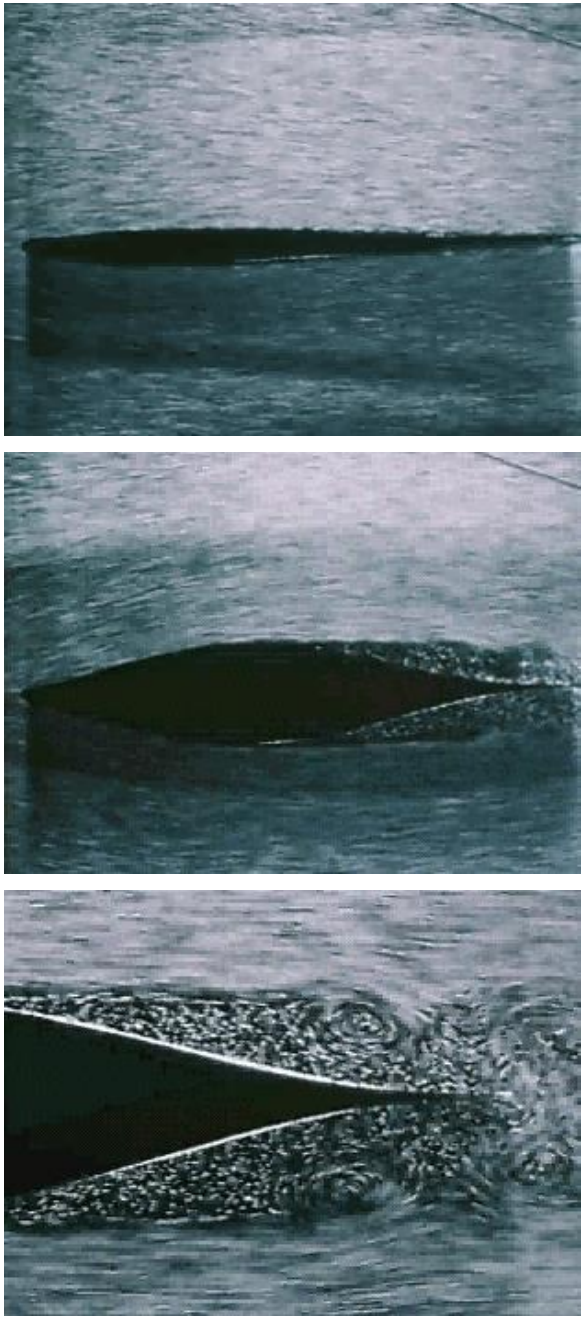
Airfoil - effect of angle of attack

- The loss in pressure in the separated flow region behind solid bodies causes an imbalance between the upstream and downstream forces, contributing greatly to an increased net drag force.
- In the case of streamlined airfoils at low angle of attack, separation occurs only at the tip, with minimal losses. As the angle of attack increases, the separation point moves upstream, leading to increased drag.

Images: Homsy et al. [2]

Airfoil - effect of shape

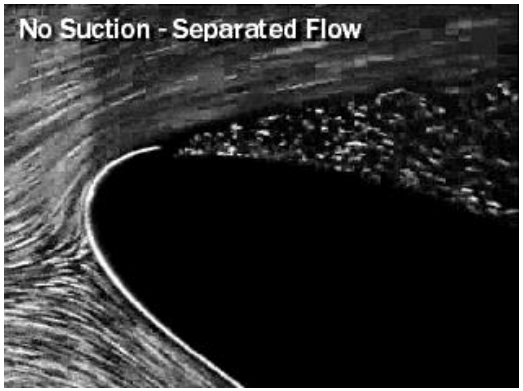
- The pressure field is changed by changing the thickness of a streamlined body placed in the flow. The acceleration and deceleration caused by a finite body width creates favorable and unfavorable pressure gradients.
- When the body is thin, there are only weak pressure gradients, and the flow remains attached. As the body is made thicker, the adverse pressure gradient resulting from the deceleration near the rear leads to flow separation, recirculation, and vortex shedding.
- Focusing in on the rear region of the flow, it is seen that as the body is again reduced in thickness, the separated region disappears as the strengths of the adverse pressure gradient is diminished.

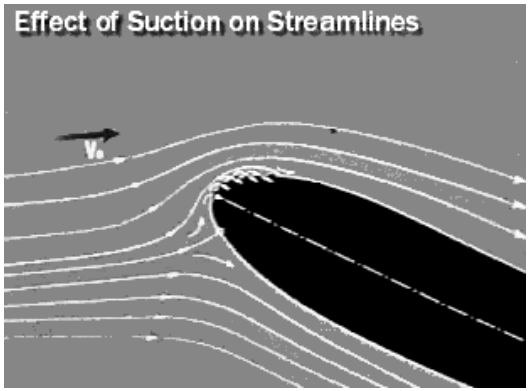


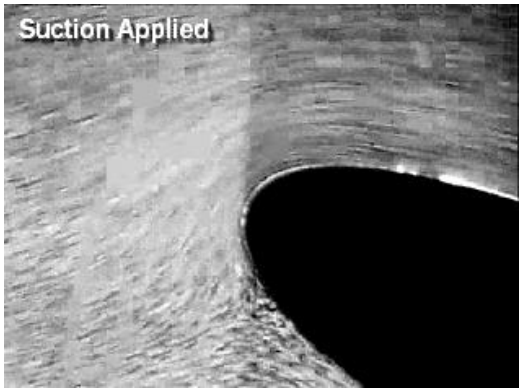
Images: Homsy et al. [2]

Suction

- Just as flow separation can be understood in terms of the combined effects of viscosity and adverse pressure gradients, separated flows can be reattached by the application of a suitable modification to the boundary conditions.
- In this example, suction is applied to the leading edge of the airfoil at a sharp angle of attack, removing the early separation zone, and moving the separation point much farther downstream.







Images: Homsy et al. [2]

Blowing

- Separation in external flows, such as the flow past a sudden expansion can be controlled not only by suction but also by blowing.
- In this experiment, the region of separated flow is eliminated by the introduction of high momentum fluid at a point near the separation point.
- This acts to eliminate the adverse pressure gradient by accelerating the fluid close to the boundary, leading to re-attachment of the flow.

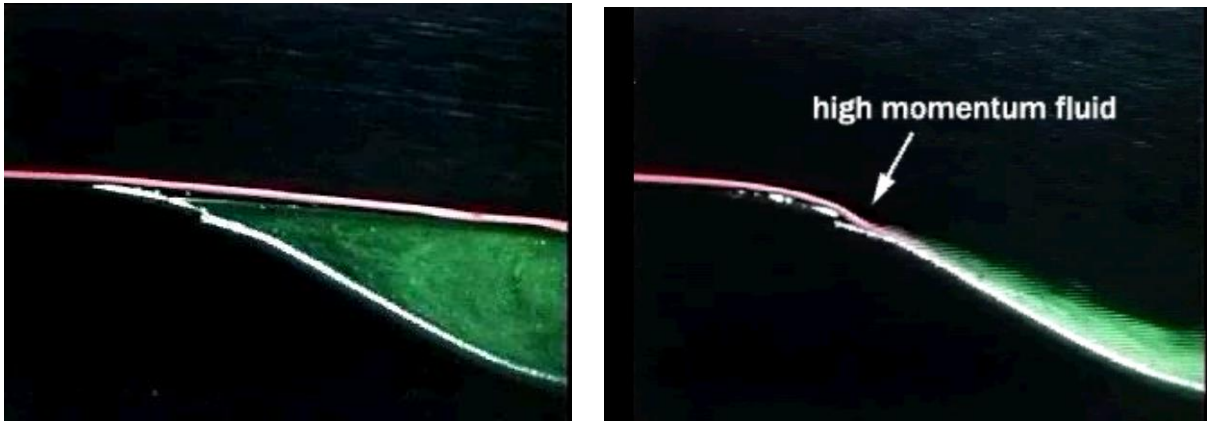
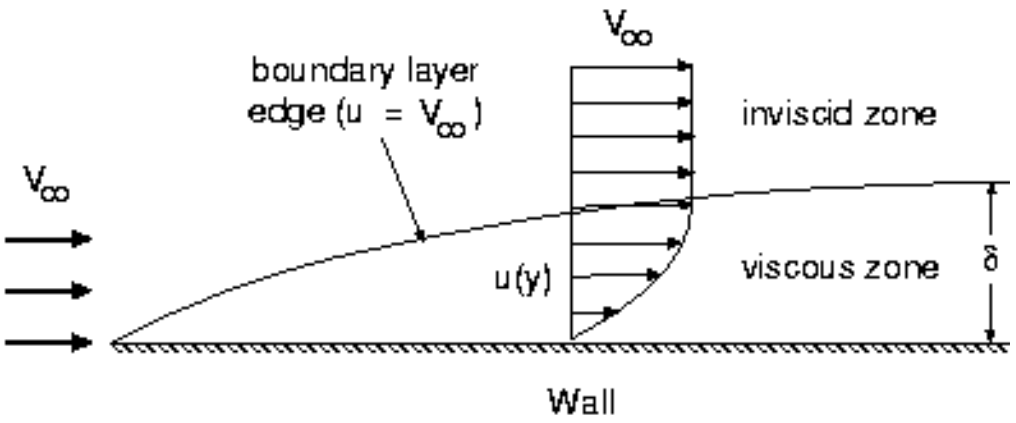


Image: Homsy et al. [2]

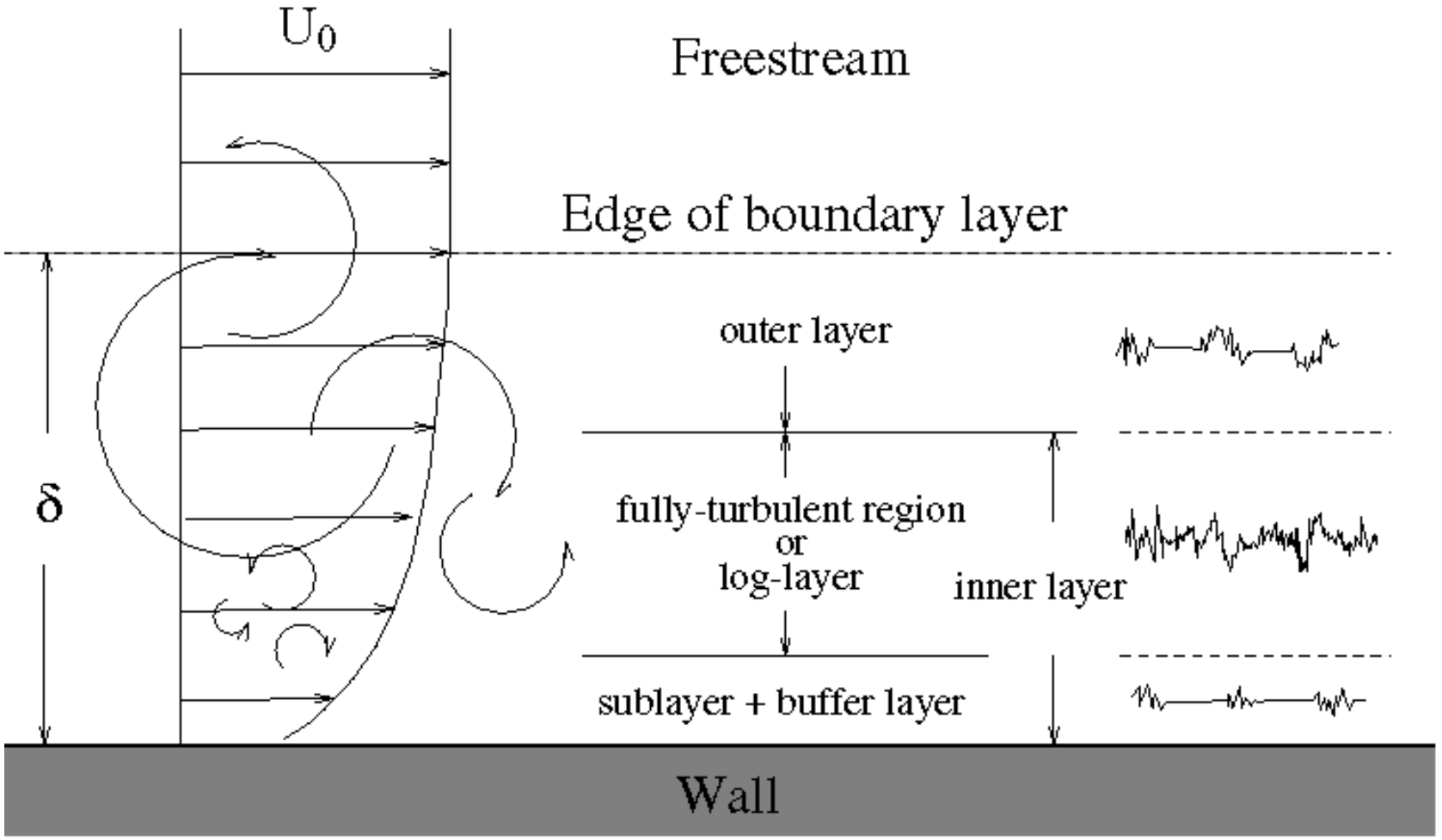
The turbulent boundary layer

- In turbulent flow, the boundary layer is defined as the thin region on the surface of a body in which viscous effects are important.
- The boundary layer allows the fluid to transition from the free stream velocity U_τ to a velocity of zero at the wall.
- The velocity component normal to the surface is much smaller than the velocity parallel to the surface: v << u.
- The gradients of the flow across the layer are much greater than the gradients in the flow direction.
- The boundary layer thickness δ is defined as the distance away from the surface where the velocity reaches 99% of the free-stream velocity.



$$\delta = y, \; where \; {u}/{U} = 0.99$$

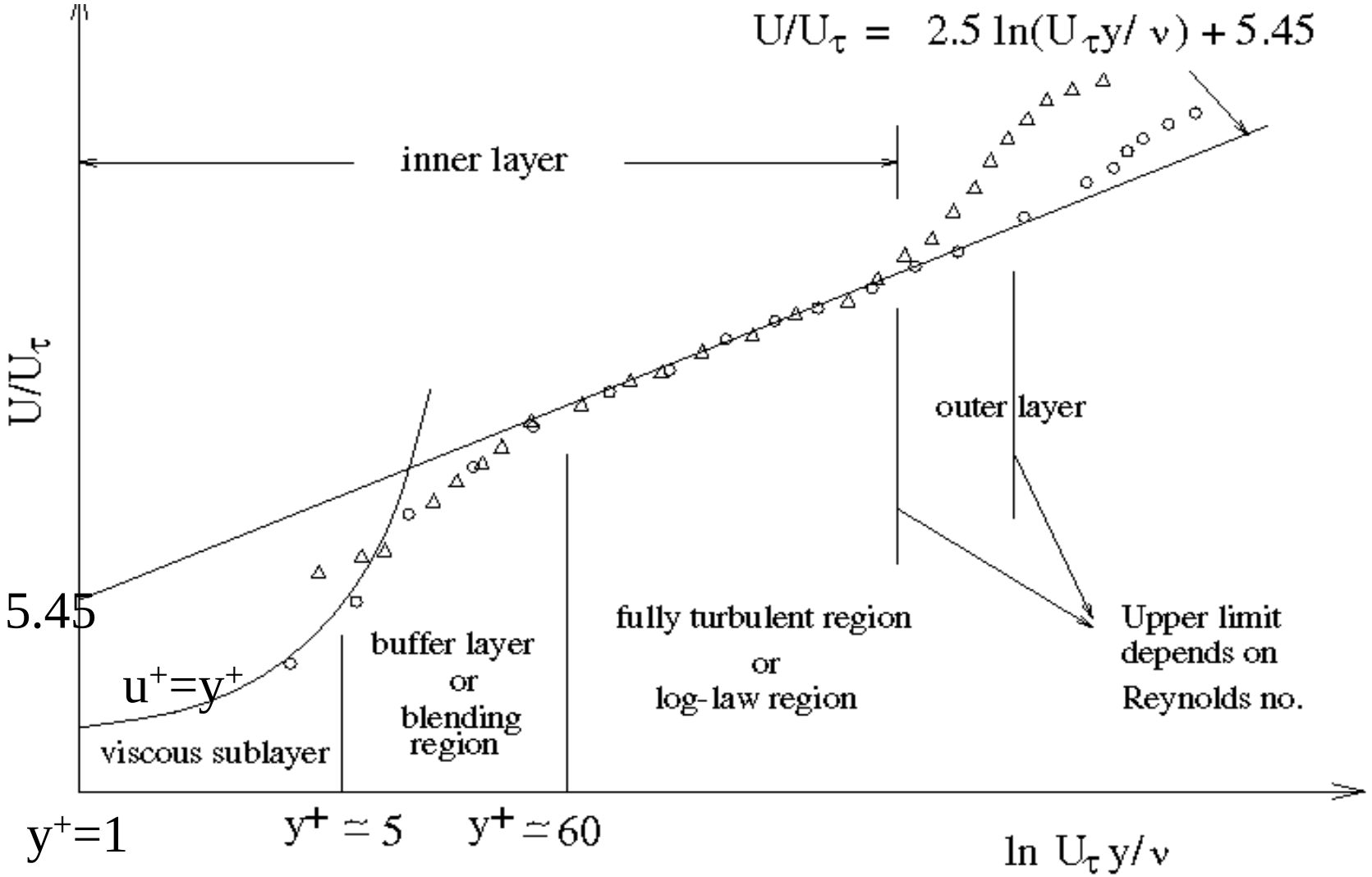
The turbulent boundary layer



The turbulent boundary layer

- Important variables:
  - Distance from the wall: y.
  - Wall shear stress: τ_w. The force exerted on a flat plate is the area times the wall shear stress.
  - Density: ρ.
  - Dynamic viscosity: μ.
  - Kinematic viscosity: ν.
  - Velocity at y: U.
  - The friction velocity: $u_\tau = (\tau_w/\rho)^{1/2}$.
- We can define a Reynolds number based on the distance to the wall using the friction velocity: $y^+ = yu_\tau/\nu$.
- We can also make the velocity at y dimensionless using the friction velocity: $u^+ = U/ u_\tau$.

Boundary layer structure



Standard wall functions

- The experimental boundary layer profile can be used to calculate τ_w. However, this requires y^+ for the cell adjacent to the wall to be calculated iteratively.
- In order to save calculation time, the following explicit set of correlations is usually solved instead:

$$y^* = \frac{\rho C_\mu^{1/4} k_P^{1/2} y_P}{\mu} \Rightarrow \left\{ \begin{array}{l} y^* \geq 11.225 \Rightarrow U^* = \frac{1}{\kappa} \ln\left(E y^*\right) \\ y^* < 11.225 \Rightarrow U^* = y^* \end{array} \right\} \Rightarrow \tau_w = \frac{U_P C_\mu^{1/4} k_P^{1/2}}{U^* / \rho}$$

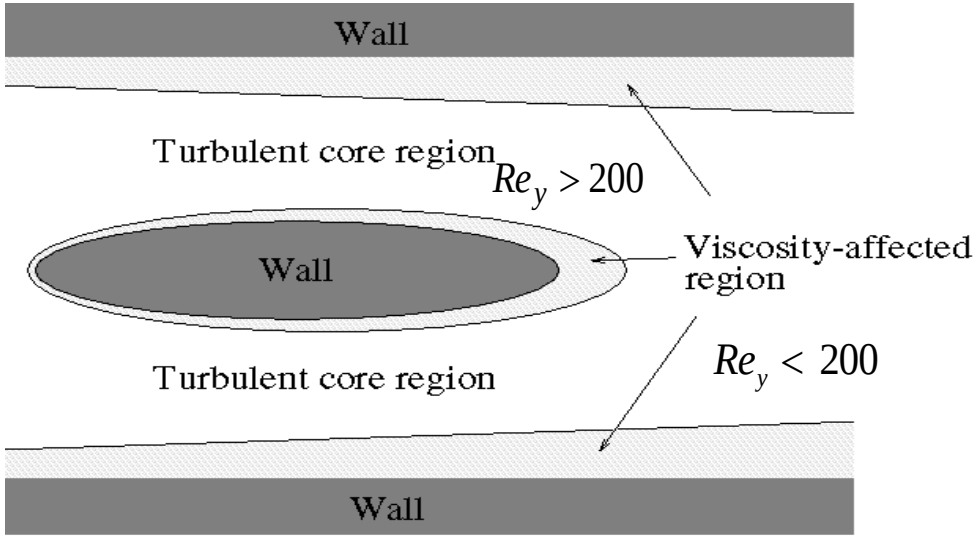
- Here:
  - U_p is the velocity in the center of the cell adjacent to the wall.
  - y_p is the distance between the wall and the cell center.
  - k_p is the turbulent kinetic energy in the cell center.
  - κ is the von Karman constant (0.42).
  - E is an empirical constant that depends on the roughness of the walls (9.8 for smooth surfaces).

Near-wall treatment - momentum equations

- The objective is to take the effects of the boundary layer correctly into account without having to use a mesh that is so fine that the flow pattern in the layer can be calculated explicitly.
- Using the no-slip boundary condition at wall, velocities at the nodes at the wall equal those of the wall.
- The shear stress in the cell adjacent to the wall is calculated using the correlations shown in the previous slide.
- This allows the first grid point to be placed away from the wall, typically at $50 < y^+ < 500$, and the flow in the viscous sublayer and buffer layer does not have to be resolved.
- This approach is called the “standard wall function” approach.
- The correlations shown in the previous slide are for steady state (“equilibrium”) flow conditions. Improvements, “non-equilibrium wall functions,” are available that can give improved predictions for flows with strong separation and large adverse pressure gradients.

Two-layer zonal model

- A disadvantage of the wall-function approach is that it relies on empirical correlations.
- The two-layer zonal model does not. It is used for low-Re flows or flows with complex near-wall phenomena.



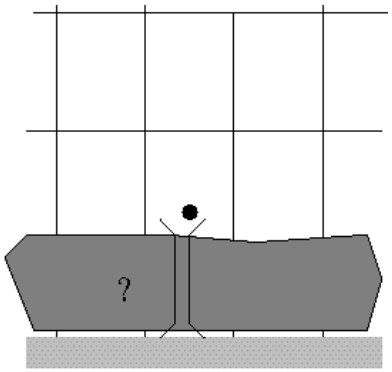
- Zones distinguished by a wall-distance-based turbulent Reynolds number: $Re_y \equiv \frac{\rho\sqrt{k}y}{\mu}$
- The flow pattern in the boundary layer is calculated explicitly.
- Regular turbulence models are used in the turbulent core region.
- Only *k* equation is solved in the viscosity-affected region.
- ε is computed using a correlation for the turbulent length scale.
- Zoning is dynamic and solution adaptive.

Near-wall treatment - turbulence

- The turbulence structure in the boundary layer is highly anisotropic.
- ε and k require special treatment at the walls.
- Furthermore, special turbulence models are available for the low Reynolds number region in the boundary layer.
- These are aptly called “low Reynolds number” models.
- This is still a very active area of research, and we will not discuss those here in detail.

Computational grid guidelines

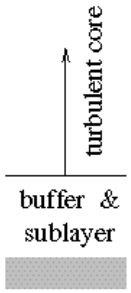
Wall Function Approach



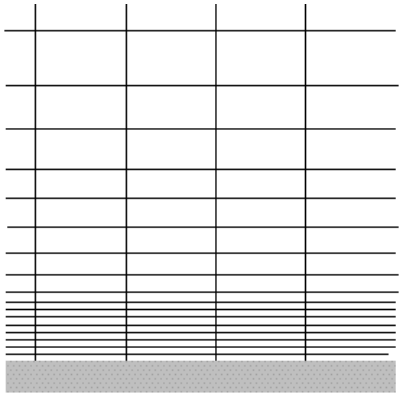
- First grid point in log-law region:

$$50 \le y^+ \le 500$$

- Gradual expansion in cell size away from the wall.
- Better to use stretched quad/hex cells for economy.



Two-Layer Zonal Model Approach



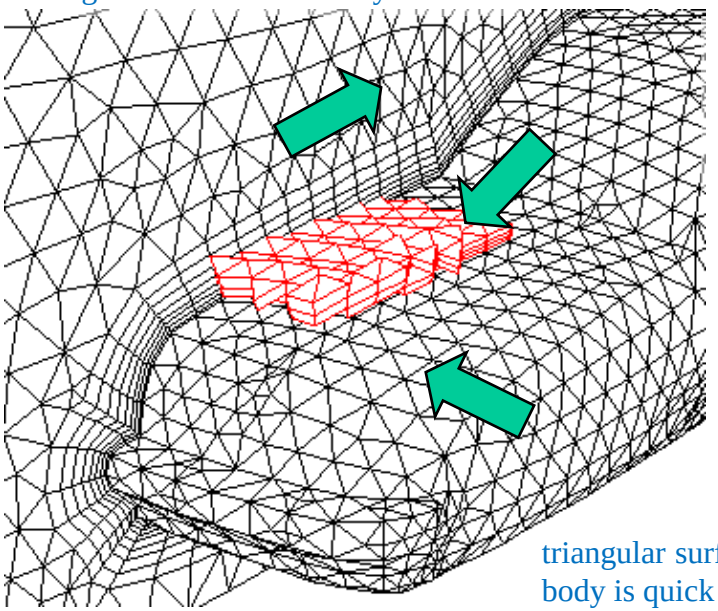
- First grid point at $y^+ \approx 1$.
- At least ten grid points within buffer and sublayers.
- Better to use stretched quad/hex cells for economy.

Comparison of near-wall treatments

Approach	Strengths	Weaknesses
Standard wall-functions	Robust, economical, reasonably accurate	Empirically based on simple high- Re flows; poor for low-Re effects, massive transpiration, PGs, strong body forces, highly 3D flows
Non-equilibrium wall-functions	Accounts for pressure gradient (PG) effects. Improved predictions for separation, reattachment, impingement	Poor for low-Re effects, massive transpiration (blowing, suction), severe PGs, strong body forces, highly 3D flows
Two-layer zonal model	Does not rely on empirical law-of-the-wall relations, good for complex flows, applicable to low-Re flows	Requires finer mesh resolution and therefore larger cpu and memory resources

Obtaining accurate solutions

- When very accurate (say 2%) drag, lift, or torque predictions are required, the boundary layer and flow separation require accurate modeling.
- The following practices will improve prediction accuracy:
  - Use boundary layer meshes consisting of quads, hexes, or prisms. Avoid using pyramid or tetrahedral cells immediately adjacent to the wall.
  - After converging the solution, use the surface integral reporting option to check if y^+ is in the right range, and if not refine the grid using adaption.
  - For best predictions use the two-layer zonal model and completely resolve the flow in the whole boundary layer.



Summary

- The concept of the boundary layer was introduced.
- Boundary layers require special treatment in the CFD model.
- The influence of pressure gradient on boundary layer attachment showed that an adverse pressure gradient gives rise to flow separation.
- For accurate drag, lift, and torque predictions, the boundary layer and flow separation need to be modeled accurately.
- This requires the use of:
  - A suitable grid.
  - A suitable turbulence model.
  - Higher order discretization.
  - Deep convergence using the force to be predicted as a convergence monitor.

Lecture 12 - Large Eddy Simulation

Applied Computational Fluid Dynamics

André Bakker

Outline

- Brief summary of turbulence models.
- Introduction to large eddy simulation (LES).
- Examples:
  - HEV static mixer.
  - Mixing tank with Rushton turbine.
  - Mixing tank with high efficiency impeller.

Modeling turbulence

- Turbulence is a 3D transient phenomenon.
  - Fluctuations cover a wide range of time and length scales.
- Turbulence models range from approximate to highly rigorous:
  - Steady-state isotropic models.
  - Transient 3D models of entire spectrum.
- Models are incorporated into the Navier-Stokes equations using a variety of methods.

The turbulence spectrum

- Many scales of turbulent eddies exist:
  - Large eddies contain most of the turbulent kinetic energy.
    - Scale sizes are on the order of the flow passages.
  - Energy cascades from large to small eddies.
  - Small eddies dissipate the energy they receive from larger eddies in the spectrum.
- Difficulty in turbulence modeling is trying to accurately capture the contributions of all scales in the spectrum.

Direct numerical simulation (DNS)

- Navier-Stokes equations are solved on a fine grid using a small time-step.
- Goal is to capture the smallest turbulence scales.
  - large-scales are captured as well.
- Result is accurate, 3D, transient behavior.
- Great for simple flows, but computationally intensive.
  - Not suited to industrial applications with CPU resources available today.

The cost of DNS

- The number of grid points per dimension needed to resolve the small-scales is:

$$N_{1D} \sim \mathrm{Re}_t^{3/4}, \quad \mathrm{Re}_t = \frac{\rho\sqrt{k}\ell}{\mu}$$

- The number of grid points needed for a 3D DNS simulation is:

$$N_{3D} \sim \mathrm{Re}_t^{9/4}$$

- The overall cost, including time step, of the computational effort is proportional to $\mathrm{Re}_t^{3.}$

RANS turbulence models (1/2)

- Velocities are described by an equilibrium (v_o) and fluctuating (v') contribution:

$$v_i = v_{oi} + v_i'.$$

- Momentum equations are rewritten, then time-averaged (Reynolds Averaged Navier-Stokes equations).
  - Averaging eliminates terms with v' as a factor.
  - Terms with $\overline{v_i' v_j'}$ remain.
  - These Reynolds stresses are computed with a turbulence model.
  - Impact on transport equations is through the effective viscosity:

    $\mu_{eff} \sim \mu_t + \mu_o$ (1 and 2 equation models).

RANS turbulence models (2/2)

- Many flavors exist, such as:
  - k-ε: Robust, popular 2-equation model using constants taken from simple, high Re flows.
    - isotropic turbulence effects: μ_{eff} is a scalar.
  - RSM: 5-equation (2D) or 7-equation (3D) model.
    - non-isotropic turbulence effects makes this suitable for highly swirling flows.

Large eddy simulation (LES)

- LES is midway between DNS and RANS in terms of:
  - Rigor.
  - Computational requirement.
- Spectrum of turbulent eddies in the Navier-Stokes equations is “filtered”:
  - The filter is a function of the grid size.
  - Small eddies are removed and modeled using a *subgrid-scale (SGS)* model.
  - Large eddies are retained and solved for directly using a transient calculation.

Filtered variables

- A variable, $\phi(x')$, is filtered using a filter function, G.

$$\tilde{\phi}(\mathbf{x}) = \int_D \phi(\mathbf{x}')G(\mathbf{x},\mathbf{x}')d\mathbf{x}'$$

- G is a function of the cell volume.

Thus:

$$G(\mathbf{x},\mathbf{x}') = \begin{cases} 1/\mathrm{V} & \text{for } \mathbf{x}' \in \mathcal{V} \\ 0 & \text{otherwise} \end{cases}$$

$$\tilde{\phi}(\mathbf{x}) = \frac{1}{V}\int_{\nu} \phi(\mathbf{x}')d\mathbf{x}', \qquad \mathbf{x}' \in V$$

Filtered transport equations

- The filtered continuity and momentum equations use filtered variables:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \tilde{u}_j}{\partial x_j} = 0$$

and:

$$\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_j}$$

τ_{ij} is the filtered stress tensor.

σ_{ij} are the subgrid-scale Reynolds stresses.

Subgrid-scale (SGS) modeling

- SGS Reynolds stresses are modeled by:

$$\sigma_{ij}^{s} - \frac{1}{3}\delta ij\,\sigma_{kk}^{s} = -2\mu_{t}S_{ij}$$

where μ_t is the subgrid-scale eddy viscosity and S_{ij} is the rate of strain tensor.

- Two common models are:

Smagorinsky SGS model

$$\mu_{t} = \rho L^{2}\sqrt{2S_{ij}S_{ij}}$$

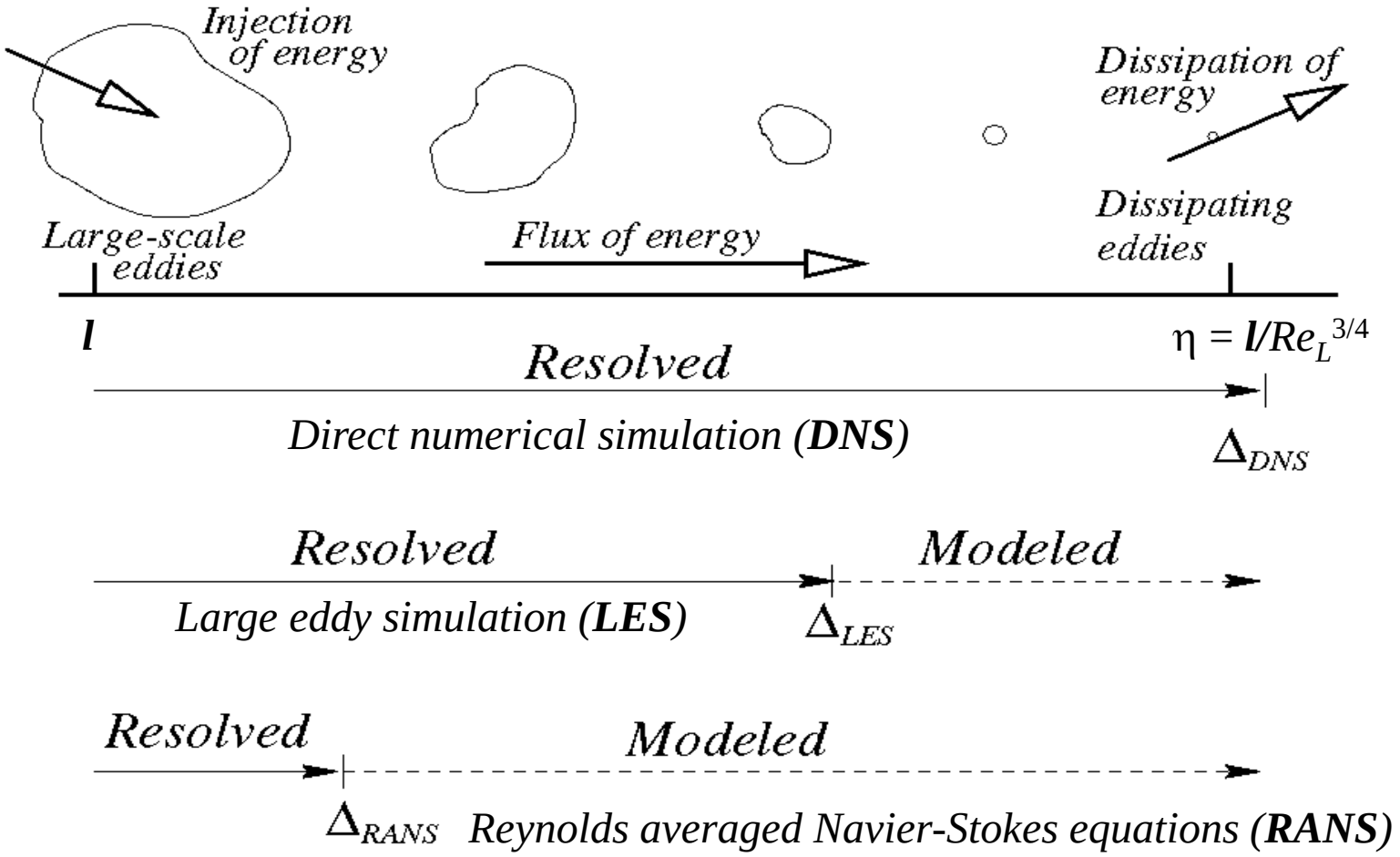
$$L = \min\left(\kappa\,\mathrm{d}, \mathrm{C_s}\,\mathrm{V}^{\frac{1}{3}}\right)$$

RNG SGS model

$$\mu_{t} = \mu\left[1 + \mathrm{H}\left(\frac{\mu_s^{2}\mu_{\mathrm{tot}}}{\mu^{3}} - C\right)\right]^{1/3}$$

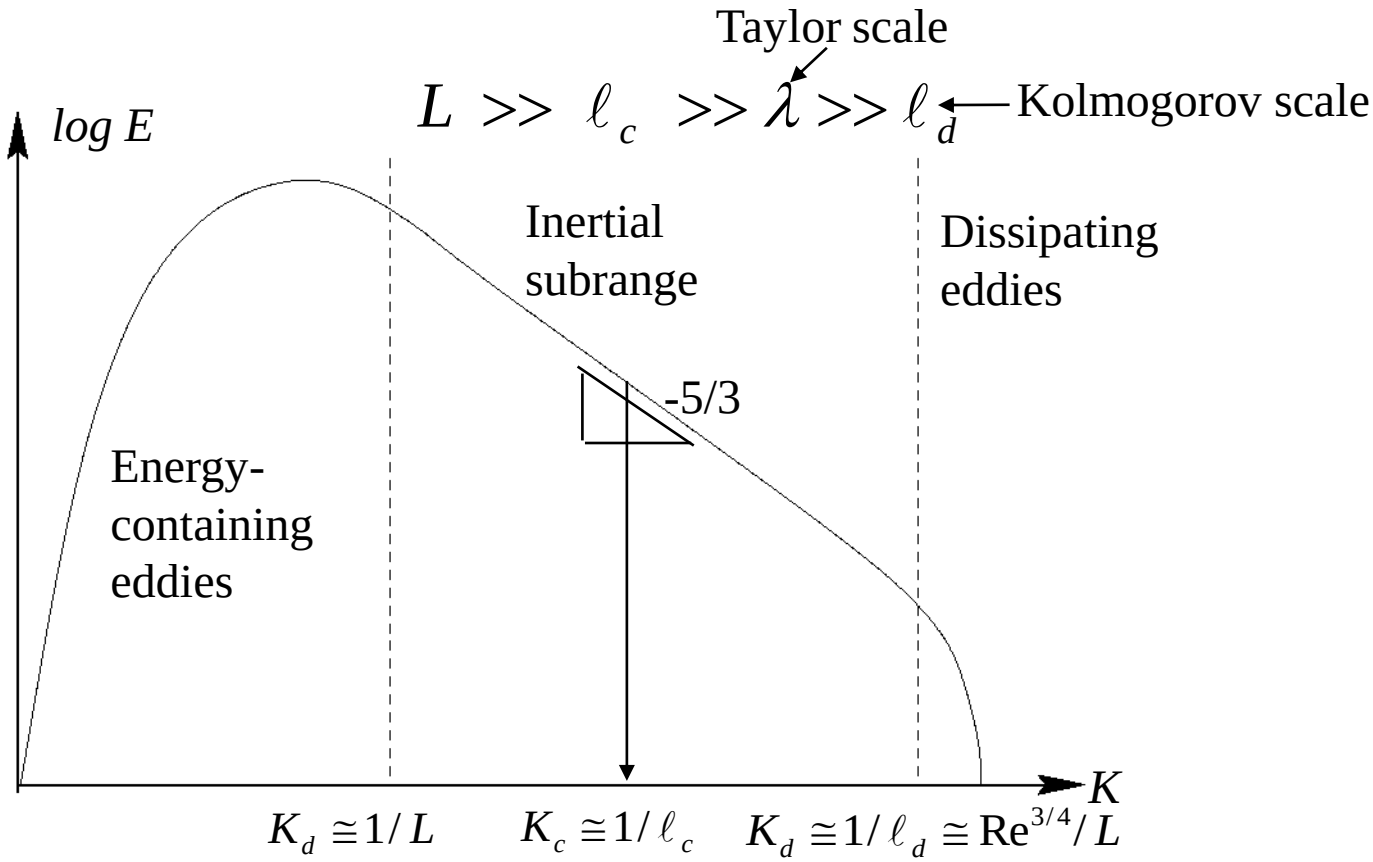
$$\mu_{s} = \left(0.157V^{\frac{1}{3}}\right)^{2}\sqrt{2S_{ij}S_{ij}}$$

Prediction Methods



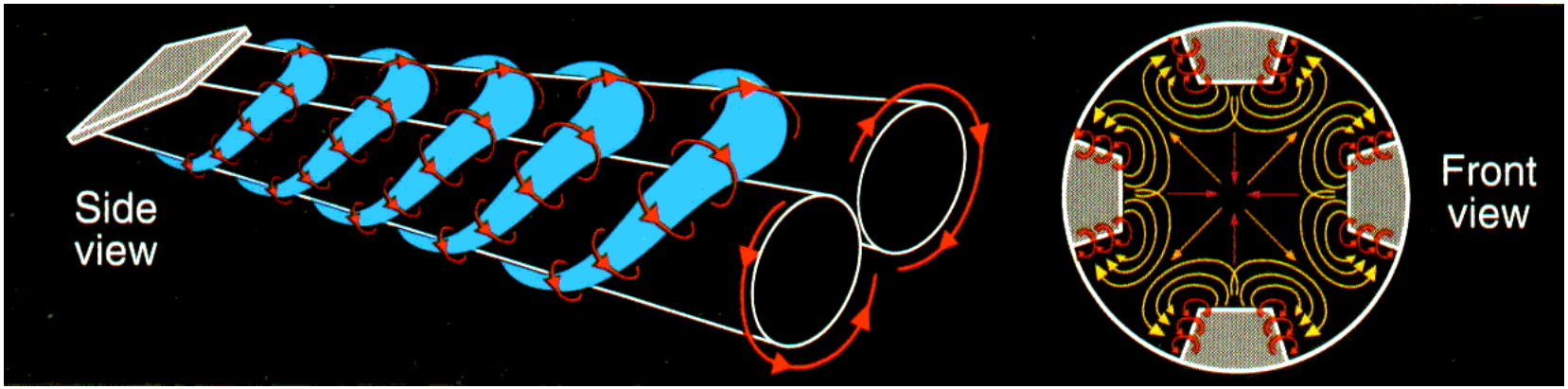
LES - what does it take?

- Requires 3-D transient modeling.
- Requires spatial and temporal resolution of scales in “inertial subrange”.



Example: HEV static mixer

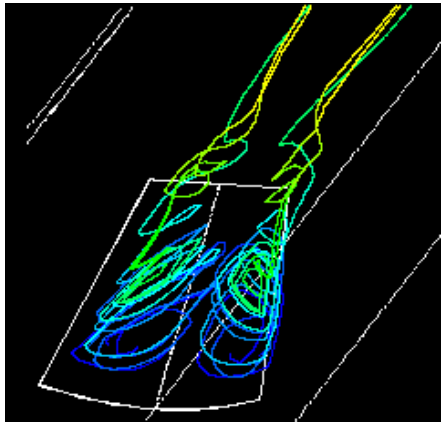
- Circular or square cross-section pipe with sets of tabs mounted on the walls.
- Flow around tabs is unsteady, with counter-rotating longitudinal vortices, and hairpin vortices.



