



Computational Aerodynamics

III B. Tech VI semester (Autonomous IARE R-16)

BY

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CO's	Course outcomes
CO1	Understand the applications of CFD in various engineering fields and to generate governing equations in conservative and non-conservative form.
CO2	Understand the mathematical behaviour of partial differential equations and classify into hyperbolic, parabolic and elliptical natures.
CO3	Acquire the concepts of finite difference method through discretization and grid generation techniques.
CO4	Identify different CFD techniques available for different partial differential equations.
CO5	Explore the concepts of finite volume methods, and its difference from finite difference method.

UNIT - I



INTRODUCTION TO CFD

UNIT - I

CLOs	Course Learning Outcome
CLO1	Understand the necessity of CFD tool as both research and design areas in modern computational world.
CLO2	Explain the applications of computational fluid dynamics tool in various engineering branches other than aerospace engineering.
CLO3	Recognize the selection of type of flow from the finite control volume and infinitesimal small fluid element depending upon the requirements.
CLO4	Develop the governing equations required for computational aerodynamics in both conservation and non-conservation forms.

Outline



- Approaches
- Introduction-Benefits
- Modeling of fluid
- Non Dimensional Representation
- Classification of PDE
- Finite Difference
- Consistency, Stability, Error analysis of schemes

Approaches

Approach	Advantages	Disadvantages
Experimental	Capable of being most realistic	Equipment required, Scaling problems, Measurement Difficulty, Operating Cost
Theoretical	General Information in Formula form	Restricted to simple geometry and physics, Usually for Linear problems
Computational	Complicated Physics, Details of Flow	Truncation Errors, Computer Costs, Boundary conditions

Introduction



What is CFD?

- ⦿ CFD: A methodology for obtaining a discrete solution of real world fluid flow problems.
- ⦿ Discrete Solution: Solution is obtained at a finite collection of space points and at discrete time levels
- ⦿ For a reasonably accurate solution, the number of space points that need to be involved is of the order of few millions. Solution is achievable only through modern high speed computers

The Benefits of CFD

◎ **Insight**

- Difficult to prototype or test through experimentation
- Better Details

◎ **Foresight**

- Better prediction: In a short time

◎ **Efficiency**

- Design better and faster, economical, meet environmental regulations and ensure industry compliance.
- CFD analysis leads to shorter design cycles and your products get to market faster.
- In addition, equipment improvements are built and installed with minimal downtime.
- CFD is a tool for compressing the design and development cycle allowing for rapid prototyping.

Why use CFD?

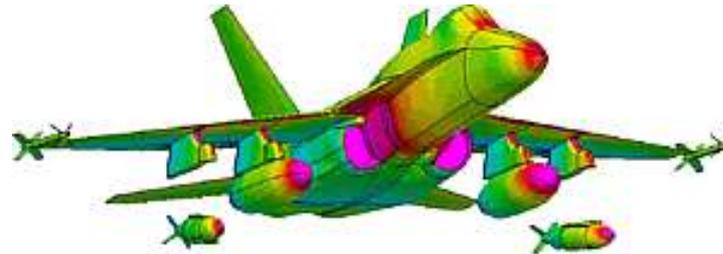
Analysis and Design

- ◎ Simulation-based design instead of “build & test”
 - More cost effective and more rapid than EFDCFD provides high-fidelity database for diagnosing flow field
- ◎ Simulation of physical fluid phenomena that are difficult for experiments
 - Full scale simulations (e.g., ships and airplanes)
 - Environmental effects (wind, weather, etc.)
 - Hazards (e.g., explosions, radiation, pollution)
 - Physics (e.g., planetary boundary layer, stellar evolution)
- ◎ **Knowledge and exploration of flow physics**

Where is CFD used?

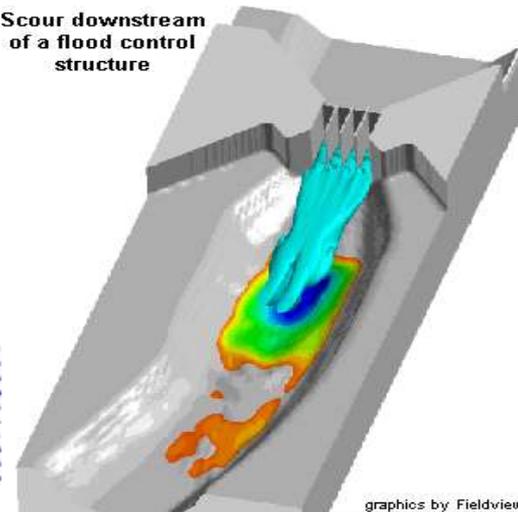
- Where is CFD used?
- **Aerospace**
- **Automotive**
- **Biomedical**
- Chemical Processing
- HVAC
- Hydraulics
- Marine
- Oil & Gas
- Power Generation
- Sports
- Pollutant Monitoring

Aerospace



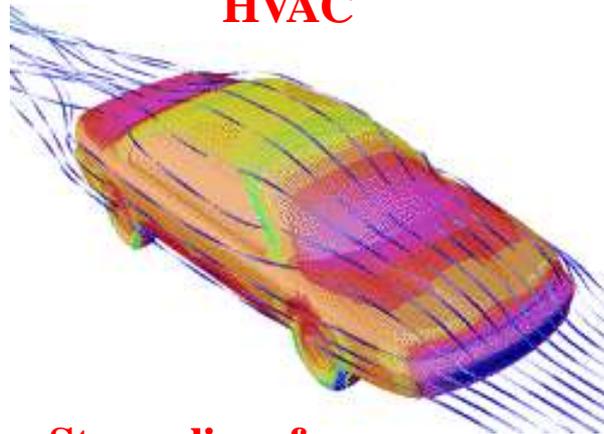
Hydraulics

Scour downstream
of a flood control
structure



graphics by Fieldview

HVAC

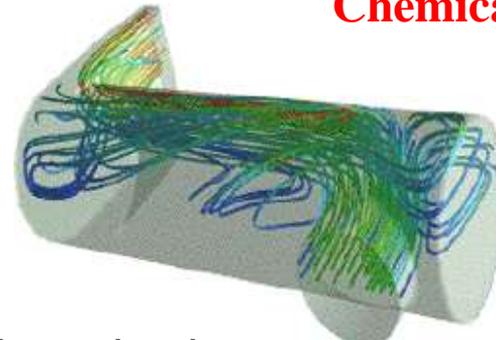


**Streamlines for
workstation ventilation**

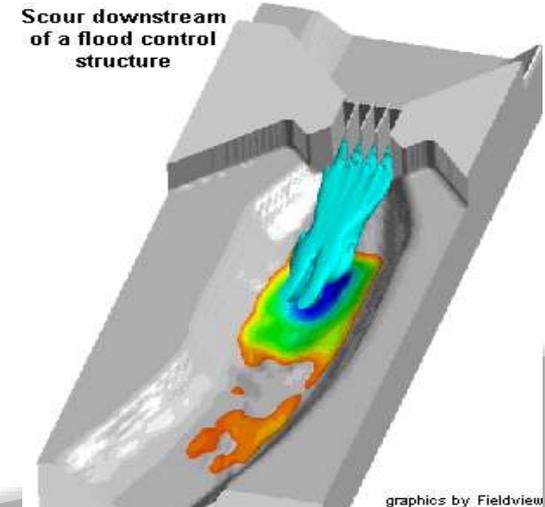
Where is CFD used?

- ◎ Where is CFD used?
- Aerospace
- Automotive
- Biomedical
- **Chemical Processing**
- **HVAC**
- **Hydraulics**
- Marine
- Oil & Gas
- Power Generation
- Sports

Chemical Processing



Polymerization reactor vessel - prediction of flow separation and residence time effects.



graphics by Fieldview

Where is CFD used?

Where is CFD used?

- Aerospace
- Automotive
- Biomedical
- Chemical Processing
- HVAC
- Hydraulics
- *Marine*
- *Oil & Gas*
- *Power Generation*
- *Sports*

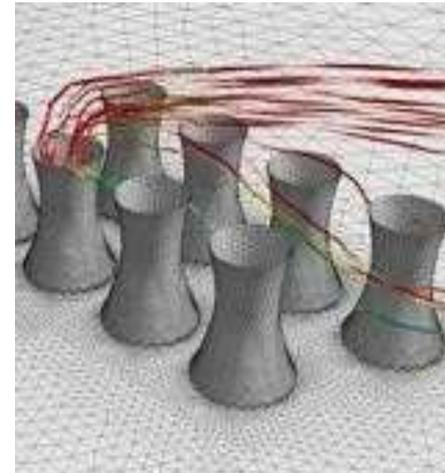


Oil & Gas



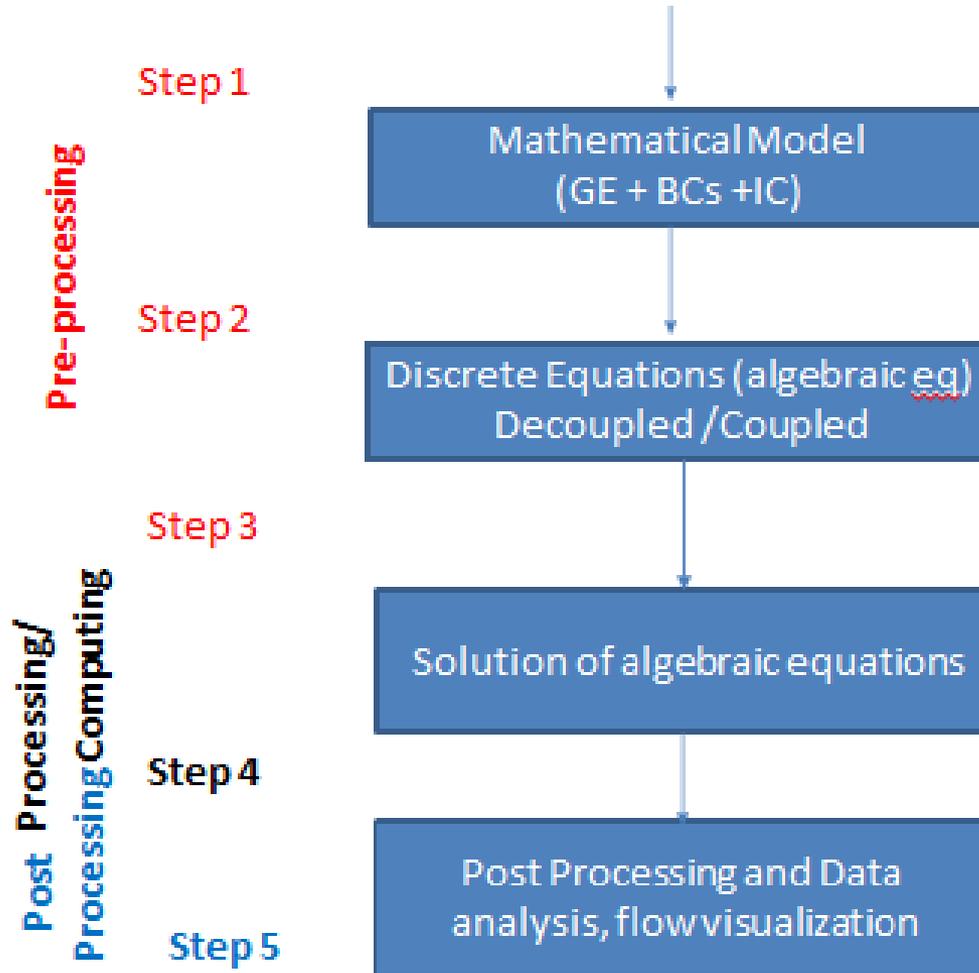
Sports

Power Generation



Flow around cooling towers

Steps in CFD Analysis



Physical Laws,
Levels of approximation:

Constitutive Behavior,
Simplifying approximation, Semi-empirical models

Discretization of flow domain: Grid/Mesh Generation

Discretization of GE+BCs:

Numerical Methodology

Modelling of Fluid Flow

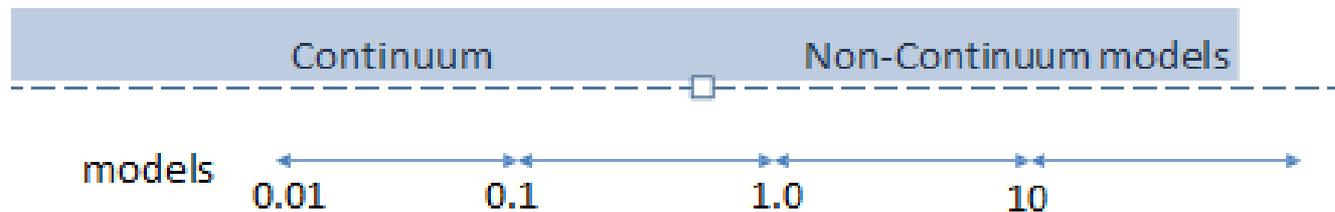
Continuum models

- Each Macroscopic property = $f(r, t)$

Non Continuum models

- Micro, slip flow, molecular Based on the

Knudsen number=Ratio of Mean free path/length scale



Overlap region: 0.01 to 0.1

- Levels of approximation: temp and velocity jump at solid-fluid interface

Continuum Model

- Materials , such as solids, liquids and gases, are composed of molecules separated by space.
- On a microscopic scale, materials have cracks and discontinuities. However, certain physical phenomena can be modeled assuming the materials exist as a continuum, meaning the matter in the body is continuously distributed and fills the entire region of space it occupies.
- A continuum is a body that can be continually sub-divided into infinitesimal elements with properties being those of the bulk material.

