Motivation

Introduction

- The physical aspects of fluid flow are governed by three principles:
  - Mass is conserved.
  - Force = mass \times acceleration (Newton's second law).
  - Energy is conserved (not considered in this lecture).
- Principles can be described with integral equations or partial differential equations.
- In CFD, these governing equations are replaced by discretized algebraic forms.
- Algebraic forms provide quantities at discrete points in time and space, no closed-form analytical solution.

Continuous Quantities

- \( x, y, z \) - 3D coordinate system
- \( t \) - time
- \( \rho (x,y,z,t) \) - density
- \( \mathbf{v} (x,y,z,t) \) - velocity
- \( \mathbf{v} (x,y,z,t) = (u(x,y,z,t), v(x,y,z,t), w(x,y,z,t))^T \)

Problem

- \( \mathbf{v} (x,y,z,t) \)
- \( \rho (x,y,z,t) \)
- \( \mathbf{v} (x,y,z,t+\Delta t) \)
- \( \rho (x,y,z,t+\Delta t) \)
Outline

- introduction
- pre-requisites
- governing equations
  - continuity equation
  - momentum equation
- summary
- solution techniques
  - Lax-Wendroff
  - MacCormack
- numerical aspects
- recent research in graphics

Substantial Derivative of $\rho$

Taylor series at point 1

$$\rho_{1} - \rho_{2} = \left( \frac{\partial \rho}{\partial x} \right) \left( x_{2} - x_{1} \right) + \left( \frac{\partial \rho}{\partial y} \right) \left( y_{2} - y_{1} \right) + \left( \frac{\partial \rho}{\partial z} \right) \left( z_{2} - z_{1} \right) + \left( \frac{\partial \rho}{\partial t} \right) \left( t_{2} - t_{1} \right)$$

$\to$

$$\rho_{1} - \rho_{2} = \left( \frac{\partial \rho}{\partial x} \right) \left( x_{2} - x_{1} \right) + \left( \frac{\partial \rho}{\partial y} \right) \left( y_{2} - y_{1} \right) + \left( \frac{\partial \rho}{\partial z} \right) \left( z_{2} - z_{1} \right) + \left( \frac{\partial \rho}{\partial t} \right) \left( t_{2} - t_{1} \right)$$

$\rho_{1} - \rho_{2} = \left( \frac{\partial \rho}{\partial x} \right) \left( x_{2} - x_{1} \right) + \left( \frac{\partial \rho}{\partial y} \right) \left( y_{2} - y_{1} \right) + \left( \frac{\partial \rho}{\partial z} \right) \left( z_{2} - z_{1} \right) + \left( \frac{\partial \rho}{\partial t} \right) \left( t_{2} - t_{1} \right)$$

Substantial Derivative

- infinitesimally small fluid element moving with the flow
- $(x_{1}, y_{1}, z_{1})$ - position at time $t_{1}$
- $(x_{2}, y_{2}, z_{2})$ - position at time $t_{2}$

$v_{1}(x_{1}, y_{1}, z_{1}, t_{1}) = (u(x_{1}, y_{1}, z_{1}, t_{1}), v(x_{1}, y_{1}, z_{1}, t_{1}), w(x_{1}, y_{1}, z_{1}, t_{1}))^{T}$

$v_{2}(x_{2}, y_{2}, z_{2}, t_{2}) = (u(x_{2}, y_{2}, z_{2}, t_{2}), v(x_{2}, y_{2}, z_{2}, t_{2}), w(x_{2}, y_{2}, z_{2}, t_{2}))^{T}$

$\rho_{1} (x_{1}, y_{1}, z_{1}, t_{1})$

$\rho_{2} (x_{2}, y_{2}, z_{2}, t_{2})$

Substantial Derivative

- substantial derivative of $\rho$
  $$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial x} u + \frac{\partial \rho}{\partial y} v + \frac{\partial \rho}{\partial z} w + \frac{\partial \rho}{\partial t}$$

- substantial derivative = local derivative + convective derivative
  $$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + (\nabla \cdot \mathbf{V}) \cdot \nabla = \left( \frac{\partial \rho}{\partial x} \right) \frac{\partial}{\partial x} + \left( \frac{\partial \rho}{\partial y} \right) \frac{\partial}{\partial y} + \left( \frac{\partial \rho}{\partial z} \right) \frac{\partial}{\partial z}$$

- local derivative - time rate of change at a fixed location
- convective derivative - time rate of change due to fluid flow
- subst. derivative = total derivative with respect to time
Divergence of $v$:

- divergence of velocity $v = \text{time rate of change of the volume } \delta V$ of a moving fluid element per unit volume

$$\nabla \cdot v = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = \frac{1}{\delta V} \frac{D(\delta V)}{Dt}$$