Source: “Kenics Static Mixers” brochure, 1996.

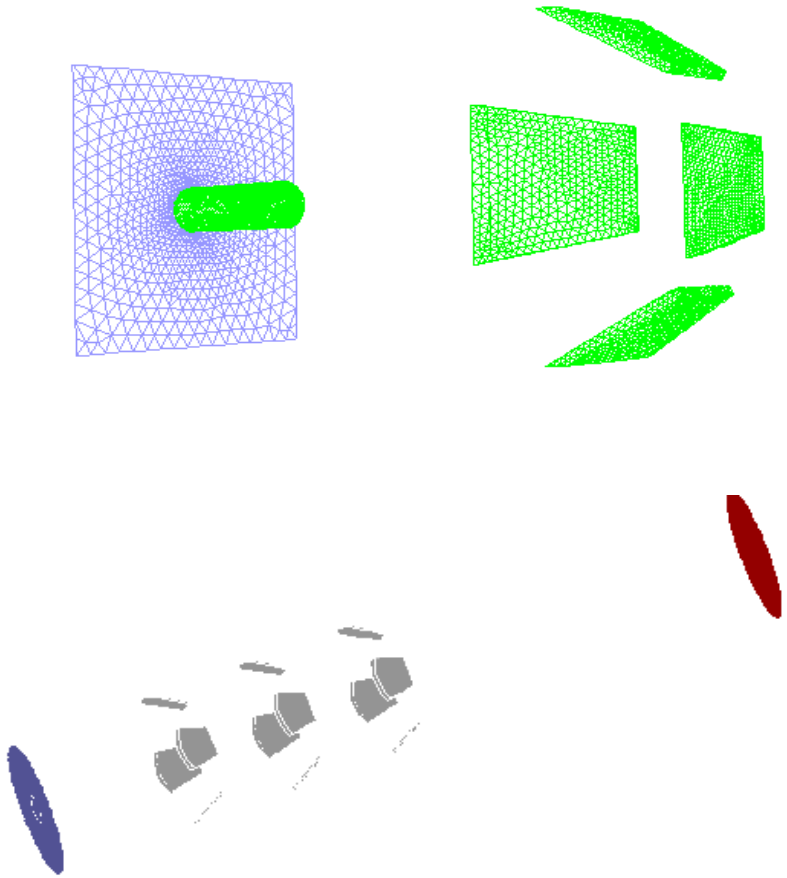
Previous models

- Assumptions:
  - Eight-fold symmetry.
  - Steady state flow with RANS model.
- Results:
  - Longitudinal vortices observed.
- Disadvantages:
  - Hairpin vortices not observed.
  - Under-prediction of mixing near center.
  - No material exchange between areas surrounding tabs.



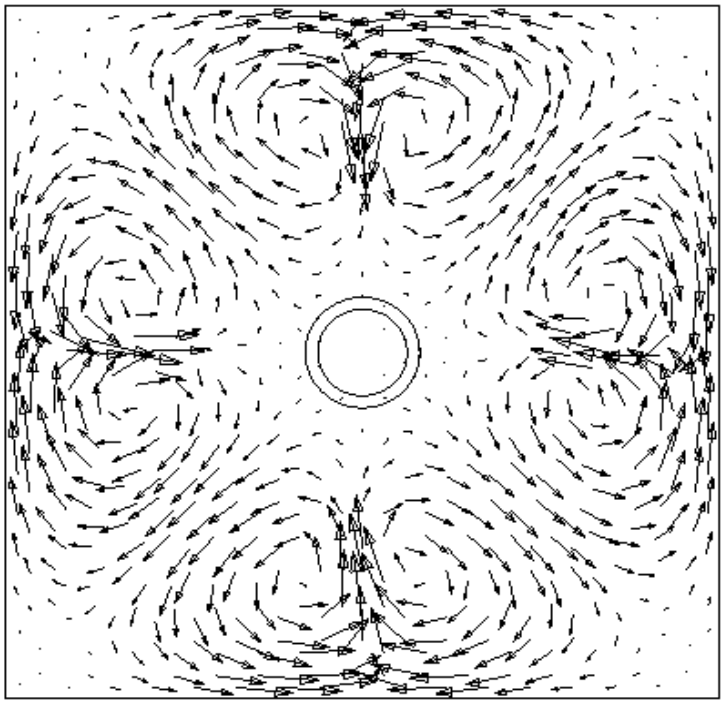
Geometries studied

- Two models studied.
  - Square duct.
    - 0.1x0.1x1 $m^{3.}$
    - Air at 30 m/s.
    - Re ~ 200k.
  - Cylindrical pipe.
    - D = 0.05 m.
    - Water at 0.12 m/s.
    - Re ~ 5000.
- Both models:
  - 500k cells.
  - Unstructured grid.

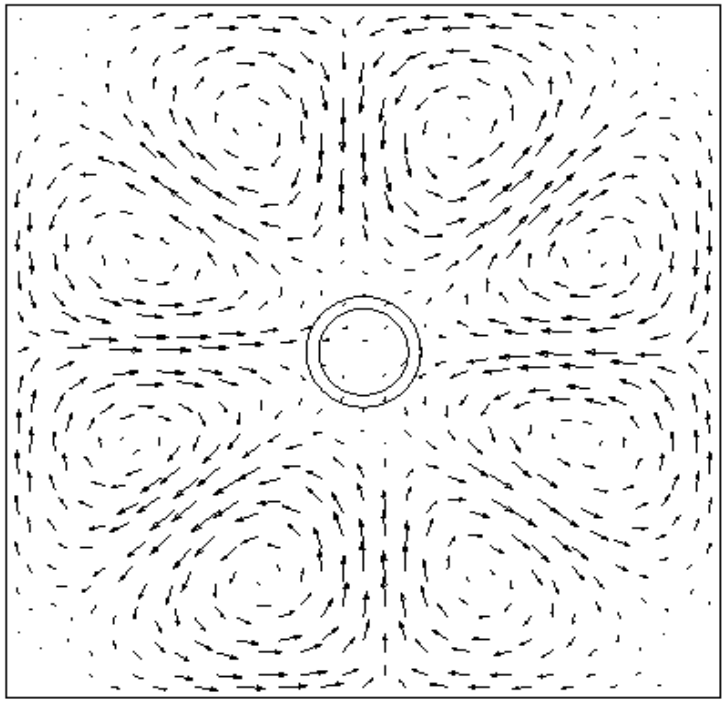


Square duct results: RNG k-ε

When using the RNG k-ε model, the longitudinal vortices are symmetric and stable.

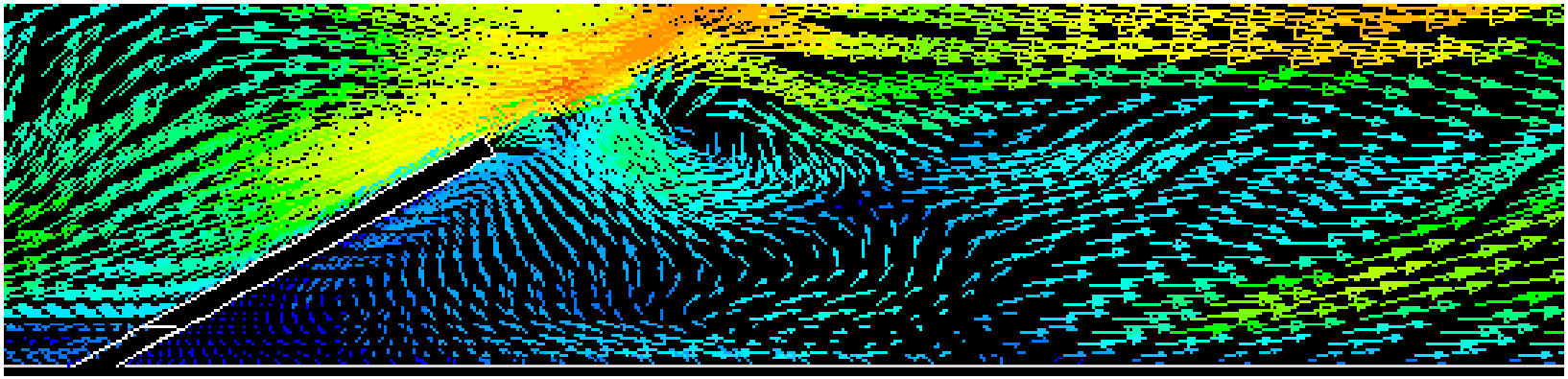


Between 3rd and 4th tabs

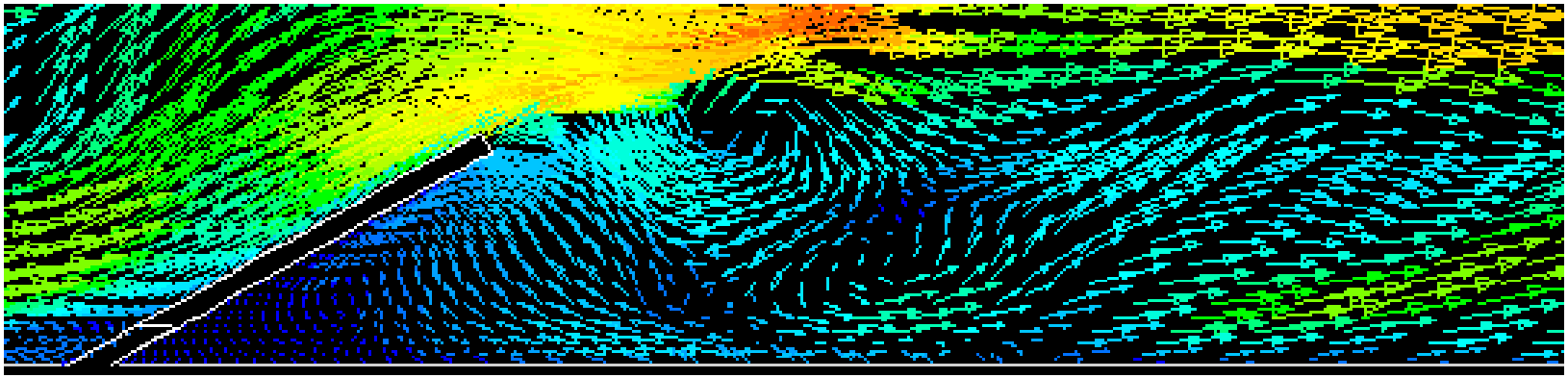


Two widths downstream of last tabs

Cylindrical pipe: LES hairpin vortices - 1



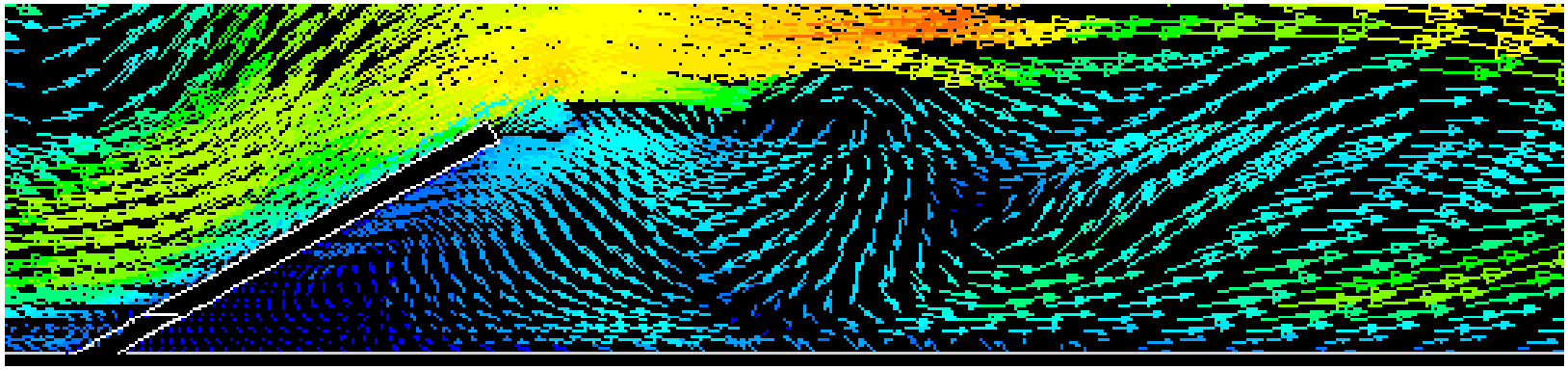
T = 6.40 s



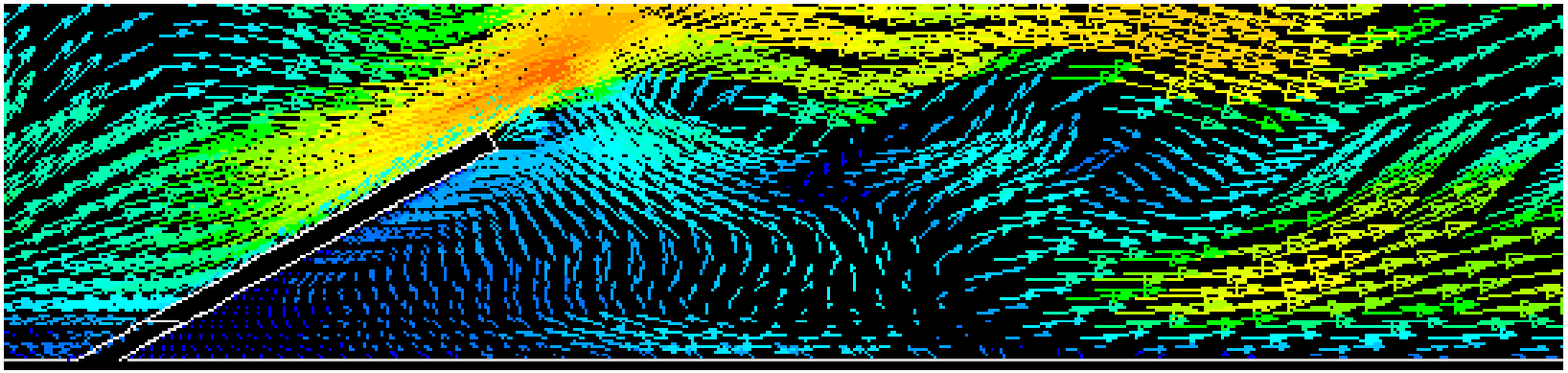
T = 6.43 s

When using the LES model, the vortices are unsteady, similar to what is seen in experiments.

Cylindrical pipe: LES hairpin vortices - 2



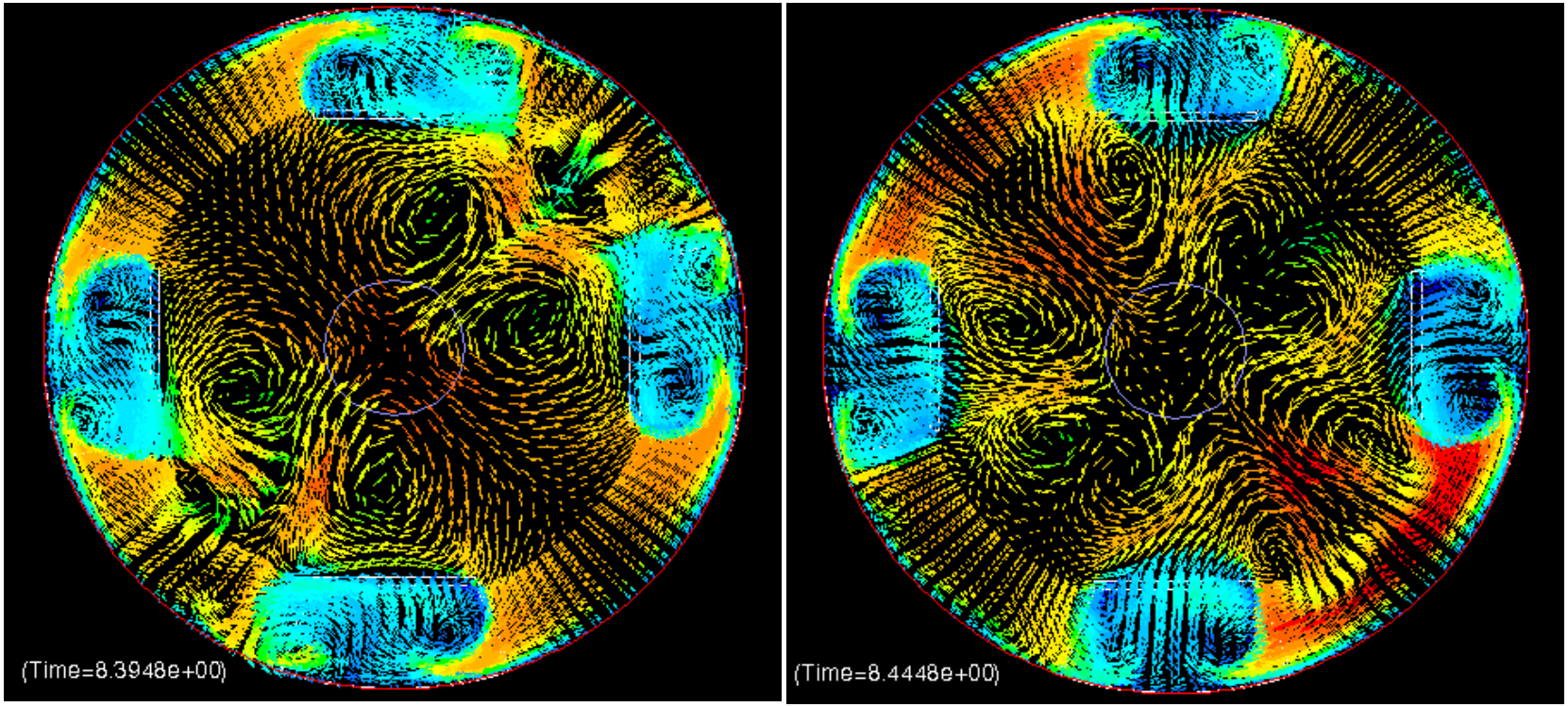
T = 6.46 s



T = 6.53 s

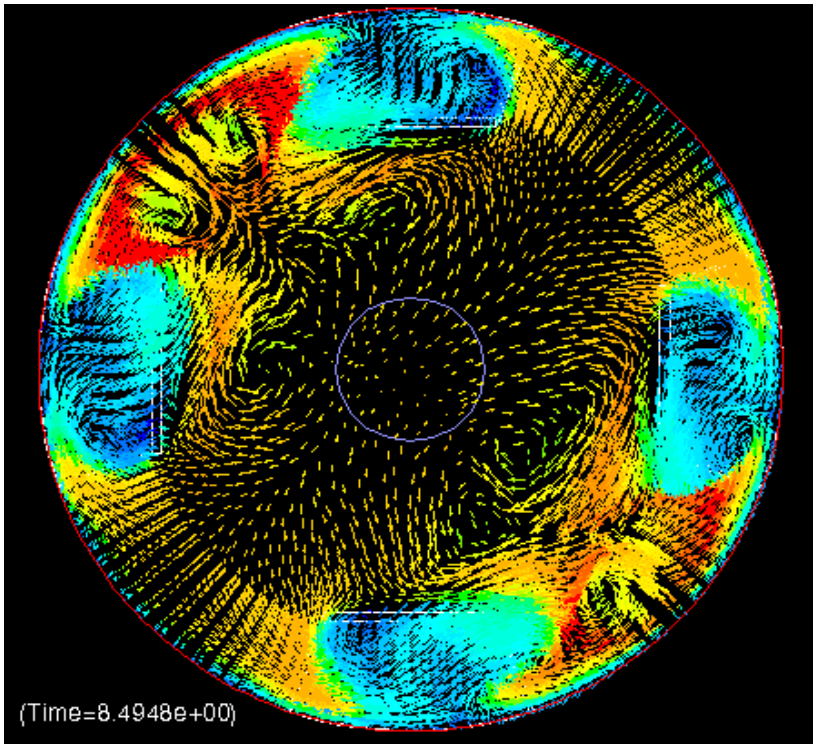
Cylindrical pipe: LES longitudinal vortices - 1

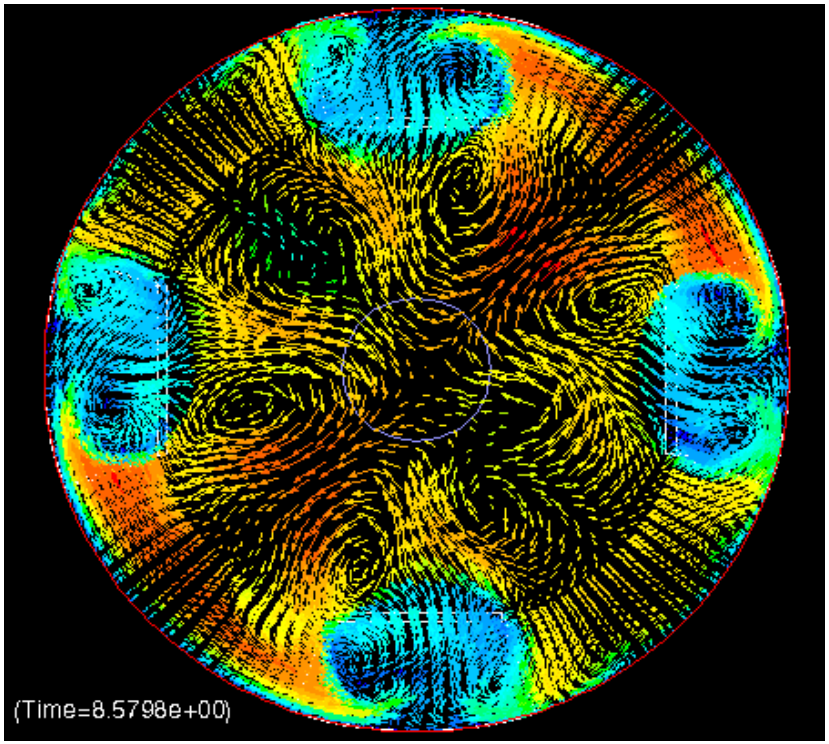
Cylindrical. At tip of last set of tabs.



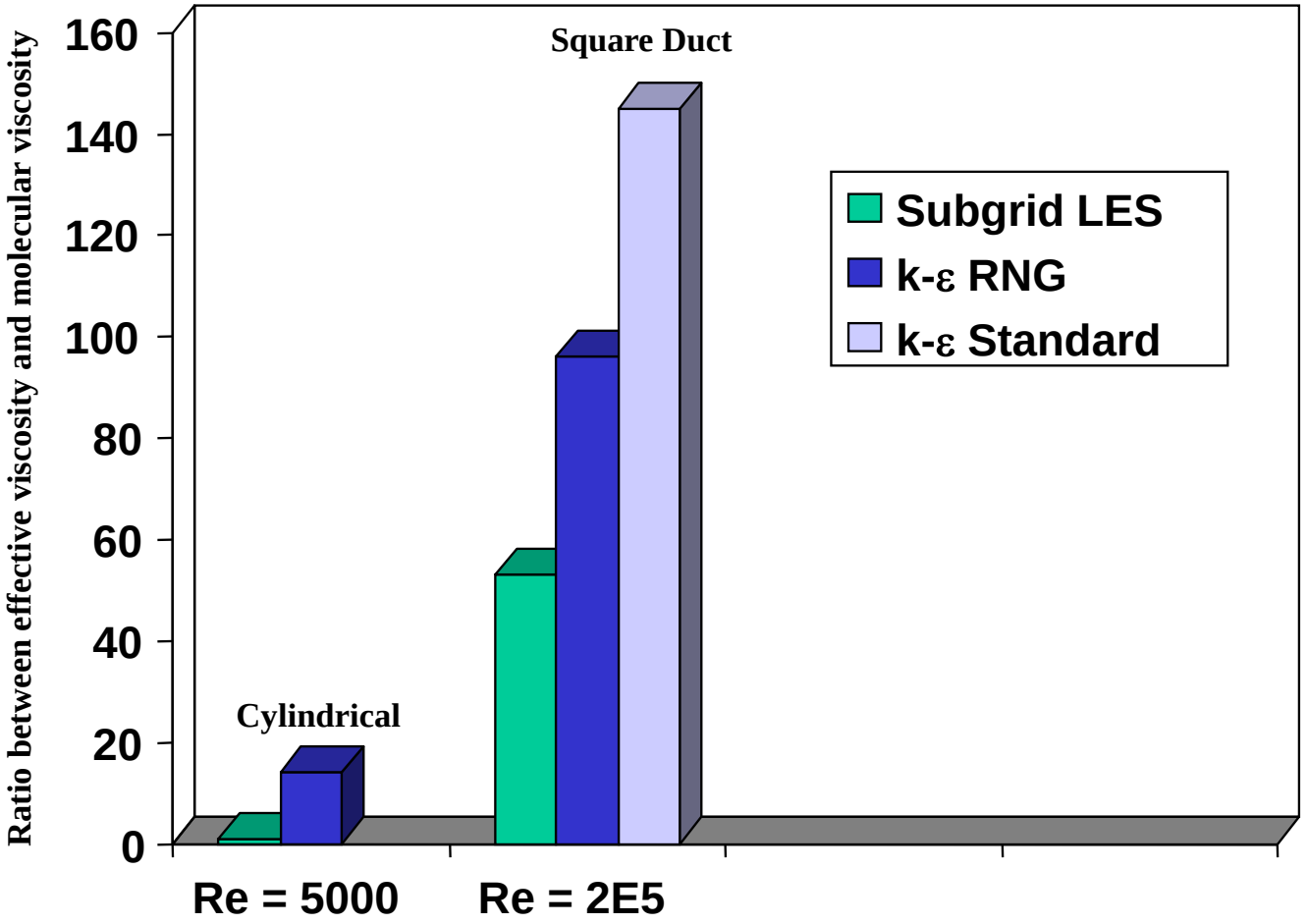
Cylindrical pipe: LES longitudinal vortices - 2

Cylindrical. At tip of last set of tabs.





Effective viscosity comparison

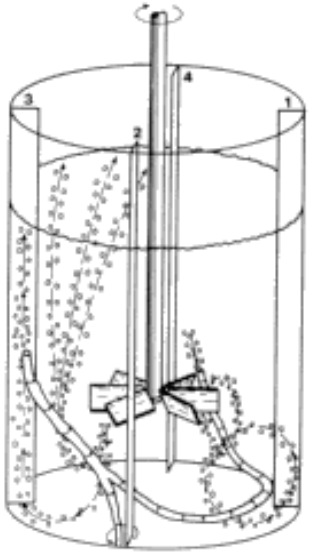


The effective viscosity is lower with the LES model than with the *k*-ε models, allowing the vortices in the simulation to become unsteady.

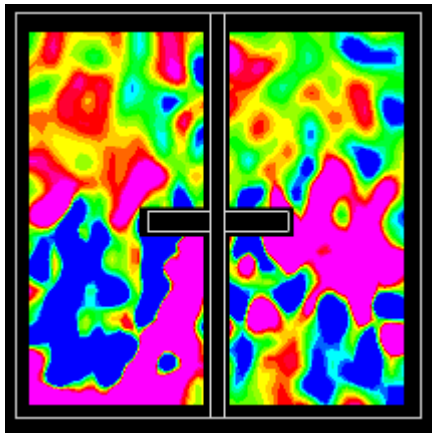
HEV mixer conclusion

- LES predicts unsteady vortex system including transient hairpin vortices, as also seen in experiments.
- Interaction between vortices causes material exchange between tabs, and between the center and tabs.

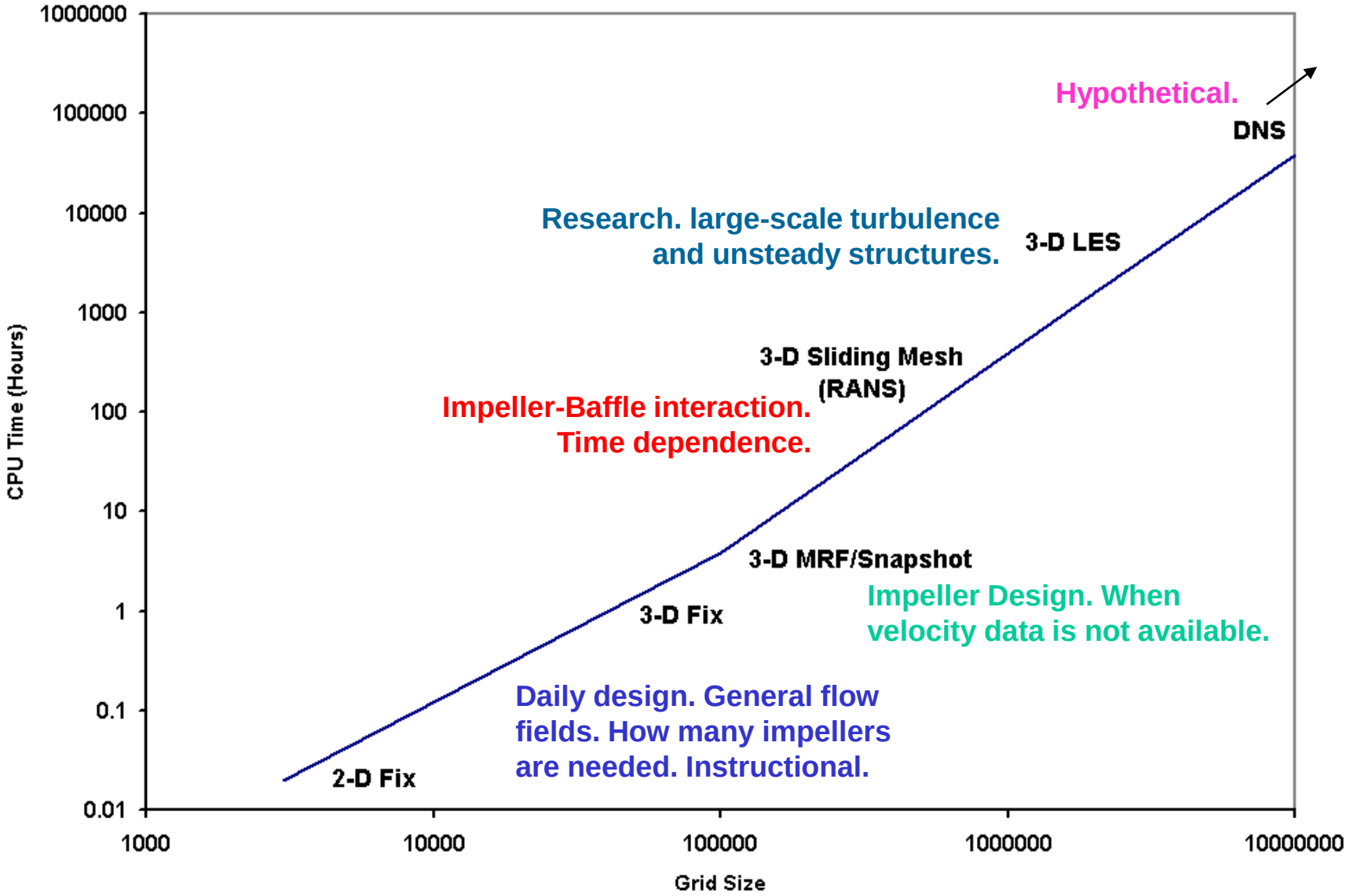
Example: mixing tank flow instabilities



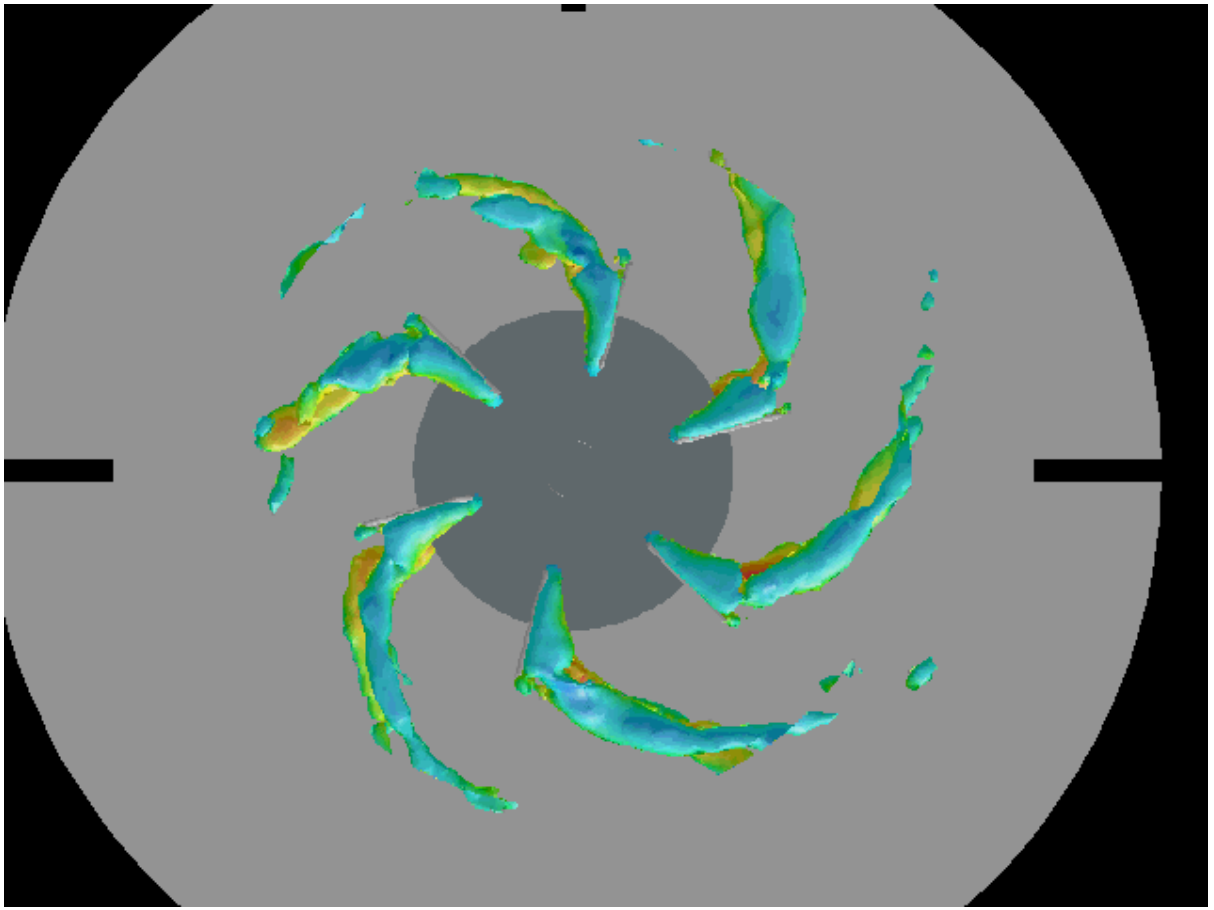
- Experimental work suggests that large-scale, time-dependent structures, with periods much longer than the time of an impeller revolution, are involved in many of the fundamental hydrodynamic processes in stirred vessels.
- Local velocity data histograms may be bi-modal or tri-modal.
- The gas holdup distribution may be asymmetric and oscillating.
- In solids suspension processes, solids can be swept from one side of the vessel to the other in a relatively slow oscillating pattern, even in dilute suspensions.
- Digital particle image velocimetry experiments have shown large-scale asymmetries with periods up to several minutes.



Mixing tank modeling options



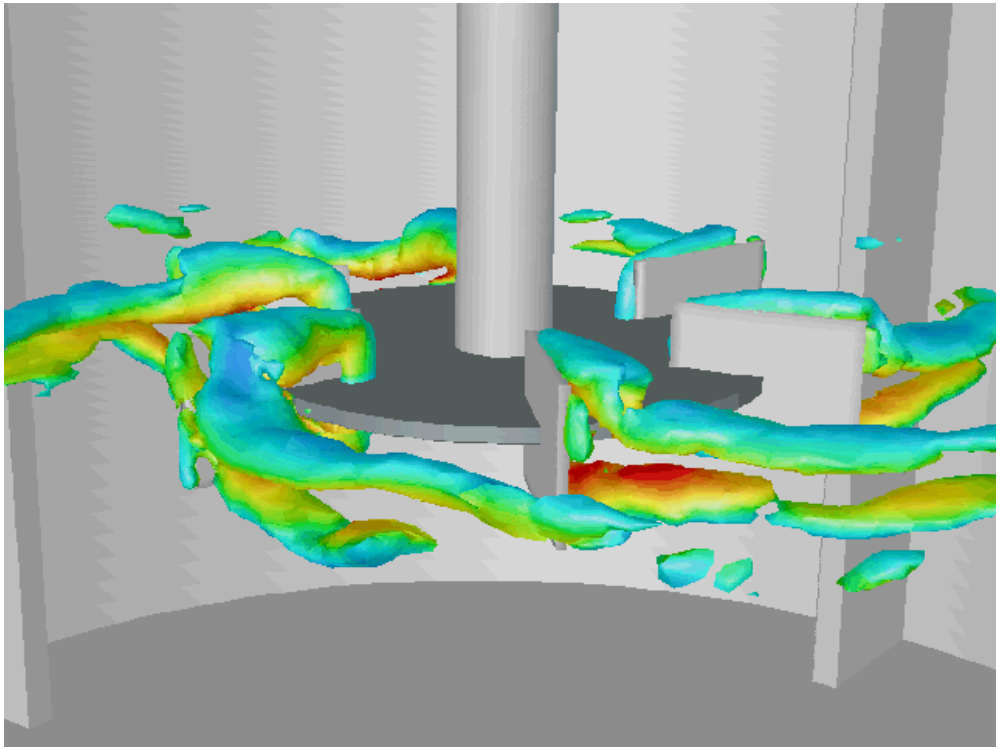
Rushton turbine - trailing vortices (LES)



Iso-Surface of Vorticity Magnitude (550 s^{-1})

Colored by velocity magnitude

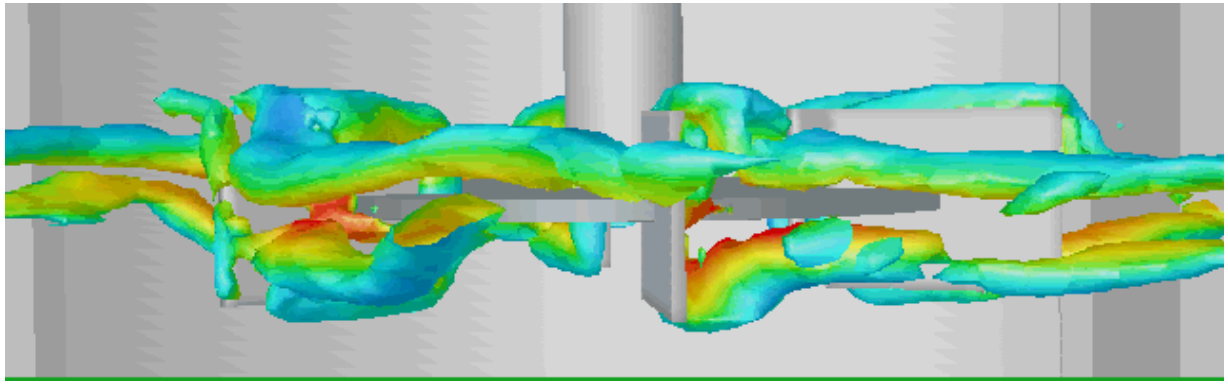
Rushton turbine - trailing vortices (LES)



Iso-Surface of Vorticity Magnitude (550 s^{-1})

Colored by velocity magnitude

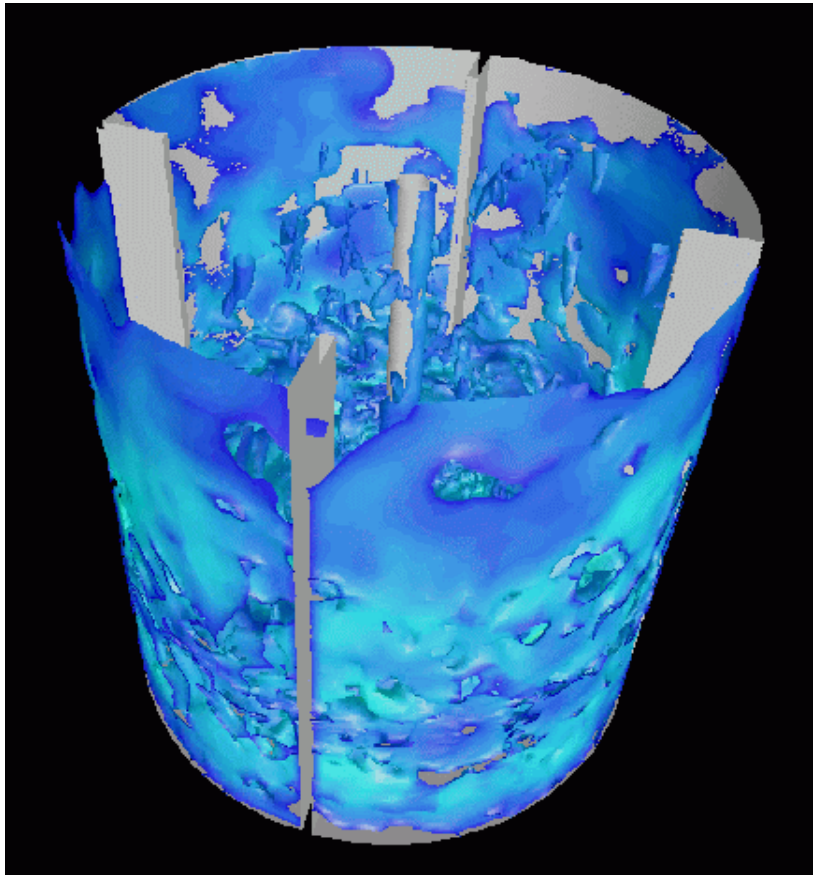
Rushton turbine - trailing vortices (LES)



Iso-Surface of Vorticity Magnitude (550 s^{-1})