Conservative form

All conservative forms are considered most suitable for CFD

- The conservative properties can be easily preserved at discrete level.
- For high speed flows having discontinuous features like shock waves, the fluxes in the conservation equations remain well behaved across these almost discontinuous features, and therefore the flow behavior is better captured at the discrete level.

Governing equations

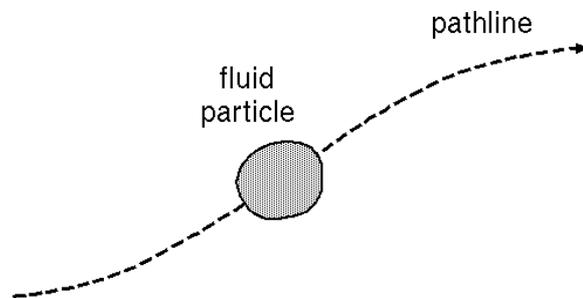
The governing equations include the following conservation laws of physics:

- 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.

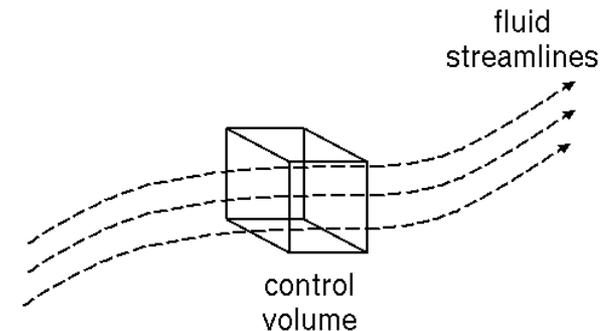
The fluid is treated as a continuum. For length scales of, say, $1\mu\text{m}$ and larger, the molecular structure and motions may be ignored.

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:

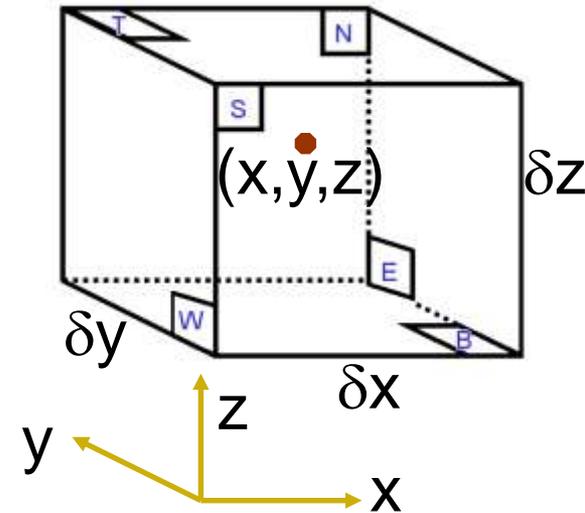
- Velocity u .
- Pressure p .
- Density ρ .
- Temperature T .
- Energy E .

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.

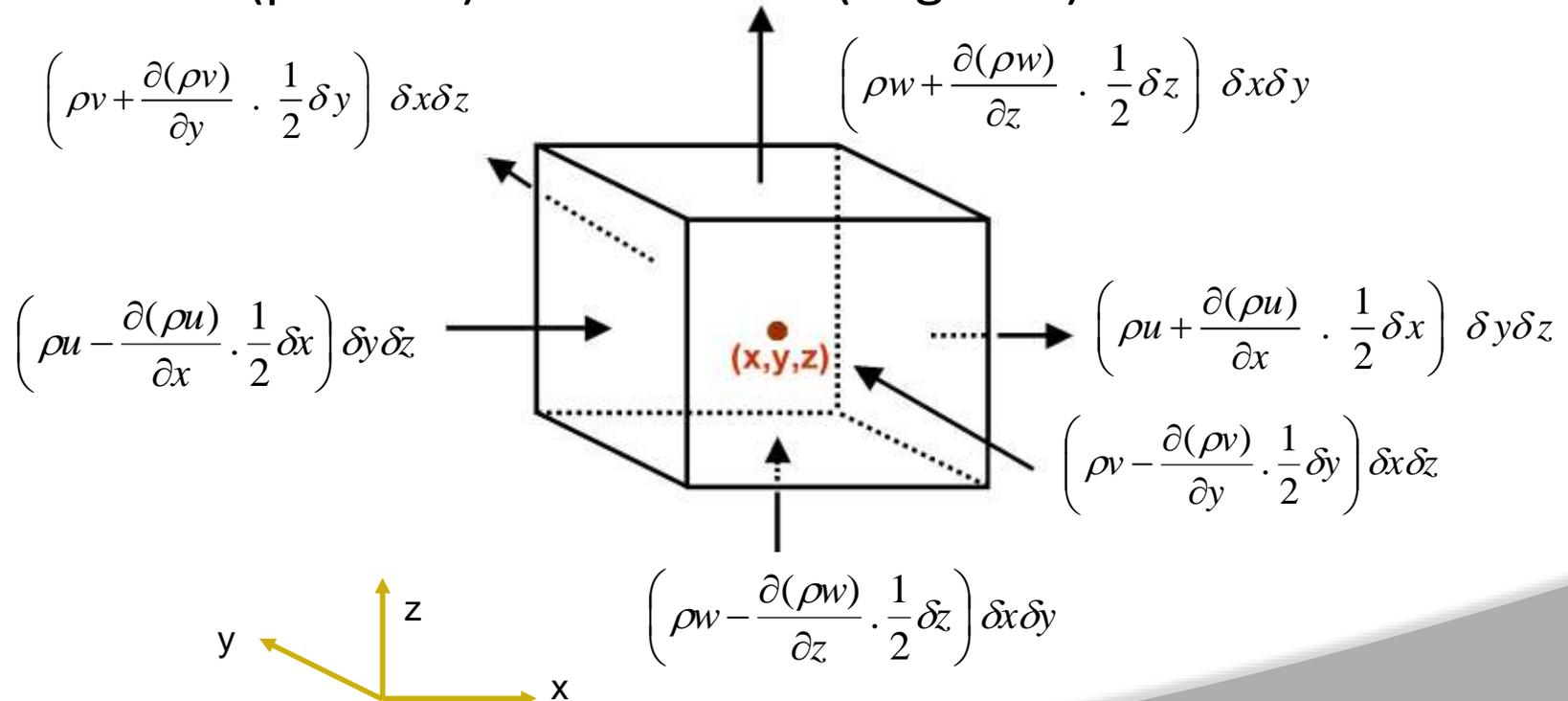
Fluid element for conservation laws



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

Mass balance

- Rate of increase of mass in fluid element equals the net rate of flow of mass into element.
- Rate of increase is:
- 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:

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

Change in density

Net flow of mass across boundaries

Convective term

- For incompressible fluids $\partial \rho / \partial t = 0$, and the equation becomes:
 $\text{div} \mathbf{u} = 0$.

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



Finite control volume
fixed in space

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

Integral form

Conservation form



Finite control volume fixed
mass moving with flow

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

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

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:

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

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 f is given by:

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

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

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

Continuity equation

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

Arbitrary property

Rate of change for a stationary fluid element

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- ⊙ However, some equations are easier derived for fluid particles. For a moving fluid particle, the total derivative per unit volume of this property f is given by:

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

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

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

Continuity equation

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

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:

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

zero because of continuity

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

Rate of increase of f of fluid element + Net rate of flow of f out of fluid element = Rate of increase of f 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	$\rho \frac{Du}{Dt}$	$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \mathbf{u})$
y-momentum	v	$\rho \frac{Dv}{Dt}$	$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v \mathbf{u})$
z-momentum	w	$\rho \frac{Dw}{Dt}$	$\frac{\partial(\rho w)}{\partial t} + \text{div}(\rho w \mathbf{u})$
Energy	E	$\rho \frac{DE}{Dt}$	$\frac{\partial(\rho E)}{\partial t} + \text{div}(\rho E \mathbf{u})$

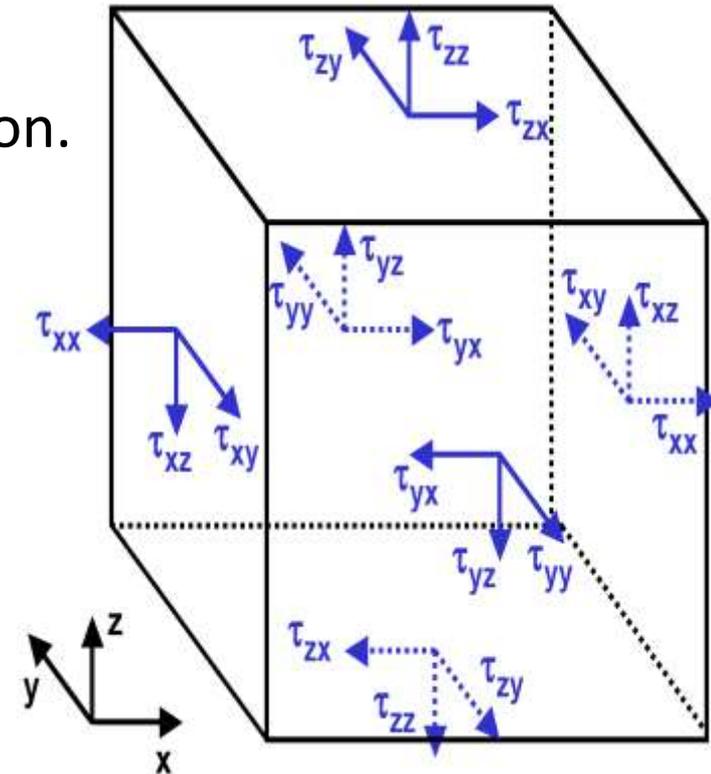
Momentum equation in three dimensions

- ⦿ 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:

$$\rho \frac{Du}{Dt} \quad \rho \frac{Dv}{Dt} \quad \rho \frac{Dw}{Dt}$$
- ⦿ 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