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**Continuity Equation**

- mass is conserved
- infinitesimally small fluid element moving with the flow
- fixed mass $\delta m$, variable volume $\delta V$, variable density $\rho$
  $$\delta m = \rho \cdot \delta V$$
- time rate of change of the mass of the moving fluid element is zero
  $$\frac{D\delta m}{Dt} = \frac{D(\rho \cdot \delta V)}{Dt} = \delta V \frac{D\rho}{Dt} + \rho \frac{D\delta V}{Dt} = 0$$

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

- substantial derivative - time rate of change of density of a moving fluid element
- divergence of velocity - time rate of change of volume of a moving fluid element per volume
**Continuity Equation**

- non-conservation form (considers moving element)
  \[ \frac{Dp}{Dt} + \rho \nabla \cdot \mathbf{v} = 0 \]

- manipulation
  \[ \frac{Dp}{Dt} + \rho \nabla \cdot \mathbf{v} = \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \right) \]

- conservation form (considers element at fixed location)
  \[ \frac{Dp}{Dt} + \nabla \cdot \left( \rho \mathbf{v} \right) = 0 \]

**Motivation for Conservation Form**

- infinitesimally small element at a fixed location
- mass flux through element
- difference of mass inflow and outflow = net mass flow
- net mass flow = time rate of mass increase

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \right) = 0 \]

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**Momentum Equation**

- consider a moving fluid element
- physical principle: \( F = m \cdot a \) (Newton’s second law)
- two sources of forces
  - body forces
    - gravity
  - surface forces
    - based on pressure distribution on the surface
    - based on shear and normal stress distribution on the surface due to deformation of the fluid element
**Body Force**

- \( f = \text{body force per unit mass} \)
- gravity: \( f = \delta m g / \delta m = g \)
  - body force on fluid element
- \( \rho f (\text{dx dy dz}) \)

**Pressure Force**

- consider the \( x \) component
- pressure force acts orthogonal to surface into the fluid element
- net pressure force in \( x \) direction
  \[
  
  \left[ p - \left( p + \frac{\partial p}{\partial x} dx \right) \right] dy \ dz = -\frac{\partial p}{\partial x} \ dx \ dy \ dz
  
  \]

**Stress**

- normal stress - related to the time rate of change of volume
- shear stress - related to the time rate of change of the shearing deformation
- \( \tau_{jk} \) - stress in \( k \) direction applied to a surface perpendicular to the \( j \) axis
- \( \tau_{xx} \) - normal stress in \( x \) direction
- \( \tau_{xz}, \tau_{yx} \) - shear stresses in \( x \) directions

- normal stress is related to pressure orthogonal to surface
- shear stress is related to friction parallel to surface
- friction and pressure are related to the velocity gradient
  - friction (shear stress) models viscosity (viscous flow)
  - in contrast to inviscid flow, where friction is not considered
Momentum Equation

- viscous flow, non-conversation form
- Navier-Stokes equations

\[
\rho \frac{Du}{Dt} = \frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho \ f_x
\]

\[
\rho \frac{Dv}{Dt} = \frac{\partial p}{\partial y} + \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + \rho \ f_y
\]

\[
\rho \frac{Dw}{Dt} = \frac{\partial p}{\partial z} + \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho \ f_z
\]
Momentum Equation

- Navier-Stokes equations in conservation form

\[
\frac{\partial (p u)}{\partial t} + \nabla \cdot (p u v) = - \frac{\partial p}{\partial x} + \frac{\partial \tau_{ux}}{\partial x} + \frac{\partial \tau_{uy}}{\partial y} + \frac{\partial \tau_{uz}}{\partial z} + p f_x
\]

\[
\frac{\partial (p v)}{\partial t} + \nabla \cdot (p u v) = - \frac{\partial p}{\partial y} + \frac{\partial \tau_{ux}}{\partial x} + \frac{\partial \tau_{vy}}{\partial y} + \frac{\partial \tau_{uz}}{\partial z} + p f_y
\]

\[
\frac{\partial (p w)}{\partial t} + \nabla \cdot (p u v) = - \frac{\partial p}{\partial z} + \frac{\partial \tau_{ux}}{\partial x} + \frac{\partial \tau_{uy}}{\partial y} + \frac{\partial \tau_{uz}}{\partial z} + p f_z
\]

