Lecture 1 - Introduction to CFD

Applied Computational Fluid Dynamics

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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.
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: \( F = m \cdot a \).
  – 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.
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.
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 number, and more.
- Theodore von Karman (1881-1963) analyzed what is now known as the von Karman vortex street.
Lewis Fry Richardson (1881-1953)

• In 1922, Lewis Fry Richardson 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).

• 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, citing: “a considerable amount of labour and endurance.”
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).
  - $k$-$\varepsilon$ 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 $k$-$\varepsilon$ 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).
  - CFX (UK and Canada).
  - Fidap (US).
  - Polyflow (Belgium).
  - Phoenix (UK).
  - Star CD (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

- 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.
CFD - how it works (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.).
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.

\[
\frac{\partial}{\partial t} \int_V \rho \phi \, dV + \oint_{\partial V} \rho \phi \mathbf{V} \cdot d\mathbf{A} = \int_A \Gamma \nabla \phi \cdot d\mathbf{A} + \int_V S_\phi \, dV
\]

- unsteady
- convection
- diffusion
- generation

<table>
<thead>
<tr>
<th>Eqn.</th>
<th>( \phi )</th>
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<tbody>
<tr>
<td>continuity</td>
<td>1</td>
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<tr>
<td>x-mom.</td>
<td>( u )</td>
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<tr>
<td>y-mom.</td>
<td>( v )</td>
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<td>energy</td>
<td>( h )</td>
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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.
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.
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 $A = 2.91 \text{ m}^2$.
- The drag coefficient is:

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

- 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

- 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 can not be (easily) tested, e.g. hypersonic flow.
  - CFD provides the ability to theoretically simulate any physical condition.
Advantages of CFD (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

• 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)

• 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.