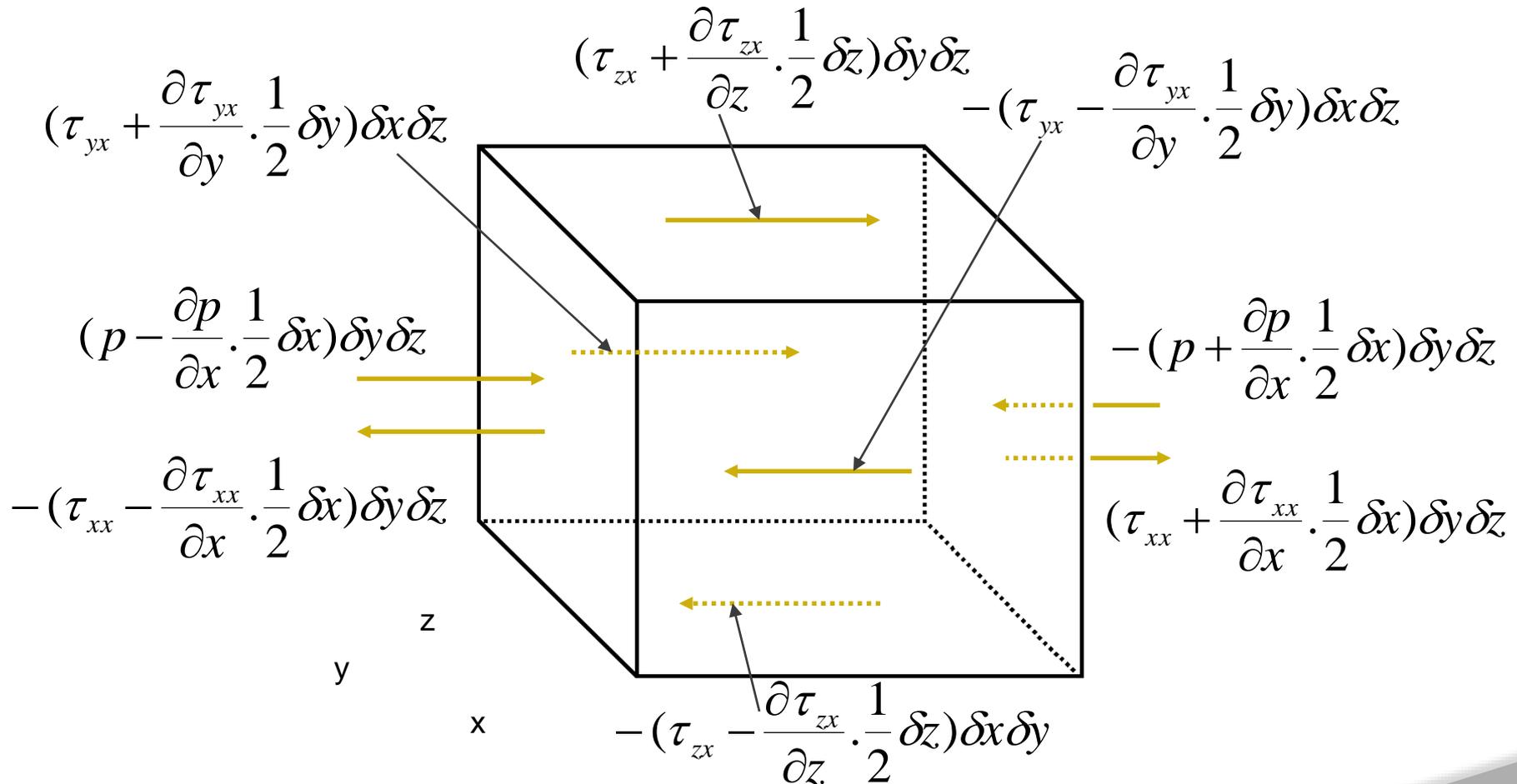
- Stresses are forces per area. Unit is N/m^2 or Pa.
- Viscous stresses denoted by t .
- Suffix notation t_{ij} is used to indicate direction.
- Nine stress components.
 - t_{xx} , t_{yy} , t_{zz} are normal stresses.
E.g. t_{zz} is the stress in the z-direction on a z-plane.
 - Other stresses are shear stresses. E.g. t_{zy} is the stress in the y-direction on a z-plane.



Fig

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:

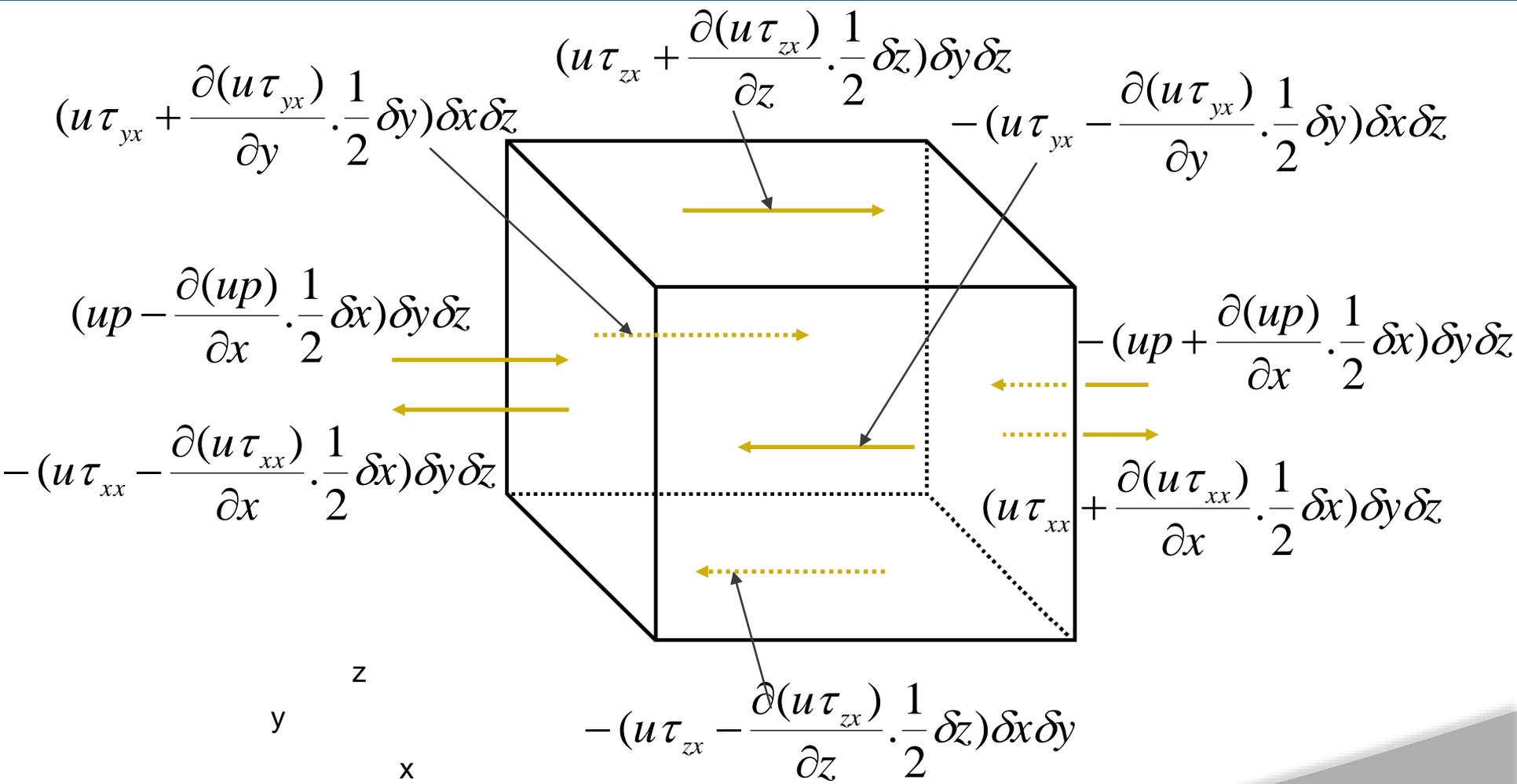
$$\rho \frac{Dv}{Dt} = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial(-p + \tau_{yy})}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + S_{My}$$

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

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.

Work done by surface stresses in x-direction



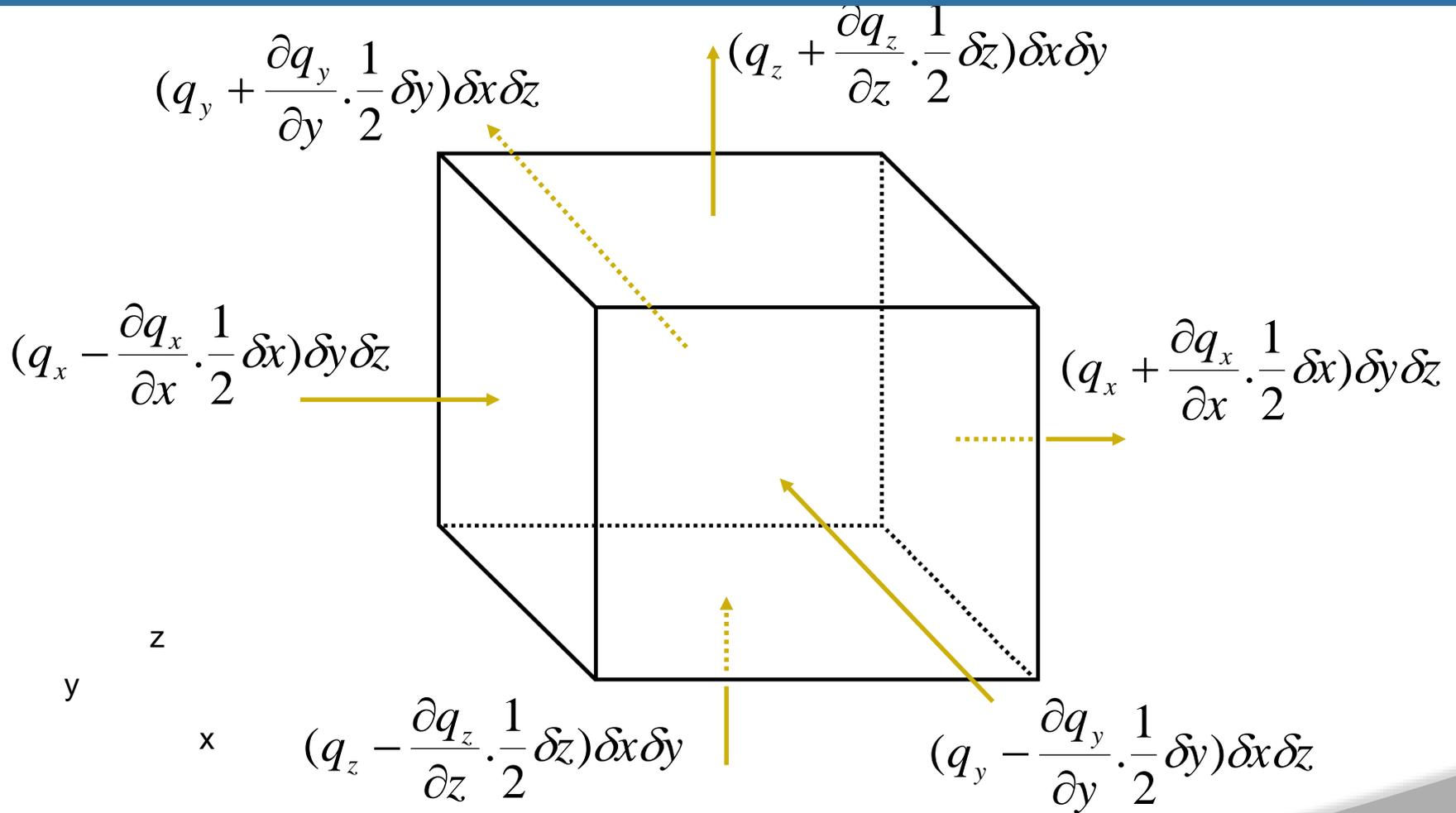
Work done is force times velocity.

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:

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

Energy flux due to heat conduction



The heat flux vector \mathbf{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:

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

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

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

$$\mathbf{q} = -k \text{ grad } T$$

In vector form:

$$-\text{div } \mathbf{q} = \text{div}(k \text{ grad } T)$$

- Thus, energy flux due to conduction:
- 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:

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

- 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:

$$\rho \frac{D[\frac{1}{2}(u^2 + v^2 + w^2)]}{Dt} = -\mathbf{u} \cdot \mathbf{grad} p + u \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) + v \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) + w \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) + \mathbf{u} \cdot \mathbf{S}_M$$

Internal energy equation

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

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

Enthalpy equation

An often used alternative form of the energy equation is the total enthalpy equation.

- **Specific enthalpy** $h = i + p / \rho$.
- **Total enthalpy** $h_0 = h + \frac{1}{2} (u^2 + v^2 + w^2) = E + p / \rho$.

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

Viscous stresses

- ⊙ A model for the viscous stresses t_{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.