Colored by velocity magnitude

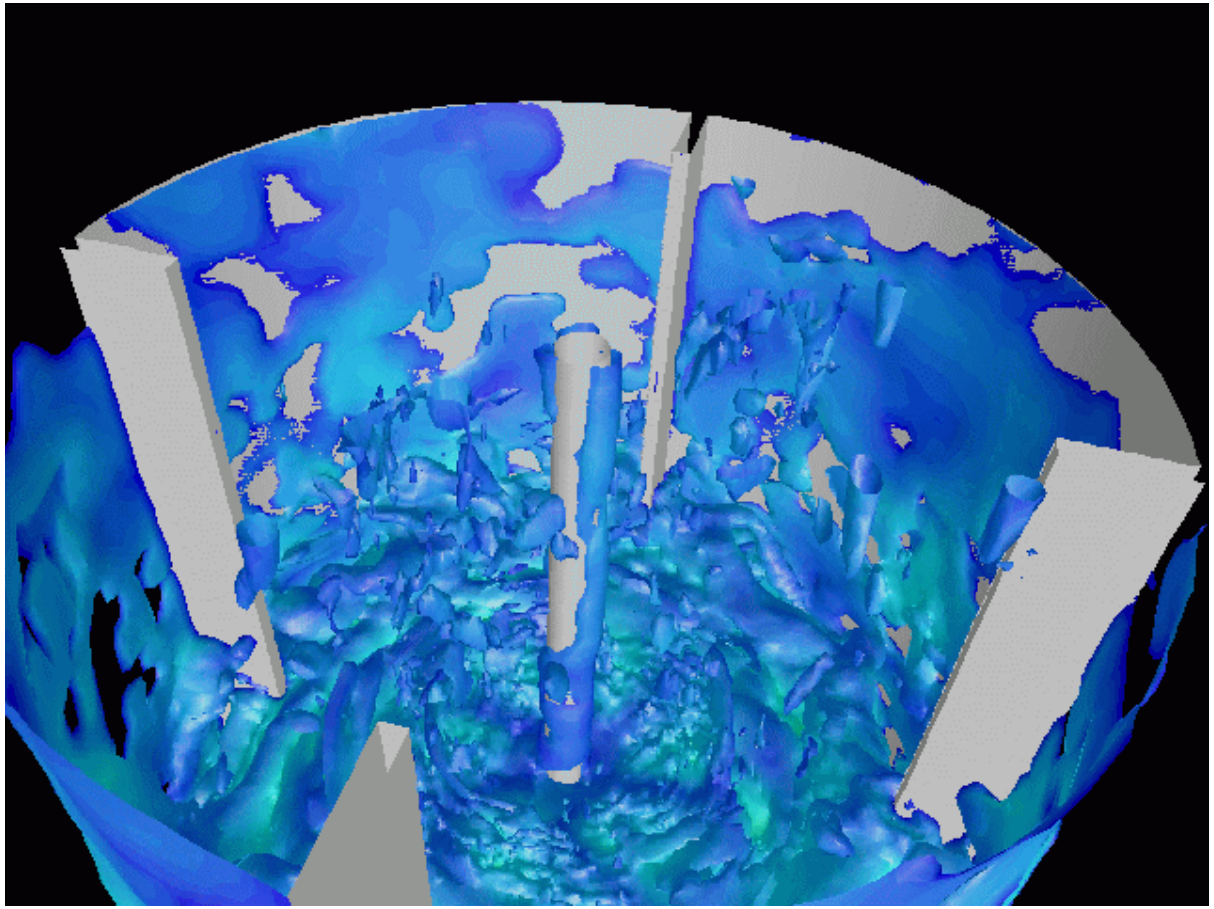
Rushton turbine - vorticity (LES)



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

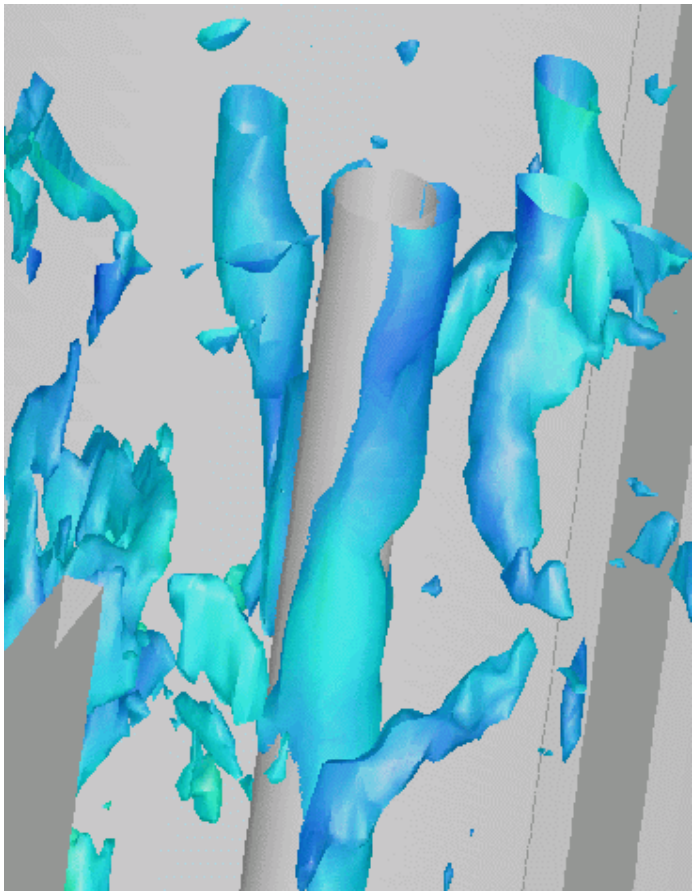
Rushton turbine - vorticity (LES)



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

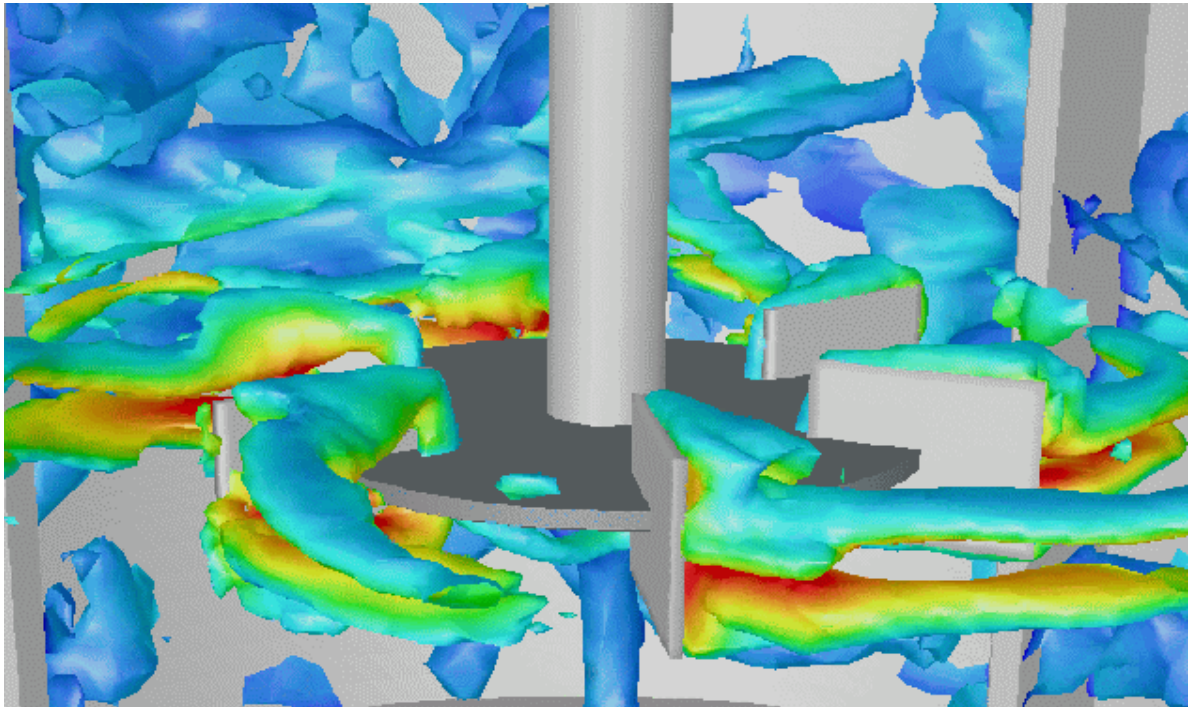
Rushton turbine - vortices at surface (LES)



Iso-Surface of Vorticity Magnitude (80 s^{-1})

Colored by velocity magnitude

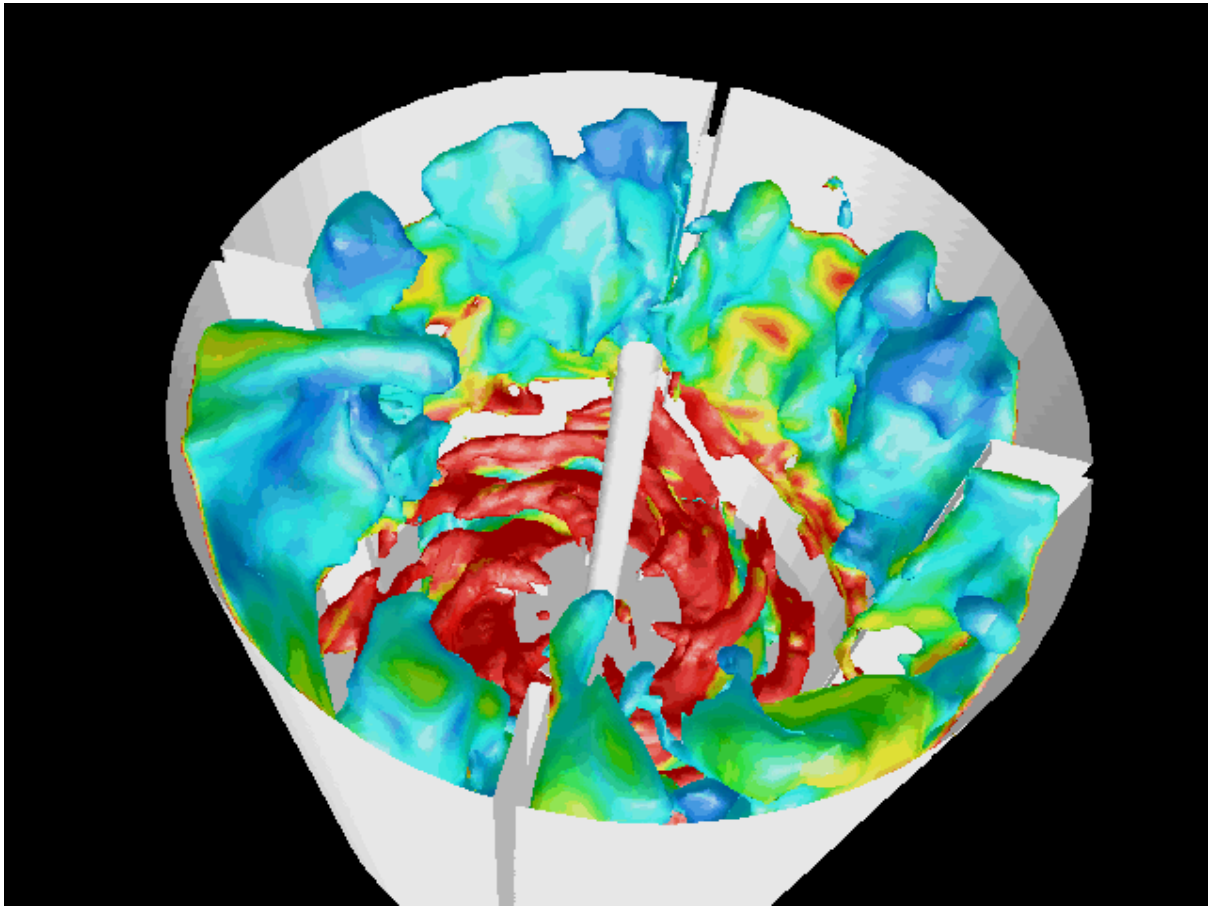
Rushton turbine - trailing vortices (LES)



Iso-Surface of Vorticity Magnitude (550 and 80 s^{-1})

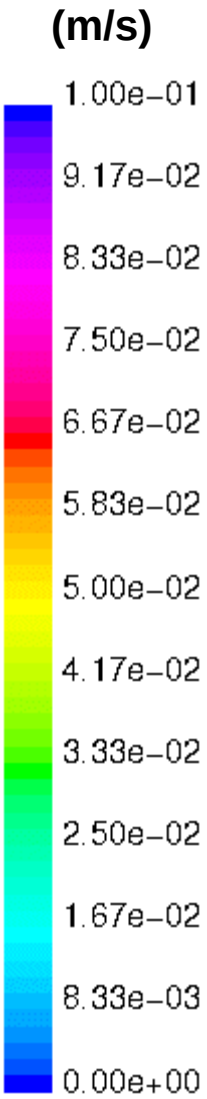
Colored by velocity magnitude

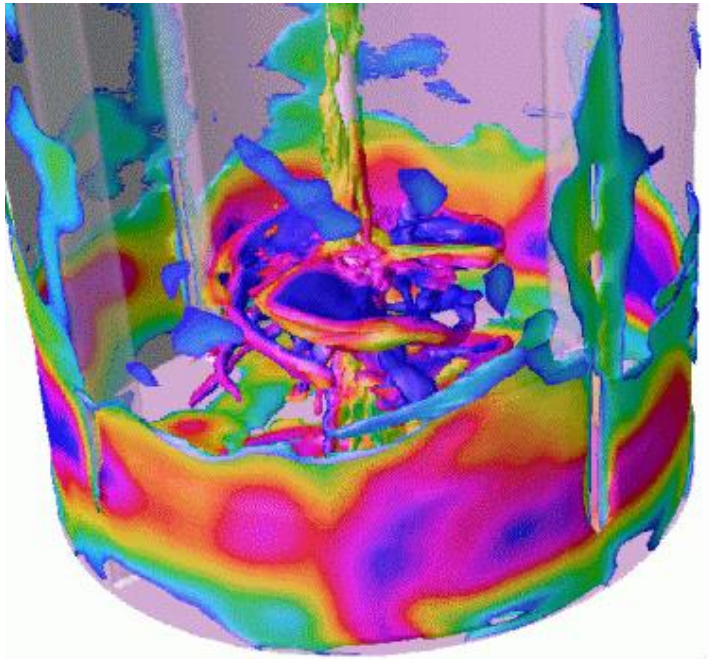
Rushton turbine - axial velocity (LES)



Iso-surface of axial velocity of 0.1m/s. The velocity is directed upwards in the regions enclosed by the iso-surface. The surface is colored by strain rate on a scale of 0 to 100 1/s.

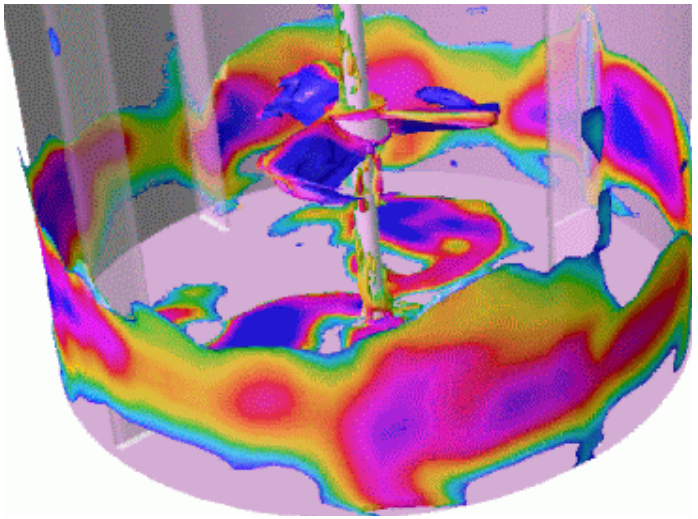
Velocity on vorticity iso-surfaces (LES)





Iso-Surface of Vorticity Magnitude (15 s^{-1})

15.5 revs.

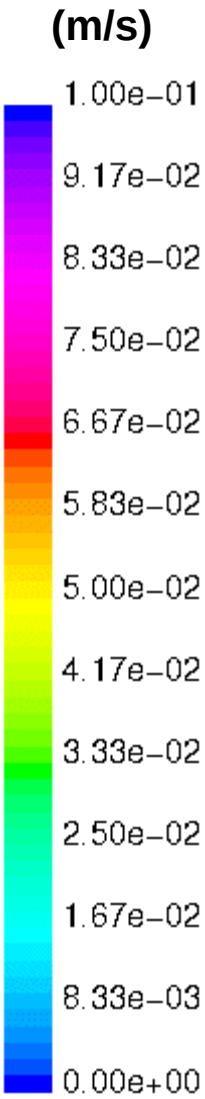


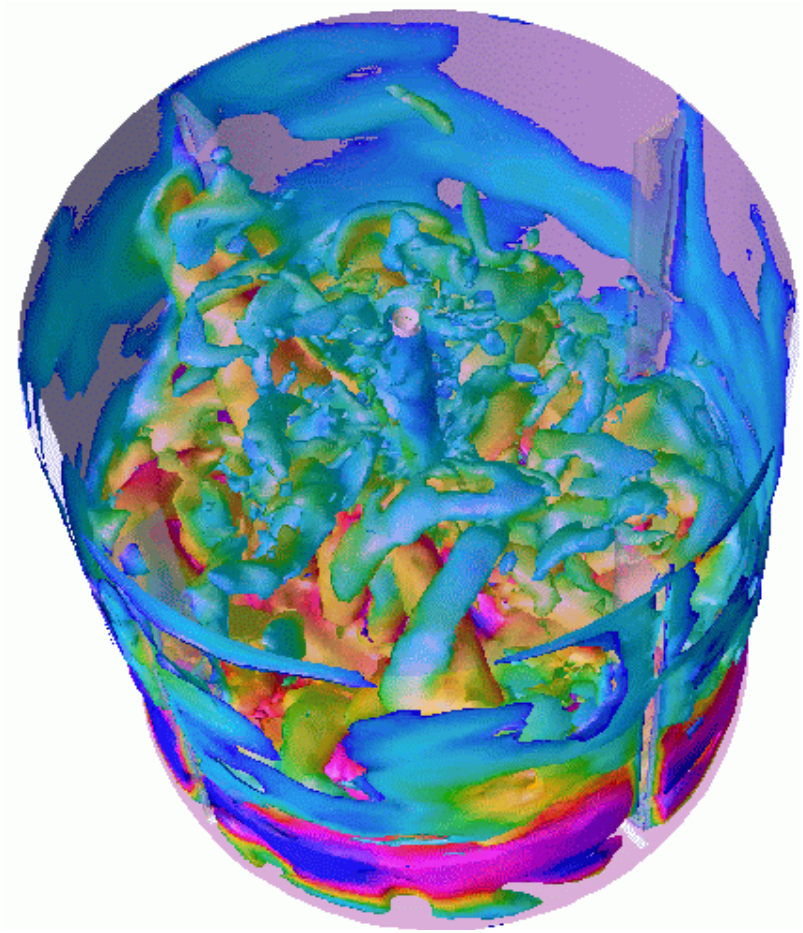
Iso-Surface of Vorticity Magnitude (30 s^{-1})

Vorticity is: $\nabla x V$

Shear rate is: ∇V

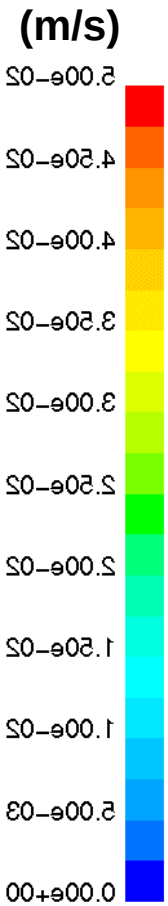
Velocity on vorticity iso-surfaces (LES)

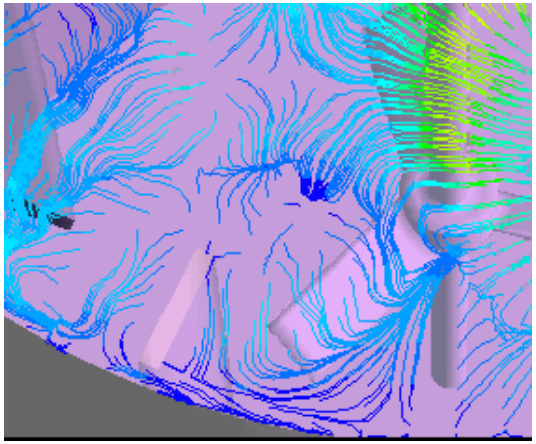




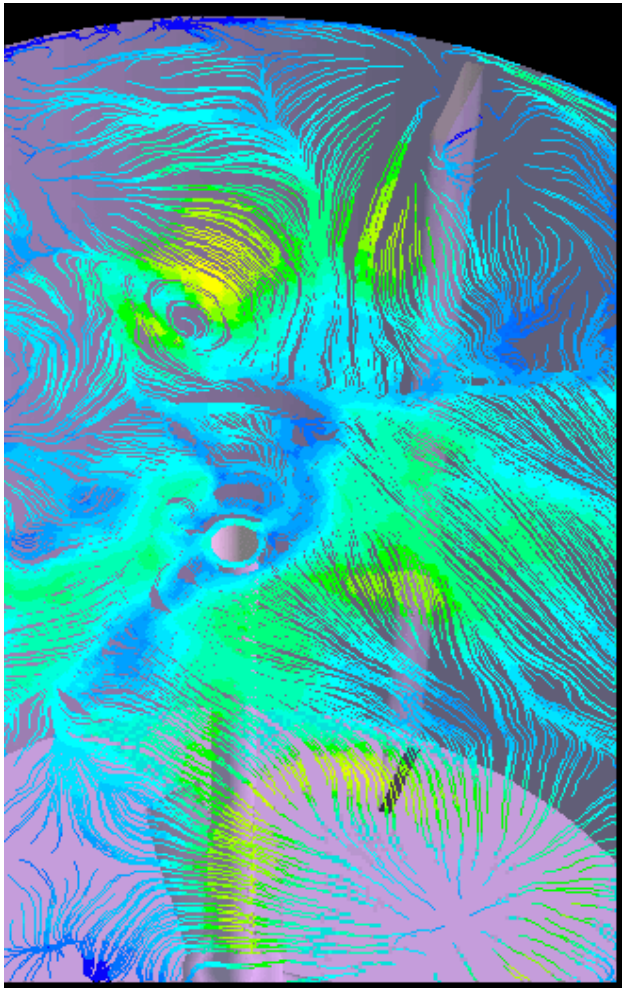
Iso-Surface of Vorticity Magnitude (5 s^{-1})
3.9 revs.

Flow at the surface (LES)



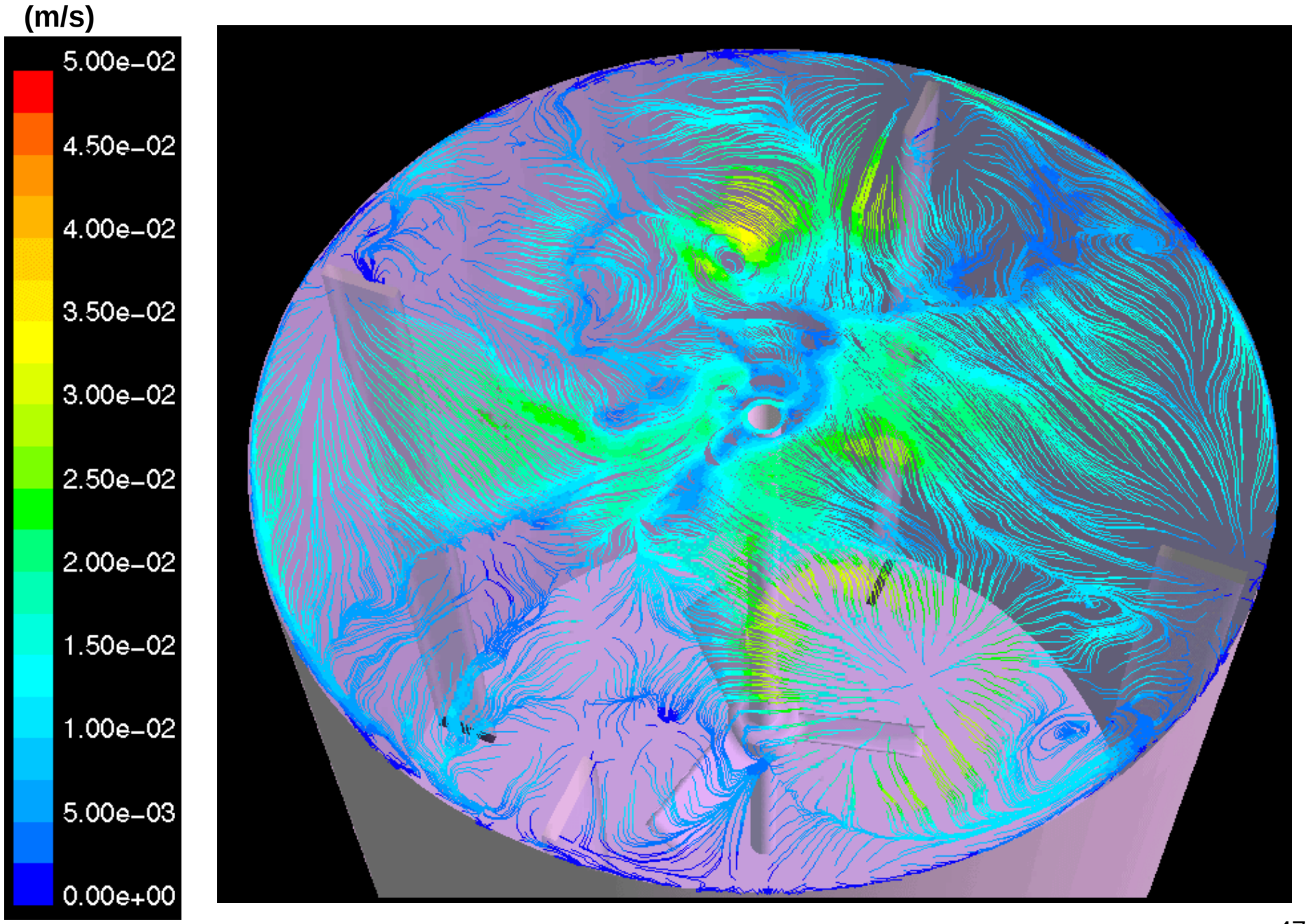


HE-3 “oilflow” lines at liquid surface (8.8 revolutions)

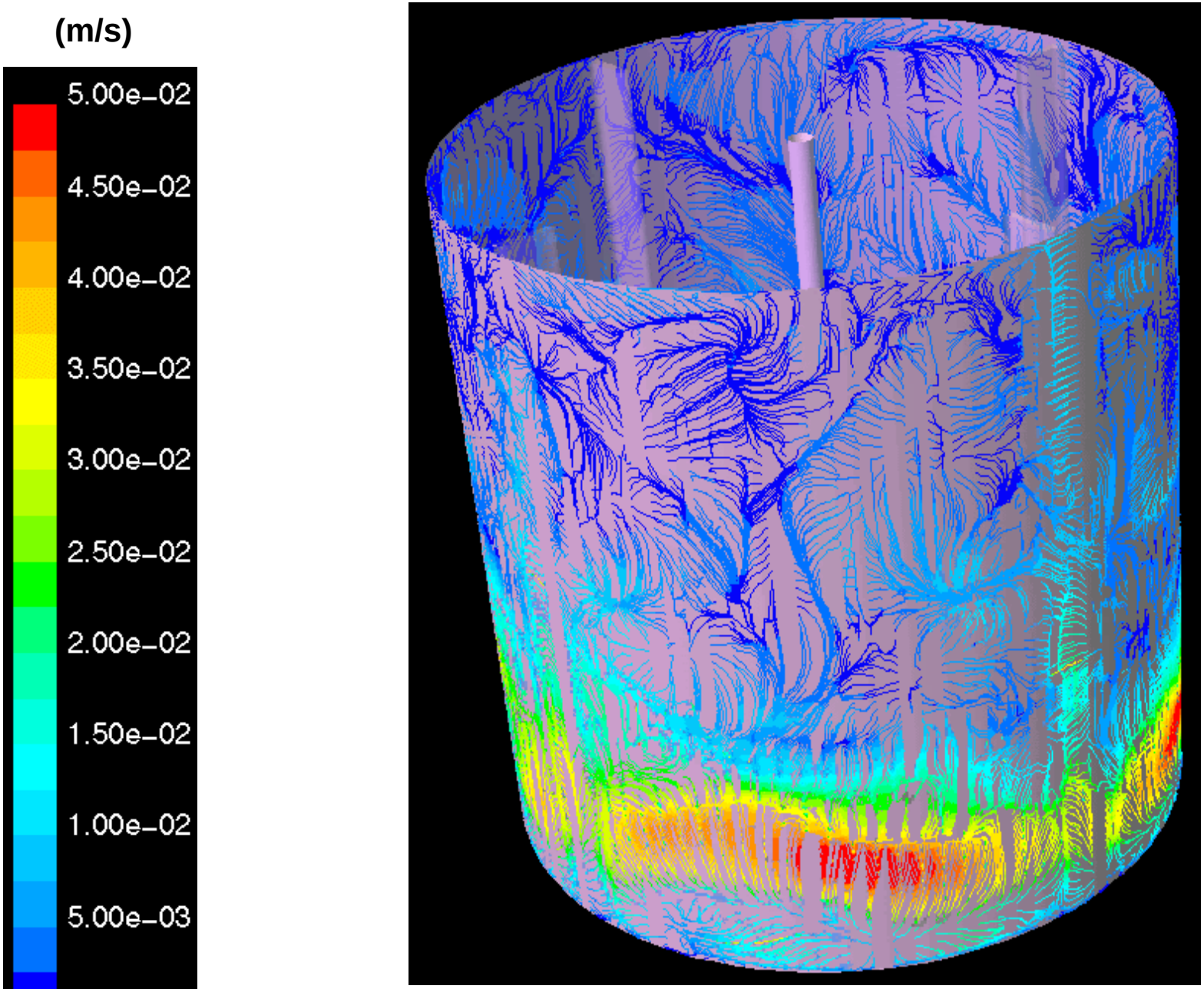


“Oilflow” lines are pathlines constrained to the surface from which they are released.

HE-3 “oilflow” lines at liquid surface (12.3 revolutions) (LES)



HE-3 “oilflow” at vessel wall (18 revolutions) (LES)



Summary mixing tanks

- LES is a transient turbulence model that falls midway between RANS and DNS models.
- The differences between predicted mixing patterns with RANS and LES are clear.
- The predicted flow patterns for the HE-3 and PBT compared well with digital particle image velocimetry data reported in the literature and exhibited the long-time scale instabilities seen in the experiments.
- The results of these studies open the way to a renewed interpretation of many previously unexplained hydrodynamic phenomena that are observed in stirred vessels.
- However, 2-D fix, 3-D fix, and MRF models are much faster computationally and still have their place, especially in design.

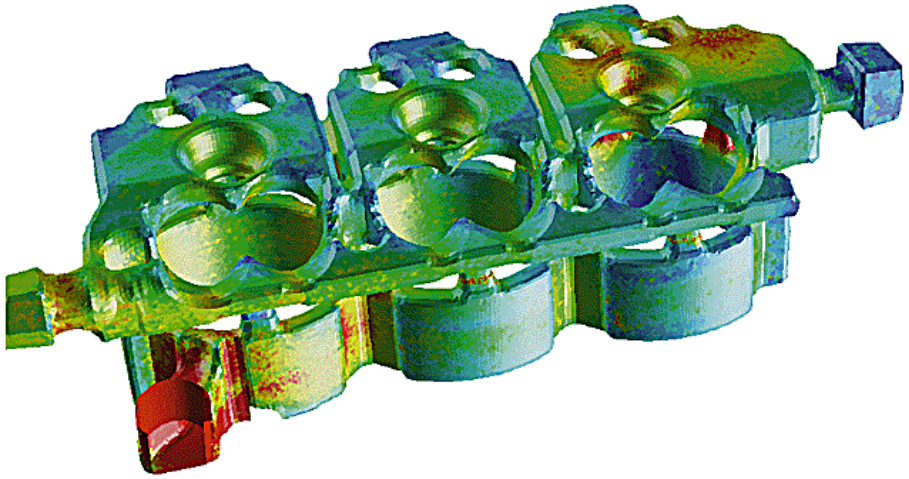
Lecture 13 - Heat Transfer

Applied Computational Fluid Dynamics

André Bakker

Introduction

- Typical design problems involve the determination of:
  - Overall heat transfer coefficient, e.g., for a car radiator.
  - Highest (or lowest) temperature in a system, e.g., in a gas turbine, chemical reaction vessels, food ovens.
  - Temperature distribution (related to thermal stress), e.g., in the walls of a spacecraft.
  - Temperature response in time dependent heating/cooling problems, e.g., engine cooling, or how fast does a car heat up in the sun and how is it affected by the shape of the windshield?



Overview dimensionless numbers

- Nusselt number: $Nu = hL/k_f$. Ratio between total heat transfer in a convection dominated system and the estimated conductive heat transfer.
- Grashof number: $Gr = L^3 g\Delta\rho / \nu^2 \rho_w$. Ratio between buoyancy forces and viscous forces.
- Prandtl number: $Pr = \mu c_p / k$. Ratio between momentum diffusivity and thermal diffusivity. Typical values are Pr = 0.01 for liquid metals; Pr = 0.7 for most gases; Pr = 6 for water at room temperature.
- Rayleigh number: $Ra = Gr\,Pr = L^3 \rho^2 g\beta c_p \Delta T / \mu k = L^3 \rho g \beta \Delta T / \mu\alpha$

  The Rayleigh number governs natural convection phenomena.
- Reynolds number: $Re = \rho UL / \mu$. Ratio between inertial and viscous forces.

Enthalpy equation

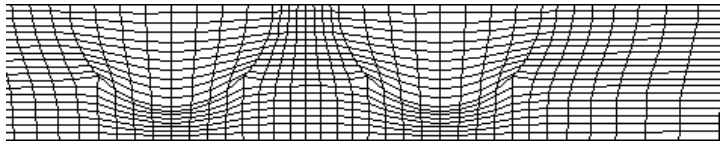
- In CFD it is common to solve the enthalpy equation, subject to a wide range of thermal boundary conditions.
  - Energy sources due to chemical reaction are included for reacting flows.
  - Energy sources due to species diffusion are included for multiple species flows.
  - The energy source due to viscous heating describes thermal energy created by viscous shear in the flow. This is important when the shear stress in the fluid is large (e.g., lubrication) and/or in high-velocity, compressible flows. Often, however, it is negligible.
  - In solid regions, a simple conduction equation is usually solved, although convective terms can also be included for moving solids.

Modes of heat transfer

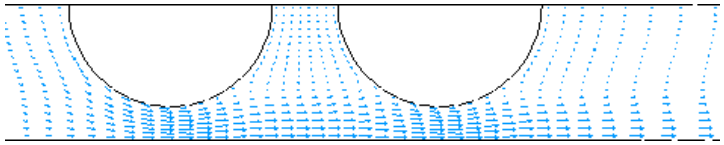
- Conduction: diffusion of heat due to temperature gradients. A measure of the amount of conduction for a given gradient is the heat conductivity.
- Convection: when heat is carried away by moving fluid. The flow can either be caused by external influences, forced convection; or by buoyancy forces, natural convection. Convective heat transfer is tightly coupled to the fluid flow solution.
- Radiation: transfer of energy by electromagnetic waves between surfaces with different temperatures, separated by a medium that is at least partially transparent to the (infrared) radiation. Radiation is especially important at high temperatures, e.g., during combustion processes, but can also have a measurable effect at room temperatures.

Conjugate heat transfer

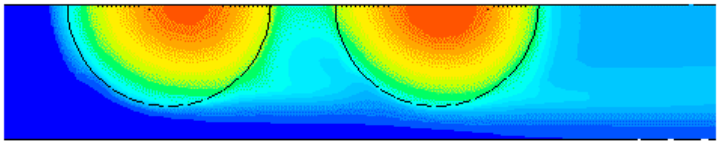
- “Conjugate heat transfer” refers to the ability to compute conduction of heat through solids, coupled with convective heat transfer in a fluid.
- Coupled boundary conditions are available for wall zones that separate two cell zones.
- Either the solid zone or the fluid zone, or both, may contain heat sources.
- The example here shows the temperature profile for coolant flowing over fuel rods that generate heat.



Grid



Velocity vectors



Temperature contours

Example: Cooling flow over fuel rods

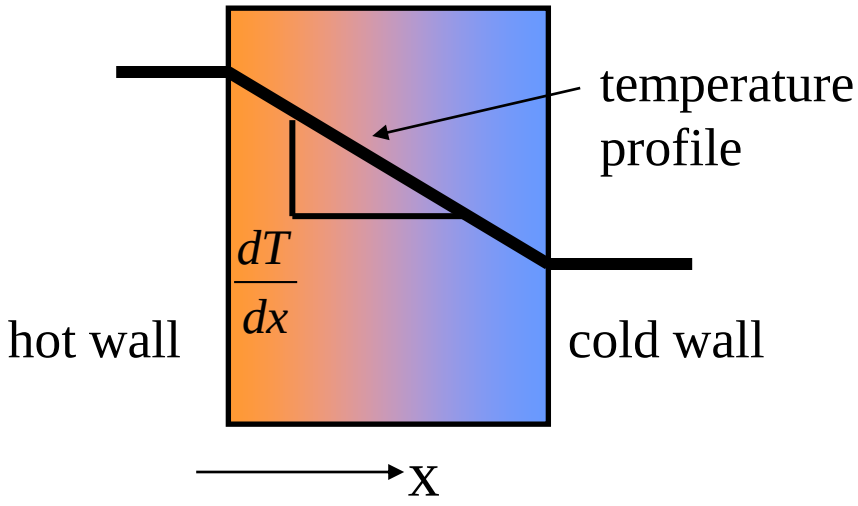
Heat conduction - Fourier's law

- The heat flux is proportional to the temperature gradient:

$$\frac{Q}{A} = q = -k\nabla T$$

where *k(x,y,z,T)* is the thermal conductivity.

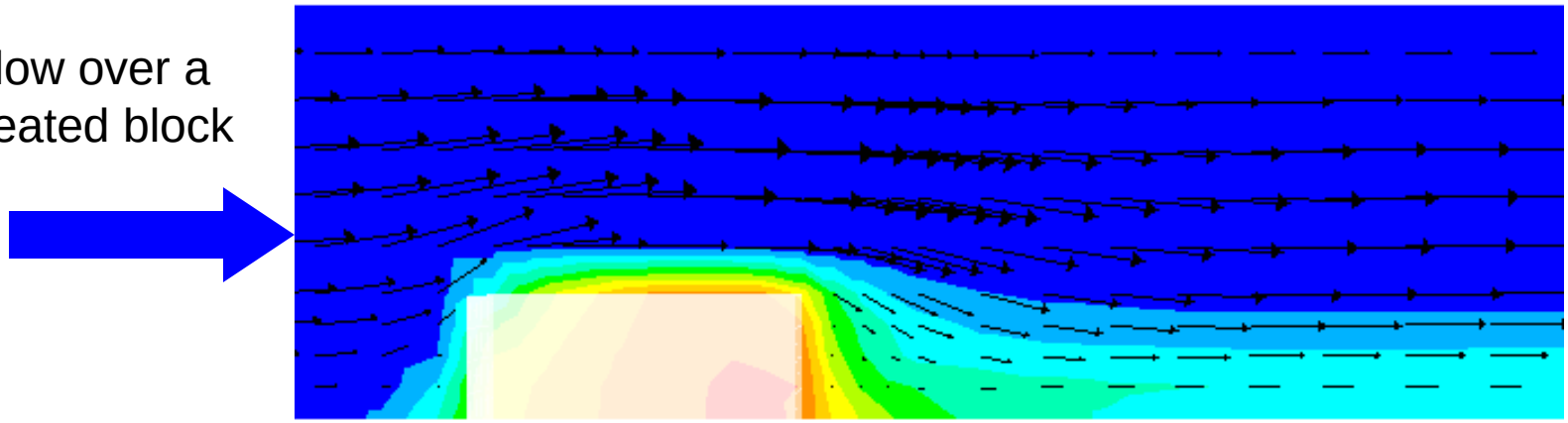
- In most practical situations, conduction, convection, and radiation appear in combination. Also, for convection, the heat transfer coefficient is important, because a flow can only carry heat away from a wall when that wall is conducting.