Newtonian Fluids

- Newton: shear stress in a fluid is proportional to velocity gradients
- most fluids can be assumed to be newtonian, but blood is a popular non-newtonian fluid
- Stokes:
  \[
  \tau_{ux} = \lambda (\nabla \cdot v) + 2 \mu \frac{\partial u}{\partial x} \quad \tau_{uv} = \lambda (\nabla \cdot v) + 2 \mu \frac{\partial v}{\partial y} \quad \tau_{uw} = \lambda (\nabla \cdot v) + 2 \mu \frac{\partial w}{\partial z}
  \]

  \[
  \tau_{ux} = \mu \left[ \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right] \quad \tau_{uv} = \tau_{uv} = \mu \left[ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right] \quad \tau_{uw} = \mu \left[ \frac{\partial w}{\partial z} + \frac{\partial \tau_{ux}}{\partial x} \right]
  \]

- \( \mu \) is the molecular viscosity coefficient
- \( \lambda \) is the second viscosity coefficient with \( \lambda = -2/3 \cdot \mu \)

Perfect Gas

- intermolecular forces are negligible
- \( R \) - specific gas constant
- \( T \) - temperature
- termal equation of state \( p = \rho R T \)

Momentum Equation in x

\[
\frac{\partial (p u)}{\partial t} + \nabla \cdot (p u v) = - \frac{\partial p}{\partial x} + \frac{\partial \tau_{ux}}{\partial x} + \frac{\partial \tau_{uy}}{\partial y} + \frac{\partial \tau_{uz}}{\partial z} + p f_x
\]

- now,
  \( p \) can be expressed using density and
  \( \tau \) can be expressed using velocity gradients,
  \( f_x \) is user-defined (e.g. gravity)
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Governing Equations – Viscous Compressible Flow

- thus, four equations and four unknowns \( p, u, v, w \)
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \\
  \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \mathbf{v}) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + \rho f_x \\
  \frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \mathbf{v}) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + \rho f_y \\
  \frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{v}) = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \\
  \]

Governing Equations – Inviscid Compressible Flow

- Euler equations
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \\
  \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u \mathbf{v}) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} + \rho f_x \\
  \frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho v \mathbf{v}) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} + \rho f_y \\
  \frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{v}) = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \\
  \]

Comments on the Governing Equations

- coupled system of nonlinear partial differential equations
- normal and shear stress terms are functions of the velocity gradients
- pressure is a function of the density
- only momentum equations are Navier-Stokes equations, however the name is commonly used for the full set of governing equations (plus energy equation)
Governing Equations in Conservation Form

- can be obtained directly from a control volume fixed in space
- consider flux of mass, momentum (and energy) into and out of the volume
- have a divergence term which involves the flux of mass \( \rho v \), momentum in x, y, z \( \rho u v, \rho v v, \rho w v \)
- can be expressed in a generic form

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = J
\]

Generic Form

- U - solution vector (to be solved for)
- F, G, H - flux vectors
- J - source vector (external forces, energy changes)

\[
\frac{\partial U}{\partial t} = J - \frac{\partial F}{\partial x} - \frac{\partial G}{\partial y} - \frac{\partial H}{\partial z}
\]

Motivation for Different Forms of the Governing Equations

- in many real-world problems, discontinuous changes in the flow-field variables \( \rho, v \) occur (shocks, shock waves)
- problem: differential form of the governing equations assumes differentiable (continuous) flow properties
- simple 1-D shock wave: \( \rho_1, U_1 = \rho_2, U_2 \)

conservation form solves for \( \rho u \), sees no discontinuity
- positive effect on numerical accuracy and stability
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Lax-Wendroff Technique

- flow-field variables \( \rho, u, v, w \) are known at each discrete spatial position \((x, y, z)\) at time \(t\)
- Lax-Wendroff computes all information at time \(t+\Delta t\)
- second-order accuracy in space and time

- explicit, finite-difference method
- particularly suited to marching solutions
- marching suited to hyperbolic, parabolic PDEs
- unsteady (time-dependent), compressible flow is governed by hyperbolic PDEs

Lax-Wendroff Example

- 2D, inviscid flow, no body force, in non-conservation form

\[
\frac{\partial \rho}{\partial t} = -\left( \rho \frac{\partial u}{\partial x} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial v}{\partial y} + v \frac{\partial \rho}{\partial y} \right)
\]

\[
\frac{\partial u}{\partial t} = -\left( u \frac{\partial u}{\partial x} + \frac{u}{\rho} \frac{\partial p}{\partial x} + RT \frac{\partial v}{\partial x} \right)
\]

\[
\frac{\partial v}{\partial t} = -\left( u \frac{\partial v}{\partial x} + \frac{v}{\rho} \frac{\partial p}{\partial y} + RT \frac{\partial v}{\partial y} \right)
\]