Viscous stress tensor

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

$$\boldsymbol{\tau} = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix} = \begin{pmatrix} 2\mu \frac{\partial u}{\partial x} - \frac{2}{3}\mu \operatorname{div} \mathbf{u} & \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) \\ \mu \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) & 2\mu \frac{\partial v}{\partial y} - \frac{2}{3}\mu \operatorname{div} \mathbf{u} & \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) \\ \mu \left(\frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right) & \mu \left(\frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right) & 2\mu \frac{\partial w}{\partial z} - \frac{2}{3}\mu \operatorname{div} \mathbf{u} \end{pmatrix}$$

Note: $\operatorname{div} \mathbf{u} = 0$ for incompressible fluids

Navier-Stokes equations

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

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

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

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

Viscous dissipation

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

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

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

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

Summary of equations in conservation form

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

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

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

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

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

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

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

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:

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

- 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
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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 \mathbf{a} states:

$$\int_{CV} \text{div} \mathbf{a} dV = \int_A \mathbf{n} \cdot \mathbf{a} dA$$

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

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

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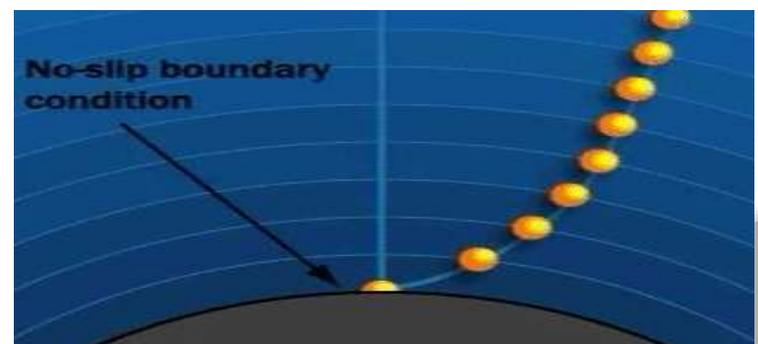
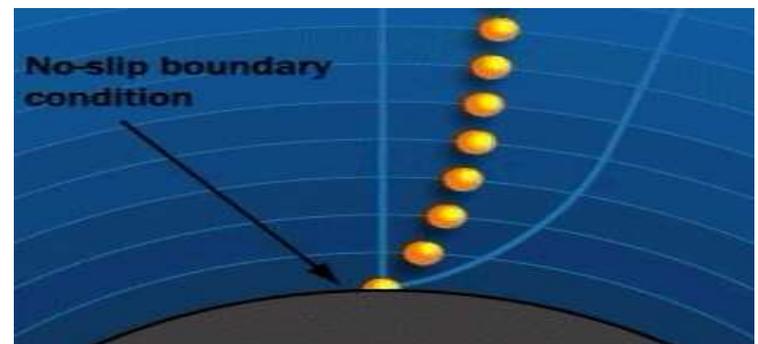
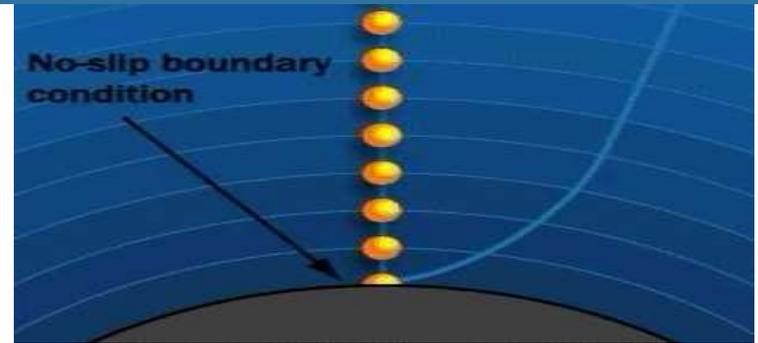
- This is the actual form of the conservation equations solved by finite volume based CFD programs to calculate the flow pattern and associated scalar fields.

Boundary conditions

- ◎ 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.

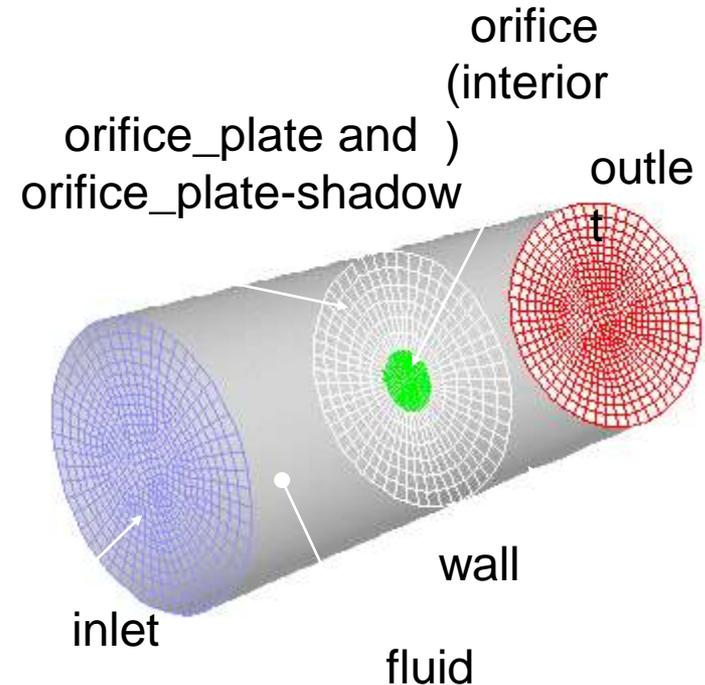
Boundary conditions

- 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.



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. $u(x) = \text{constant}$.
- ⦿ When using a Neumann boundary condition, one prescribes the gradient normal to the boundary of a variable at the boundary, e.g. $\partial_n u(x) = \text{constant}$.
- ⦿ When using a mixed boundary condition a function of the form $au(x) + b\partial_n u(x) = \text{constant}$ 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.

Flow inlets and outlets



General guidelines:

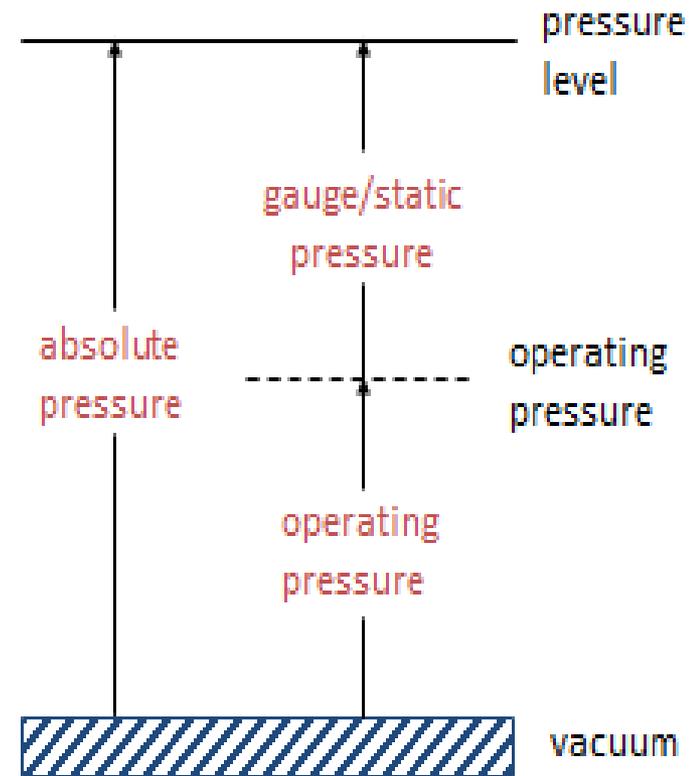
- Select boundary location and shape such that flow either goes in or out. Not mandatory, but will typically result in better convergence.
- Should not observe large gradients in direction normal to boundary near inlets and outlets. This indicates an incorrect problem specification.
- Minimize grid skewness 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:

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

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

- 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.

Pressure inlet boundary (2)

- ⦿ Outflow can occur at pressure inlet boundaries. In that case the flow direction is taken from the interior solution.
- ⦿ 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.

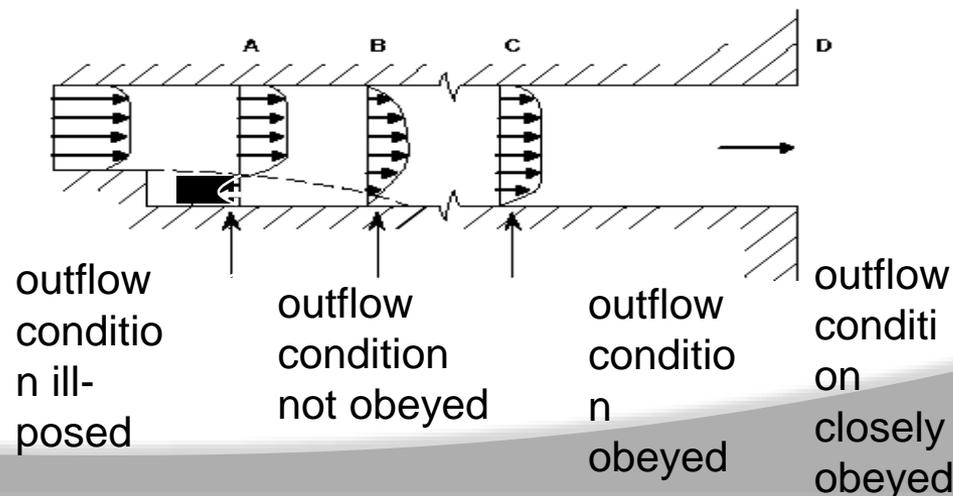
Restrictions on outflow boundaries

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.

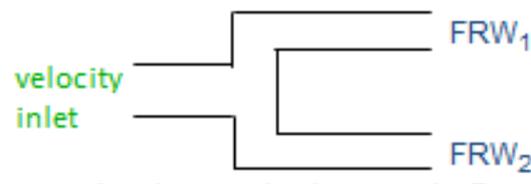
Do not use outflow boundaries where:

- 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.

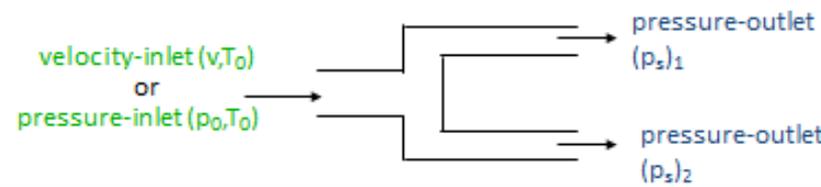


Modeling multiple exits

- 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: $m_i = FRW_i / \sum FRW_i$.
 - 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.

Other inlet and outlet boundary conditions

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:

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

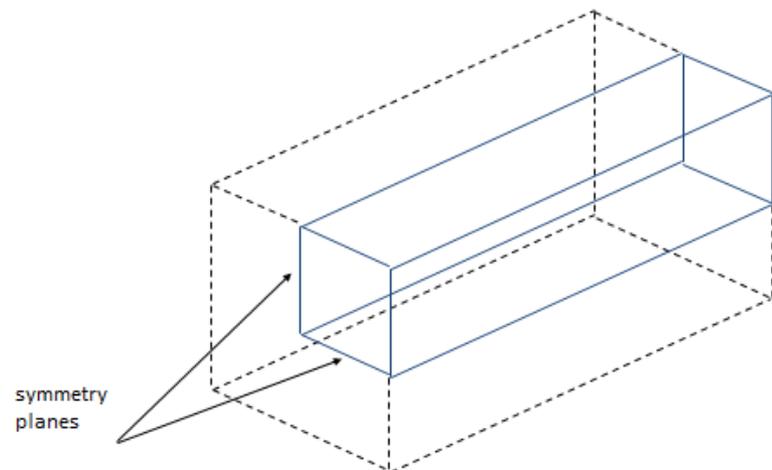
- ⊙ Here k is the turbulent kinetic energy and u is the local velocity magnitude.
- ⊙ Intensity and length scale depend on conditions upstream:
 - Exhaust of a turbine.
Intensity = 20%. Length scale = 1 - 10 % of blade span.
 - Downstream of perforated plate or screen.
Intensity = 10%. Length scale = 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

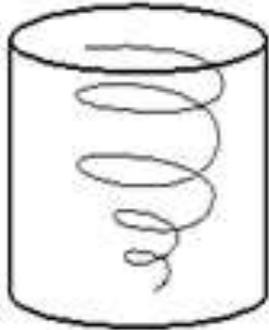
- ⊙ Used when physical geometry of interest and expected flow pattern and the thermal solution are of a periodically repeating nature.
 - Reduces computational effort in problem.