Convection heat transfer

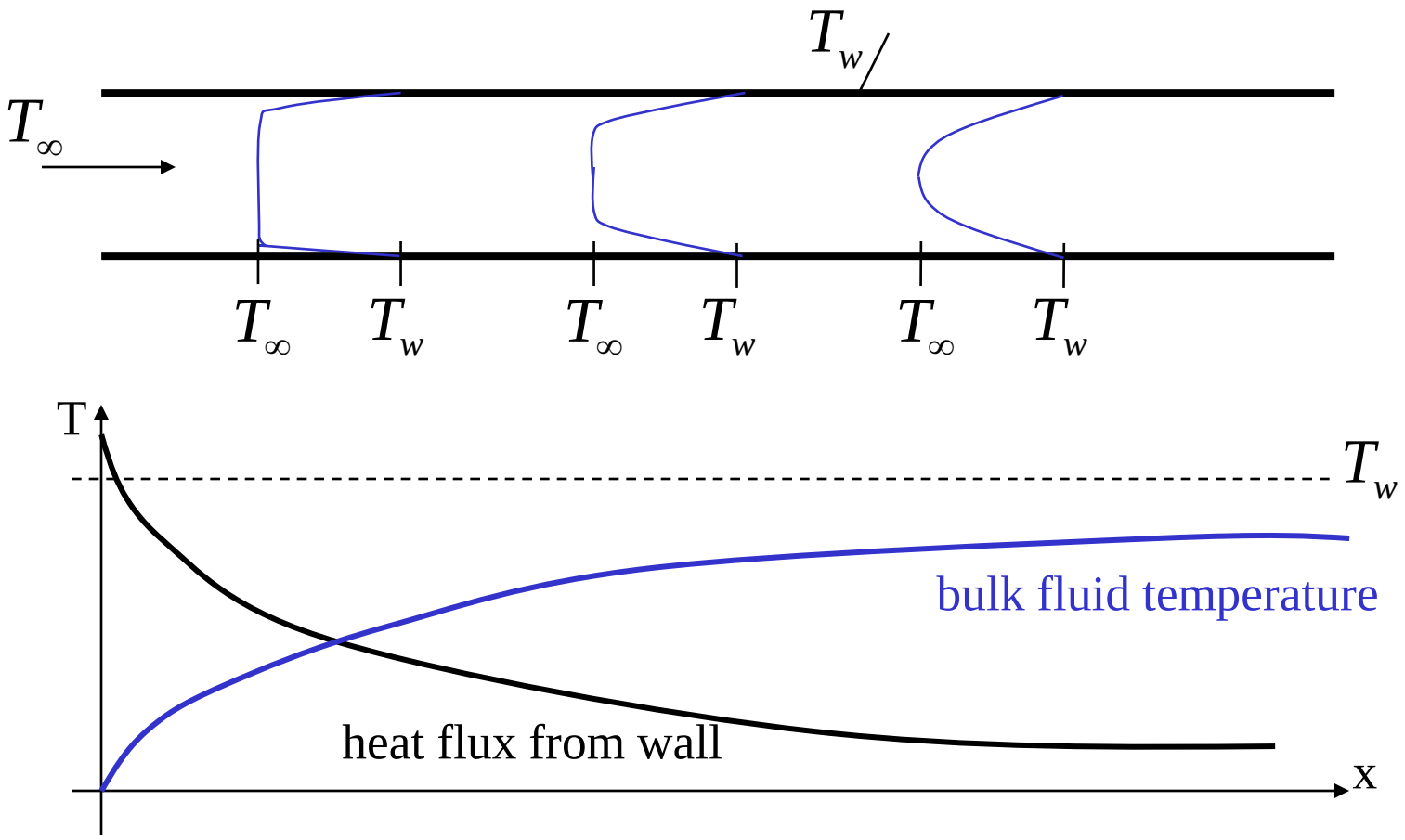
- Convection is movement of heat with a fluid.
- E.g., when cold air sweeps past a warm body, it draws away warm air near the body and replaces it with cold air.

Flow over a heated block



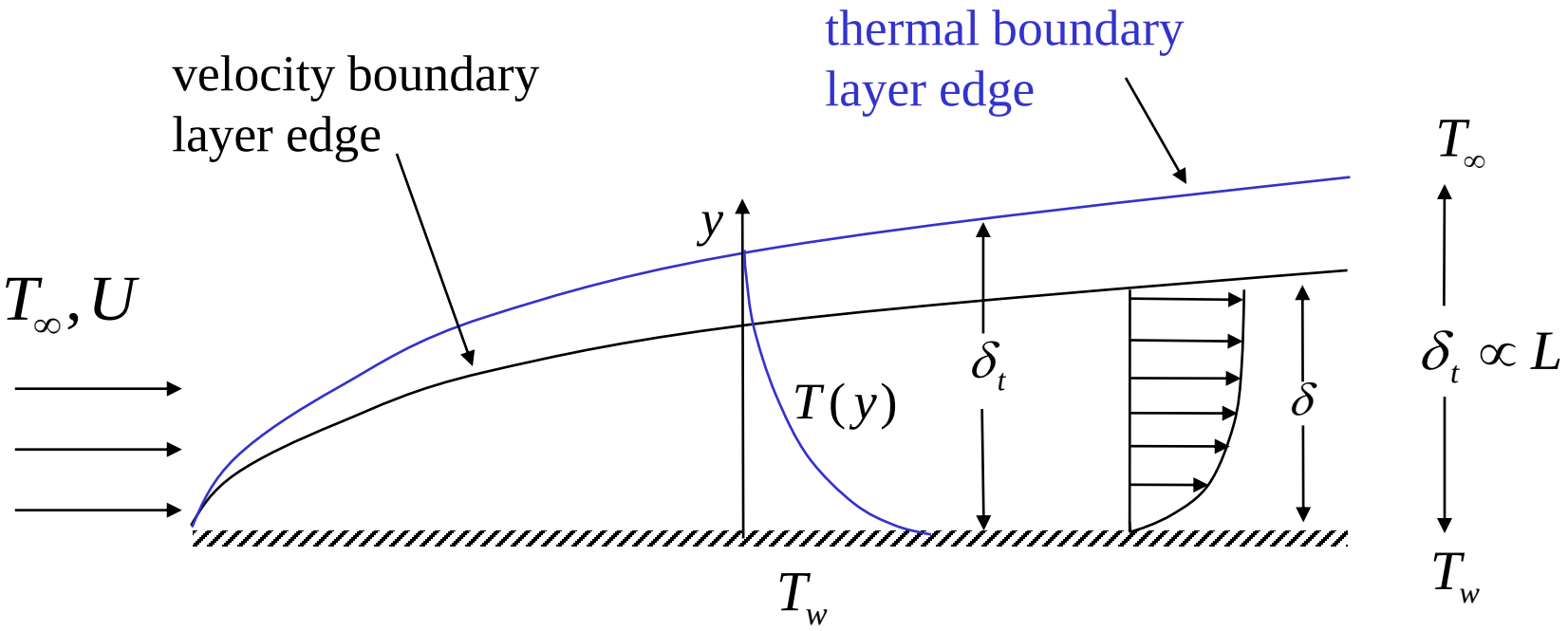
Forced convection example

- Developing flow in a pipe (constant wall temperature).



Thermal boundary layer

- Just as there is a viscous boundary layer in the velocity distribution, there is also a thermal boundary layer.
- Thermal boundary layer thickness is different from the thickness of the (momentum) viscous sublayer, and fluid dependent. The thickness of the thermal sublayer for a high-Prandtl-number fluid (e.g., water) is much less than the momentum sublayer thickness. For fluids of low Prandtl numbers (e.g., liquid metal), it is much larger than the momentum sublayer thickness.

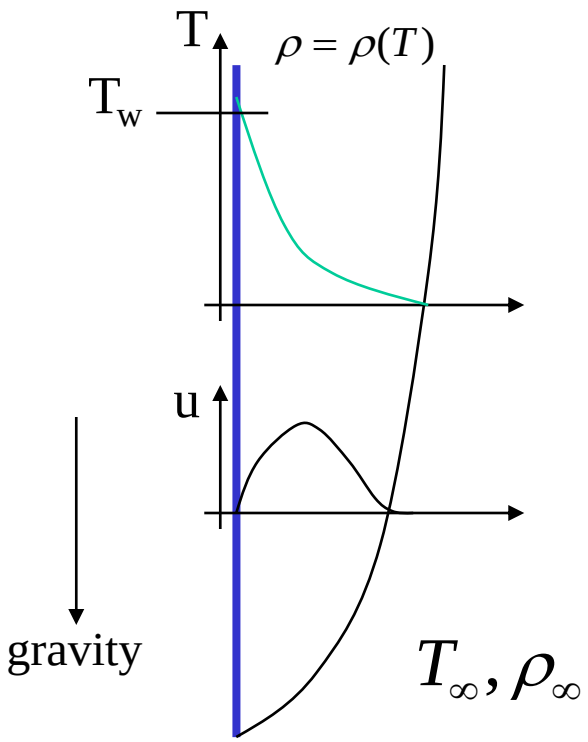


Natural convection

- Natural convection (from a heated vertical plate).
- As the fluid is warmed by the plate, its density decreases and a buoyant force arises which induces flow in the vertical direction. The force is proportional to $(\rho - \rho_\infty)g$.
- The dimensionless group that governs natural convection is the Rayleigh number:

$$Ra = Gr.Pr = \frac{g\beta\Delta TL^3}{\alpha\upsilon}$$

- Typically: $Nu \propto Ra^x \quad \frac{1}{4} < x < \frac{1}{3}$



Natural convection around a person

- Light weight warm air tends to move upward when surrounded by cooler air.
- Thus, warm-blooded animals are surrounded by thermal plumes of rising warm air.
- This plume is made visible by means of a Schlieren optical system that is based on the fact that the refraction of light through a gas is dependent on the density of the gas.
- Although the velocity of the rising air is relatively small, the Reynolds number for this flow is on the order of 3000.

Image: Homsy et al. [2]

Natural convection - Boussinesq model

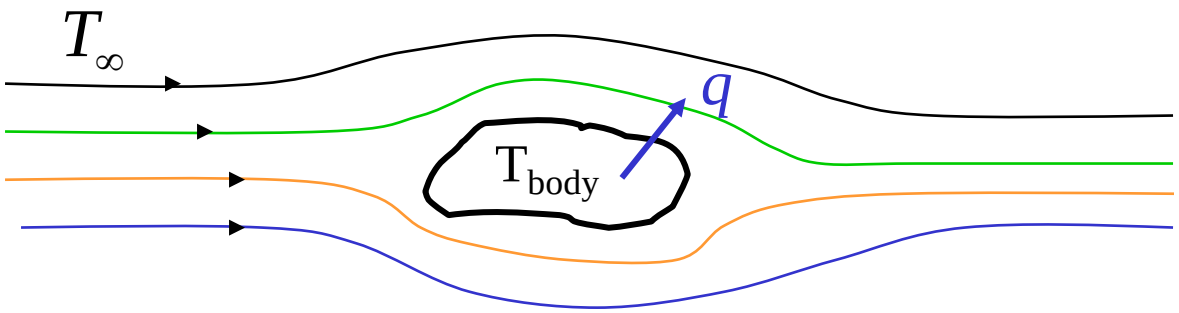
- Makes simplifying assumption that density is uniform.
  - Except for the body force term in the momentum equation, which is replaced by:

$$(\rho - \rho_0)g = -\rho_0 \beta (T - T_0)g$$

  - Valid when density variations are small (i.e., small variations in *T*).
- Provides faster convergence for many natural-convection flows than by using fluid density as function of temperature because the constant density assumptions reduces non-linearity.
- Natural convection problems inside closed domains:
  - For steady-state solver, Boussinesq model must be used. Constant density ρ_o allows mass in volume to be defined.
  - For unsteady solver, Boussinesq model or ideal gas law can be used. Initial conditions define mass in volume.

Newton's law of cooling

- Newton described the cooling of objects with an arbitrary shape in a pragmatic way. He postulated that the heat transfer *Q* is proportional to the surface area *A* of the object and a temperature difference ΔT.
- The proportionality constant is the heat transfer coefficient *h*(W/m^2-K). This empirical constant lumps together all the information about the heat transfer process that we don't know or don't understand.



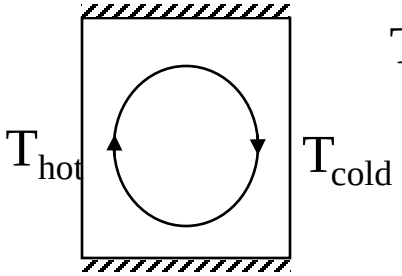
$$Q = qA = \bar{h}\,A(T_{body} - T_\infty) = \bar{h}\,A\Delta T$$

$\bar{h}$ = average heat transfer coefficient (W/m^2-K)

Heat transfer coefficient

- *h* is not a constant, but *h = h(ΔT).*
- Three types of convection.
- Natural convection. Fluid moves due to buoyancy.

$$h \propto \Delta T^{x} \qquad \frac{1}{4} < x < \frac{1}{3}$$

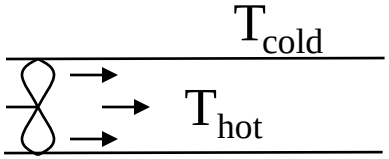


Typical values of *h:*

4 - 4,000 W/m^2-K

- Forced convection: flow is induced by external means.

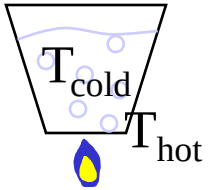
$$h = const$$



80 - 75,000

- Boiling convection: body is hot enough to boil liquid.

$$h \propto \Delta T^{2}$$

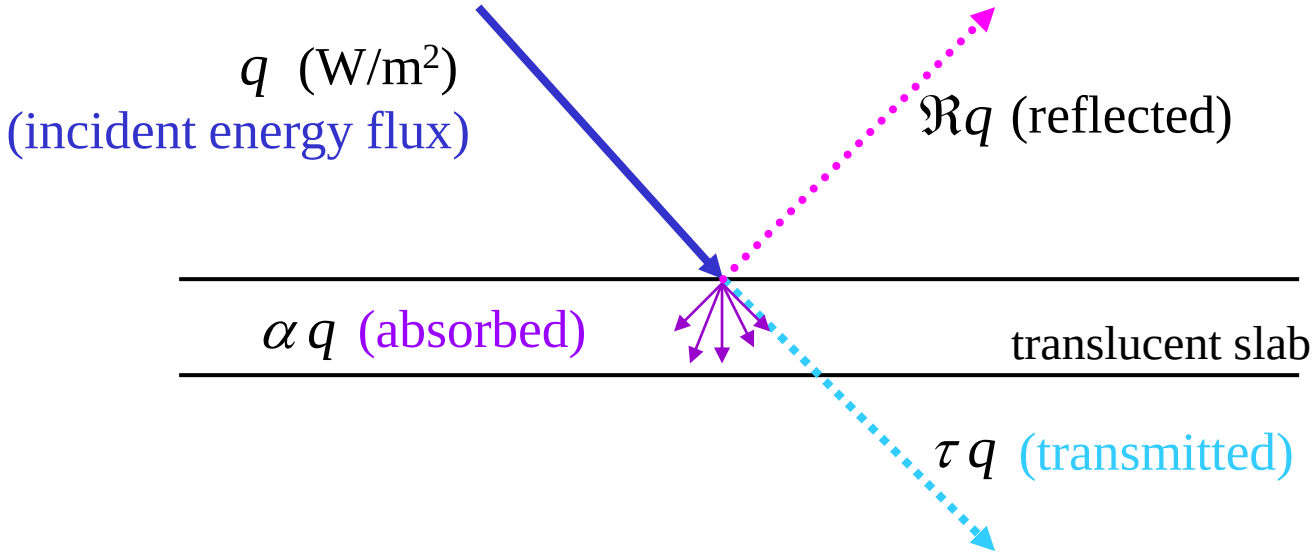


300 - 900,000

Radiation heat transfer

- Thermal radiation is emission of energy as electromagnetic waves.
- Intensity depends on body temperature and surface characteristics.
- Important mode of heat transfer at high temperatures, e.g., combustion.
- Can also be important in natural convection problems.
- Radiation properties can be strong functions of chemical composition, especially CO_2, H_2O.
- Radiation heat exchange is difficult solve (except for simple configurations). We must rely on computational methods.

Surface characteristics



$$1 = \alpha + \Re + \tau$$

absorptance

reflectance

transmittance

Black body radiation

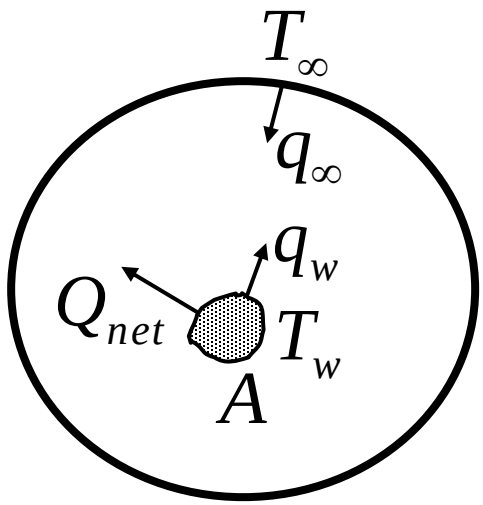
- A “black body”:
  - Is a model of a perfect radiator.
  - Absorbs all energy that reaches it; reflects nothing.
  - Therefore $\alpha = 1,\ \Re = \tau = 0.$
- The energy emitted by a black body is the theoretical maximum:

$$q = \sigma T^4$$

- This is Stefan-Boltzmann law; σ is the Stefan-Boltzmann constant (5.6697E-8 W/m^{2}K^4).
- The wavelength at which the maximum amount of radiation occurs is given by Wien’s law: $\lambda_{\max} T = 2.898\text{E} - 3\ [\text{mK}]$
- Typical wavelengths are $\lambda_{\max}$ = 10 μm (far infrared) at room temperature and $\lambda_{\max}$ = 0.5 μm (green) at 6000K.

Real bodies

- Real bodies will emit less radiation than a black body: $q = \varepsilon \sigma T^4$
- Here ε is the emissivity, which is a number between 0 and 1. Such a body would be called “gray” because the emissivity is the average over the spectrum.
- Example: radiation from a small body to its surroundings.
  - Both the body and its surroundings emit thermal radiation.
  - The net heat transfer will be from the hotter to the colder.
- The net heat transfer is then: $Q_{net} = \varepsilon A \sigma (T_w^4 - T_\infty^4)$
- For small ΔT the term (T_w^{4}-T_∞^{4}) can be approximated as $4\overline{T}^3 (T_w - T_\infty)$ and $Q_{net} = A h_r \Delta T$ with h_r as an effective radiation heat transfer coefficient.



The radiative heat transfer equation (RTE)

$$\frac{dI(\vec{r},\vec{s})}{ds} + (a+\sigma_s)I(\vec{r},\vec{s}) = an^2\frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi}\int_0^{4\pi} I(\vec{r},\vec{s}\,')\,\Phi(\vec{s}\cdot\vec{s}\,')\,d\Omega'$$

where $\vec{r}$ = position vector

$\vec{s}$ = direction vector

$\vec{s}\,'$ = scattering direction vector

s = path length

a = absorption coefficient

n = refractive index

σ_s = scattering coefficient

σ = Stefan-Boltzmann constant (5.672×10^{-8} W/m^2-K^4)

I = radiation intensity, which depends on position ($\vec{r}$)

and direction ($\vec{s}$)

T = local temperature

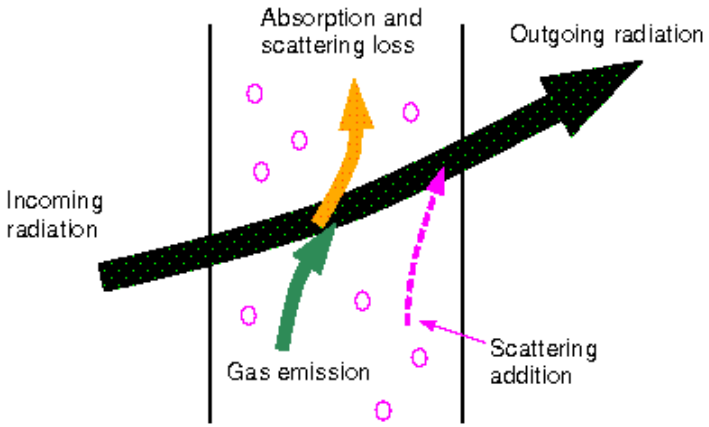
Φ = phase function

Ω' = solid angle

$(a+\sigma_s)s$ is the optical thickness or opacity of the medium. The refractive index n is important when considering radiation in semi-transparent media.

Radiation

- Radiation intensity transport equations (RTE) are solved.
  - Local absorption by fluid and at boundaries links energy equation with RTE.
- Radiation intensity is directionally and spatially dependent.
  - Intensity along any direction can be reduced by:
    - Local absorption.
    - Out-scattering (scattering away from the direction).
  - Intensity along any direction can be augmented by:
    - Local emission.
    - In-scattering (scattering into the direction).
- Common radiation models are:
  - Discrete Ordinates Model (DOM).
  - Discrete Transfer Radiation Model (DTRM)
  - P-1 Radiation Model.
  - Rosseland Model.
  - Surface-to-surface radiation (S2S)
  - Monte-Carlo Model



Discrete ordinates model

- The radiative transfer equation is solved for a discrete number of finite solid angles:

$$\frac{\partial I_{si}}{\partial x_i} + \underbrace{(a+\sigma_s)I(r,s)}_{\text{absorption}} = \underbrace{an^2\frac{\sigma T^4}{\pi}}_{\text{emission}} + \underbrace{\frac{\sigma_s}{4\pi}\int_0^{4\pi} I(r,s')\Phi(s\cdot s')d\Omega'}_{\text{scattering}}$$

- Advantages:
  - Solution method similar to that for the other conservation equations.
  - Conservative method leads to heat balance for coarse discretization.
  - Accuracy can be increased by using a finer discretization.
  - Accounts for scattering, semi-transparent media, specular surfaces.
  - Banded-gray option for wavelength-dependent transmission.
- Limitations:
  - Solving a problem with a large number of ordinates is CPU-intensive.

Discrete transfer radiation model (DTRM)

- Main assumption: radiation leaving surface element in a specific range of solid angles can be approximated by a single ray.
- Uses ray-tracing technique to integrate radiant intensity along each ray:

$$\frac{dI}{ds} = -\alpha\ I + \alpha\ \frac{\sigma T^4}{\pi}$$

- Advantages:
  - Relatively simple model.
  - Can increase accuracy by increasing number of rays.
  - Applies to wide range of optical thicknesses.
- Limitations:
  - Assumes all surfaces are diffuse (isotropic reflection).
  - Effect of scattering not included.
  - Solving a problem with a large number of rays is CPU-intensive.

P-1 model

- Main assumption: radiation intensity can be decomposed into series of spherical harmonics. Only first term in this (rapidly converging) series used in P-1 model.
- Advantages:
  - Radiative transfer equation easy to solve with little CPU demand.
  - Works reasonably well for combustion applications where optical thickness is large.
  - Easily applied to complicated geometries with curvilinear coordinates.
  - Effects of particles, droplets, and soot can be included.
- Limitations:
  - Assumes all surfaces are diffuse.
  - May result in loss of accuracy, depending on complexity of geometry, if optical thickness is small.
  - Tends to overpredict radiative fluxes from localized heat sources or sinks.
- A further simplified (and faster but less accurate) version of this model is the Rosseland model.

Choosing a radiation model

- For certain problems, one radiation model may be more appropriate in general.
  - Computational effort: P-1 gives reasonable accuracy with less effort.
  - Accuracy: DTRM and DOM more accurate.
  - Optical thickness: DTRM/DOM for optically thin media (optical thickness << 1); P-1 sufficiently accurate and faster for optically thick media.
  - Scattering: P-1 and DOM account for scattering.
  - Particulate effects: P-1 and DOM account for radiation exchange between gas and particulates.
  - Localized heat sources: DTRM/DOM with sufficiently large number of rays/ordinates is more appropriate.
  - Surface-to-surface radiation is commonly used in electronics cooling and similar applications.

Wall heat flux calculation

heat flux : $q = h_f (T_w - T_f) + q_{rad}$

for laminar flows : $h_f = \frac{k_f}{\Delta y}$

for turbulent flows : h_f follows from correlations describing the thermal boundary layer profile

external wall radiation : $q_{rad} = \varepsilon_{ext} \sigma (T_\infty^4 - T_w^4)$

$T_w =$ wall temperature

$T_f =$ fluid cell temperature

$T_\infty =$ user specified temperature

$\varepsilon_{ext} =$ emissivity of external wall surface

$\sigma =$ Stefan – Boltzmann constant

$h_f =$ fluid side local heat transfer coefficient

$\Delta y =$ normal distance fluid cell center to wall

Heat transfer optimization

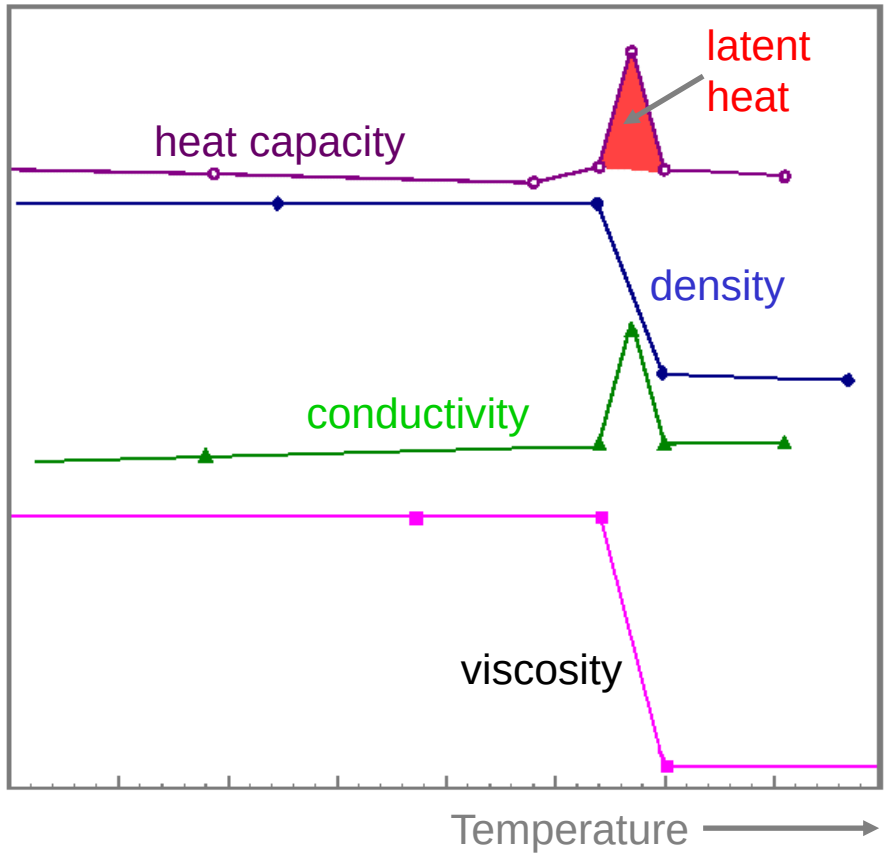
- We have the following relations for heat transfer:
  - Conduction: $Q = A\Delta T\, k_f / d$
  - Convection: $Q = Ah\Delta T$
  - Radiation: $Q = Ah_r\, \Delta T$
- As a result, when equipment designers want to improve heat transfer rates, they focus on:
  - Increasing the area A, e.g., by using profiled pipes and ribbed surfaces.
  - Increasing ΔT (which is not always controllable).
  - For conduction, increasing k_f/d.
  - Increase h by not relying on natural convection but introducing forced convection.
  - Increase h_r, by using “black” surfaces.

Fluid properties

- Fluid properties such as heat capacity, conductivity, and viscosity can be defined as:
  - Constant.
  - Temperature-dependent.
  - Composition-dependent.
  - Computed by kinetic theory.
  - Computed by user-defined functions.
- Density can be computed by ideal gas law.
- Alternately, density can be treated as:
  - Constant (with optional Boussinesq modeling).
  - Temperature-dependent.
  - Composition-dependent.
  - User defined functions.

Phase change

- Systems in which phase change occurs (e.g., melting, solidification, and sometimes evaporation) can be modeled as a single-phase flow with modified physical properties.
- In that case, the medium gets the properties of one phase state below a certain critical temperature, and the properties of the other phase state above a second critical temperature.
- Linear transitions for μ and ρ.
- A “spike” in c_p is added, the area of which corresponds to the latent heat.



- A second spike is added to the heat conductivity curve, to keep the ratio between heat capacity and thermal conductivity constant. This is necessary to conduct the heat without the computations becoming unstable.

Thermal boundary conditions

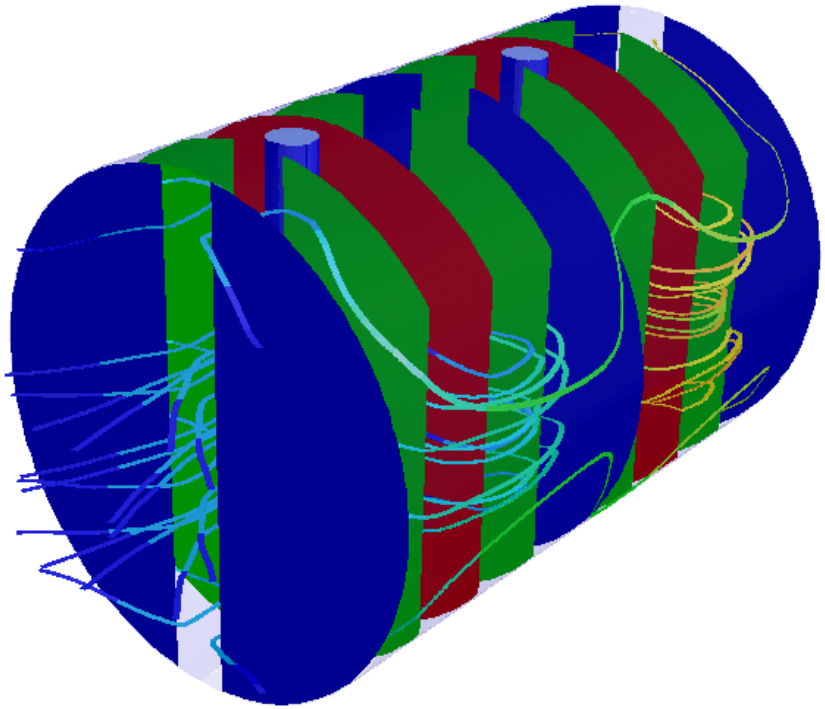
- At flow inlets and exits.
  - At flow inlets, must supply fluid temperature.
  - At flow exits, fluid temperature extrapolated from upstream value.
  - At pressure outlets, where flow reversal may occur, “backflow” temperature is required.
- Thermal conditions for fluids and solids.
  - Can specify energy source.
- Thermal boundary conditions at walls.
  - Specified heat flux.
  - Specified temperature.
  - Convective heat transfer.
  - External radiation.
  - Combined external radiation and external convective heat transfer.

Notes on convergence

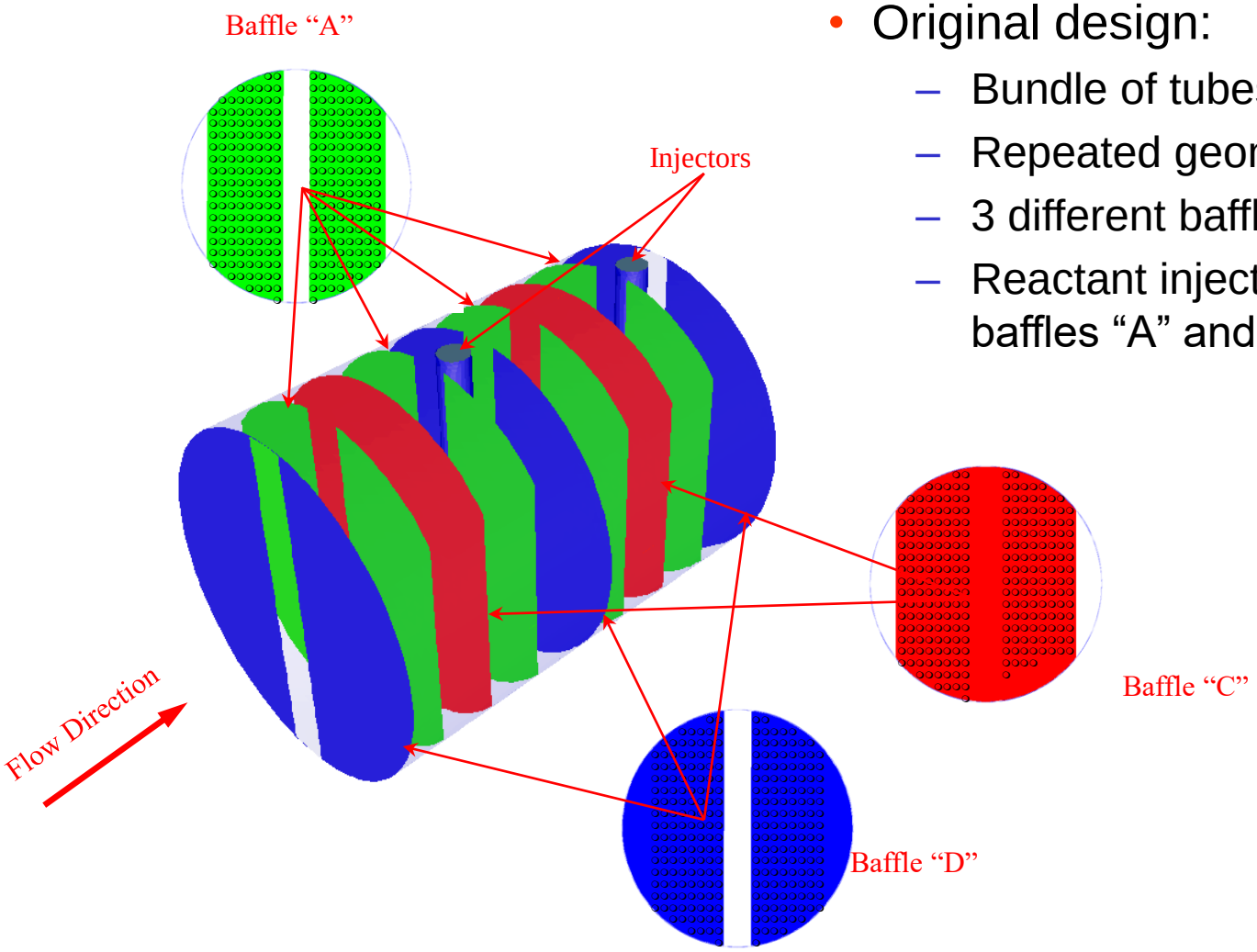
- Heat transfer calculations often converge slowly. It is recommended to use underrelaxation factors of 0.9 or larger for enthalpy. If lower underrelaxation factors are used, obtaining a good solution may take prohibitively long.
- If underrelaxation factors of 0.2 or lower have to be used to prevent divergence, it usually means that the model is ill-posed.
- Deep convergence is usually required with scaled residuals having to be of the order 1E-6 or smaller.

Example: heat exchanger efficiency

- Problem: improve the efficiency of a tube-cooled reactor.
- Non-standard design, i.e., traditional correlation-based methods not applicable.
- Solution: more uniform flow distribution through the shell that will result in a higher overall heat transfer coefficient and improved efficiency.



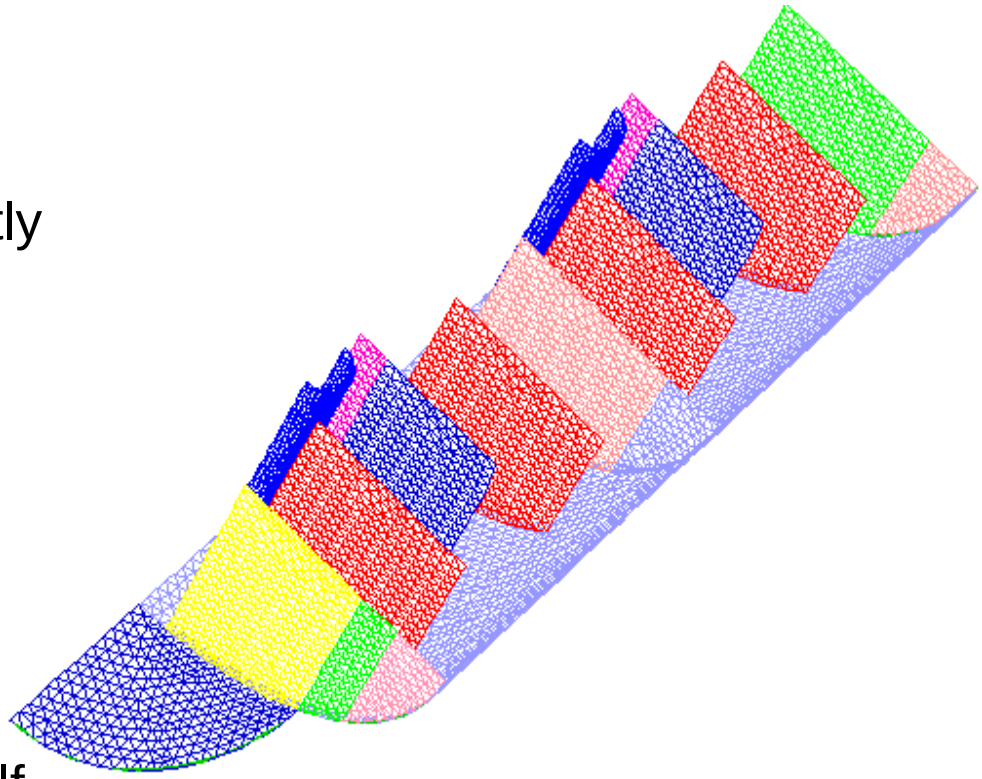
Heat exchanger - original design



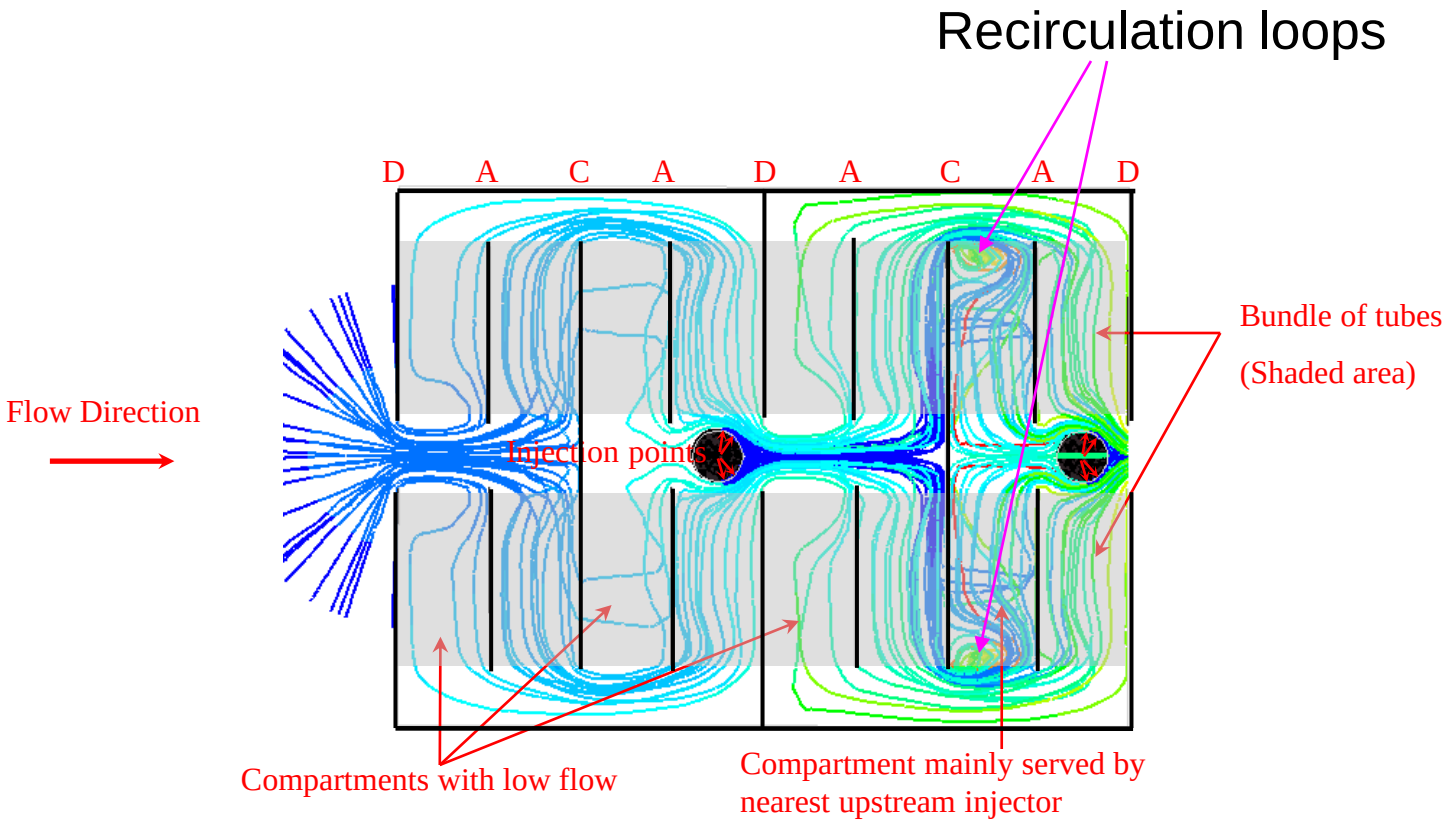
- Original design:
  - Bundle of tubes as shown.
  - Repeated geometry.
  - 3 different baffles, A, C, and D.
  - Reactant injectors between baffles “A” and “D”.

Heat exchanger - modeling approach

- 3-dimensional, steady, turbulent, incompressible, isothermal.
- Bundle of tubes modeled as a non-isotropic porous medium. Two symmetry planes significantly reduce domain size.
- Hybrid, unstructured mesh of 330,000 cells.
- Zero thickness walls for baffles.
- Leakage between baffles and shell wall (0.15” gap) modeled using thin prism cells.
- Uniform inflow applied over a half-cylindrical surface upstream of the first baffle.