Taylor Series Expansions

- \( \rho_{i,j} \) - density at position \((i, j)\) and time \(t\)
- \( \rho_{i,j}, u_{i,j}, v_{i,j} \) are known

\[
\rho_{i,j}^{t+\Delta t} = \rho_{i,j}^t + \left( \frac{\partial \rho}{\partial t} \right)_{i,j} \Delta t + \left( \frac{\partial^2 \rho}{\partial t^2} \right)_{i,j} \frac{(\Delta t)^2}{2} + ...
\]

\[
u_{i,j}^{t+\Delta t} = u_{i,j}^t + \left( \frac{\partial u}{\partial t} \right)_{i,j} \Delta t + \left( \frac{\partial^2 u}{\partial t^2} \right)_{i,j} \frac{(\Delta t)^2}{2} + ...
\]

\[
u_{i,j}^{t+\Delta t} = v_{i,j}^t + \left( \frac{\partial v}{\partial t} \right)_{i,j} \Delta t + \left( \frac{\partial^2 v}{\partial t^2} \right)_{i,j} \frac{(\Delta t)^2}{2} + ...
\]
\( \partial^2 \rho / \partial t^2 \) can be obtained by differentiating the governing equation with respect to time.

\[
\frac{\partial^2 \rho}{\partial t^2} = - \left( \rho \frac{\partial^2 u}{\partial x^2} + 2 \rho \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} + \rho \frac{\partial^2 v}{\partial y^2} \right)
\]

Mixed second derivatives can be obtained by differentiating the governing equations with respect to a spatial variable, e.g.

\[
\frac{\partial^2 u}{\partial x^2} = \rho \frac{\partial^2 u}{\partial x^2} + \left( \rho \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right) + \frac{\partial^2 v}{\partial y^2}
\]

Brackets missing on pp. 219, 220 in Anderson's book!
**MacCormack Technique**

- same characteristics like Lax-Wendroff
- second-order accuracy in space and time
- requires only first time derivative
- predictor - corrector
- illustrated for density

\[ p_{i,j}^{n+1} = p_{i,j}^{n} + \left( \frac{\partial p}{\partial t} \right)_{i,j} \Delta t \]

**MacCormack Technique**

- predictor step for density

\[ \frac{\partial p}{\partial t} \left|_{i,j} \right. = \left( \frac{p_{i+1,j}^{n} - 2p_{i,j}^{n} + p_{i-1,j}^{n}}{2\Delta x} + \frac{p_{i,j+1}^{n} - p_{i,j-1}^{n}}{2\Delta y} \right) \frac{1}{\Delta t} \]

- \( u, v \) are predicted the same way

**MacCormack Technique**

- corrector step for density

\[ p_{i,j}^{n+1} = p_{i,j}^{n} + \frac{1}{2} \left( \frac{\partial p}{\partial t} \right)_{i,j} \Delta t + \frac{1}{2} \left( \frac{\partial p}{\partial t} \right)_{i,j} \Delta t \]

- corresponds to Heun scheme for ODEs
- other higher-order schemes, e.g., Runge-Kutta 2 or 4, could be used as well

**Comments**

- Lax-Wendroff and MacCormack can be used for unsteady flow
  - non-conservation form
  - conservation form
  - viscous flow
  - inviscid flow
- higher-order accuracy required to avoid numerical dissipation, artificial viscosity, numerical dispersion
- note that viscosity is represented by second partial derivatives in the governing equations
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Numerical Effects

- truncation error causes dissipation and dispersion
- numerical dissipation is caused by even-order terms of the truncation error
- numerical dispersion is caused by odd-order terms
- leading term in the truncation error dominates the behavior

Numerical Effects

- artificial viscosity compromises the accuracy, but improves the stability of the solution
- adding artificial viscosity increases the probability of making the solution less accurate, but improves the stability
- similar to iterative solution schemes for implicit integration schemes, where a smaller number of iterations introduces "artificial viscosity", but improves the stability

Summary

- governing equations for compressible flow
  - continuity equation, momentum equation
  - Navier-Stokes (viscous flow) and Euler (inviscid flow)
  - discussion of conservation and non-conservation form
- explicit time-marching techniques
  - Lax-Wendroff
  - MacCormack
  - numerical aspects
- recent research in graphics
Recent Research

Rigid Fluid: Animating the Interplay Between Rigid Bodies and Fluid
Mark Carlson
Peter J. Mucha
Greg Turk
Georgia Institute of Technology
Sound FX by Andrew Lackey, M.P.S.E.


Recent Research

"A Method for Animating Viscoelastic Fluids"
Tolga G. Goktekin
Adam W. Bargteil
James F. O’Brien
ACM SIGGRAPH 2004
University of California, Berkeley