Two types available:

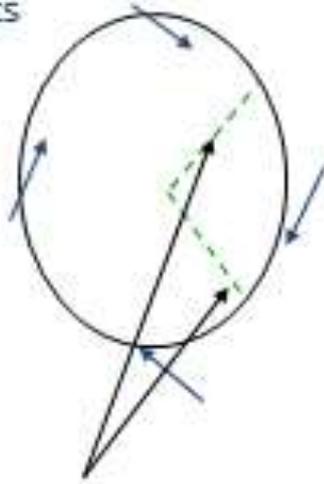
- $\Delta p = 0$ across periodic planes.
 - Rotationally or translationally periodic.
 - Rotationally periodic boundaries require axis of rotation be defined in fluid zone.
- Δp is finite across periodic planes.
 - Translationally periodic only.
 - Models fully developed conditions.
 - Specify either mean Δp per period or net mass flow rate.

Periodic boundaries: examples

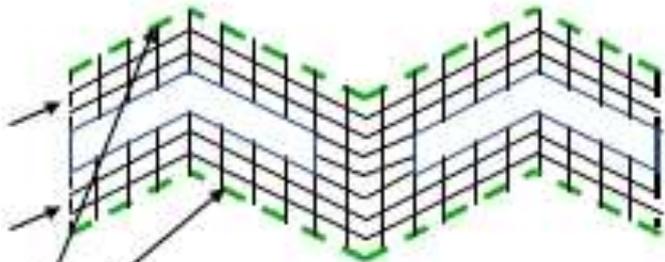
• $\Delta p = 0$:



4 tangential inlets



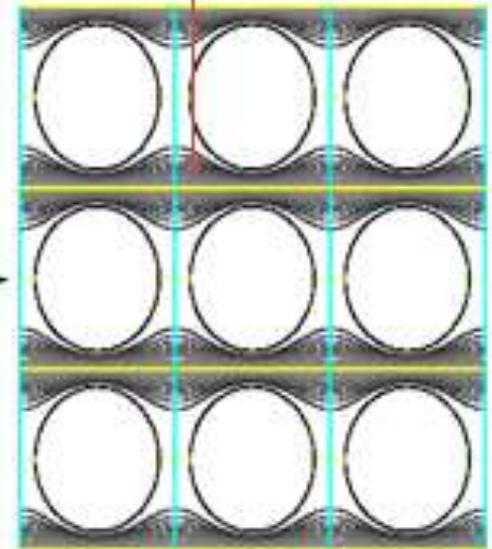
Rotationally periodic boundaries



Translationally periodic boundaries

• $\Delta p > 0$:

computational domain

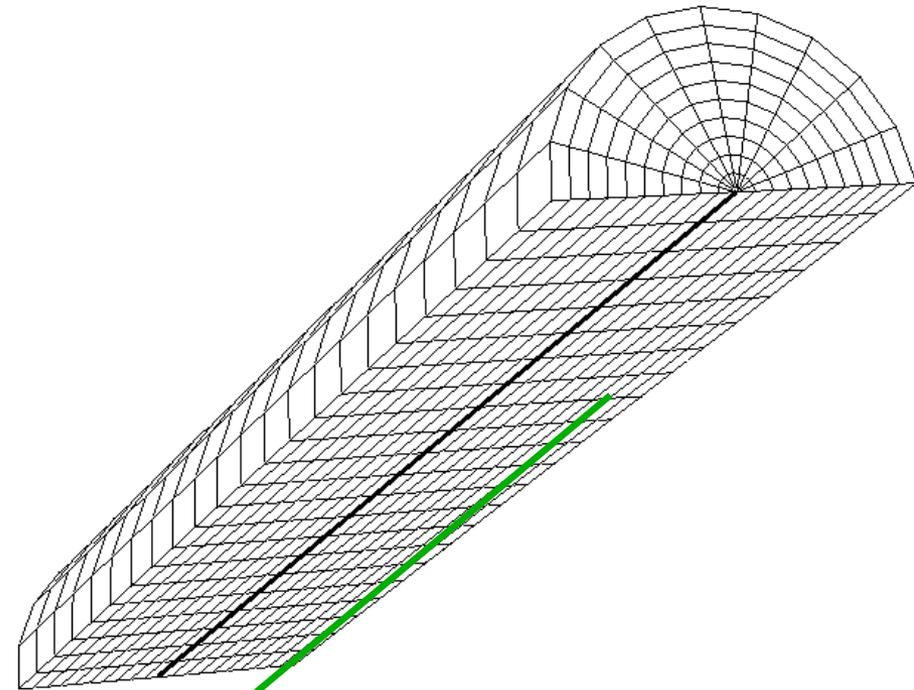
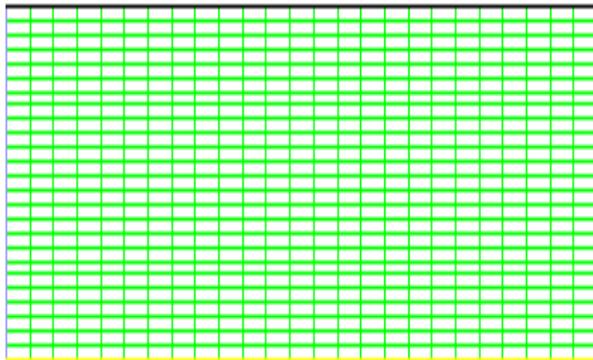


flow direction

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.



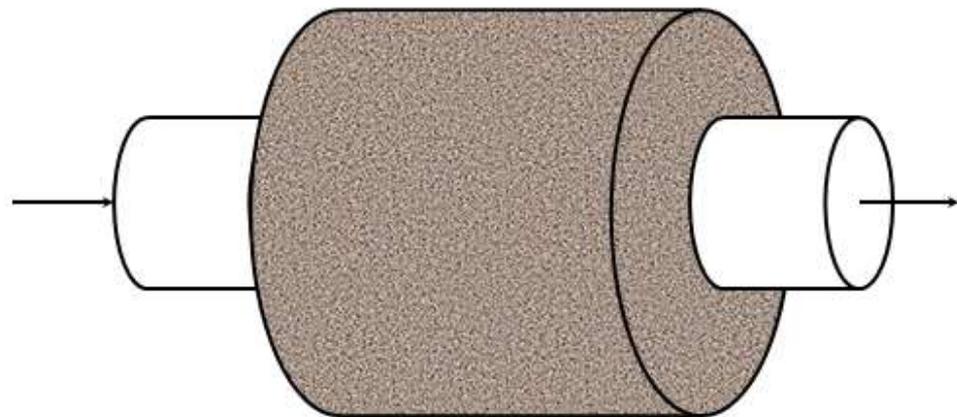
AXIS
boundary

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.

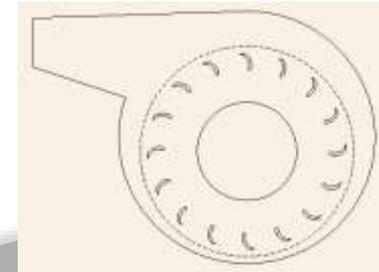
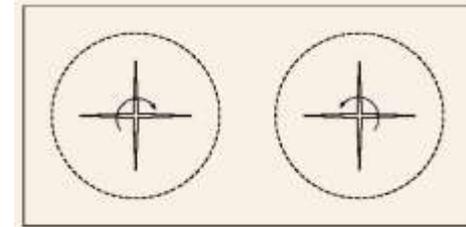
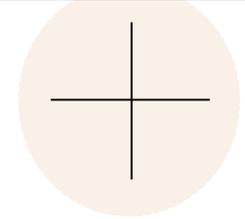
Porous media conditions

- ⦿ 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: $\rho = \text{constant}$.
- ⦿ For compressible flow: $\rho = p_{\text{absolute}}/RT$.
- ⦿ 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: $\rho = p_{\text{operating}}/RT$.
- ⦿ Generally speaking, one should set $p_{\text{operating}}$ close to the mean pressure in the domain to avoid round-off errors.
- ⦿ However, for high Mach number flows using the coupled solver, set $p_{\text{operating}}$ to zero.

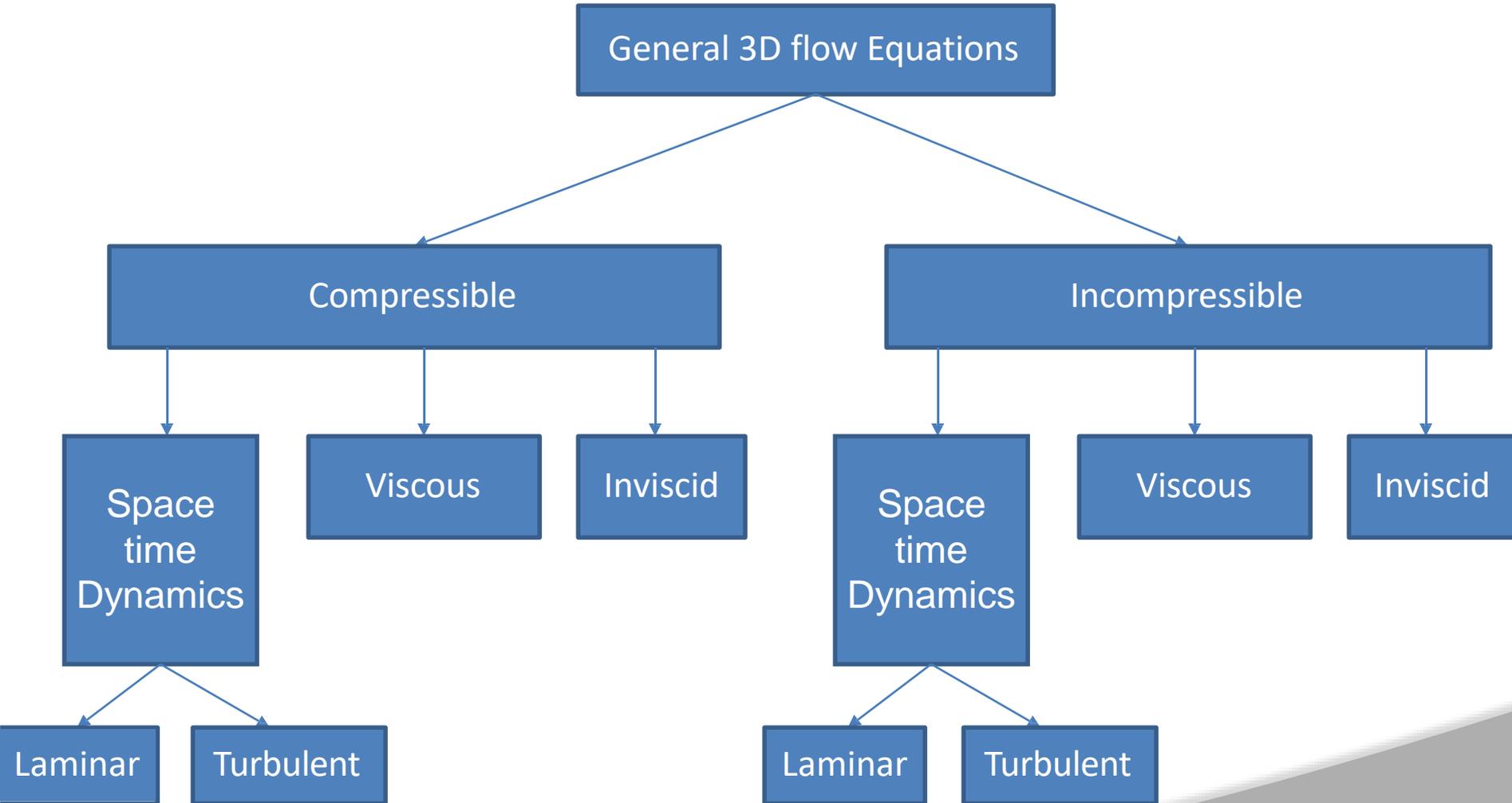
When is a problem properly specified?

- ⦿ 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.