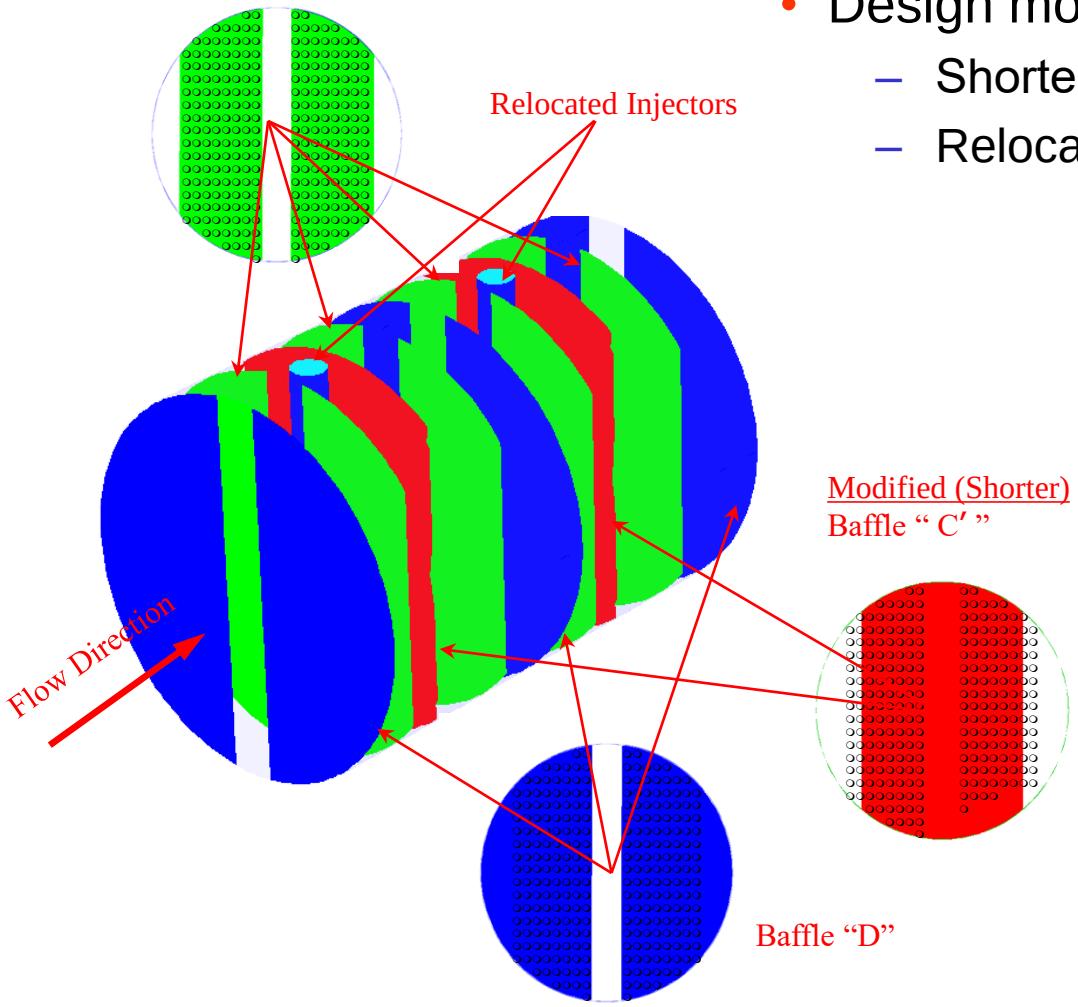


Heat exchanger - flow pattern



Non-uniform flow distribution means low efficiency

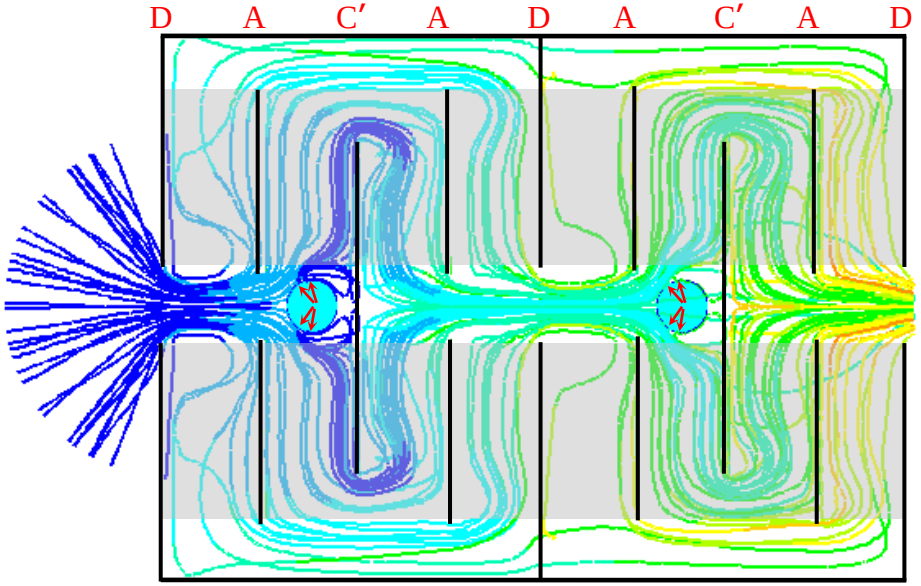
Heat exchanger - modifications



- Design modifications:
  - Shorter baffles " C' ".
  - Relocated and rotated injectors.

Heat exchanger - improved flow pattern

- Flow distribution after modifications.
- No recirculating fluid between baffles C’ and A.
- Almost uniform flow distribution.
- Problem has unique flow arrangement that does not allow traditional methods to be of any help.
- A simplified CFD model leads to significantly improved performance of the heat exchanger/reactor.



Conclusion

- Heat transfer is the study of thermal energy (heat) flows: conduction, convection, and radiation.
- The fluid flow and heat transfer problems can be tightly coupled through the convection term in the energy equation and when physical properties are temperature dependent.
- Chemical reactions, such as combustion, can lead to source terms to be included in the enthalpy equation.
- While analytical solutions exist for some simple problems, we must rely on computational methods to solve most industrially relevant applications.

Lecture 14 - Multiphase Flows

Applied Computational Fluid Dynamics

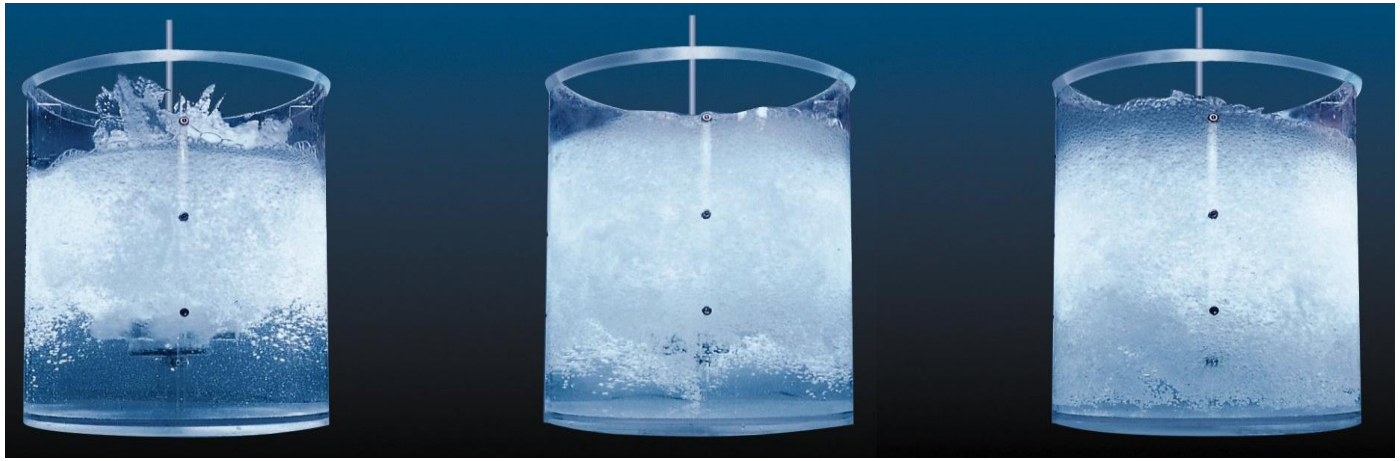
André Bakker

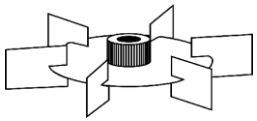
Multiphase flow

- Simultaneous flow of:
  - Materials with different states or phases (i.e., gas, liquid or solid).
  - Materials with different chemical properties but in the same state or phase (i.e., liquid-liquid systems such as oil droplets in water).
- Volume fraction:
  - Volume fraction of a phase = $\frac{\text{Volume of the phase in a cell/domain}}{\text{Volume of the cell/domain}}$
- Laminar versus turbulent:
  - Each phase can be laminar or turbulent.
  - Fluid flow (primary phase) may be turbulent with respect to the secondary phase (e.g., in the wake of a bubble) but may be laminar with respect to the domain.

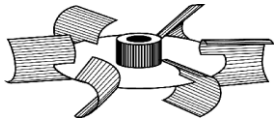
Why model multiphase flow?

- Multiphase flow is important in many industrial processes:
  - Riser reactors.
  - Bubble column reactors.
  - Fluidized bed reactors.
  - Scrubbers, dryers, etc.
- Typical objectives of a modeling analysis:
  - Maximize the contact between the different phases, typically different chemical compounds.
  - Flow dynamics.





Rushton



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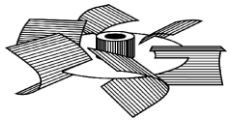
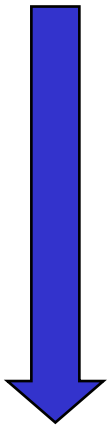


BT-6

Images: Chemineer Inc. gas-liquid mixing brochure

Modeling approach

- Empirical correlations.
- Lagrangian.
  - Track individual point particles.
  - Particles do not interact.
- Algebraic slip model.
  - Dispersed phase in a continuous phase.
  - Solve one momentum equation for the mixture.
- Two-fluids theory (multi-fluids).
  - Eulerian models.
  - Solve as many momentum equations as there are phases.
- Discrete element method.
  - Solve the trajectories of individual objects and their collisions, inside a continuous phase.
- Fully resolved and coupled.

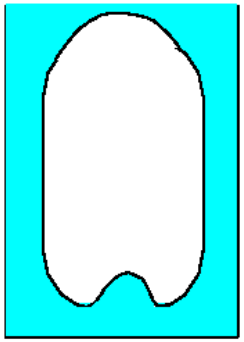


Increased complexity

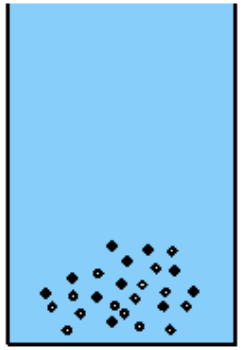
Focus of this lecture

Multiphase flow regimes

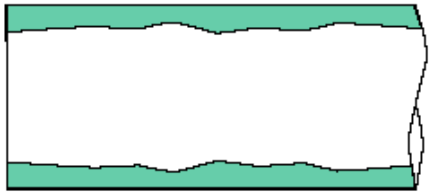
- Bubbly flow: discrete gaseous bubbles in a continuous liquid.
- Droplet flow: discrete fluid droplets in a continuous gas.
- Particle-laden flow: discrete solid particles in a continuous fluid.
- Slug flow: large bubbles in a continuous liquid.
- Annular flow: continuous liquid along walls, gas in core.
- Stratified and free-surface flow: immiscible fluids separated by a clearly-defined interface.



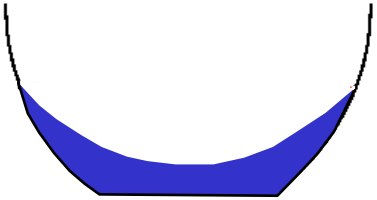
slug flow



bubbly flow
droplet flow
particle-laden flow



annular flow



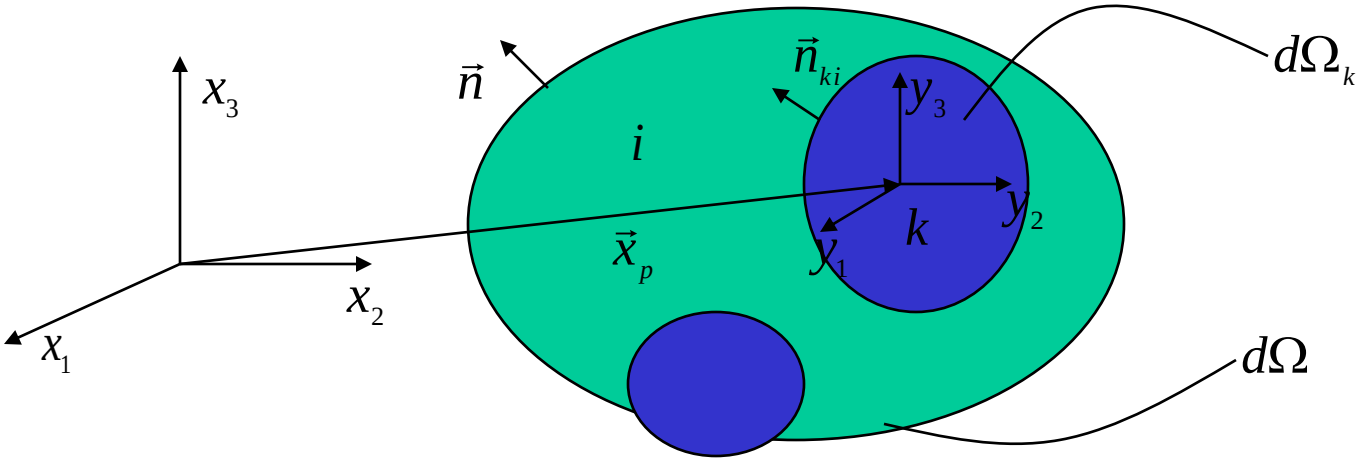
free-surface flow

Multiphase flow regimes

- User must know a priori the characteristics of the flow.
- Flow regime, e.g., bubbly flow, slug flow, annular flow, etc.
- Only model one flow regime at a time.
- Predicting the transition from one regime to another easiest if the flow regimes can be predicted by the same model. This is not always the case.
- Laminar or turbulent.
- Dilute or dense.
- Secondary phase diameter for drag considerations.

Spatial averaging

- Consider an elementary control volume $d\Omega$ bounded by the surface dS.
  - Length scales: $L >> l >> d_k \sim l_t$
  - Volumes: $d\Omega = \sum_{i=1}^{n} d\Omega_i(t)$
  - Averaging volume and coordinate system:



Phases

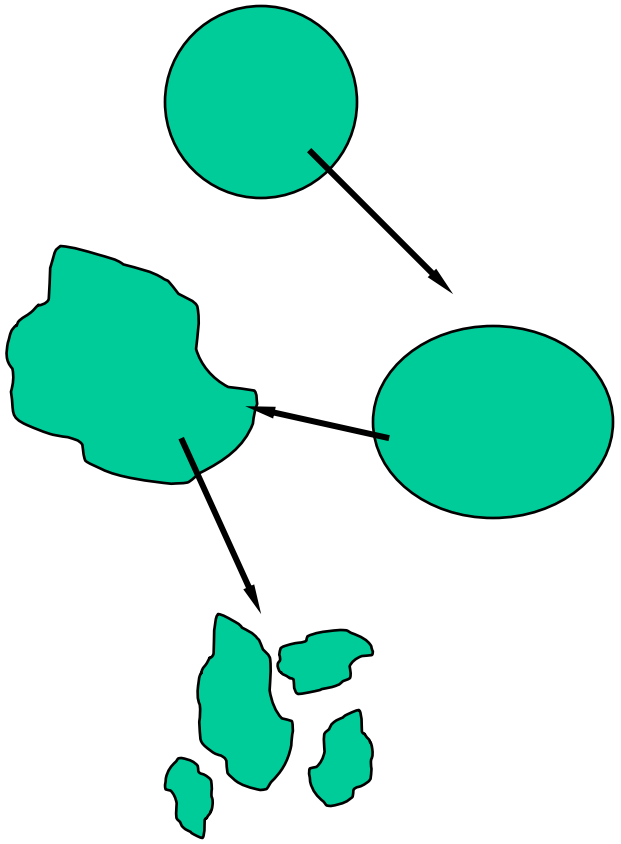
- The primary and secondary phases:
  - One of the phases is continuous (primary) while the other(s) (secondary) are dispersed within the continuous phase.
  - A diameter has to be assigned for each secondary phase to calculate its interaction (drag) with the primary phase.
  - A secondary phase with a particle size distribution is modeled by assigning a separate phase for each particle diameter.

Coupling between phases

- One-way coupling:
  - Fluid phase influences particulate phase via aerodynamic drag and turbulence transfer.
  - No influence of particulate phase on the gas phase.
- Two-way coupling:
  - Fluid phase influences particulate phase via aerodynamic drag and turbulence transfer.
  - Particulate phase reduces mean momentum and turbulent kinetic energy in fluid phase.
- Four-way coupling:
  - Includes all two-way coupling.
  - Particle-particle collisions create particle pressure and viscous stresses.

Physical effects in dispersed systems

- Hydrodynamics:
  - Change in shape.
  - Diameter.
  - Particle-wall collision.
  - Particle-particle collision.
  - Coalescence.
  - Dispersion and breakup.
  - Turbulence.
  - Inversion.
- Other transport phenomena:
  - Heat transfer.
  - Mass transfer.
  - Change in composition.
  - Heterogeneous reactions.



Algebraic slip model (ASM)

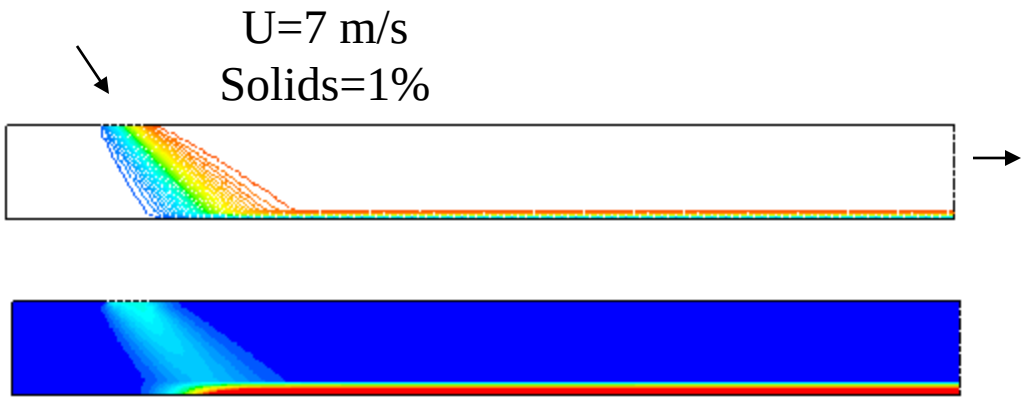
- Solves one set of momentum equations for the mass averaged velocity and tracks volume fraction of each fluid throughout domain.
- Assumes an empirically derived relation for the relative velocity of the phases.
- For turbulent flows, single set of turbulence transport equations solved.
- This approach works well for flow fields where both phases generally flow in the same direction.

Eulerian-granular/fluid model features

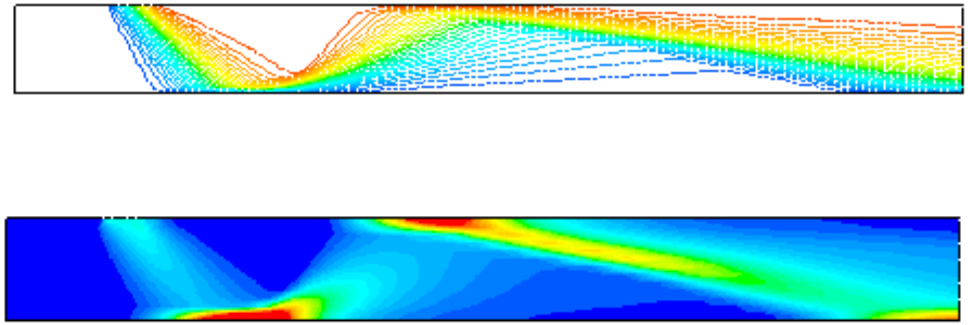
- Solves momentum equations for each phase and additional volume fraction equations.
- Appropriate for modeling fluidized beds, risers, pneumatic lines, hoppers, standpipes, and particle-laden flows in which phases mix or separate.
- Granular volume fractions from 0 to ~60%.
- Several choices for drag laws. Appropriate drag laws can be chosen for different processes.

Test case for Eulerian granular model

- Contours of solid stream function and solid volume fraction when solving with Eulerian-Eulerian model.



- Contours of solid stream function and solid volume fraction when solving with Eulerian-Granular model (EGM). EGM takes solid particle specific effects into account.



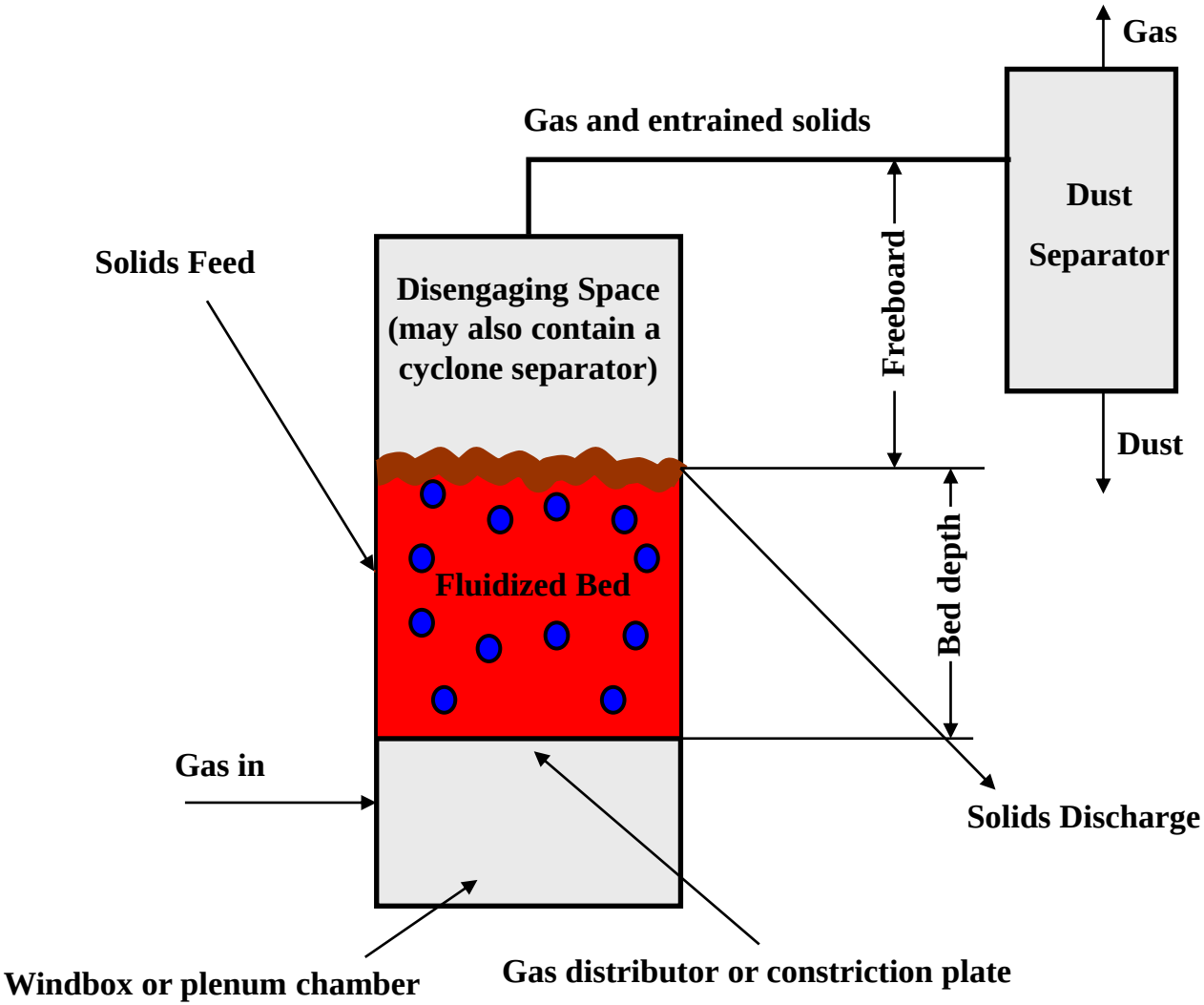
Fluidized-bed systems

- When a fluid flows upward through a bed of solids, beyond a certain fluid velocity the solids become suspended. The suspended solids:
  - has many of the properties of a fluid,
  - seeks its own level (“bed height”),
  - assumes the shape of the containing vessel.
- Bed height typically varies between 0.3m and 15m.
- Particle sizes vary between 1 μm and 6 cm. Very small particles can agglomerate. Particle sizes between 10 μm and 150 μm typically result in the best fluidization and the least formation of large bubbles. Addition of finer size particles to a bed with coarse particles usually improves fluidization.
- Superficial gas velocities (based on cross sectional area of empty bed) typically range from 0.15 m/s to 6 m/s.

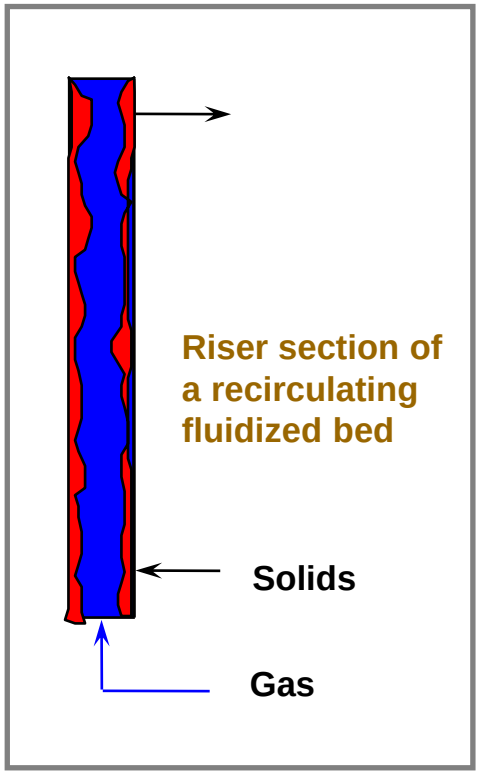
Fluidized bed uses

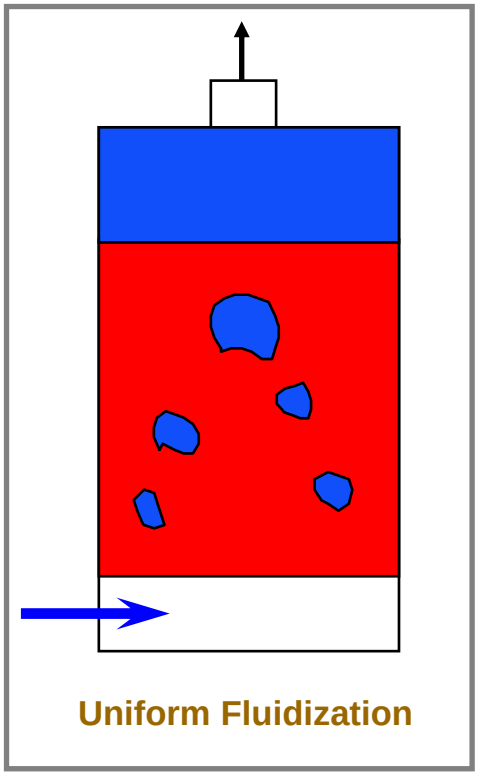
- Fluidized beds are generally used for gas-solid contacting. Typical uses include:
  - Chemical reactions:
    - Catalytic reactions (e.g., hydrocarbon cracking).
    - Noncatalytic reactions (both homogeneous and heterogeneous).
  - Physical contacting:
    - Heat transfer: to and from fluidized bed; between gases and solids; temperature control; between points in bed.
    - Solids mixing.
    - Gas mixing.
    - Drying (solids or gases).
    - Size enlargement or reduction.
    - Classification (removal of fines from gas or fines from solids).
    - Adsorption-desorption.
    - Heat treatment.
    - Coating.

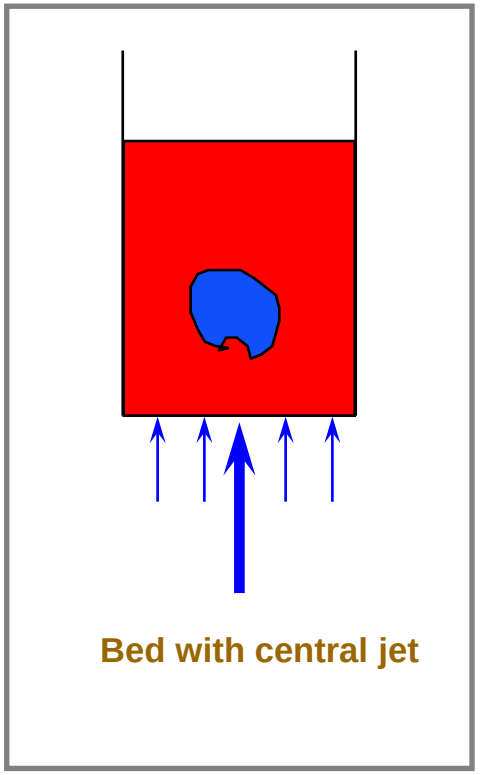
Typical fluidized bed systems - 1



Typical fluidized bed systems - 2







Fluidized bed design parameters

- Main components are the fluidization vessel (bed portion, disengagement space, gas distributor), solids feeder, flow control, solids discharge, dust separator, instrumentation, gas supply.
- There is no single design methodology that works for all applications. The design methodologies to be used depend on the application.
- Typical design parameters are bed height (depends on gas contact time, solids retention time, L/D for staging, space required for internal components such as heat exchangers).
- Flow regimes: bubbling, turbulent, recirculating, slugs. Flow regime changes can affect scale-up.
- Heat transfer and flow around heat exchanger components.
- Temperature and pressure control.
- Location of instrumentation, probes, solids feed, and discharges.

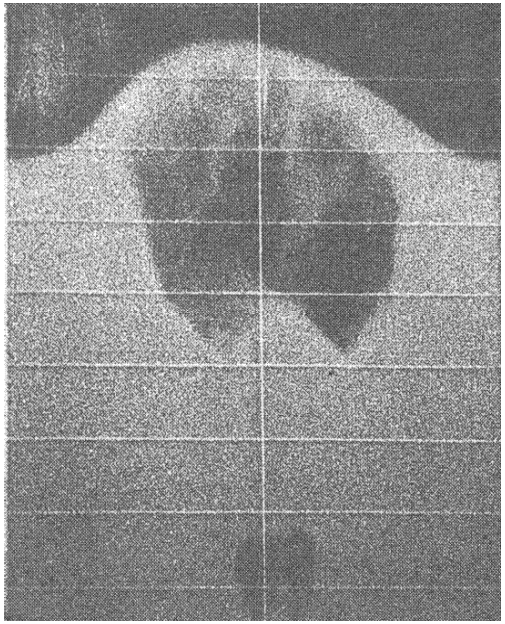
Fluidized bed - input required for CFD

- CFD cannot be used to predict the:
  - minimum fluidization velocity,
  - and the minimum bubbling velocity.
- These depend on the:
  - particle shape,
  - particle surface roughness,
  - particle cohesiveness, and the
  - particle size distribution.
- All these effects are lumped into the drag term. Hence, we need to fine tune the drag term to match the experimental data for minimum fluidization or minimum bubbling velocity.

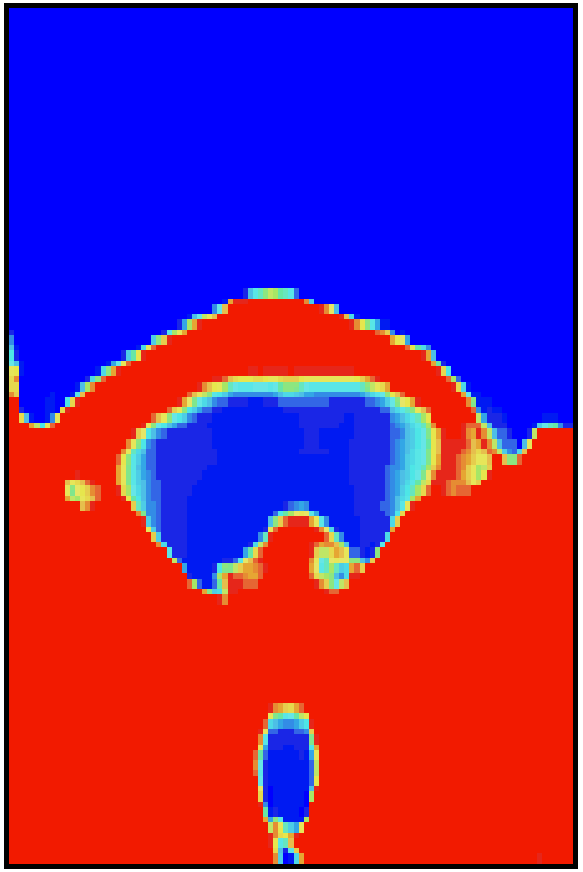
Fluidized bed - when to use CFD

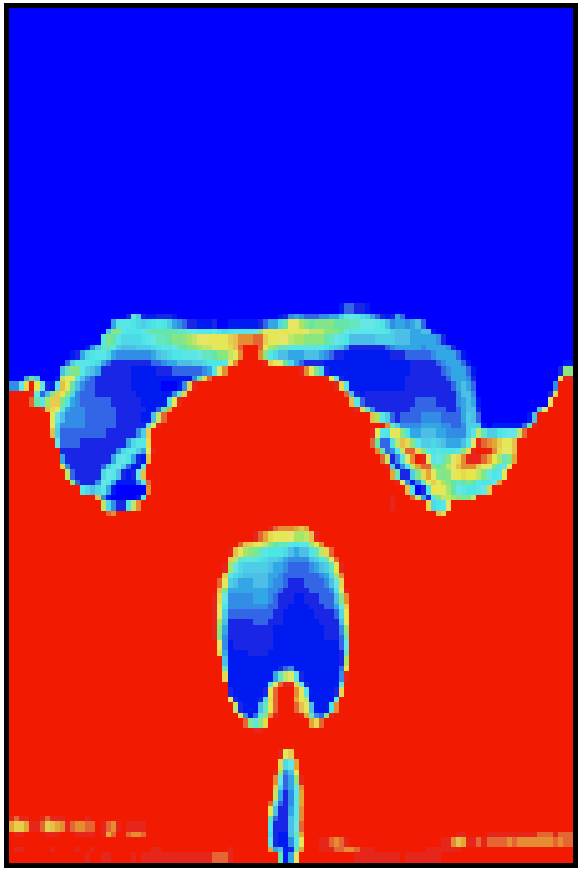
- If the drag term is tuned to match the minimum fluidization velocity, CFD then can be used to predict:
  - Bed expansion
  - Gas flow pattern
  - Solid flow pattern
  - Bubbling size, frequency and population
  - Short circuiting
  - Effects of internals
  - Effects of inlet and outlets
  - Hot spots
  - Reaction and conversion rates
  - Mixing of multiple particle size
  - Residence times of solids and gases
  - Back mixing and downflows (in risers)
  - Solids distribution/segregation

Fluidized bed simulation



Experiment: Gidaspow [11]





Simulation using FLUENT

Solution recommendations

- Use unsteady models for dense gas-solid flows (fluidized beds as well as dense pneumatic transport lines/risers). These flows typically have many complex features, and a steady state solution may not be numerically feasible unless a diffusive turbulence model (e.g., k-ε) is used.
- Use small time steps (0.001 to 0.1s) to capture important flow features.
- Always tune the drag formula for the specific applications, to match the minimum fluidization velocity.
- Higher order discretization schemes give more realistic bubble shapes, as do finer grids.

Conclusion

- In this lecture we discussed the:
  - The algebraic slip model solves one momentum equation for the mixture.
  - Eulerian model solves one momentum equation per phase.
- In the next lectures we will discuss particle tracking and free surface models.

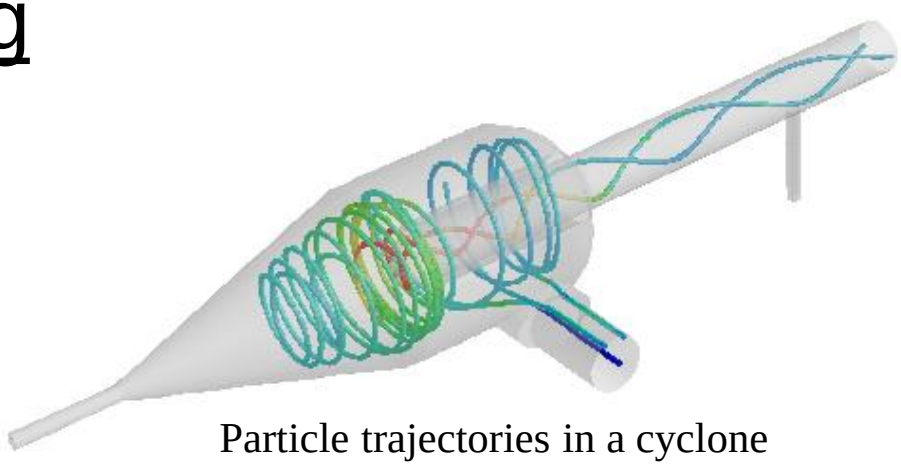
Lecture 15 - Discrete Phase Modeling

Applied Computational Fluid Dynamics

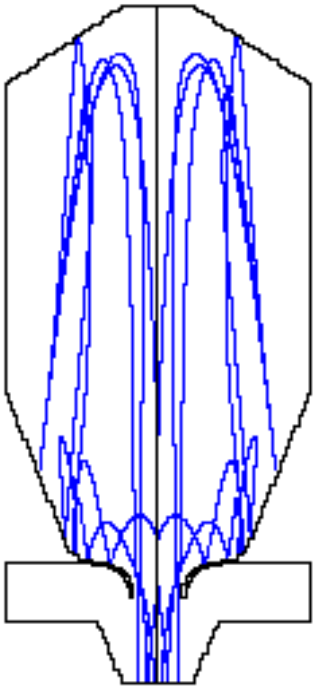
André Bakker

Discrete phase modeling

- Particle tracking.
- Steady vs. unsteady.
- Coupled vs. uncoupled.
- Advantages and limitations.
- Time stepping.
- Discretization.
- Other methods:
  - Discrete element method.
  - Macroscopic particles.



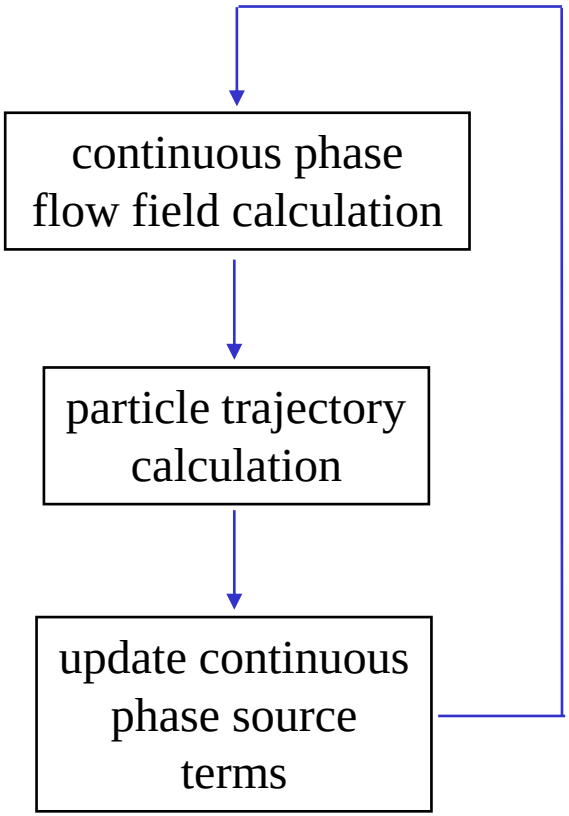
Particle trajectories in a cyclone



Particle trajectories in a spray dryer

Discrete phase model

- Trajectories of particles/droplets are computed in a Lagrangian frame.
  - Exchange (couple) heat, mass, and momentum with Eulerian frame gas phase.
- Discrete phase *volume* fraction should preferably be less than 10%.
  - *Mass* loading can be large (+100%).
  - No particle-particle interaction or break up.
- Turbulent dispersion modeled by:
  - Stochastic tracking.
  - Particle cloud model.
- Model particle separation, spray drying, liquid fuel or coal combustion, etc.



DPM theory

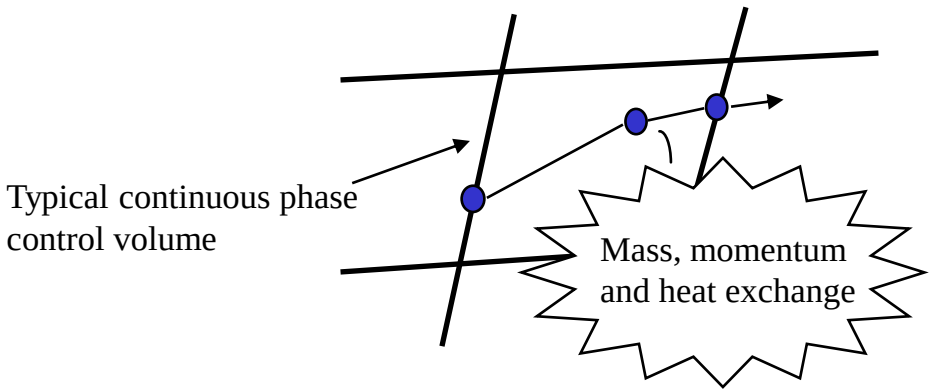
Trajectory is calculated by integrating the particle force balance equation:

$$\frac{du_i^p}{dt} = F_D\left(u_i - u_i^p\right) + g_i(\rho_p - \rho)/\rho_p + F_i/\rho_p$$

Drag force is a function of the relative velocity

Gravity force

Additional forces:
- Pressure gradient
- Thermophoretic
- Rotating reference frame
- Brownian motion
- Saffman lift
- Other (user defined)



Coupling between phases

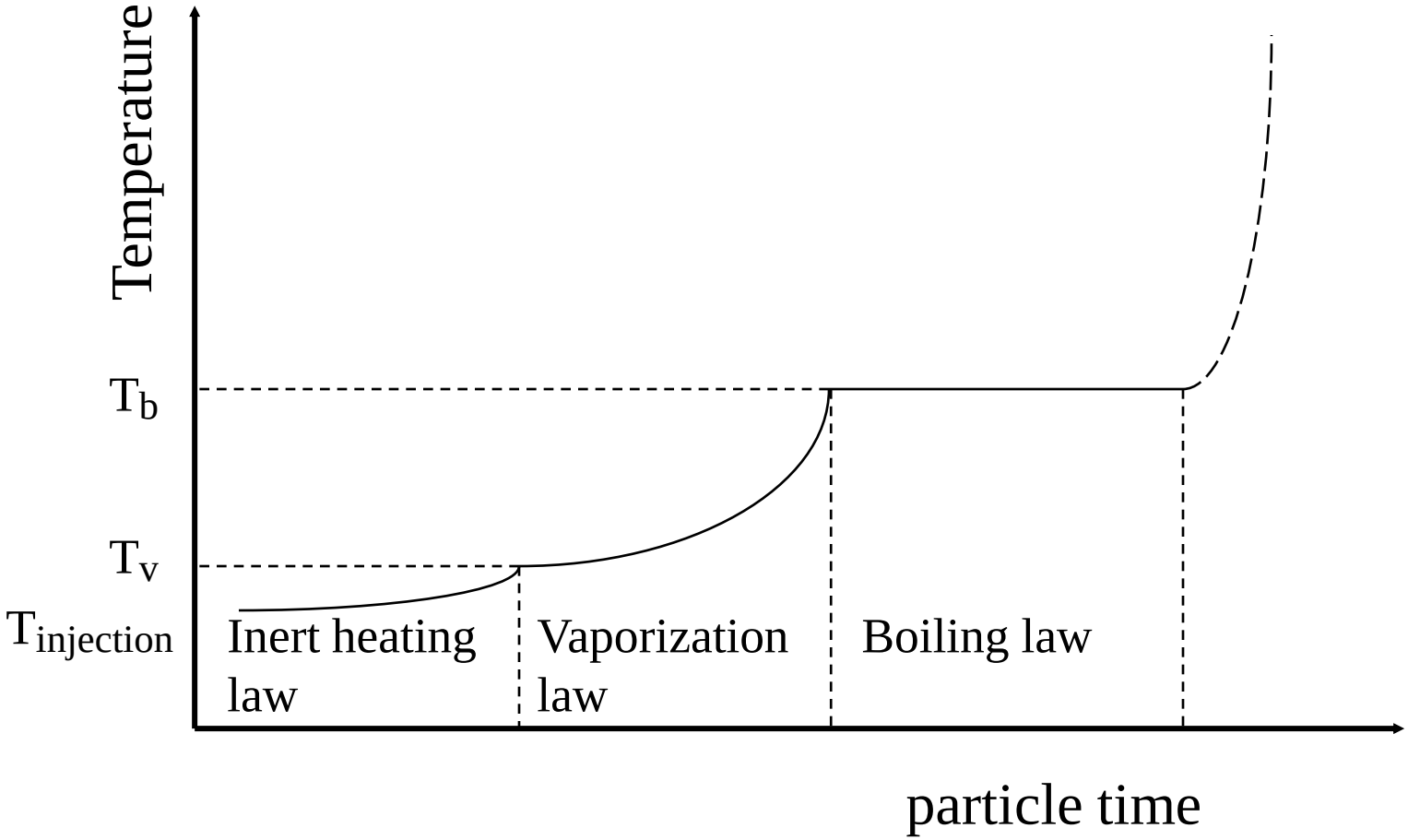
- One-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase has no influence on the gas phase.
- Two-way coupling:
  - Fluid phase influences particulate phase via drag and turbulence.
  - Particulate phase influences fluid phase via source terms of mass, momentum, and energy.
  - Examples include:
    - Inert particle heating and cooling.
    - Droplet evaporation.
    - Droplet boiling.
    - Devolatilization.
    - Surface combustion.