Simplified Models



MATHEMATICAL BEHAVIOR OF PARTIAL DIFFERENTIAL EQUATIONS AND THEIR IMPACT ON COMPUTATIONAL AERODYNAMICS

UNIT - II

CLOs

Course Learning Outcome

CLO5	Explain the need of classification of quasi linear partial differential equations by Cramer's rule and Eigen Value Method.
CLO6	Understand the concepts of range of influence and domain of dependence for a flow field.
CLO7	Explain the general behavior of the partial differential equations which falls in hyperbolic, parabolic and elliptic equations.
CLO8	Demonstrate the CFD aspects of the hyperbolic, parabolic and elliptic equations in aerodynamic problems and physical problems.

Numerical Integration of Partial Differential Equations (PDEs)



- ⦿ Introduction to PDEs.
- ⦿ Semi-analytic methods to solve PDEs.
- ⦿ Introduction to Finite Differences.
- ⦿ Stationary Problems, Elliptic PDEs.
- ⦿ Time dependent Problems.
- ⦿ Complex Problems in Solar System Research.

Differential Equations



- ⦿ A differential equation is an equation for an unknown function of one or several variables that relates the values of the function itself and of its derivatives of various orders.
- ⦿ Ordinary Differential Equation: Function has 1 independent variable.
- ⦿ Partial Differential Equation: At least 2 independent variables.

PDEs definitions

- General (implicit) form for one function $u(x,y)$:

$$F \left(x, y, u(x, y), \frac{\partial u(x, y)}{\partial x}, \frac{\partial u(x, y)}{\partial y}, \dots, \frac{\partial^2 u(x, y)}{\partial x \partial y}, \dots \right) = 0,$$

- Highest derivative defines order of PDE
- Explicit PDE => We can resolve the equation to the highest derivative of u .
- Linear PDE => PDE is linear in $u(x,y)$ and for all derivatives of $u(x,y)$
- Semi-linear PDEs are nonlinear PDEs, which are linear in the highest order derivative.

Linear PDEs of 2. Order



$a(x,y)c(x,y) - b(x,y)^2 / 4 > 0$ **Elliptic**

⊙ $a(x,y)c(x,y) - b(x,y)^2 / 4 = 0$ **Parabolic**

⊙ $a(x,y)c(x,y) - b(x,y)^2 / 4 < 0$ **Hyperbolic**

Quasi-linear: coefficients depend on u and/or first derivative of u , but NOT on second derivatives.

- Quadratic equations in the form describe cone sections.

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + F = 0$$

$a(x,y)c(x,y) - b(x,y)^2 / 4 > 0$ Ellipse

$a(x,y)c(x,y) - b(x,y)^2 / 4 = 0$ Parabola

$a(x,y)c(x,y) - b(x,y)^2 / 4 < 0$ Hyperbola

PDEs and Quadratic Equations

With coordinate transformations these equations can be written in the standard forms:

Ellipse: $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$

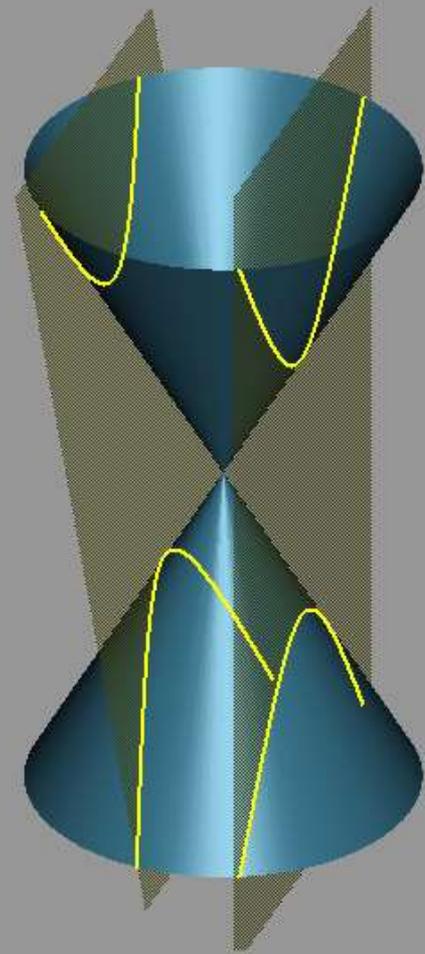
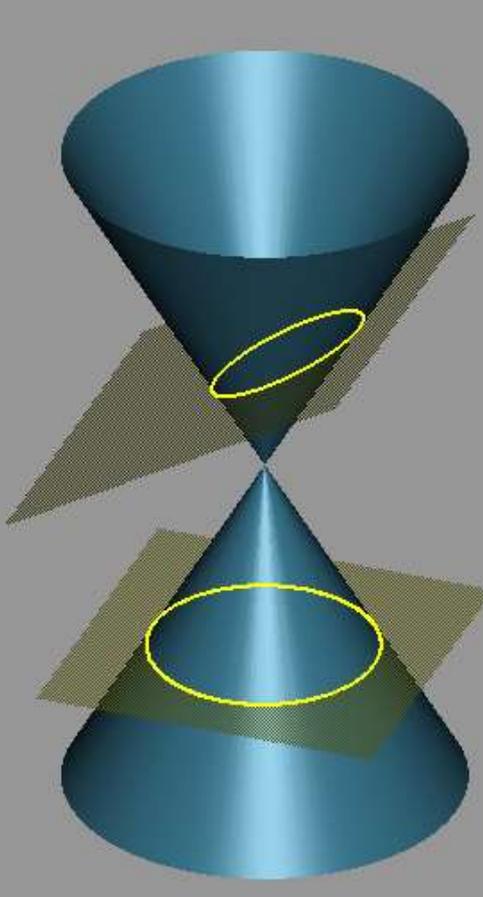
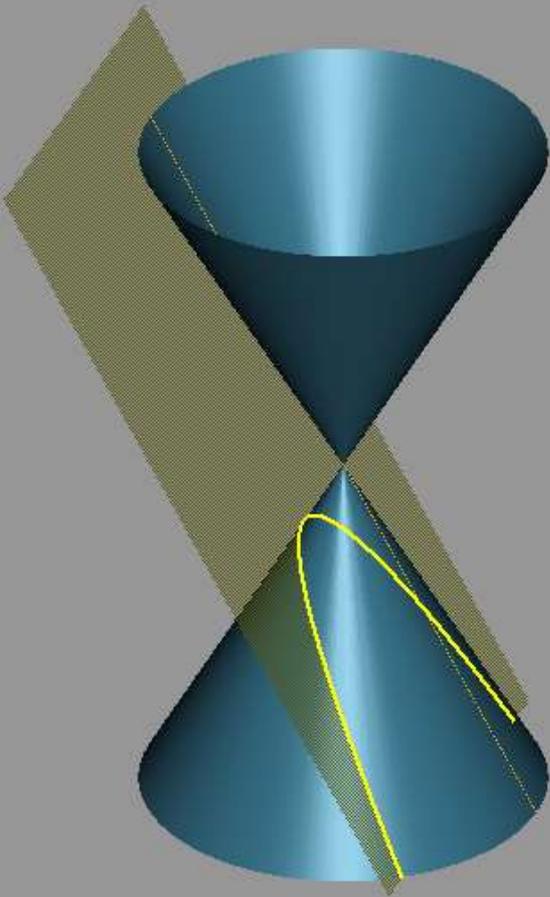
Parabola: $y^2 = 4ax$

Hyperbola: $\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1$

Coordinate transformations can be also applied to get rid of the mixed derivatives in PDEs.

(For space dependent coefficients this is only possible locally, not globally)

PDEs and Quadratic Equations



Parabola- cutting plane parallel to side of cone.

Circle and Ellipse

Hyperbolas

Second Order PDEs with more than 2 independent variables



Classification by eigen values of the coefficient matrix:

- ⦿ Elliptic: All eigen values have the same sign. [Laplace-Eq.]
- ⦿ Parabolic: One eigen value is zero. [Diffusion-Eq.]
- ⦿ Hyperbolic: One eigen value has opposite sign. [Wave-Eq.]
- ⦿ Ultra hyperbolic: More than one positive and negative eigenvalue.

Mixed types are possible for non-constant coefficients, appear frequently in science and are often difficult to solve.

Classifications

- ⦿ Classification of partial differential equations
- ⦿ A general partial differential equation in coordinates x and y : Characterization depends on the roots of the higher order (here Second order) terms:
 - **$b^2 - 4ac > 0$ then the equation is called hyperbolic.**
 - **$b^2 - 4ac = 0$ then the equation is called parabolic.**
 - **$b^2 - 4ac < 0$ 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.

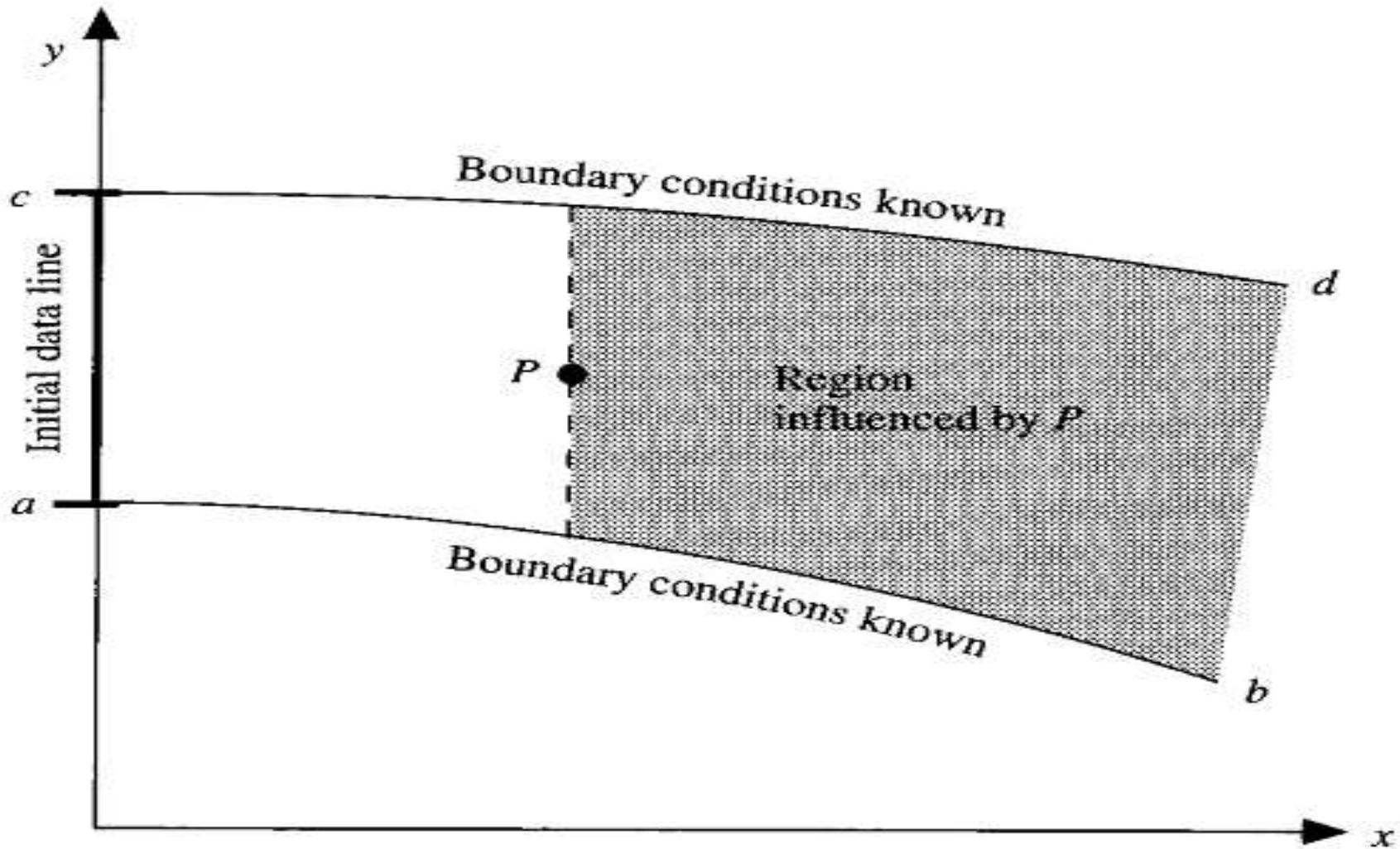
ELLIPTIC PROBLEMS

- ⦿ 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: $u = \nabla\phi$. Because the flow is incompressible, $\nabla \cdot u = 0$, which results in $\nabla^2\phi = 0$. This is also known as Laplace's equation
- ⦿ 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: 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.