Particle types

- Particle types are inert, droplet and combusting particle.

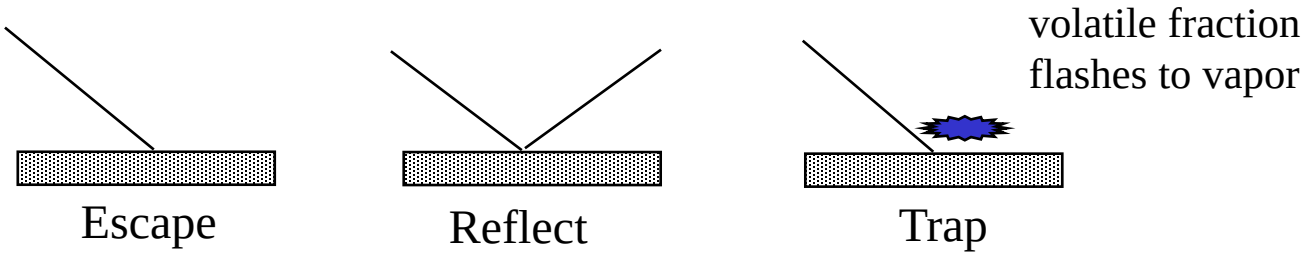
Particle Type	Description
Inert	inert/heating or cooling
Droplet (oil)	heating/evaporation/boiling
Combusting (coal)	heating; evolution of volatiles/swelling; heterogeneous surface reaction

Heat and mass transfer to a droplet



Particle-wall interaction

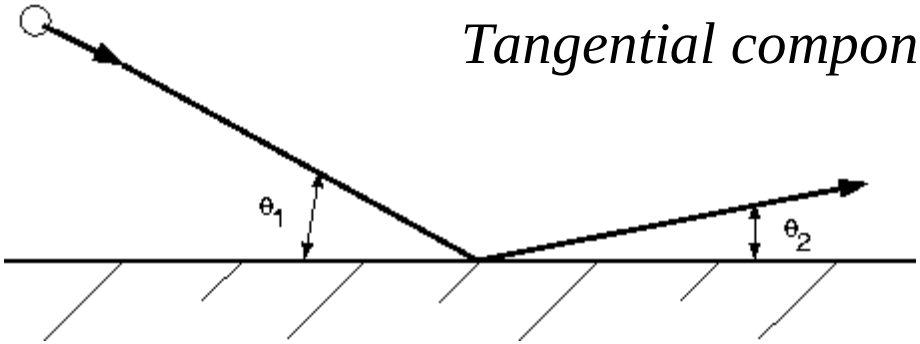
- Particle boundary conditions at walls, inlets, and outlets:



- For particle reflection, a restitution coefficient e is specified:

$$\textit{Normal component: } e_n = \frac{v_{2,n}}{v_{1,n}}$$

$$\textit{Tangential component: } e_t = \frac{v_{2,t}}{v_{1,t}}$$



Particle fates

- “Escaped” trajectories are those that terminate at a flow boundary for which the “escape” condition is set.
- “Incomplete” trajectories are those that were terminated when the maximum allowed number of time steps was exceeded.
- “Trapped” trajectories are those that terminate at a flow boundary where the “trap” condition has been set.
- “Evaporated” trajectories include those trajectories along which the particles were evaporated within the domain.
- “Aborted” trajectories are those that fail to complete due to numerical/round-off reasons. If there are many aborted particles, try to redo the calculation with a modified length scale and/or different initial conditions.

Turbulence: discrete random walk tracking

- Each injection is tracked repeatedly in order to generate a statistically meaningful sampling.
- Mass flow rates and exchange source terms for each injection are divided equally among the multiple stochastic tracks.
- Turbulent fluctuations in the flow field are represented by defining an instantaneous fluid velocity:

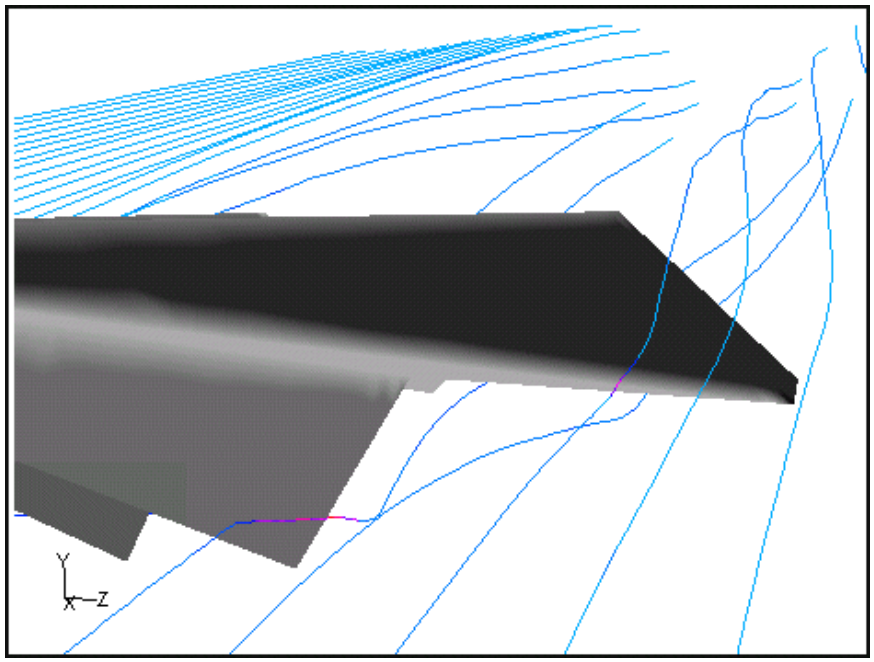
$$u_i = \overline{u}_i + u'_i$$

- where u'_i is derived from the local turbulence parameters:

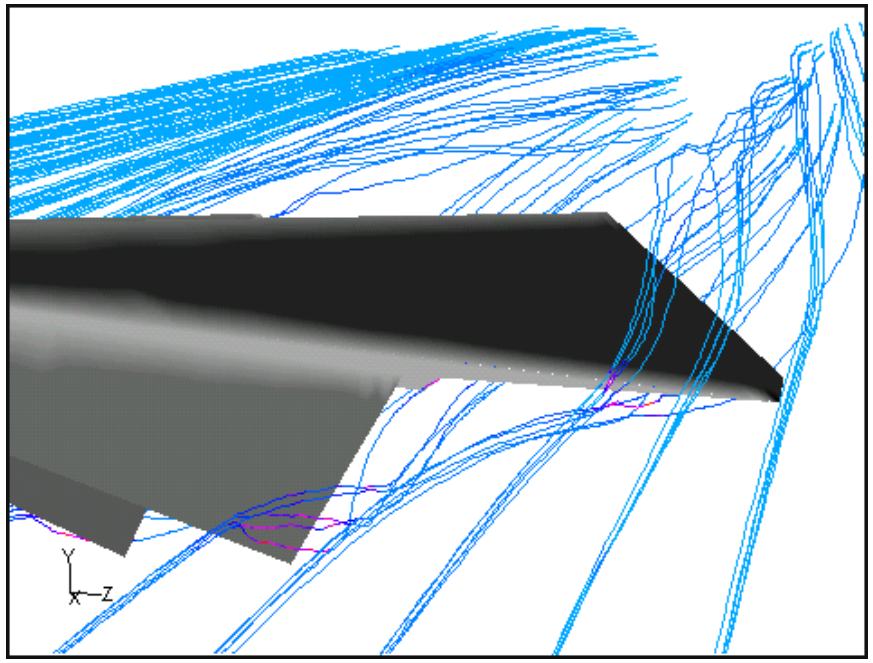
$$u'_i = \zeta \sqrt{\frac{2k}{3}}$$

- and ζ is a normally distributed random number.

Stochastic tracking example - paper plane



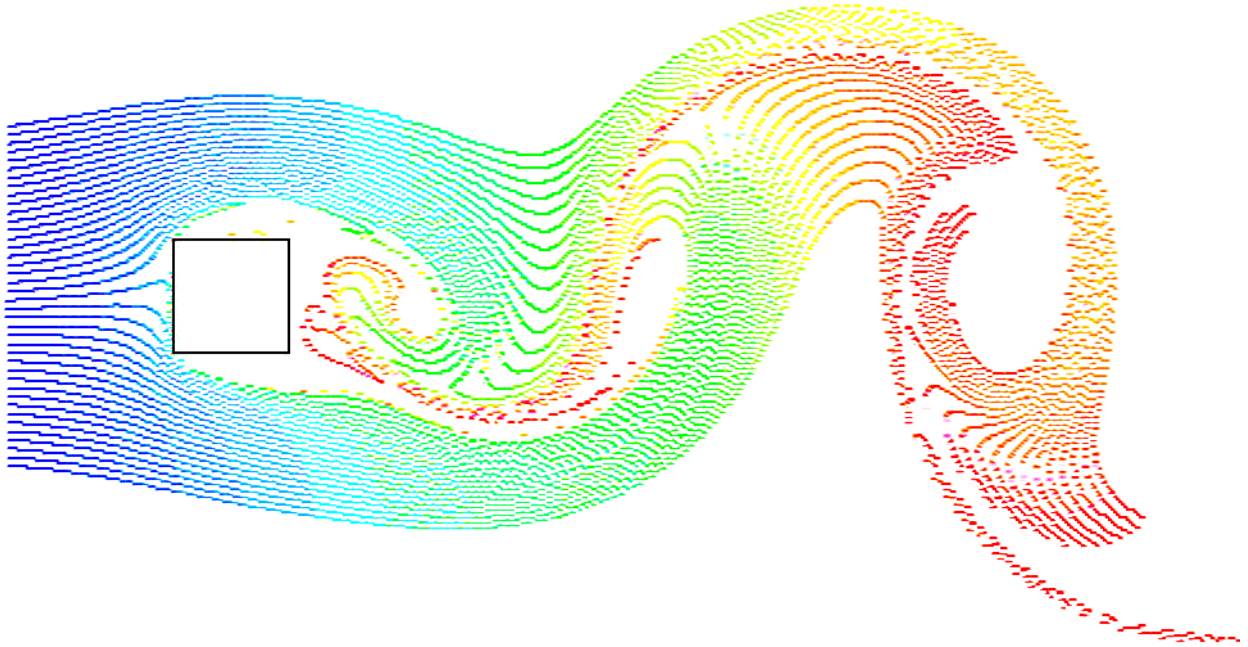
- Stochastic tracking turned off.
- One track per injection point.
- Uses steady state velocities only and ignores effect of turbulence.



- Stochastic tracking turned on.
- Five tracks per injection point.
- Adds random turbulent dispersion to each track.
- Tracks that start in the same point are all different.

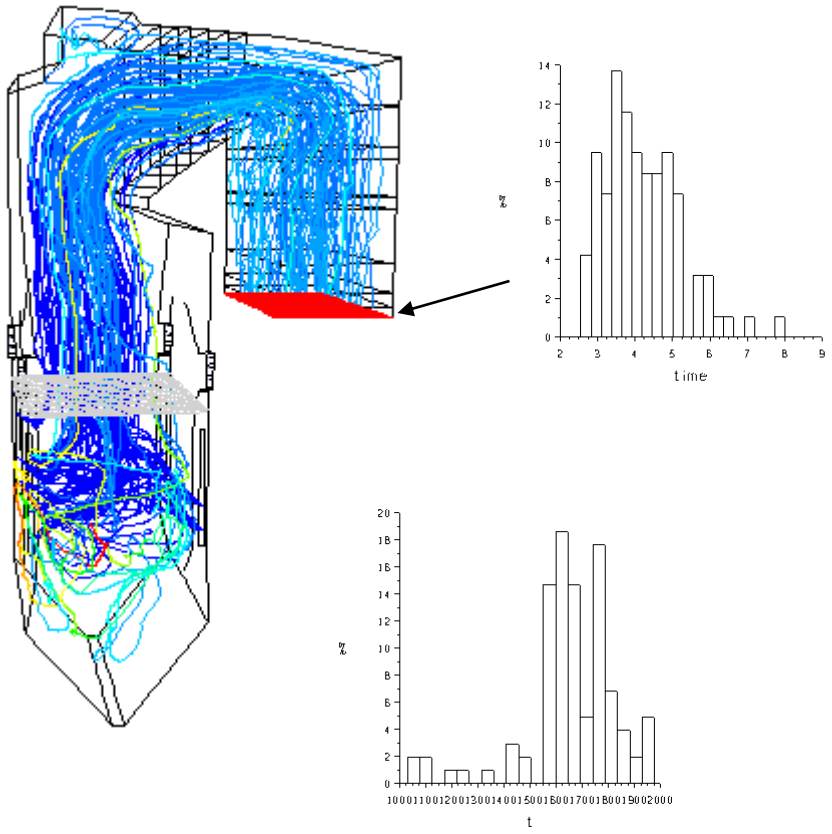
Particle tracking in unsteady flows

- Each particle advanced in time along with the flow.
- For coupled flows using implicit time stepping, sub-iterations for the particle tracking are performed within each time step.
- For non-coupled flows or coupled flows with explicit time stepping, particles are advanced at the end of each time step.



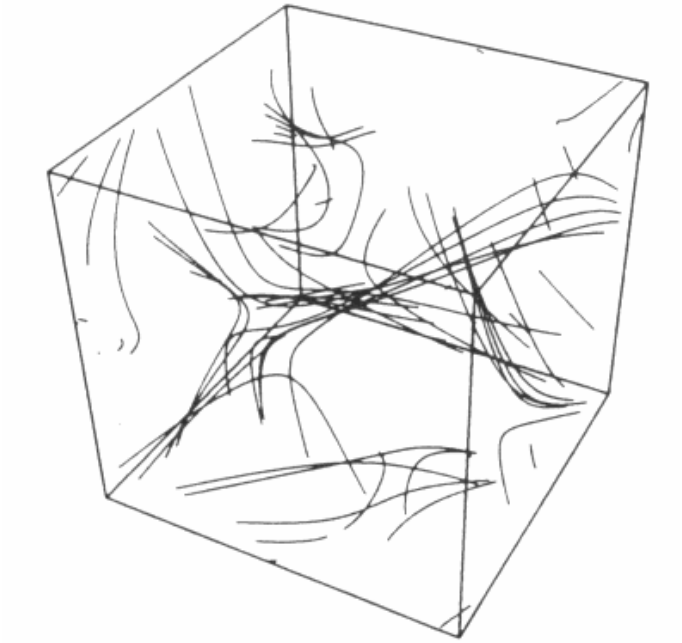
Sample planes and particle histograms

- Track mean particle trajectory as particles pass through sample planes (lines in 2D), properties (position, velocity, etc.) are written to files.
- These files can then be read into the histogram plotting tool to plot histograms of residence time and distributions of particle properties.
- The particle property mean and standard deviation are also reported.

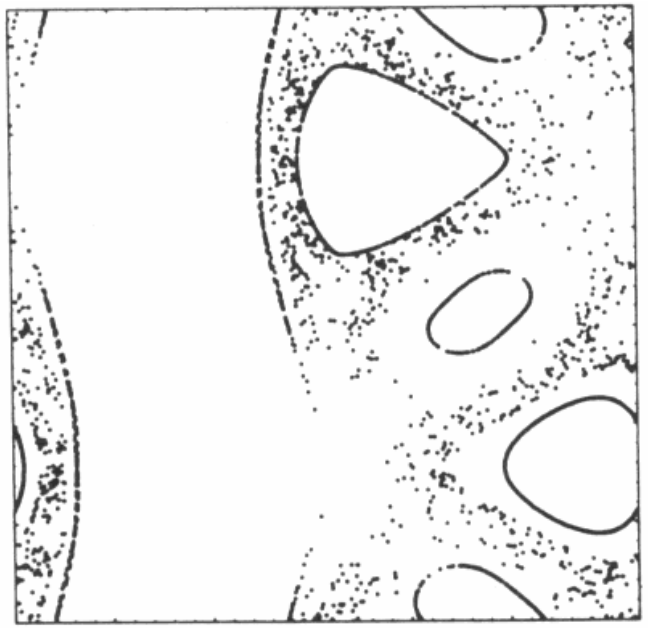


Poincaré plots

- Poincaré plots are made by placing a dot on a given surface every time a particle trajectory hits or crosses that surface.
- Here it is shown for a flow inside a closed cavity with tangentially oscillating walls.



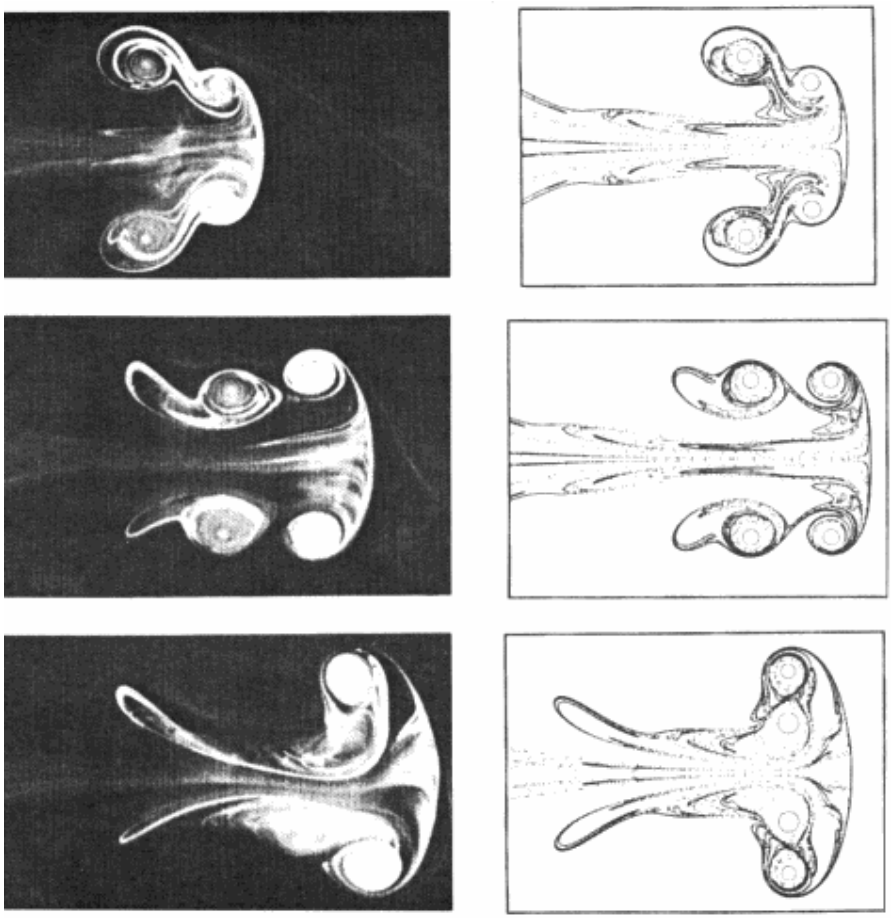
- The figure on the left shows streamlines.
- The figure on the right shows a Poincaré plot for the top surface.
- This method can be used to visualize flow structures.



Aref and Naschie. Chaos applied to fluid mixing. Page 187. 1995.

Leapfrogging vortex rings

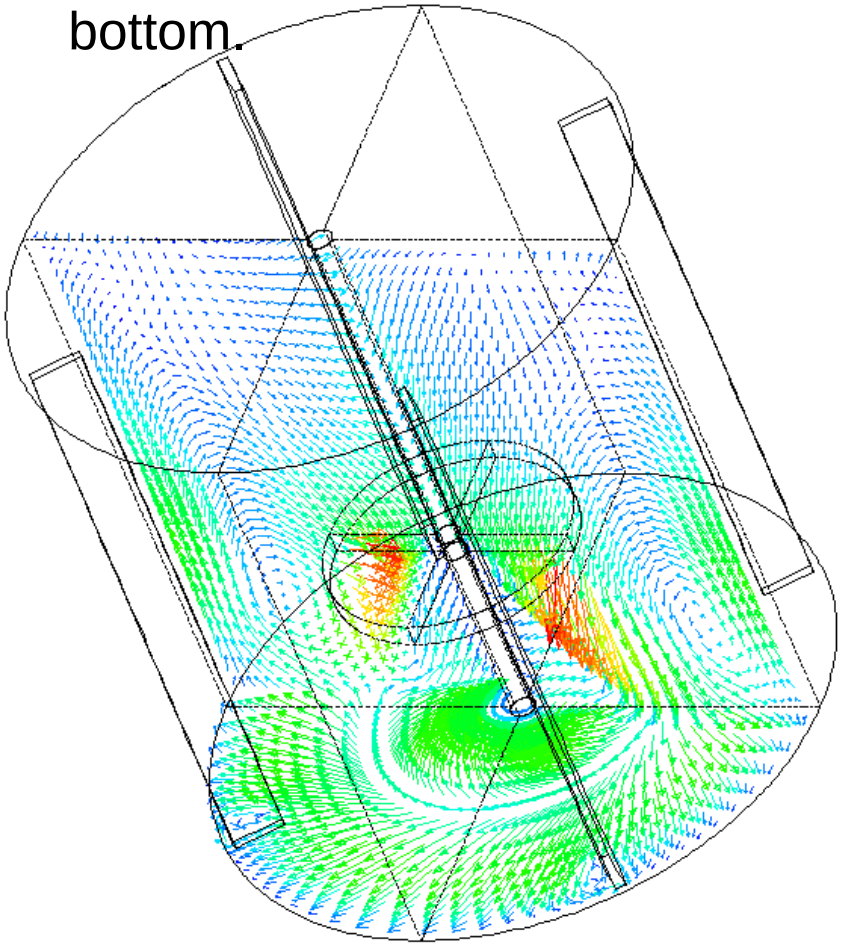
- Two ideal coaxial vortex rings with the same sense of rotation will leapfrog each other.
- The forward vortex increases in diameter and slows down. The rearward vortex shrinks and speeds up.
- Once the vortices traded places, the process repeats.
- The photographs on the left are experimental visualizations using smoke rings, and the figures on the right are Poincaré plots from a CFD simulation showing the same structures.



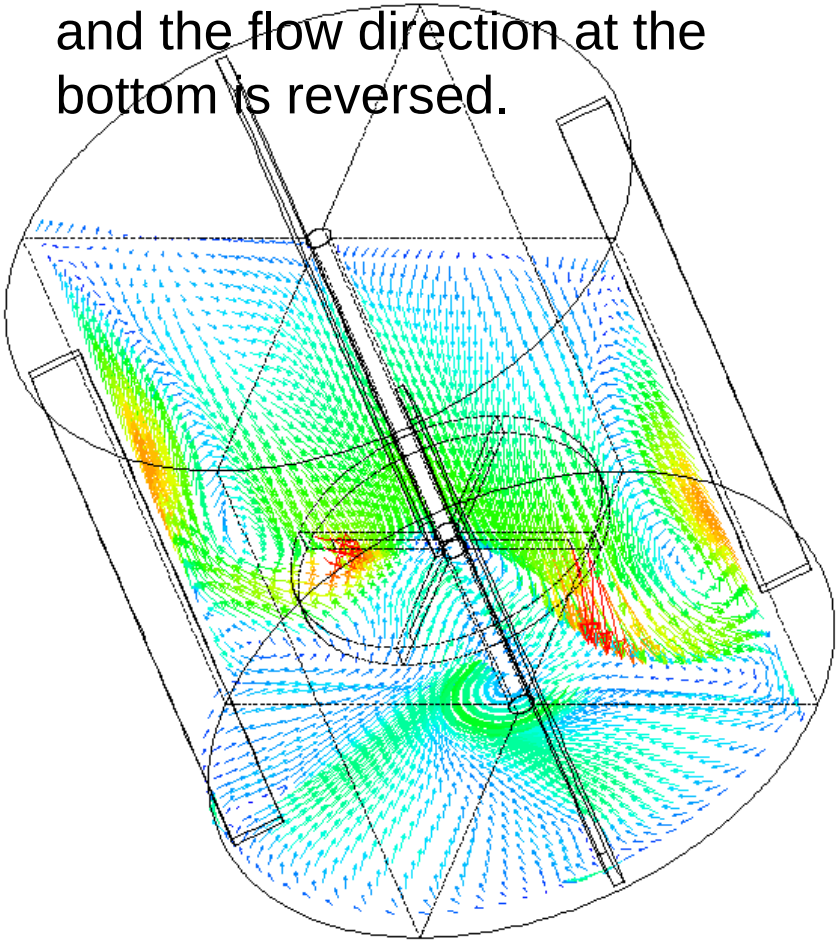
Aref and Naschie. Chaos applied to fluid mixing. Page 33 187. 1995.

Mixing vessel - velocity vectors

- Smaller diameter impeller (40% of vessel diameter).
- Impeller jet extends to the vessel bottom.

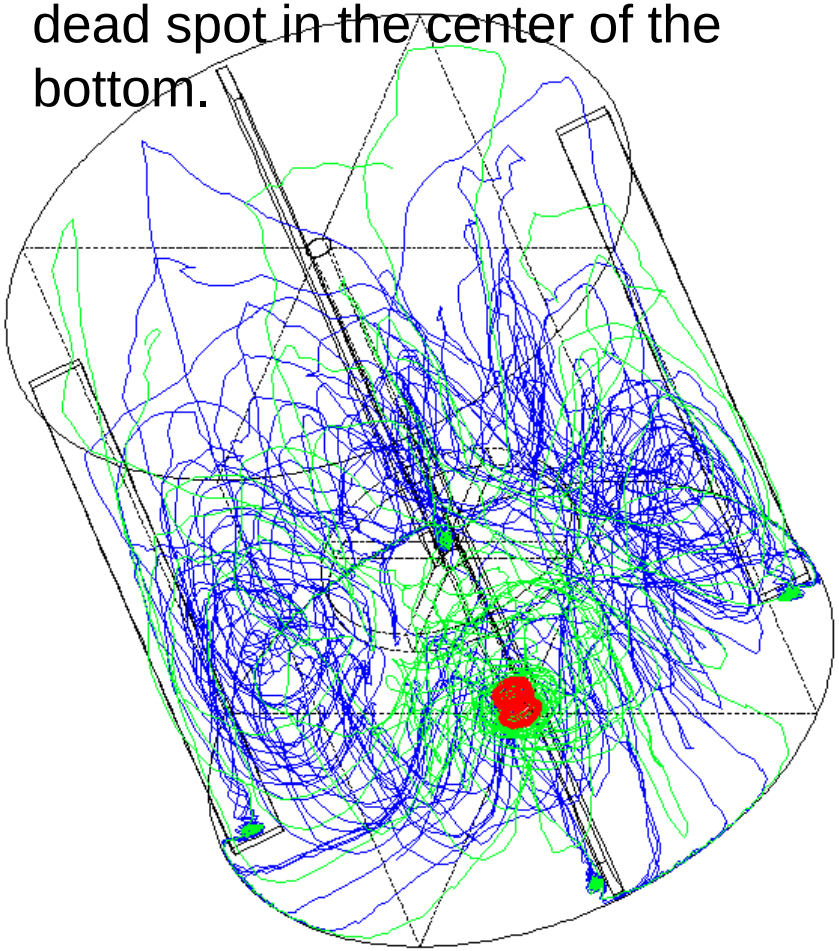


- Larger diameter impeller (50% of vessel diameter).
- Impeller jet bends off to the wall and the flow direction at the bottom is reversed.

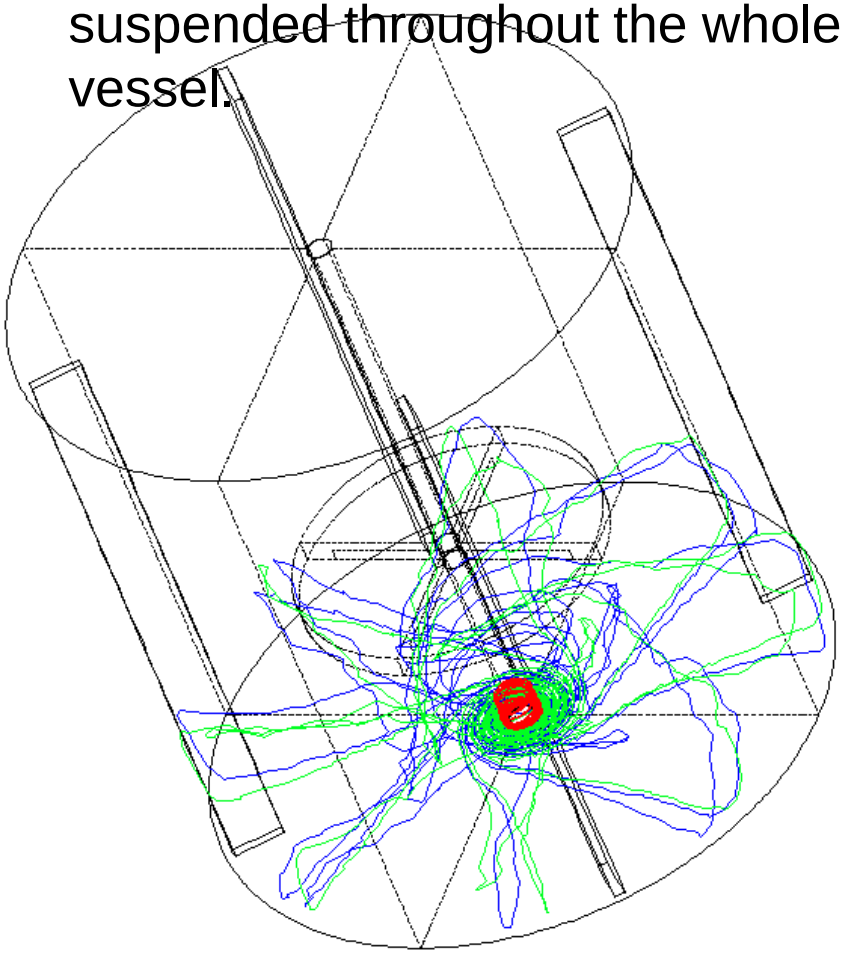


Mixing vessel - tracking of sand particles

- Smaller diameter impeller.
- The sand is dispersed throughout the whole vessel with a small dead spot in the center of the bottom.



- Larger diameter impeller.
- Due to the reversed flow pattern at the bottom, sand does not get suspended throughout the whole vessel.



Question: are particle trajectories closed?

- Not in turbulent flows.
- Viscous, periodic flows may have periodic points. These are points where the particle returns to its initial position after a certain amount of time.
- Brouwer's fixed-point theorem:

  Under a continuous mapping $f : S \rightarrow S$ *of an n- dimensional simplex into itself there exists at least one point* $x \in S$ *such that* $f(x)=x$.

- Application to particle tracks:
  - In viscous periodic flows in closed, simply connected domains there will always be at least one periodic point where a particle returned to its original location.
  - In other situations, there is no guarantee that there is any closed trajectory, and there may be none at all.

Question: how fast do particles separate?

- If we place two particles infinitesimally close together, will they stay together, or separate?
- The separation distance δ is governed by the Lyapunov exponent λ of the flow, which states that the particles will separate exponentially as a function of time t:

$$\delta(t) = \delta(0)e^{\lambda t}$$

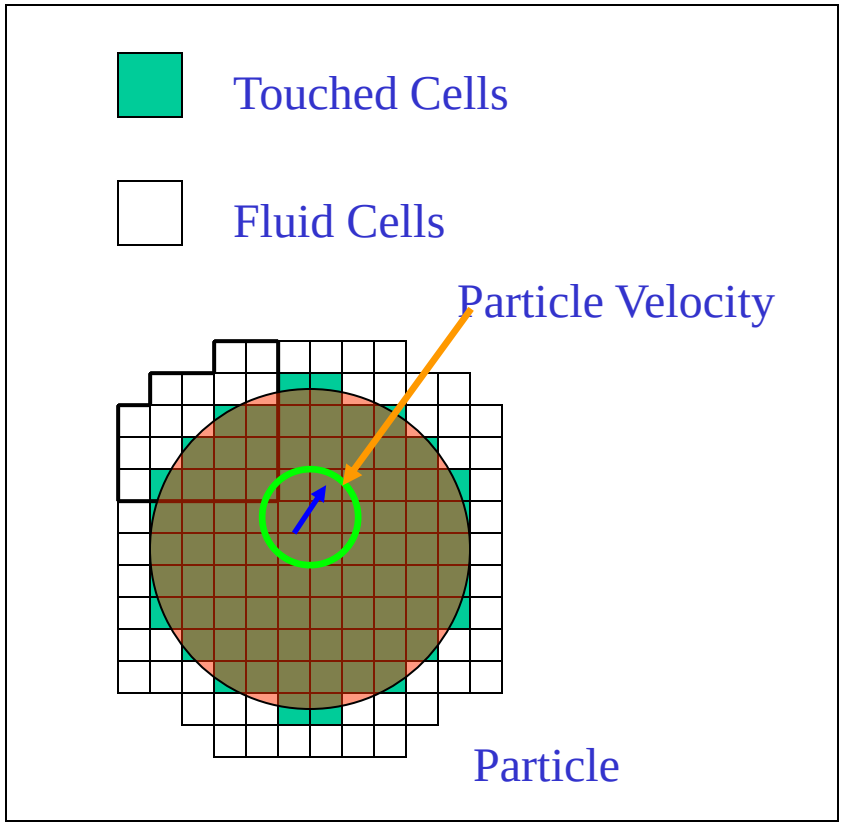
- The higher the Lyapunov exponent, the more chaotic the flow and the more stretching occurs.
- Lyapunov exponents can have any value, most of the time between 0 and 10, and usually between 0.5 and 1.

Particle tracking accuracy

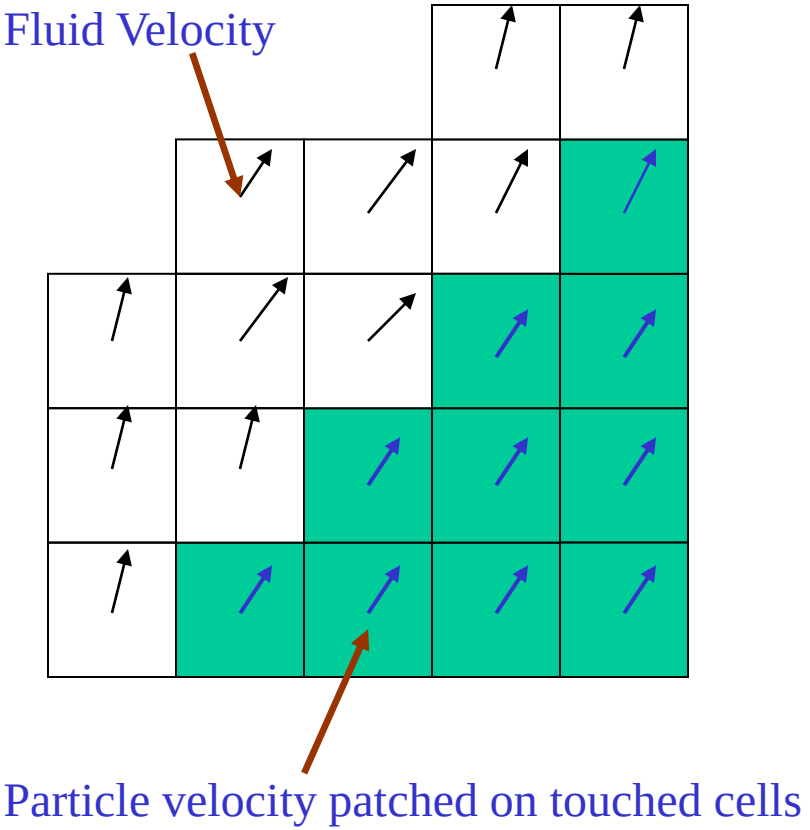
- There are three types of errors: discretization, time integration, and round-off.
- Research has shown that in regular laminar flows the error in the particle location increases as t^2, and in chaotic flows almost exponentially.
- Errors tend to align with the direction of the streamlines in most flows.
- As a result, even though errors multiply rapidly (e.g., 0.1% error for 20,000 steps is $1.001^{20,000}$ = 4.8E8), qualitative features of the flow as shown by the deformation of material lines can be properly reproduced. But the length of the material lines may be of by as much as 100%.
- Overall, particle tracking, when properly done, is less diffusive than solving for species transport, but numerical diffusion does exist.

Big particles: macroscopic particle model

- Large particles that cover multiple grid cells.
- Particles affect the flow field and collide.



- Special model implemented in FLUENT with user defined functions.



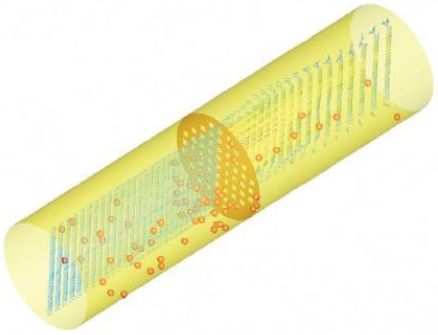
Tracking Big Particles

Particle tracking models in most commercial CFD software, such as the discrete phase model (DPM) in FLUENT, assume that particles are point masses that do not interact. Large particles immersed in the fluid flow cannot be modeled using this type of approach. The modeling of large (macroscopic) particles requires special treatment to take into account effects such as the blockage of fluid volume, the proper evolution of the drag force and torque experienced by the particles, particle-particle as well as particle-wall collisions, and friction dynamics.

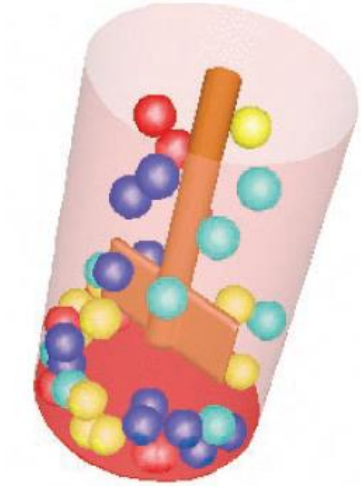
To account for these effects, a macroscopic particle model (MPM) has been developed for FLUENT 6 using user-defined functions (UDFs) and a customized graphical user interface (GUI). In the MPM approach, particles are treated in a Lagrangian frame of reference. Each particle is assumed to span several computational cells. A solid body velocity that describes the particle motion (translational and rotational) is patched in these cells. The volume fraction of the particle is also taken into account. By patching the rigid body motion of the particle, momentum is effectively added to the fluid. The integral of the momentum change, linear as well angular, gives the drag force and torque for each particle. These are used to compute the new positions and velocities of the particles at the next time-step. Additional forces, such as body forces, can also be included in the model. To detect a particle-wall collision, the model identifies the boundary faces (wall surfaces) the particle intersected during the previous time-step, if any. If a collision with a stationary wall is detected, the incoming particle velocity is projected onto the normal and tangential components of the reflected particle velocity, applying the coefficient of restitution and friction factor, as appropriate. In the same way, the model detects particle-particle collisions, and applies the principle of conservation of momentum to obtain the final velocities of both particles. The particle-wall collision algorithm also takes into account rotating or moving walls, so it can be used with both the sliding and deforming mesh models in FLUENT. The MPM UDF has been parallelized and works well with the FLUENT parallel solver.

The customized GUI is used to define all user inputs for the macroscopic particle model. The initial particle properties (positions, velocities, mass, radius) for each particle stream can be entered in the panel or read from a formatted ASCII file. MPM postprocessing tools have been coupled with FLUENT's DPM visualization tools, which allow particles to be displayed as shaded spheres with a defined radius. Transient particle data can also be saved in a Fieldview data file format.

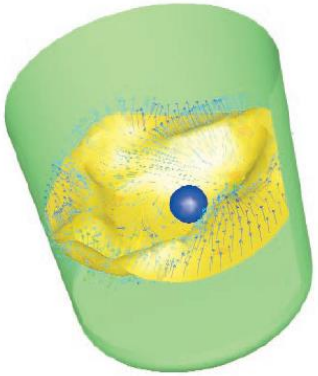
The macroscopic particle model has many industrial applications, especially in the pharmaceutical, chemical, material handling, and sports industries. Several validations have been performed. The tests have shown that a large number of particles (up to 1000) can easily be handled without the need for excessive computation time. ■



Macroscopic particles continuously injected through a filter element

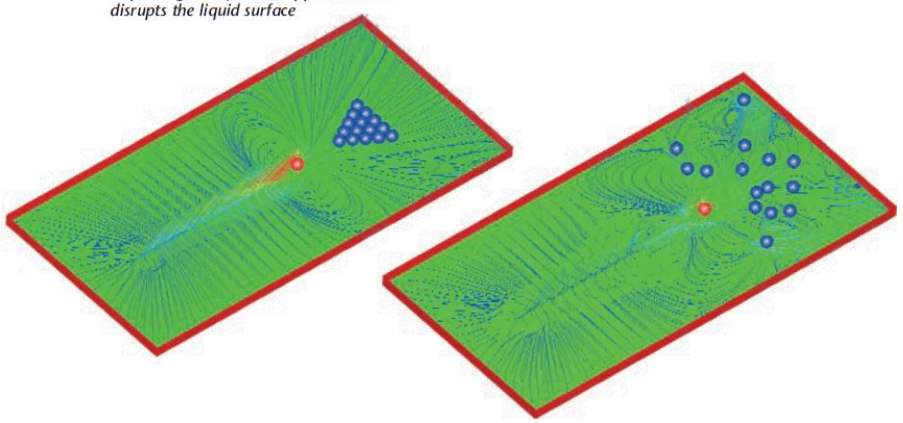


Balls of different mass continuously injected into a rotating paddle-type mixer



A spinning heavy ball dropped in water disrupts the liquid surface

Agrawal M., Bakker A., Prinkey M.T. (2003) Tracking Big Particles, Fluent Newsletter, Fall 2003, page 11.



Pathlines show the air flow (including recirculation) generated by the cue ball as it rolls towards the rack on a pool table (left) and just after it strikes and disperses the balls (right)

Summary

- Easy-to-use model.
- Clear and simple physics.
- Restricted to volume fractions < 10 %.
- Particle tracking can be used for a variety of purposes:
  - Visualization.
  - Residence time calculations.
  - Combustion.
  - Chemical reaction.
  - Drying.
  - Particle formation processes.
- Other methods exist for large particles.

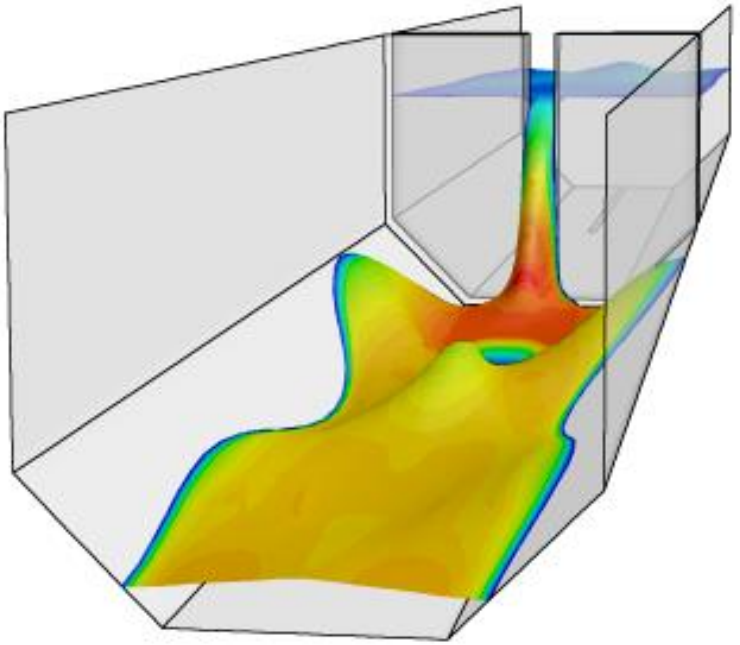
Lecture 16 - Free Surface Flows

Applied Computational Fluid Dynamics

André Bakker

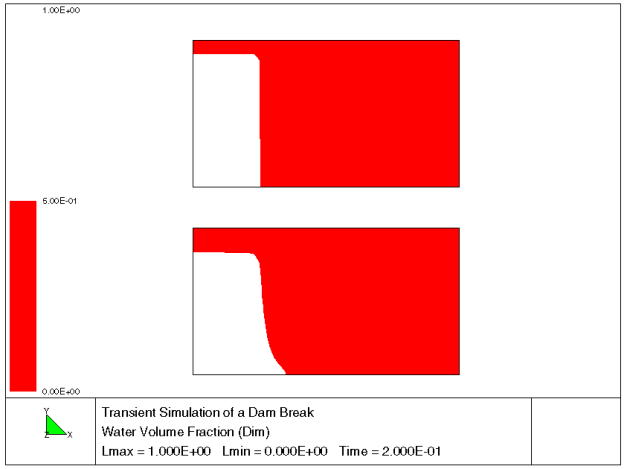
Free surface flow modeling techniques

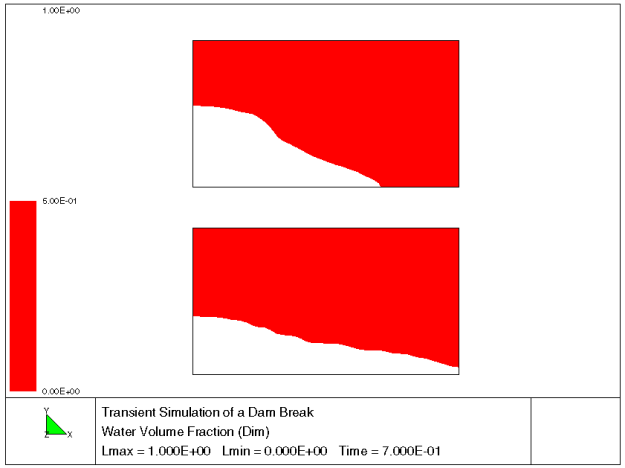
- Lagrangian methods:
  - The grid moves and follows the shape of the interface.
  - Interface is specifically delineated and precisely followed.
  - Suited for viscous, laminar flows.
  - Problems of mesh distortion, resulting in instability and internal inaccuracy.
- Eulerian methods:
  - Fluid travels between cells of the fixed mesh and there is no problem with mesh distortion.
  - Adaptive grid techniques.
  - Fixed grid techniques, e.g., volume of fluid (VOF) method.



Volume of fluid (VOF) model

- Immiscible fluids with clearly defined interface.
  - Shape of the interface is of interest.
- Typical problems:
  - Jet breakup.
  - Motion of large bubbles in a liquid.
  - Motion of liquid after a dam break.
  - Steady or transient tracking of any liquid-gas interface.
- Inappropriate if bubbles are small compared to a control volume (bubble columns).





VOF

- Assumes that each control volume contains just one phase (or the interface between phases).
- Solves one set of momentum equations for all fluids.

$$\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_i}\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \rho g_j + F_j$$

- Surface tension and wall adhesion modeled with an additional source term in momentum equation.
- For turbulent flows, single set of turbulence transport equations solved.
- Solves a volume fraction conservation equation for the secondary phase.

VOF solution strategies: time dependence

- Time-stepping for the VOF equation:
  - Automatic refinement of the time step for VOF equation using Courant number C:

$$C = \frac{\Delta t}{\Delta x_{cell} / u_{fluid}}$$

  - Δt is the minimum transit time for any cell near the interface.
- Calculation of VOF for each time-step:
  - Full coupling with momentum and continuity (VOF updated once per iteration within each time-step): more CPU time, less stable.
  - No coupling (default): VOF and properties updated once per time step. Very efficient, more stable but less accurate for very large time steps.

Volume fraction

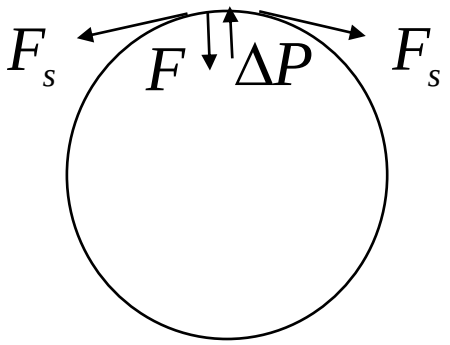
- Defines a step function ε equal to unity at any point occupied by fluid and zero elsewhere such that:

$$\varepsilon_k(_{cell}) = \frac{\iiint_{cell} \varepsilon_k(x,y,z)dxdydz}{\iiint_{cell} dxdydz}$$

- For volume fraction of kth fluid, three conditions are possible:
  - $\varepsilon_k = 0$ if cell is empty (of the k^{th} fluid).
  - $\varepsilon_k = 1$ if cell is full (of the k^{th} fluid).
  - $0 < \varepsilon_k < 1$ if cell contains the interface between the fluids.

Surface tension

- Surface tension along an interface arises from attractive forces between molecules in a fluid (cohesion).
- Near the interface, the net force is radially inward. Surface contracts and pressure increases on the concave side.
- At equilibrium, the opposing pressure gradient and cohesive forces balance to form spherical bubbles or droplets.



$$\Delta P = \sigma \left(\frac{1}{R_1} + \frac{1}{R_2} \right)$$

Surface tension - when important

- To determine significance, first evaluate the Reynolds number.

$$\boldsymbol{Re} = \frac{\rho U L}{\mu}$$

- For Re << 1, evaluate the Capillary number.

$$\boldsymbol{Ca} = \frac{\mu U}{\sigma}$$

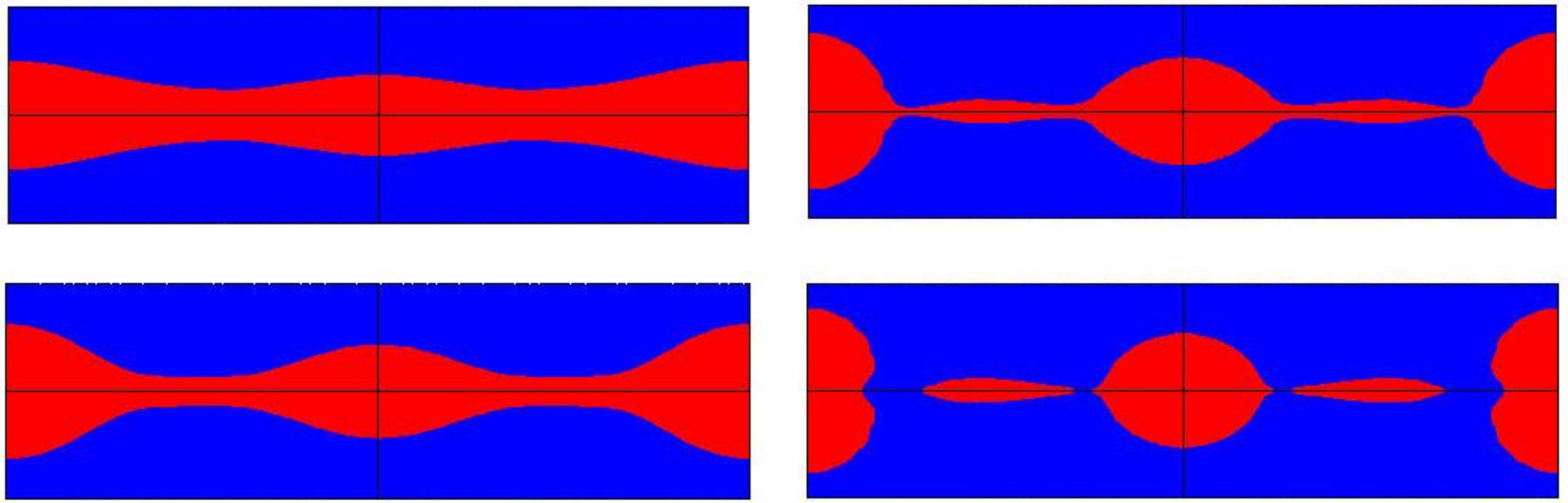
- For Re >> 1, evaluate the Weber number.

$$\boldsymbol{We} = \frac{\sigma}{\rho L U^2}$$

- Surface tension important when We >>1 or Ca<< 1.
- Surface tension modeled with an additional source term in momentum equation.

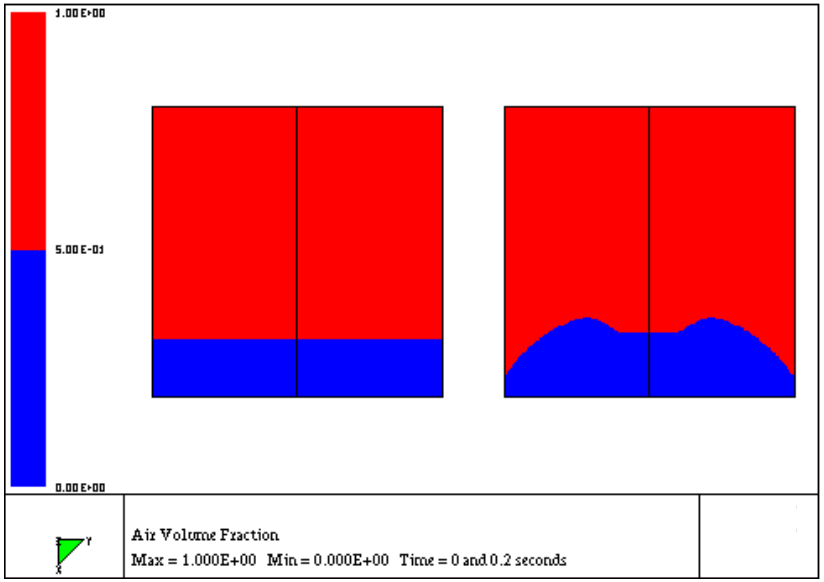
Surface tension example

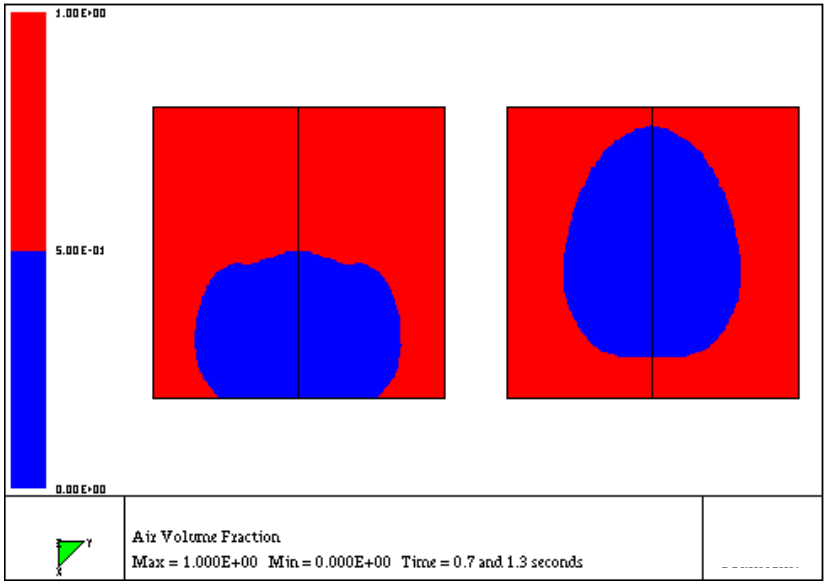
- Cylinder of water (5 x 1 cm) is surrounded by air in no gravity.
- Surface is initially perturbed so that the diameter is 5% larger on ends.
- The disturbance at the surface grows by surface tension.



Wall adhesion

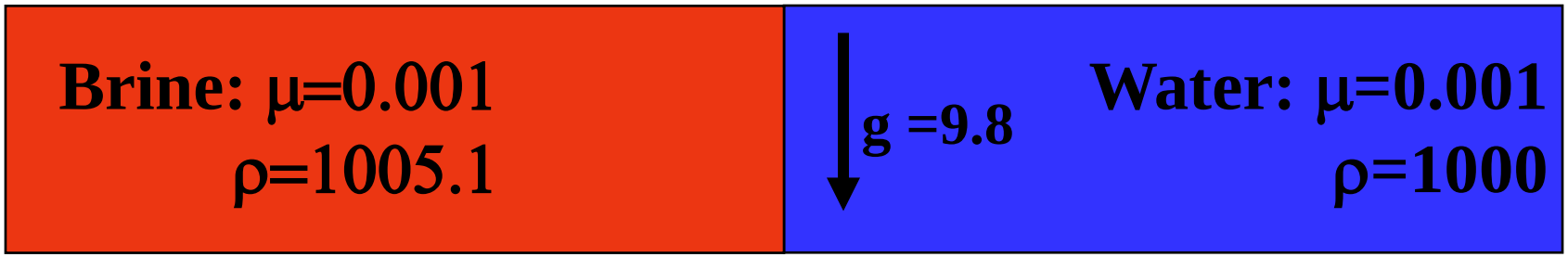
- Large contact angle (> 90°) is applied to water at bottom of container in zero-gravity field.
- An obtuse angle, as measured in water, will form at walls.
- As water tries to satisfy contact angle condition, it detaches from bottom and moves slowly upward, forming a bubble.



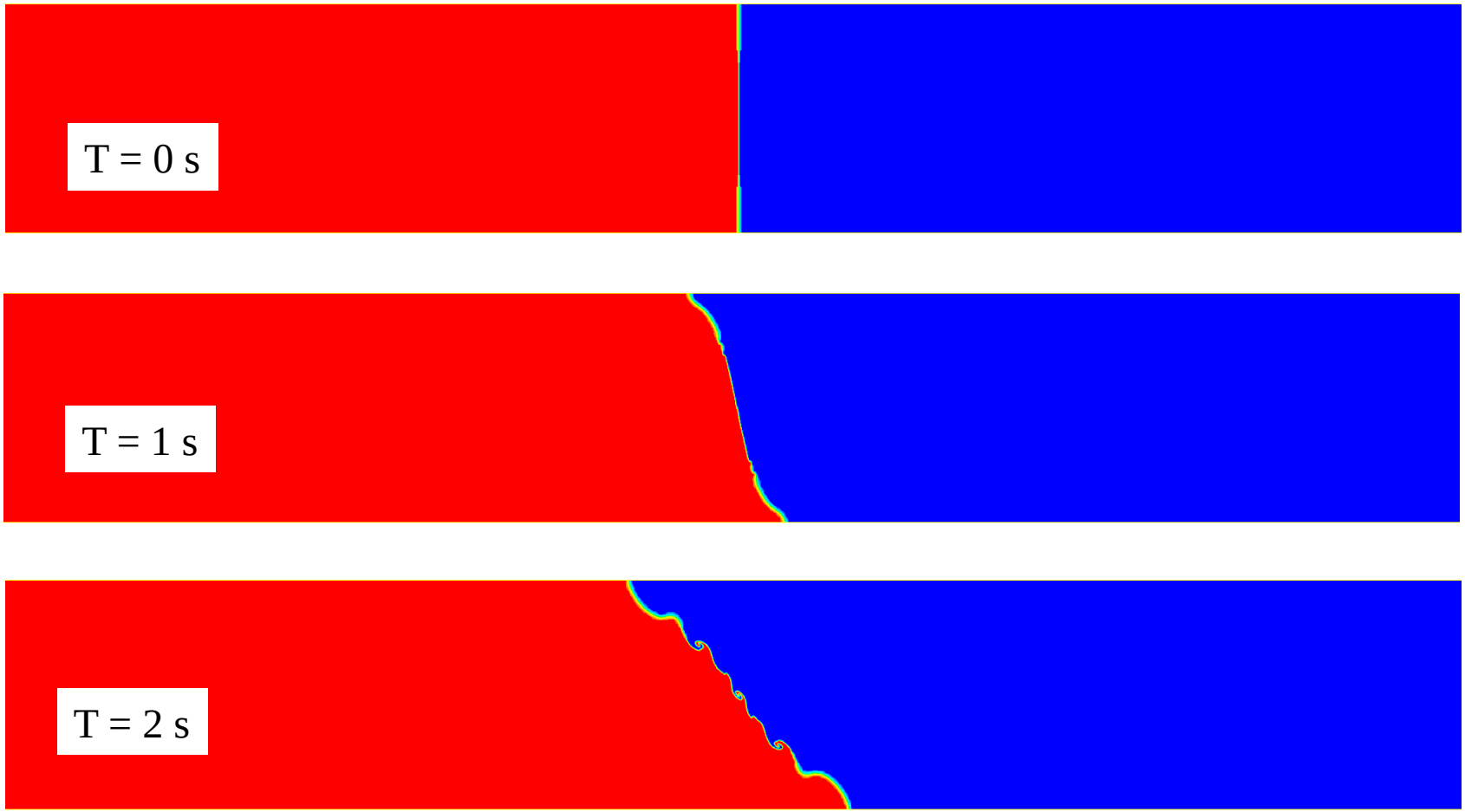


Example: modeling of the gravity current

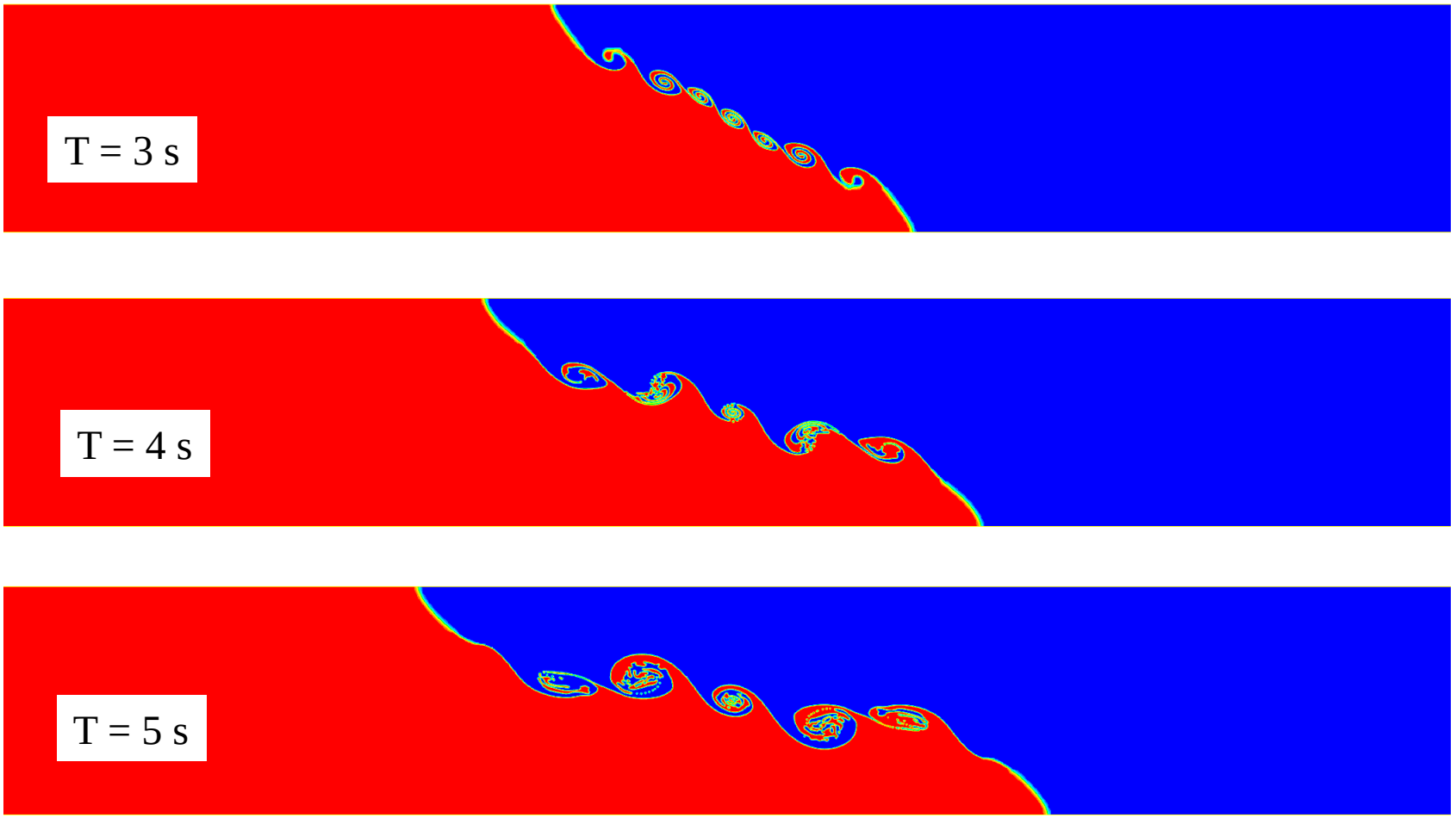
- Mixing of brine and fresh water.
  - 190K cells with hanging nodes.
  - Domain: length 1m, height 0.15m.
  - Time step: 0.002 s.
  - PISO algorithm.
  - Geometric reconstruction scheme.
  - QUICK scheme for momentum.



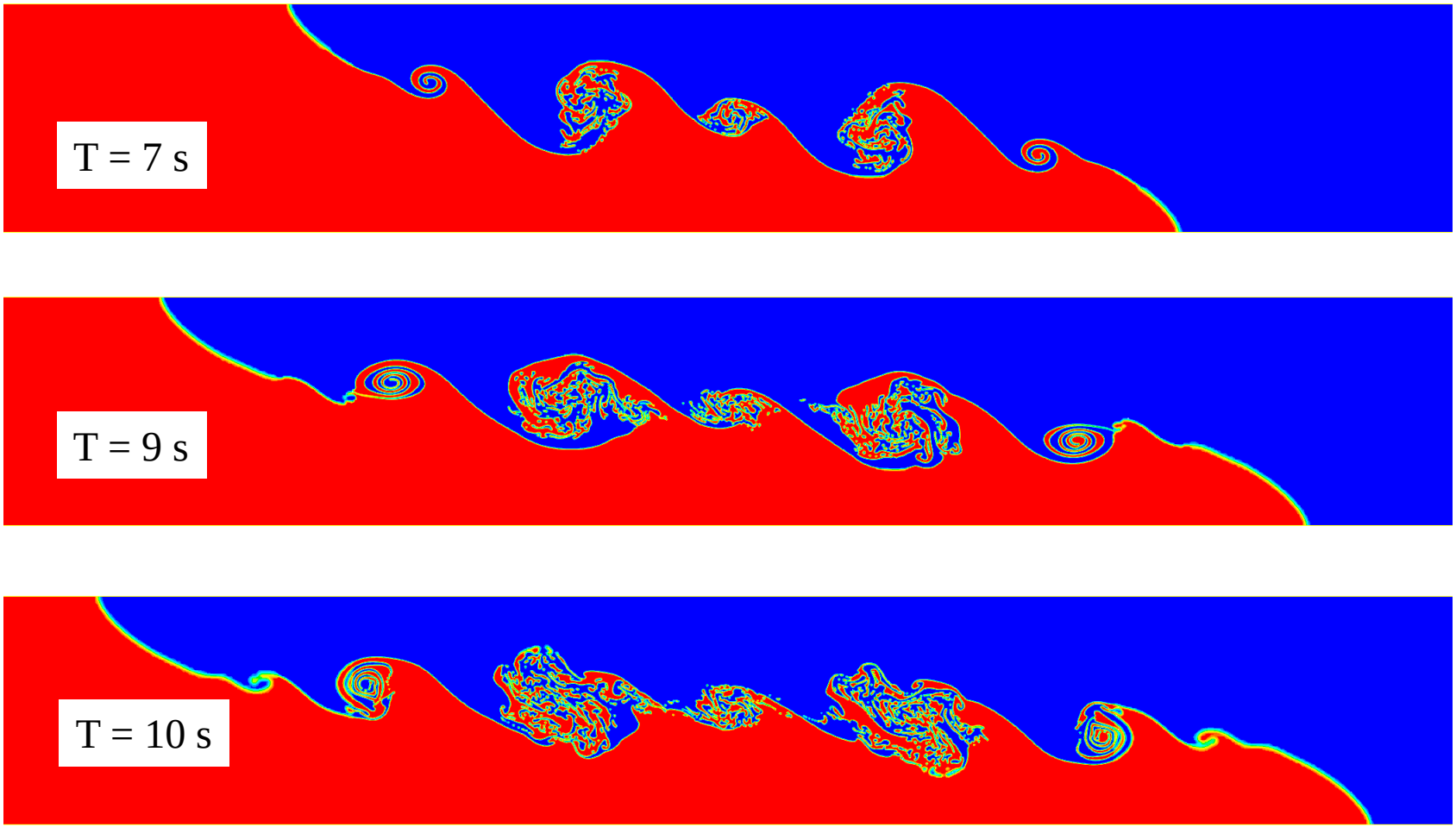
Gravity current (1)



Gravity current (2)

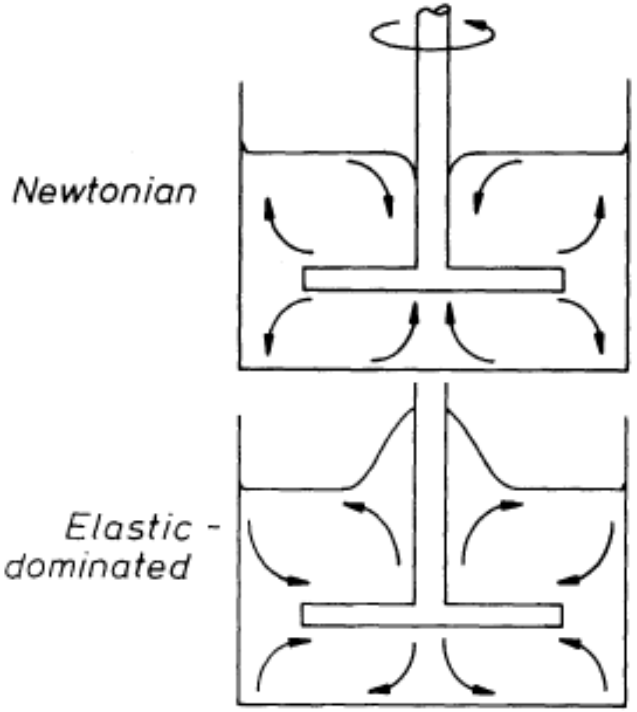


Gravity current (3)



Visco-elastic fluids - Weissenberg effect

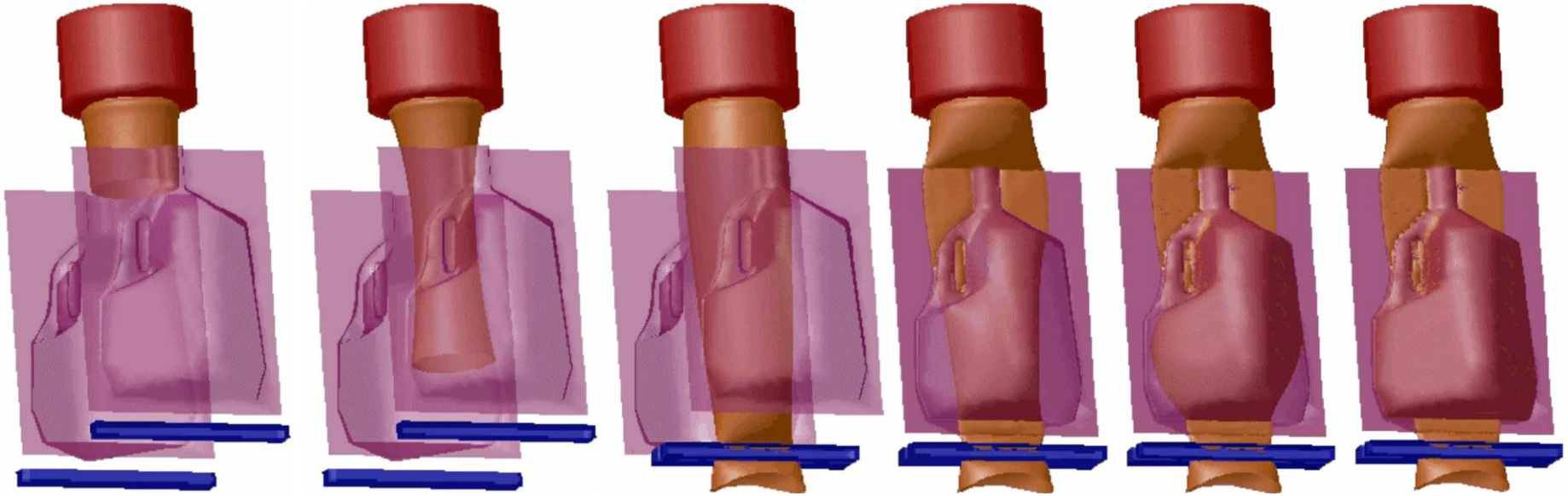
- Visco-elastic fluids, such as dough and certain polymers, tend to climb up rotating shafts instead of drawing down a vortex.
- This is called the Weissenberg effect and is very difficult to model.
- The photograph shows the flow of a solution of polyisobutylene.



Images: Barnes et al. [1]

Example: visco-elastic fluids - blow molding

- Blow molding is a commonly used technique to manufacture bottles, canisters, and other plastic objects.
- Important parameters to model are local temperature and material thickness.



Summary

- Free surface flows are encountered in many different applications:
  - Flow around a ship.
  - Blow molding.
  - Extrusion.
  - Mold filling.
- There are two basic ways to model free surface flows:
  - Lagrangian: the mesh follows the interface shape.
  - Eulerian: the mesh is fixed, and a local volume fraction is calculated.
- The most common method used in CFD programs based on the finite volume method is the volume-of-fluid (VOF) model.

Conservation Equations Overview

Applied Computational Fluid Dynamics

André Bakker

OVERVIEW BALANCE EQUATIONS ISOTHERMAL SINGLE-PHASE FLOW AND TURBULENCE MODELS

André Bakker

CONTENTS

The continuity equation:

$$\vec{\nabla}.\vec{U} = 0$$

The momentum balance:

$$\vec{\nabla}.(\vec{U}\vec{U}) = \vec{\nabla}.(\vec{\vec{\pi}} + \vec{\vec{\pi}}_T)$$

The molecular stress tensor:

$$\vec{\vec{\pi}} = -\frac{P}{\rho}\vec{\vec{I}} + \nu(\vec{\nabla}\vec{U} + (\vec{\nabla}\vec{U})^T)$$

The Reynolds stress tensor:

$$\vec{\vec{\pi}}_T = -\overline{\vec{u}\vec{u}}$$

k-ε model:

$$\vec{\vec{\pi}}_T = -\frac{2}{3}k\vec{\vec{I}} + \nu_t(\vec{\nabla}\vec{U} + (\vec{\nabla}\vec{U})^T)$$

Turbulent viscosity:

$$\nu_t = c_\mu k^2/\varepsilon$$

Model equation for k:

$$\vec{U}.\vec{\nabla}k = \vec{\nabla}.((\nu + \nu_t/\sigma_k)\vec{\nabla}k) + P_k - \varepsilon$$

$$P_k = -\overline{\vec{u}\vec{u}}:(\vec{\nabla}\vec{U})$$

Model equation for ε:

$$\vec{U}.\vec{\nabla}\varepsilon = \vec{\nabla}.((\nu + \nu_t/\sigma_\varepsilon)\vec{\nabla}\varepsilon) + c_{\varepsilon 1}\frac{\varepsilon}{k}P_k - c_{\varepsilon 2}\frac{\varepsilon^2}{k}$$

Algebraic stress model:

$$\vec{\vec{\pi}}_T = \frac{2}{3}k\vec{\vec{I}}\left[1 - \frac{(1-c_2)\frac{P_k}{\varepsilon}}{\frac{P_k}{\varepsilon}-(1-c_1)}\right] + \frac{1-c_2}{\frac{P_k}{\varepsilon}-(1-c_1)}\frac{k}{\varepsilon}\left(\vec{\vec{P}} - \frac{2}{3}P_k\vec{\vec{I}}\right)$$

$$\vec{\vec{P}} = -\left(\overline{\vec{u}\vec{u}}.(\vec{\nabla}\vec{U}) + (\overline{\vec{u}\vec{u}}.(\vec{\nabla}\vec{U}))^T\right)$$

CONTINUITY EQUATION

$$\frac{\partial \hat{\rho}}{\partial t} + \frac{\partial}{\partial x_i}(\hat{\rho}\,\hat{U}_i) = 0$$

MOMENTUM BALANCE

$$\frac{\partial}{\partial t}(\hat{\rho}\hat{U}_i) + \frac{\partial}{\partial x_k}(\hat{\rho}\hat{U}_i\hat{U}_k) = -\frac{\partial \hat{P}}{\partial x_i} + \frac{\partial}{\partial x_k}\left(\mu\left(\frac{\partial \hat{U}_i}{\partial x_k} + \frac{\partial \hat{U}_k}{\partial x_i} - \frac{2}{3}\frac{\partial \hat{U}_m}{\partial x_m}\delta_{ik}\right)\right) + \hat{\rho} g_i$$

$$\frac{2}{3}\frac{\partial \hat{U}_m}{\partial x_m}\delta_{ik} = 0 \quad \text{for incompressible flows}$$

MEAN MOTION - CONTINUITY

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho\, U_i) = 0$$

For incompressible flows:

$$\frac{\partial U_i}{\partial x_i} = 0$$

MEAN MOTION - MOMENTUM

$$\frac{\partial}{\partial t}(\rho U_i) + \frac{\partial}{\partial x_j}(\rho U_i U_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_k}\left(\mu\frac{\partial U_k}{\partial x_k} - \mu\frac{2}{3}\frac{\partial U_m}{\partial x_m}\delta_{ik} - \rho\overline{u_i u_k}\right) + \rho g_i$$

For incompressible flows:

$$\frac{\partial U_i}{\partial t} + U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_k}\left(\nu\frac{\partial U_k}{\partial x_k} - \overline{u_i u_k}\right) + g_i$$

DEFINITIONS REYNOLDS AVERAGING

$$\hat{U}_i = U_i + u_i$$

$$\overline{\hat{U}_i\hat{U}_j} = U_i U_j + \overline{u_i u_j}$$

$$\overline{\hat{U}_i} = U_i$$

$$\overline{u_i} = 0$$

$$\hat{\Phi} = \Phi + \varphi$$

$$\overline{\hat{\Phi}} = \Phi$$

$$\overline{\varphi} = 0$$

$$\overline{\hat{\Phi}\,\hat{U}_i} = \Phi\, U_i + \overline{\varphi\, u_j}$$

$$\overline{\hat{\rho}} = \rho$$

$$\hat{P} = P + p$$

REYNOLDS STRESSES - ANALYTICAL EQUATION (incompressible flow)

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + U_k \frac{\partial}{\partial x_k}(\overline{u_i u_j}) = - \underbrace{\left(\overline{u_j u_k} \frac{\partial U_i}{\partial x_k} + \overline{u_i u_k} \frac{\partial U_j}{\partial x_k} \right)}_{\text{(A)}}$$

$$- \underbrace{\frac{\partial}{\partial x_k} \left(\overline{u_i u_j u_k} - \nu \frac{\partial}{\partial x_k}(\overline{u_i u_j}) + \overline{\frac{p}{\rho}(u_i \delta_{jk} + u_j \delta_{ik})} \right)}_{\text{(B)}}$$

$$+ \underbrace{\overline{\frac{p}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)}}_{\text{(C)}} - \underbrace{2\nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}}}_{\text{(D)}}$$

(A) Rate of generation of $\overline{u_i u_j}$ by the effects of the mean strain. Transfer of energy from the mean flow to turbulence. Symbol P_{ij}.

(B) "Diffusion" D_{ij} of $\overline{u_i u_j}$ in three components:

(1) "turbulent" diffusion involving triple products.

(2) "viscous" diffusion written in this way for convenience.

(3) "pressure" diffusion.

(C) The pressure-strain correlation. Symbol Ψ_{ij}. Appears by rearrangement of the pressure terms:

$$\overline{u_j \frac{\partial}{\partial x_i}(P+p)} = \overline{u_j \frac{\partial p}{\partial x_i}} = \frac{\partial}{\partial x_i}\overline{(p u_j)} - p \overline{\frac{\partial u_j}{\partial x_i}} = \frac{\partial}{\partial x_k}\overline{(p u_j)} - p \overline{\frac{\partial u_j}{\partial x_i}}$$

This decomposition into pressure diffusion plus pressure strain is convenient because the second component has zero trace on contraction. It is not unique.

(D) Viscous destruction of $\overline{u_i u_j}$. Symbol ε_{ij}. Appears by rearrangement of the viscous terms.

$$\overline{\nu u_j \frac{\partial^2}{\partial x_k^2}(U_i + u_i)} + \overline{\nu u_i \frac{\partial^2}{\partial x_k^2}(U_j + u_j)} = \nu \frac{\partial^2}{\partial x_k^2}\overline{(u_i u_j)} - 2\nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}}$$

Convenient because the first component has the form of viscous gradient diffusion of $\overline{u_i u_j}$. The second component has useful properties.

TURBULENT KINETIC ENERGY - ANALYTICAL EQUATION (Incompressible flow)

$$k = \frac{1}{2} \overline{u_i u_i}$$

$$\frac{\partial k}{\partial t} + U_k \frac{\partial k}{\partial x_k} = \underbrace{- \overline{u_i u_k} \frac{\partial U_i}{\partial x_k}}_{\text{(A)}} \underbrace{- \frac{\partial}{\partial x_k}\left(\frac{1}{2} \overline{u_k u_i^2} - \nu \frac{\partial k}{\partial x_k} + \overline{\frac{p}{\rho} u_k} \right)}_{\text{(B)}} \underbrace{- \nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k}}}_{\text{(C)}}$$

(A) Production rate of k by interaction with the mean strain rate. Symbol P_k.

(B) "Diffusion" of k: (1) "Turbulent", (2) "Viscous", (3) "Pressure"

(C) Viscous destruction of k, symbol ε.