PARABOLIC PROBLEMS



HYPERBOLIC PROBLEMS



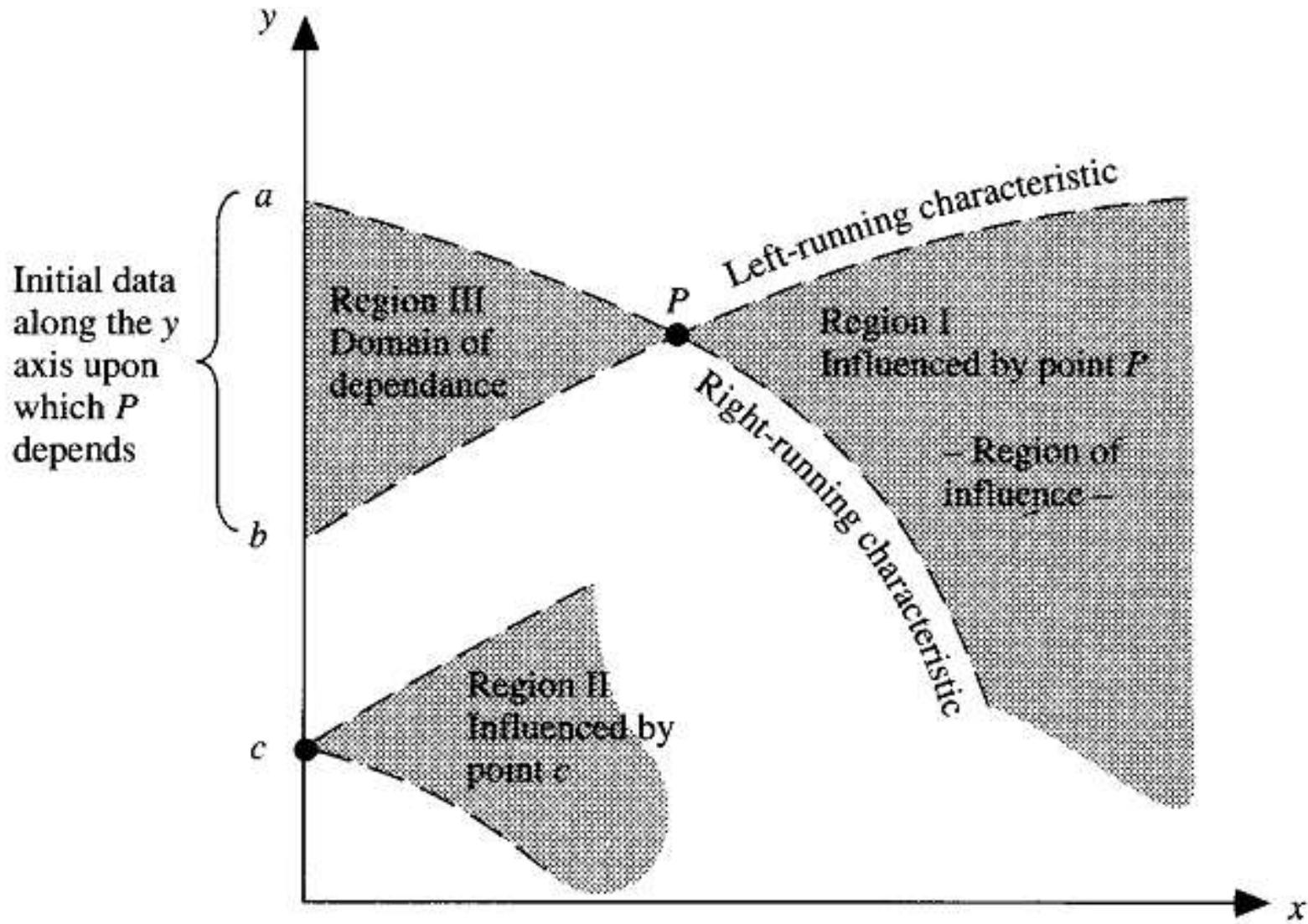
Hyperbolic equations are typical of marching problems with negligible dissipation.

An example is the wave equation:

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: 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.

HYPERBOLIC PROBLEMS



Well posed problems (as defined by Hadamard 1902)

A problem is well posed if:

- ⦿ A solution exists.
- ⦿ The solution is unique.
- ⦿ The solution depends continuously on the data (boundary and/or initial conditions).
- ⦿ Problems which do not fulfill these criteria are ill-posed.



1865-1963

Well posed problems have a good chance to be solved numerically with a stable algorithm.

Ill-posed problems

- ⦿ Ill-posed problems play an important role in some areas, for example for inverse problems like tomography.
- ⦿ Problem needs to be reformulated for numerical treatment.
- ⦿ Add additional constraints, for example smoothness of the solution.
- ⦿ Input data need to be regularized / preprocessed.

Ill-conditioned problems

- ⦿ Even well posed problems can be ill-conditioned.
- ⦿ Small changes (errors, noise) in data lead to large errors in the solution.
- ⦿ Can occur if continuous problems are solved approximately on a numerical grid.
- ⦿ PDE => algebraic equation in form $Ax = b$
- ⦿ Condition number of matrix A :

$$\kappa(A) = \left| \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \right|$$

are maximal and minimal Eigen values of A .

$\lambda_{\max}(A), \lambda_{\min}(A)$

- ⦿ Well conditioned problems have a low condition number.

How to solve PDEs?

PDEs are solved together with appropriate **Boundary conditions** and/or **Initial Conditions**.

Boundary value problem

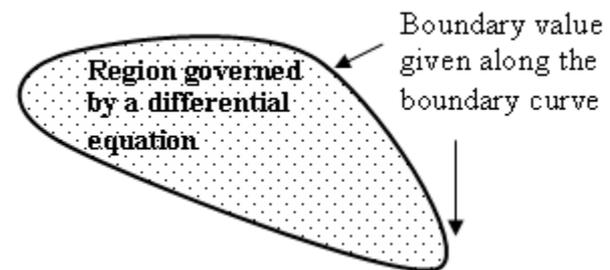
Dirichlet B.C:

Specify $u(x,y,\dots)$ on boundaries (say at $x=0$, $x=L_x$, $y=0$, $y=L_y$ in a rectangular box)

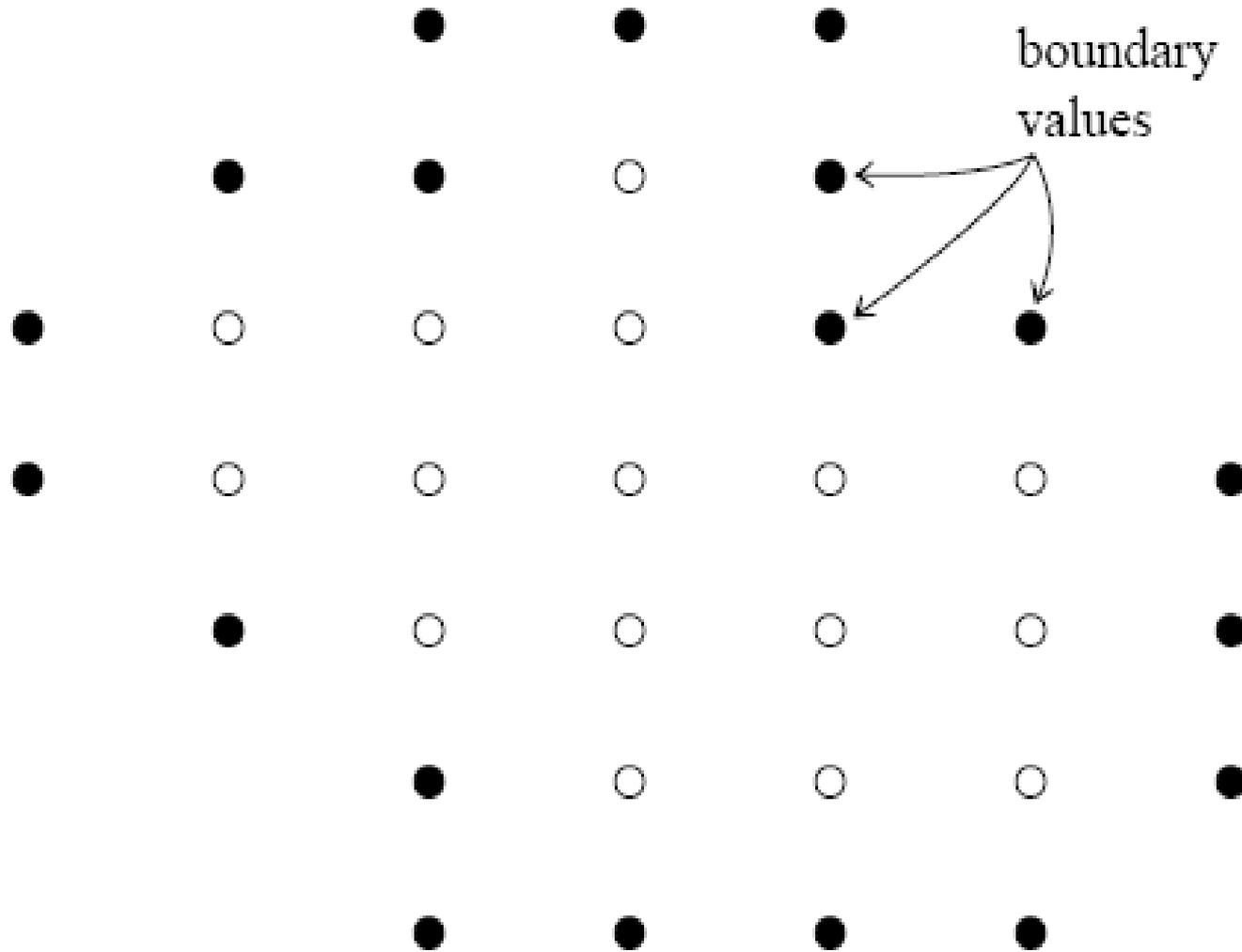
Von Neumann B.C:

Specify normal gradient of $u(x,y,\dots)$ on boundaries.

In principle boundary can be arbitrary shaped.(but difficult to implement **in computer codes**)

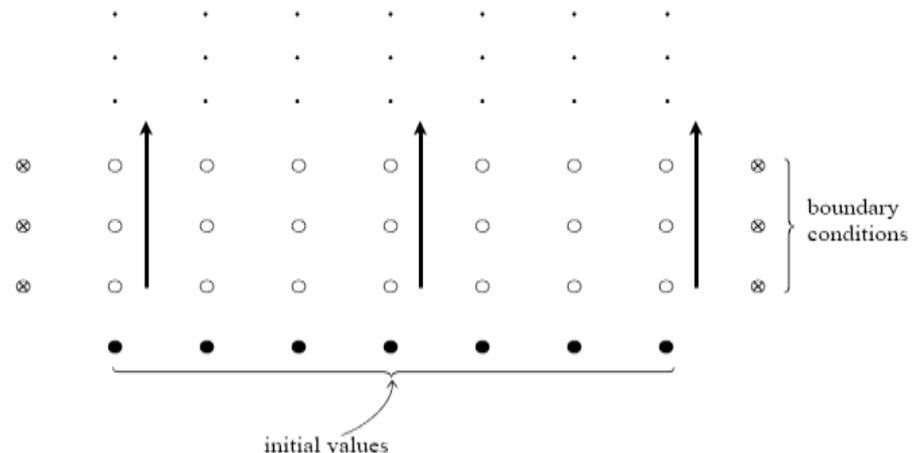


Boundary value problem



Initial value problem

- ⦿ Boundary values are usually specified on all boundaries of the computational domain.
- ⦿ Initial conditions are specified in the entire computational (spatial) domain, but only for the initial time $t=0$.
- ⦿ Initial conditions as a Cauchy problem:
 - Specify initial distribution $u(x,y,\dots,t=0)$
 [for parabolic problems like the Heat equation]
 - Specify u and du/dt for $t=0$
 [for hyperbolic problems like wave equation.]