TURBULENT KINETIC ENERGY - MODEL EQUATION (Incompressible flow)

$$\frac{\partial k}{\partial t} + U_k \frac{\partial k}{\partial x_k} = \frac{\partial}{\partial x_k}\left((\nu + \nu_t/\sigma_k) \frac{\partial k}{\partial x_k} \right) + P_k - \varepsilon$$

$$P_k = - \overline{u_i u_k} \frac{\partial U_i}{\partial x_k}$$

$$\nu_t = c_\mu k^2/\varepsilon$$

$$c_\mu = 0.09$$

$$\sigma_k = 1.0$$

This model equation is used in both the low Reynolds no. and the high Reynolds no. k-ε eddy viscosity model, as well as in higher order closure models like the ASM model and full Reynolds stress models.

ENERGY DISSIPATION RATE - ANALYTICAL EQUATION

$$\varepsilon = \nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_k}}$$

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = -\frac{\partial}{\partial x_k}\left(\nu u_k \overline{\frac{\partial u_i}{\partial x_1} \frac{\partial u_i}{\partial x_1}} + 2 \frac{\nu}{\rho} \overline{\frac{\partial p}{\partial x_i} \frac{\partial u_k}{\partial x_i}} - \nu \frac{\partial \varepsilon}{\partial x_k} \right)$$

$\{1\}$ $\{1\}$ $\{Re_l^{-1}\}$

$$- 2 \nu \frac{\partial U_i}{\partial x_k} \left(\overline{\frac{\partial u_i}{\partial x_1} \frac{\partial u_k}{\partial x_1}} + \overline{\frac{\partial u_1}{\partial x_i} \frac{\partial u_1}{\partial x_k}} \right) - 2 \nu \overline{u_k \frac{\partial u_i}{\partial x_1}} \frac{\partial^2 U_i}{\partial x_k \partial x_1}$$

$\{Re_l^{-1/2}\}$ $\{Re_l^{-1/2}\}$

$$- 2 \nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_1} \frac{\partial u_k}{\partial x_1}} - 2 \overline{\left(\nu \frac{\partial^2 u_1}{\partial x_k \partial x_1}\right)^2}$$

$\{Re_l^{+1/2}\}$ $\{Re_l^{+1/2}\}$

ENERGY DISSIPATION RATE AT HIGH REYNOLDS NUMBERS

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = \underbrace{-\frac{\partial}{\partial x_k}\left(\nu u_k \overline{\frac{\partial u_i}{\partial x_1} \frac{\partial u_i}{\partial x_1}} + 2 \frac{\nu}{\rho} \overline{\frac{\partial p}{\partial x_i} \frac{\partial u_k}{\partial x_i}} \right)}_{(A)} \underbrace{- 2\nu \overline{\frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_1} \frac{\partial u_k}{\partial x_1}}}_{(B)} \underbrace{- 2 \overline{\left(\nu \frac{\partial^2 u_i}{\partial x_k \partial x_1}\right)^2}}_{(C)}$$

Terms (B) and (C) individually vary as $Re_l^{1/2}$, i.e. become infinite, but when taken together are of order unity. When these terms are modelled they must be modelled together! However, the ε equation is in general modelled using a standard type of convection/diffusion equation assuming isotropy:

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = \frac{\partial}{\partial x_k}\left((\nu + \nu_t/\sigma_\varepsilon) \frac{\partial \varepsilon}{\partial x_k} \right) + c_{\varepsilon 1} \frac{\varepsilon}{k} P_k - c_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

$c_\varepsilon = 1.3$ $c_{\varepsilon 1} = 1.45$ $c_{\varepsilon 2} = 1.92$ $\sigma_\varepsilon = 1.3$

HIGH REYNOLDS NO. k-ε MODEL (incompressible flow)

$$\overline{u_i u_j} = -\nu_t \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + \frac{2}{3} \delta_{ij} k$$

$$\nu_t = c_\mu k^2/\varepsilon$$

$$\frac{\partial k}{\partial t} + U_k \frac{\partial k}{\partial x_k} = \frac{\partial}{\partial x_k}\left((\nu + \nu_t/\sigma_k) \frac{\partial k}{\partial x_k} \right) + P_k - \varepsilon$$

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = \frac{\partial}{\partial x_k}\left((\nu + \nu_t/\sigma_\varepsilon) \frac{\partial \varepsilon}{\partial x_k} \right) + c_{\varepsilon 1} \frac{\varepsilon}{k} P_k - c_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

$$P_k = - \overline{u_i u_k} \frac{\partial U_i}{\partial x_k}$$

$c_\mu = 0.09$ $c_{\varepsilon 1} = 1.44$ $c_{\varepsilon 2} = 1.92$ $\sigma_k = 1.0$ $\sigma_\varepsilon = 1.3$

LOW REYNOLDS NO. k-ε MODEL (incompressible flow)

$$\frac{\partial \tilde{\varepsilon}}{\partial t} + U_k \frac{\partial \tilde{\varepsilon}}{\partial x_k} = \frac{\partial}{\partial x_k}\left((\nu + \nu_t/\sigma_\varepsilon) \frac{\partial \tilde{\varepsilon}}{\partial x_k} \right) + c_{\varepsilon 1} \frac{\varepsilon}{k} P_k - c_{\varepsilon 2} \frac{\varepsilon^2}{k} + 2\nu\nu_t \left(\frac{\partial^2 U_i}{\partial x_k \partial x_1} \right)^2$$

$$\varepsilon = \tilde{\varepsilon} + 2 \nu \left(\frac{\partial \sqrt{k}}{\partial x_j} \right)^2$$

$$\nu_t = c_\mu k^2/\tilde{\varepsilon}$$

$$c_\mu = 0.09 \exp\left[-3.4/(1 + R_t/50)^2 \right]$$

$$c_{\varepsilon 2} = 1.92 \ (1 - 0.3 \exp(-R_t^2))$$

$$R_t = k^2/(\nu\tilde{\varepsilon})$$

The other equations are the same as in the high Reynolds no. k-ε model.

(Reynolds stress model)

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + U_k \frac{\partial}{\partial x_k}(\overline{u_i u_j}) = P_{ij} + D_{ij} + \Psi_{ij} - \varepsilon_{ij}$$

P_{ij} Production by mean strain rate, requires no modelling:

$$P_{ij} = - \left(\overline{u_j u_k} \frac{\partial U_i}{\partial x_k} + \overline{u_i u_k} \frac{\partial U_j}{\partial x_k} \right)$$

D_{ij} Diffusion, can be modelled using a gradient diffusion approximation:

$$D_{ij} = \frac{\partial}{\partial x_k} \left(c_s \frac{k}{\varepsilon} \overline{u_k u_l} \frac{\partial}{\partial x_l}(\overline{u_i u_j}) \right)$$

A model constant $c_s = 0.22$ has been introduced. The following simpler model is also used:

$$D_{ij} = \frac{\partial}{\partial x_k} \left(\nu_t \frac{\partial}{\partial x_k}(\overline{u_i u_j}) \right)$$

Instead of ν_t only, $(\nu + \nu_t)$ can also be used.

Ψ_{ij} The pressure-strain relation can be modelled by:

$$\Psi_{ij} = - c_1 \frac{\varepsilon}{k} \left(\overline{u_i u_j} - \frac{2}{3} k \delta_{ij} \right) - c_2 \left(P_{ij} - \frac{2}{3} P_k \delta_{ij} \right)$$

$$P_k = \frac{1}{2} P_{ii}$$

ε_{ij} Viscous destruction, can be modelled by (assuming isotropy):

$$\varepsilon_{ij} = \frac{2}{3} \delta_{ij} \varepsilon$$

The turbulent kinetic energy is calculated using the standard model equation:

$$\frac{\partial k}{\partial t} + U_k \frac{\partial k}{\partial x_k} = \frac{\partial}{\partial x_k} \left((\nu + \nu_t/\sigma_k) \frac{\partial k}{\partial x_k} \right) + P_k - \varepsilon$$

The energy dissipation rate can be calculated using the model equation from the k-ε model:

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = \frac{\partial}{\partial x_k} \left((\nu + \nu_t/\sigma_\varepsilon) \frac{\partial \varepsilon}{\partial x_k} \right) + c_{\varepsilon 1} \frac{\varepsilon}{k} P_k - c_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

or, using the information about the anisotropy in the flow, the following equation can be used:

$$\frac{\partial \varepsilon}{\partial t} + U_k \frac{\partial \varepsilon}{\partial x_k} = \frac{\partial}{\partial x_k} \left(c_\varepsilon \frac{k}{\varepsilon} \overline{u_k u_l} \frac{\partial \varepsilon}{\partial x_k} \right) + c_{\varepsilon 1} \frac{\varepsilon}{k} P_k - c_{\varepsilon 2} \frac{\varepsilon^2}{k}$$

The model constants are:

$c_s = 0.22$
$c_1 = 1.80$
$c_2 = 0.60$
$c_\varepsilon = 0.18$
$c_{\varepsilon 1} = 1.44$
$c_{\varepsilon 2} = 1.92$

MODEL EQUATION EQUATIONS ASM-MODEL (incompressible flow)

(Algebraic stress turbulence model)

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + U_k \frac{\partial}{\partial x_k}(\overline{u_i u_j}) = P_{ij} + D_{ij} + \Psi_{ij} - \varepsilon_{ij}$$

This equation can be simplified by combining the convection and diffusion terms:

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + \left[U_k \frac{\partial}{\partial x_k}(\overline{u_i u_j}) + \frac{\partial}{\partial x_k}\left(\nu_t \frac{\partial}{\partial x_k}(\overline{u_i u_j}) \right) \right] = P_{ij} + \Psi_{ij} - \varepsilon_{ij}$$

which leads to:

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + T_{ij} = P_{ij} + \Psi_{ij} - \varepsilon_{ij}$$

This equation can be simplified using Rodi's approximation. It is assumed that the transport of $\overline{u_i u_j}$ is proportional to the transport of k, with the ratio $\overline{u_i u_j}/k$ as proportionality factor:

$$\frac{\partial}{\partial t}(\overline{u_i u_j}) + T_{ij} = \frac{\overline{u_i u_j}}{k}\left(\frac{\partial k}{\partial t} + U_k \frac{\partial k}{\partial x_k} - \mathrm{Diff}(k) \right) = \frac{\overline{u_i u_j}}{k}(P_k - \varepsilon)$$

This results in the following algebraic equation for the Reynolds stresses:

$$\overline{u_i u_j} = \frac{2}{3} k \delta_{ij} \left[1 - \frac{(1-c_2)\frac{P_k}{\varepsilon}}{\frac{P_k}{\varepsilon}-(1-c_1)} \right] + \frac{1-c_2}{\frac{P_k}{\varepsilon}-(1-c_1)} \frac{k}{\varepsilon}\left(P_{ij} - \frac{2}{3} P_k \delta_{ij} + \frac{c_3}{1-c_2} A_{ij} \right)$$

The term A_{ij} is the so-called added convection term, which is zero when the equations are written out in cartesian coordinates but plays an important role when the equations are written in cylindrical-polar coordinates.

The equations used for calculating k and ε are the same as in the Reynolds stress model.

The model constants are: $c_1 = 2.50$

$c_2 = 0.55$

VECTOR NOTATION

$\vec{X}.\vec{Y} = x_i y_i$

(Scalar/dot product)

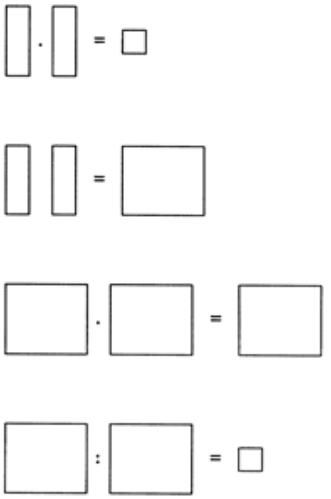
$\vec{X}\vec{Y} = \vec{\vec{Z}}$ $\quad z_{ij} = x_i y_j$

(Dyadic product)

$\vec{\vec{A}}.\vec{B} = \vec{C}$ $\quad c_{ij} = a_{ik} b_{kj}$

$\vec{\vec{A}}:\vec{\vec{B}} = a_{ij} b_{ji}$

(Double dotted product)



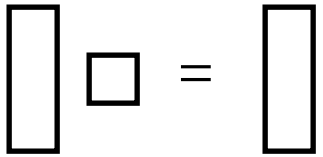
Mathematics Review

Applied Computational Fluid Dynamics

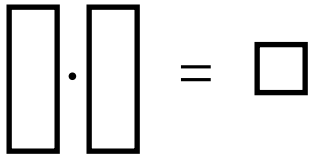
André Bakker

Vector Notation - 1

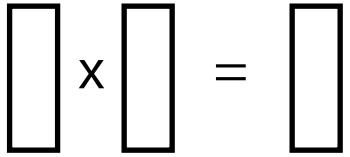
Multiplication: $\vec{X}\ f = \vec{Y}$ $\quad y_i = f x_i$



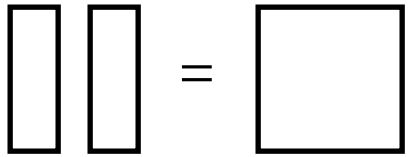
Scalar ("inner") product: $\vec{X} \cdot \vec{Y} = x_i y_i$



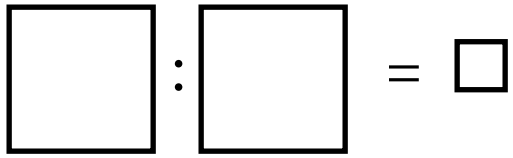
Vector ("outer") product: $\vec{X} \times \vec{Y} = \vec{Z}$



Dyadic ("tensor") product: $\vec{X}\,\vec{Y} = \vec{\vec{A}}$ $\quad a_{ij} = x_i y_j$

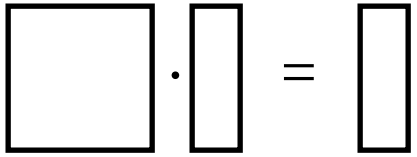


Double dot ("inner") product: $\vec{\vec{A}} : \vec{\vec{B}} = a_{ij} b_{ji}$

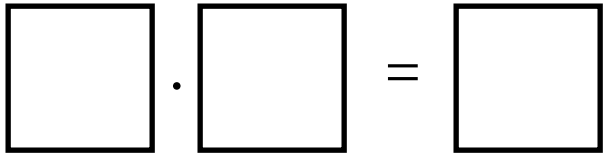


Vector Notation - 2

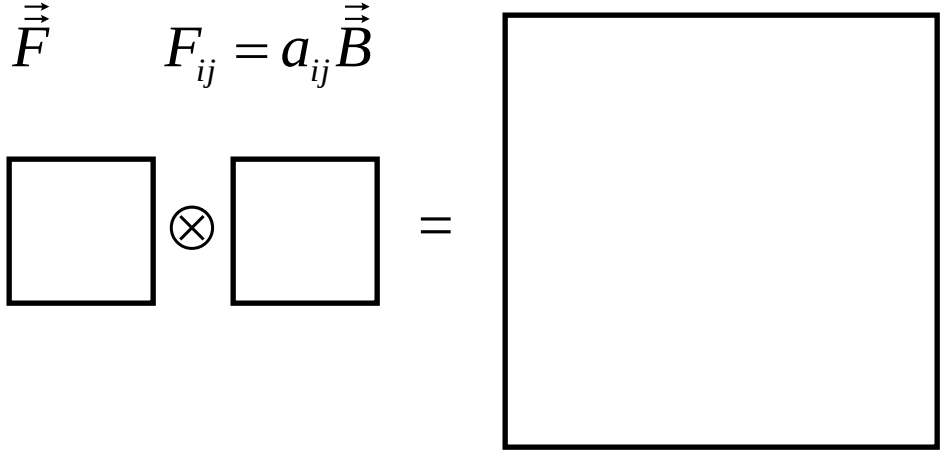
Scalar product: $\vec{\vec{A}} \cdot \vec{X} = \vec{Y}$ $\quad y_i = a_{ik} x_k$



Scalar product: $\vec{\vec{A}} \cdot \vec{\vec{B}} = \vec{\vec{C}}$ $\quad c_{ij} = a_{ik} b_{kj}$



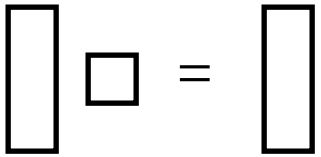
Kronecker product: $\vec{\vec{A}} \otimes \vec{\vec{B}} = \vec{\vec{\vec{F}}}$ $\quad F_{ij} = a_{ij} \vec{\vec{B}}$



Gradients and divergence

- The gradient of a scalar f is a vector:

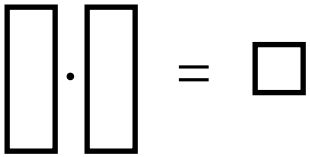
$$grad\ f = \nabla f = \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j} + \frac{\partial f}{\partial z}\mathbf{k}$$



Similarly, the gradient of a vector is a second order tensor, and the gradient of a second order tensor is a third order tensor.

- The divergence of a vector is a scalar:

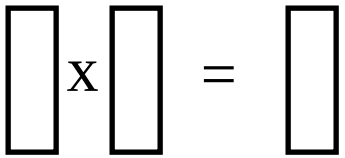
$$div\,\mathbf{A} = \nabla.\mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$



Curl

- The curl ("rotation") of a vector **v**(u,v,w) is another vector:

$$curl\ \mathbf{v} \;=\; rot\ \mathbf{v} \;=\; \nabla \times \mathbf{v} \;=\; \left(\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z},\ \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x},\ \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right)$$



Definitions - rectangular coordinates

$$\nabla f = \frac{\partial f}{\partial x}\mathbf{i} + \frac{\partial f}{\partial y}\mathbf{j} + \frac{\partial f}{\partial z}\mathbf{k}$$

$$\nabla . \mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$$

$$\nabla \times \mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\mathbf{i} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\mathbf{j} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\mathbf{k}$$

$$\nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

$$\nabla^2 \mathbf{A} = \nabla^2 A_x \mathbf{i} + \nabla^2 A_y \mathbf{j} + \nabla^2 A_z \mathbf{k}$$

Identities

$$\nabla(f\,g) = f\,\nabla g + g\nabla f$$

$$\nabla(\mathbf{A}\cdot\mathbf{B}) = (\mathbf{B}\cdot\nabla)\mathbf{A} + (\mathbf{A}\cdot\nabla)\mathbf{B} + \mathbf{B}\times(\nabla\times\mathbf{A}) + \mathbf{A}\times(\nabla\times\mathbf{B})$$

$$\nabla\cdot(f\,\mathbf{A}) = (\nabla f)\cdot\mathbf{A} + f\,(\nabla\cdot\mathbf{A})$$

$$\nabla\cdot(\mathbf{A}\times\mathbf{B}) = \mathbf{B}\cdot(\nabla\times\mathbf{A}) - \mathbf{A}\cdot(\nabla\times\mathbf{B})$$

$$\nabla\times(f\mathbf{A}) = (\nabla f)\times\mathbf{A} + f\,(\nabla\times\mathbf{A})$$

$$\nabla\times(\mathbf{A}\times\mathbf{B}) = (\mathbf{B}\cdot\nabla)\mathbf{A} - (\mathbf{A}\cdot\nabla)\mathbf{B} + (\nabla\cdot\mathbf{B})\mathbf{A} - (\nabla\cdot\mathbf{A})\mathbf{B}$$

Identities

$$\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$$

$$(\mathbf{A} \cdot \nabla)\mathbf{B} = \left[A_x \frac{\partial B_x}{\partial x} + A_y \frac{\partial B_x}{\partial y} + A_z \frac{\partial B_x}{\partial z} \right] \mathbf{i}$$
$$+ \left[A_x \frac{\partial B_y}{\partial x} + A_y \frac{\partial B_y}{\partial y} + A_z \frac{\partial B_y}{\partial z} \right] \mathbf{j}$$
$$+ \left[A_x \frac{\partial B_z}{\partial x} + A_y \frac{\partial B_z}{\partial y} + A_z \frac{\partial B_z}{\partial z} \right] \mathbf{k}$$

$$\int_\tau \nabla f \, d\tau = \int_S f \, \mathbf{da}$$

$$\int_\tau (\nabla \times \mathbf{A}) \, d\tau = -\int_S \mathbf{A} \times \mathbf{da}$$

where S is the surface which bounds volume τ

Differentiation rules

$\varphi = \varphi(\boldsymbol{r})$ en $\psi = \psi(\boldsymbol{r})$ *are differentiable scalar functions*
$\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{r})$ en $\boldsymbol{w} = \boldsymbol{w}(\boldsymbol{r})$ *are differentiable vector functions*

$$\text{grad}\ \varphi = \nabla\varphi;\ \text{div}\ \boldsymbol{v} = \nabla\cdot\boldsymbol{v};\ \text{rot}\ \boldsymbol{v} = \nabla\times\boldsymbol{v}$$

$$\begin{aligned}
\text{grad}\,(\varphi+\psi) &= \text{grad}\,\varphi + \text{grad}\,\psi \\
\text{div}\,(\boldsymbol{v}+\text{w}) &= \text{div}\,\boldsymbol{v} + \text{div}\,\boldsymbol{w} \\
\text{rot}\,(\boldsymbol{v}+\text{w}) &= \text{rot}\,\boldsymbol{v} + \text{rot}\,\boldsymbol{w} \\
\text{grad}\,(\varphi\psi) &= \psi\ \text{grad}\,\varphi + \varphi\ \text{grad}\,\psi \\
\text{div}\,(\varphi\boldsymbol{v}) &= v\cdot\text{grad}\ \varphi + \varphi\,\text{div}\ \boldsymbol{v} \\
\text{rot}\,(\varphi\boldsymbol{v}) &= \text{grad}\,\varphi\times\boldsymbol{v} + \varphi\,\text{rot}\ v \\
\text{div}\,(\boldsymbol{v}\times w) &= \boldsymbol{w}\cdot\text{rot}\ \boldsymbol{v} - \boldsymbol{v}\cdot\text{rot}\ \boldsymbol{w} \\
\text{rot}\,(\boldsymbol{v}\times w) &= (\boldsymbol{w}\cdot\nabla)\boldsymbol{v} - w\ \text{div}\ \boldsymbol{v} - (\boldsymbol{v}\cdot\nabla)\boldsymbol{w} + \boldsymbol{v}\ \text{div}\ \boldsymbol{w} \\
\text{grad}\,(\boldsymbol{v}\cdot\boldsymbol{w}) &= \boldsymbol{w}\times\text{rot}\,\boldsymbol{v} + (\boldsymbol{w}\cdot\nabla)\boldsymbol{v} + \boldsymbol{v}\times\text{rot}\,\boldsymbol{w} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{w} \\
\text{div grad}\,\varphi &= \nabla^2\varphi\ (\varphi = \varphi(\boldsymbol{r}) \\
\nabla^2 &= \nabla\cdot\nabla = \partial_x^2 + \partial_y^2 + \partial_z^2\ \text{(Laplace operator)} \\
\text{rot grad}\,\varphi &= \boldsymbol{0} \\
\text{div rot}\,\boldsymbol{v} &= 0 \qquad\qquad (\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{r})\ \textit{twice} \\
\text{rot rot}\,\boldsymbol{v} &= \text{grad div}\ v - \nabla^2\boldsymbol{v} \qquad\qquad \textit{differentiable})
\end{aligned}$$

Integral theorems

Gauss' divergence theorem: $\iint_S \mathbf{A} \cdot d\mathbf{s} = \iiint_\tau \nabla \cdot \mathbf{A}\, d\tau$

where S is the surface which bounds volume τ

Stokes' theorem: $\oint_C \mathbf{A} \cdot d\,\mathbf{l} = \iint_S (\nabla \times \mathbf{A}) \cdot d\,\mathbf{s}$

where C is the closed curve which bounds the open surface S (*i.e. S may be a* $3-D$ *surface but does not bound a volume*)

Euclidian Norm

- Various definitions exist for the norm of vectors and matrices. The most well-known is the Euclidian norm.

- The Euclidian norm ||**V**|| of a vector **V** is:

$$\|\mathbf{V}\| = \sqrt{\sum_i v_i^2}$$

- The Euclidian norm ||**A**|| of a matrix **A** is:

$$\|\mathbf{A}\| = \sqrt{\sum_{i,j} a_{ij}^2}$$

- Other norms are the spectral norm, which is the maximum of the individual elements, or the Hölder norm, which is similar to the Euclidian norm, but uses exponents p and 1/p instead of 2 and 1/2, with p a number larger or equal to 1.

Matrices - Miscellaneous

- The determinant of a matrix **A** with elements a_{ij} and i=3 rows and j=3 columns:

$$\mathbf{A} = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

$$\det \mathbf{A} = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31} - a_{12}a_{21}a_{33} - a_{11}a_{23}a_{32}$$

- A diagonal matrix is a matrix where all elements are zero except a_{11}, a_{22}, and a_{33}. For a tri-diagonal matrix also the diagonals above and below the main diagonal are non-zero, while all other elements are zero.
- Triangular decomposition is expressing **A** as the product **LU** with **L** a lower-triangular matrix (elements above diagonal are 0) and **U** an upper triangular matrix.
- The transpose $\mathbf{A}^T$ has elements $a'_{ij}=a_{ji}$. A matrix is symmetric if $\mathbf{A}^T = \mathbf{A}$.
- A sparse matrix is a matrix where the vast majority of elements is zero and only few elements are non-zero.

Matrix invariants

- An invariant is a scalar property of a matrix that is independent of the coordinate system in which the matrix is written.
- The first invariant I_1 of a matrix **A** is the trace *tr* **A**. This is simply the sum of the diagonal components: $I_1 = tr\ \mathbf{A} = a_{11} + a_{22} + a_{33}$
- The second invariant is: $$I_2 = \begin{vmatrix} a_{22} & a_{32} \\ a_{23} & a_{33} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{31} \\ a_{13} & a_{33} \end{vmatrix}$$
- The third invariant is the determinant of the matrix: $I_3 = \det \mathbf{A}$.
- The three invariants are the simplest possible linear, quadratic, and cubic combinations of the eigenvalues that do not depend on their ordering.

Gauss-Seidel method

- The Gauss-Seidel method is a numerical method to solve the following set of linear equations:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + ... + a_{1N}x_N = C_1$$
$$\vdots \qquad\qquad \vdots \qquad\qquad \vdots$$
$$a_{N1}x_1 + a_{N2}x_2 + a_{N3}x_3 + ... + a_{NN}x_N = C_N$$

- We first make an initial guess for x_1:

$$x_1^1 = \frac{C_1}{a_{11}}$$

- The superscript 1 denotes the 1st iteration.
- Next, using x_1^1:

$$x_2^1 = \frac{C_2}{a_{22}} - \frac{1}{a_{22}}(a_{21}x_1^1)$$

Gauss-Seidel method - continued

- Next, using x_1^1 and x_2^0:

$$x_3^1 = \frac{C_3}{a_{33}} - \frac{1}{a_{33}}(a_{31}x_1^1 + a_{32}x_2^1)$$

- And continue, until:

$$x_N^1 = \frac{C_N}{a_{NN}} - \frac{1}{a_{NN}}\sum_1^{n-1} a_{Ni}x_i^1$$

- For all consecutive iterations we solve for x_1^2, using x_2^1 … x_N^1, and next for x_2^2 using x_1^2, x_3^1 … x_N^1, etc.
- We repeat this process until convergence, i.e., until:

$$(x_i^k - x_i^{k-1}) < \delta$$

with δ a specified small value.

Gauss-Seidel method - continued

- It is possible to improve the speed at which this system of equations is solved by applying overrelaxation, or improve the stability if the system does not converge by applying underrelaxation.
- Say at iteration k the value of x_i equals x_i^k. If applying the Gauss-Seidel method, the value for iteration k+1 would be x_i^{k+1}, then, instead of using x_i^{k+1}, we consider this to be a *predictor*.
- We then calculate a *corrector* as follows:

$$corrector = R(x_i^{k+1} - x_i^k)$$

- Here R is the relaxation factor (R>0). If R<1 we use underrelaxation and if R>1 we use overrelaxation.
- Next we recalculate x_i^{k+1}as follows:

$$x_i^{k+1} = x_i^k + corrector$$

Gauss elimination

- Consider the same set of algebraic equations shown in the Gauss-Seidel discussion. Consider the matrix **A**:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

- The heart of the algorithm is the technique for eliminating all the elements below the diagonal, i.e., to replace them with zeros, to create an upper triangular matrix:

$$\mathbf{U} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix}$$

Gauss elimination - continued

- This is done by multiplying the first row by a_{21}/a_{11} and subtracting it from the second row. Note that C_2 then becomes C_2-C_1a_{21}/a_{11}.
- The other elements a_{31} through a_{n1} are treated similarly. Now all elements in the first column below a_{11} are 0.
- This process is then repeated for all columns.
- This process is called forward elimination.
- Once the upper diagonal matrix has been created, the last equation only contains one variable x_n, which is readily calculated as $x_n=C_n/a_{nn}$.
- This value can then be substituted in equation n-1 to calculate x_{n-1} and this process can be repeated to calculate all variables x_i. This is called backsubstitution.
- The number of operations required for this method increases proportional to n^3. For large matrices this can be a computationally expensive method.

Tridiagonal matrix algorithm (TDMA)

- TDMA is an algorithm similar to Gauss elimination for tridiagonal matrices, i.e., matrices for which only the main diagonal and the diagonals immediately above and below it are non-zero.
- This system can be written as:

$$a_{i,i-1}x_{i-1} + a_{i,i}x_i + a_{i,i+1}x_{i+1} = C_i$$

- Only one element needs to be replaced by a zero on each row to create an upper diagonal matrix.
- When the algorithm reaches the ith row, only $a_{i,i}$ and C_i need to be modified:

$$a_{i,i} = a_{i,i} - \frac{a_{i,i-1}a_{i-1,i+1}}{a_{i-1,i}} \qquad C_i = C_i - \frac{a_{i,i-1}C_{i-1}}{a_{i-1,i}}$$

- Back substitution is then used to calculate all x_i.
- The computational effort scales with n and this is an efficient method to solve this set of equations.

Differential equations

- Ordinary differential equation (ODE): an equation which, other than the one independent variable x and the dependent variable y, also contains derivatives from y to x. General form:

  $$F(x,y,y',y'' \ldots y^{(n)}) = 0$$

  The order of the equation is determined by the order n of the highest order derivative.
- A partial differential equation (PDE) has two or more independent variables. A PDE with two independent variables has the following form:

  $$F\left(x, y, z, \frac{\partial z}{\partial x}, \frac{\partial z}{\partial y}, \frac{\partial^2 z}{\partial x^2}, \frac{\partial^2 z}{\partial x \partial y}, \frac{\partial^2 z}{\partial y^2}, \ldots \right) = 0$$

  with $z=z(x,y)$. The order is again determined by the order of the highest order partial derivative in the equation. Methods such as “Laplace transformations” or “variable separation” can sometimes be used to express PDEs as sets of ODEs. These will not be discussed here.

Classification of partial differential equations

- A general partial differential equation in coordinates x and y:

$$a\frac{\partial^2\phi}{\partial x^2}+b\frac{\partial^2\phi}{\partial x\partial y}+c\frac{\partial^2\phi}{\partial y^2}+d\frac{\partial\phi}{\partial x}+e\frac{\partial\phi}{\partial y}+f\phi+g=0$$

- Characterization depends on the roots of the higher order (here second order) terms:
  - $(b^2\text{-}4ac) > 0$ then the equation is called hyperbolic.
  - $(b^2\text{-}4ac) = 0$ then the equation is called parabolic.
  - $(b^2\text{-}4ac) < 0$ then the equation is called elliptic.
- Note: if a, b, and c themselves depend on x and y, the equations may be of different type, depending on the location in x-y space. In that case the equations are of *mixed* type.

Origin of the terms

- The origin of the terms “elliptic,” “parabolic,” or “hyperbolic used to label these equations is simply a direct analogy with the case for conic sections.
- The general equation for a conic section from analytic geometry is:

$$ax^2 + bxy + cy^2 + dx + ey + f = 0$$

where if

  - (b^2-4ac) > 0 the conic is a hyperbola.
  - (b^2-4ac) = 0 the conic is a parabola.
  - (b^2-4ac) < 0 the conic is an ellipse.

Numerical integration methods

- Ordinary differential equation:

$$\frac{d\phi(t)}{dt} = f(t, \phi(t)); \quad \phi(t_0) = \phi^0$$

- Here f is a known function. Φ^0 is the initial point. The basic problem is how to calculate the solution a short time Δt after the initial point at time $t_1=t_0+\Delta t$. This process can then be repeated to calculate the solution at t_2, etc.
- The simplest method is to calculate the solution at t_1 by adding $f(t_0, \Phi^0)\,\Delta t$ to Φ^0. This is called the *explicit* or *forward* Euler method, generally expressed as:

$$\phi(t_{n+1}) = \phi^{n+1} = \phi^n + f(t_n, \phi^n)\Delta t$$

Numerical integration methods

- Another method is the trapezoid rule which forms the basis of a popular method to solve differential equations called the Crank-Nicolson method:

$$\phi^{n+1} = \phi^{n} + \frac{1}{2}\left[f(t_n, \phi^{n}) + f(t_{n+1}, \phi^{n+1}) \right] \Delta t$$

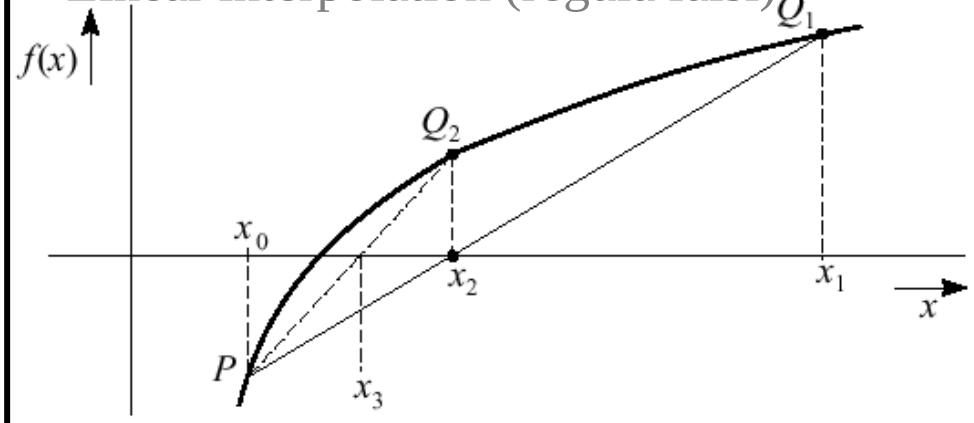
- Methods using points between t_n and t_{n+1} are called Runge-Kutta methods, which come in various forms. The simplest one is second-order Runge-Kutta:

$$\phi^{*}_{n+1/2} = \phi^{n} + \frac{\Delta t}{2} f(t_n, \phi^{n})$$

$$\phi^{n+1} = \phi^{n} + \Delta t \, f(t_{n+1/2}, \phi^{*}_{n+1/2})$$

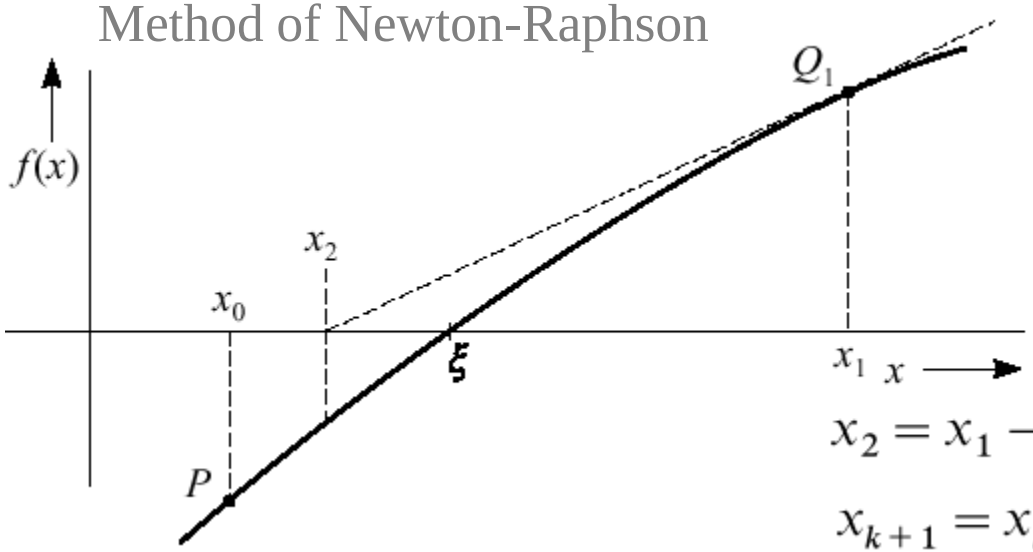
Numerically estimating zero-crossings

Linear interpolation (regula falsi)



$$x_2 = \frac{x_0 f(x_1) - x_1 f(x_0)}{f(x_1) - f(x_0)}$$ (use recursively)

Method of Newton-Raphson



$$x_2 = x_1 - f(x_1)/f'(x_1)$$

$$x_{k+1} = x_k - f(x_k)/f'(x_k)$$

Jacobian

- The general definition of the Jacobian for n functions of n variables is the following set of partial derivatives:

$$\frac{\partial(f_1, f_2, \ldots, f_n)}{\partial(x_1, x_2, \ldots, x_n)} = \begin{vmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{vmatrix}$$

- In CFD, the shear stress tensor $S_{ij} = \partial U_i / \partial x_j$ is also called “the Jacobian.”

Jacobian - continued

- The Jacobian can be used to calculate derivatives from a function in one coordinate system from the derivatives of that same function in another coordinate system.
- Equations u=f(x,y), v=g(x,y), then x and y can be determined as functions of u and v (possessing first partial derivatives) as follows:

$$u = f(x,y); \quad f_x = \partial f / \partial y; \quad f_y = \partial f / \partial x$$

$$v = g(x,y); \quad g_x = \partial g / \partial x; \quad g_y = \partial g / \partial y$$

$$\frac{\partial x}{\partial u} = \frac{g_y}{\begin{vmatrix} f_x & f_y \\ g_x & g_y \end{vmatrix}} \qquad \frac{\partial y}{\partial u} = \frac{-g_x}{\begin{vmatrix} f_x & f_y \\ g_x & g_y \end{vmatrix}}$$

- With similar functions for x_v and y_v.
- The determinants in the denominators are examples of the use of Jacobians.

Eigenvalues

- If an equation with an adjustable parameter has non-trivial solutions only for specific values of that parameter, those values are called the eigenvalues and the corresponding function the eigenfunction.
- If a differential equation with an adjustable parameter only has a solution for certain values of that parameter, those values are called the eigenvalues of the differential equation.
- For an *n*x*n* matrix **A**, for the equation $\mathbf{Az} = \lambda\mathbf{z}$, then z is an eigenvector and λ is an eigenvalue.
    - The eigenvalues are the *n* roots of the characteristic equation

      $$\det(\lambda\mathbf{I}-\mathbf{A}) = \lambda^n+p_1\lambda^{n-1}+\ldots+p_n = 0$$
    - $(\lambda\mathbf{I}-\mathbf{A})$ is the characteristic matrix of **A**.
    - The polynomial is called the characteristic polynomial of **A**.
    - The product of all the eigenvalues of **A** is equal to det **A**.
    - The sum of all the eigenvalues is equal to tr **A**.
    - The matrix is singular if at least one eigenvalue is zero.

Taylor series

- Let $f(x)$ have continuous derivatives up to the $(n+1)^{st}$ order in some interval containing the point a. Then:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + ... + \frac{f^n(a)}{n!}(x-a)^n + ...$$

Error function

- The error function is defined as:

$$Error\ \ function: \quad erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2}\, dt$$

$$Complementary\ error\ \ function: \quad erfc(z) = 1 - erf(z)$$

- It is the integral of the Gaussian ("normal") distribution. It is usually calculated from series expansions.
- Properties are:

$$erf(0) = 0$$

$$erf(\infty) = 1$$

$$erf(z) = -erf(-z)$$

$$\frac{d\, erf(z)}{dz} = \frac{2}{\sqrt{\pi}} \exp\left(-z^2\right)$$

Permutation symbol

- The permutation symbol e_{kmn} resembles a third-order tensor with k, m, and n ranging from 1 to 3.
- If the number of transpositions required to bring k, m, and n in the form 1, 2, 3 is even then e_{kmn}=1.
- If the number of transpositions required to bring k, m, and n in the form 1, 2, 3 is odd then e_{kmn}=-1.
- Otherwise e_{kmn}=0.
- Thus:

$$e_{123} = e_{231} = e_{312} = 1$$

$$e_{132} = e_{321} = e_{213} = -1$$

all other elements are zero

- Instead of e_{kmn} the permutation symbol is also often written as ε_{kmn}.

Correlation functions

- Continuous signals.
  - Let *x(t)* and *y(t)* be two signals. Then the correlation function $\Phi_{xy}(t)$ is defined as:

$$\phi_{xy}(t) = \int_{-\infty}^{\infty} x(t+\tau)\, y(\tau)\, d\tau$$

  - The function $\Phi_{xx}(t)$ is usually referred to as the autocorrelation function of the signal, while the function $\Phi_{xy}(t)$ is usually called the cross-correlation function.
- Discrete time series.
  - Let *x[n]* and *y[n]* be two real-valued discrete-time signals. The autocorrelation function $\Phi_{xx}[n]$ of *x[n]* is defined as:

$$\phi_{xx}[n] = \sum_{m=-\infty}^{+\infty} x[m+n]\, x[m]$$

  - The cross-correlation function is defined as:

$$\phi_{xy}[n] = \sum_{m=-\infty}^{+\infty} x[m+n]\, y[m]$$

Fourier transforms

- Fourier transforms are used to decompose a signal into a sum of complex exponentials (i.e., sinusoidal signals) at different frequencies.
- The general form is:

$$x(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} X(\omega)e^{i\omega t}d\omega$$

$$X(\omega) = \int_{-\infty}^{\infty} x(t)e^{-i\omega t}d\omega$$

- X(ω) is the Fourier transform of x(t). It is also called the spectrum because it shows the amplitude ("energy") associated with each frequency ω present in the signal. X(ω) is a complex function with real and imaginary parts. The magnitude |X(ω)| is also called the power spectrum.
- Slightly different forms exist for continuous, discrete, periodic, and aperiodic signals.

END