BASIC ASPECTS OF DISCRETIZATION

UNIT - III

CLOs

Course Learning Outcome

- | | |
|-------|---|
| CLO9 | Explain the need of classification of quasi linear partial differential equations by Cramer's rule and Eigen Value Method. |
| CLO10 | Understand the concepts of range of influence and domain of dependence for a flow field. |
| CLO11 | Explain the general behavior of the partial differential equations which falls in hyperbolic, parabolic and elliptic equations. |
| CLO12 | Demonstrate the CFD aspects of the hyperbolic, parabolic and elliptic equations in aerodynamic problems and physical problems. |
| CLO13 | Understand the need for generating grids for solving the finite differential equations in analyzing a flow field. |
| CLO14 | Explain the technique of pressure correction method with the need of staggered grid and its philosophy. |

Numerical methods

- ⦿ Most PDEs cannot be solved analytically.
- ⦿ Variable separation works only for some simple cases and in particular usually not for in homogenous and/or nonlinear PDEs.
- ⦿ Numerical methods require that the PDE become discretized on a grid.
- ⦿ Finite difference methods are popular/ most commonly used in science. They replace differential equation by difference equations)
- ⦿ Engineers (and a growing number of scientists too) often use Finite Elements.

Finite differences

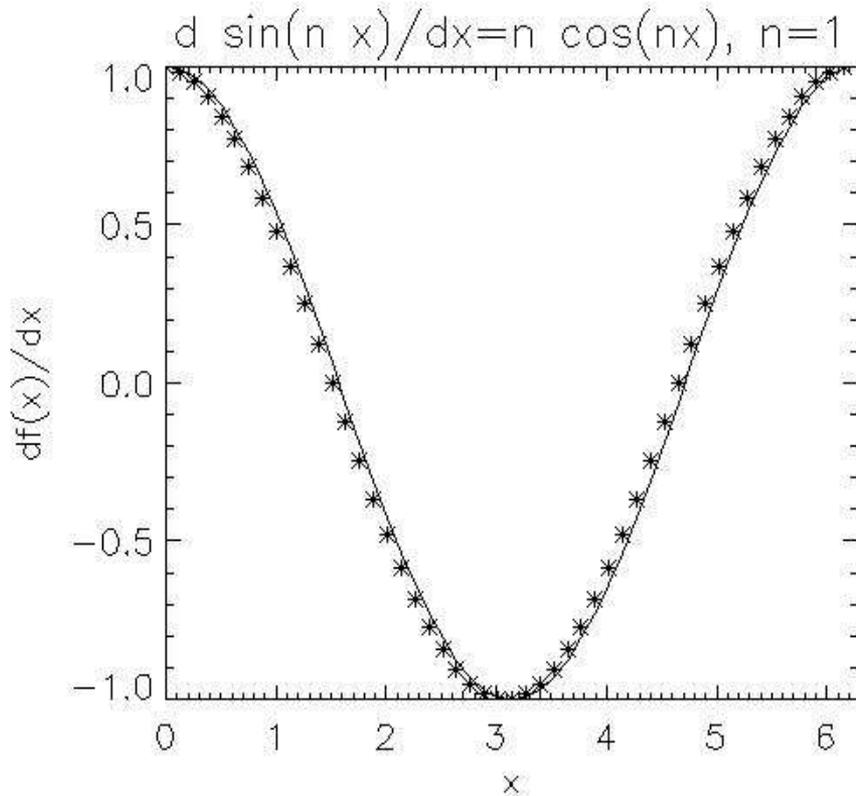
Remember the definition of differential quotient:

$$\frac{df(x)}{dx} = f'(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

- ⦿ How to compute differential quotient numerically?
- ⦿ Just apply the formular above for a finite h.
- ⦿ For simplicity we use an equidistant grid in $x=[0,h,2h,3h,\dots,(n-1) h]$ and evaluate $f(x)$ on the corresponding grid points x_i .
- ⦿ Grid resolution h must be sufficient high. Depends strongly on function $f(x)$!

Accuracy of finite differences

We approximate the derivative of $f(x)=\sin(n x)$ on a grid $x=0 \dots 2 \text{ Pi}$ with 50 (and 500) grid points by $df/dx=(f(x+h)-f(x))/h$ and compare with the exact solution $df/dx= n \cos(n x)$



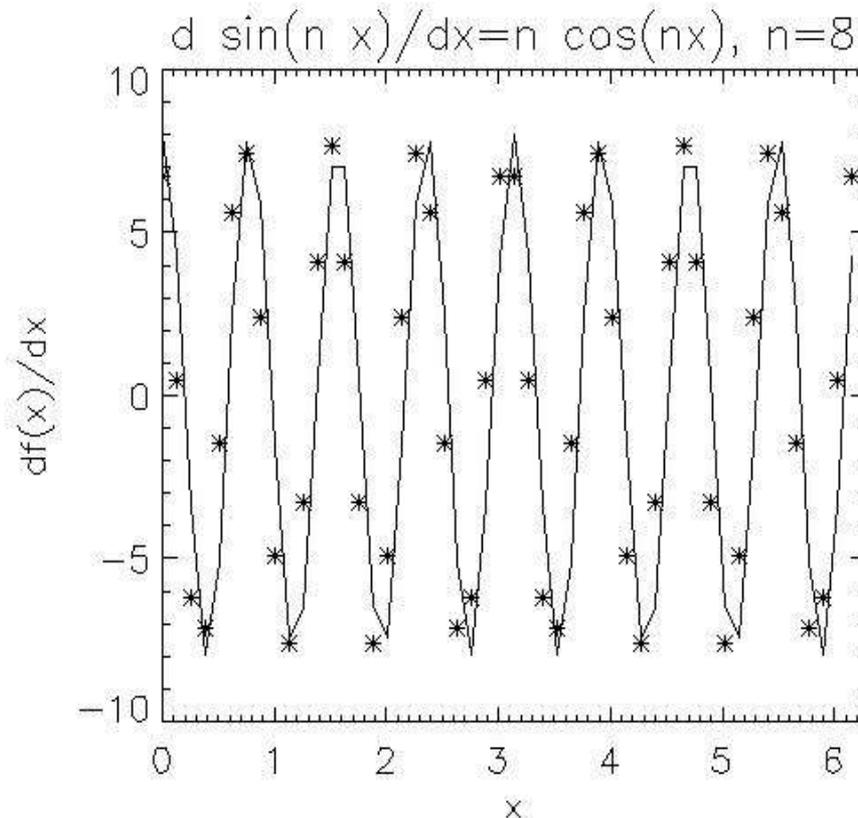
Average error done by discretization:

50 grid points: 0.040

500 grid points: 0.004

Accuracy of finite differences

We approximate the derivative of $f(x)=\sin(n x)$ on a grid $x=0 \dots 2 \text{ Pi}$ with 50 (and 500) grid points by $df/dx=(f(x+h)-f(x))/h$ and compare with the exact solution $df/dx= n \cos(n x)$

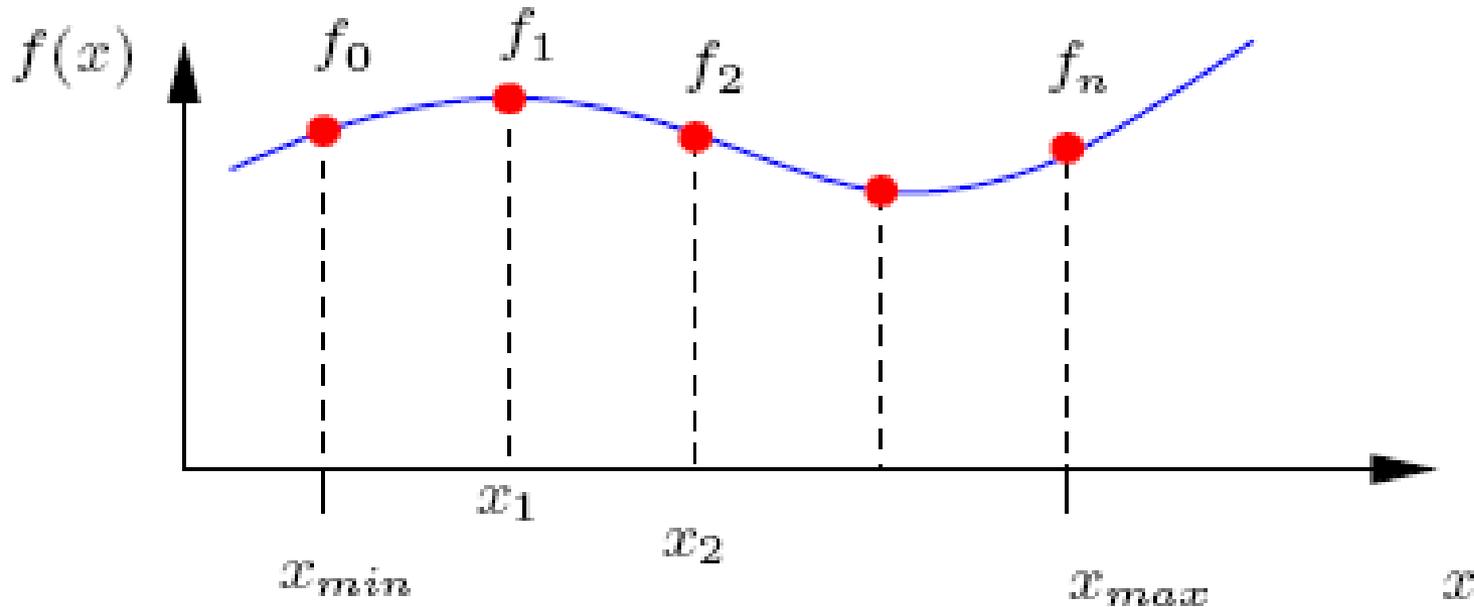


Average error done by discretization:

50 grid points: 2.49

500 grid points: 0.256

Higher accuracy methods



Can we use more points for higher accuracy?

Higher accuracy: Central differences

- ⦿ $df/dx=(f(x+h)-f(x))/h$ computes the derivative at $x+h/2$ and not exactly at x .
- ⦿ The alternative formula $df/dx=(f(x)-f(x-h))/h$ has the same shortcomings.
- ⦿ We introduce central differences: $df/dx=(f(x+h)-f(x-h))/(2h)$ which provides the derivative at x .
- ⦿ Central differences are of 2. order accuracy instead of 1. order for the simpler methods above.

How to find higher order formulas?

For sufficient smooth functions we describe the function $f(x)$ locally by polynomial of n th order. To do so $n+1$ grid points are required. n defines the **order** of the scheme.

Make a Taylor expansion (Definition $x_{i+1} = x_i + \Delta x$)

$$f_{i+1} = f_i + \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) + \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4)$$

$$f_{i-1} = f_i - \Delta x f'(x_i) + \frac{\Delta x^2}{2} f''(x_i) - \frac{\Delta x^3}{6} f'''(x_i) + O(\Delta x^4)$$

$$f_{i+2} = f_i + 2\Delta x f'(x_i) + 2\Delta x^2 f''(x_i) + \frac{4\Delta x^3}{3} f'''(x_i) + O(\Delta x^4)$$

Accuracy of finite differences

We approximate the derivative of $f(x)=\sin(n x)$ on a grid $x=0 \dots 2 \text{ Pi}$ with 50 (and 500) grid points with 1th, 2th and 4th order schemes:

	1th order	2th order	4th order
n=1, 50 pixel	0.04	0.0017	$5.4 \cdot 10^{-6}$
n=1, 500 pixel	0.004	$1.7 \cdot 10^{-5}$	$4.9 \cdot 10^{-6}$
n=8, 50 pixel	2.49	0.82	0.15
n=8, 500 pixel	0.26	0.0086	$4.5 \cdot 10^{-5}$
n=20, 50 pixel	13.5	9.9	8.1
n=20, 500 pix.	1.60	0.13	0.0017

OUTLINE OF DISCRETIZATION

- ⦿ Approximations to partial derivatives
- ⦿ Finite difference representation of Partial Differential Equations
- ⦿ Discretization
 - Consistency
 - Stability
 - Convergence
- ⦿ Explicit and implicit approaches
- ⦿ The finite volume technique
- ⦿ Boundary conditions
- ⦿ Stability analysis

THE WAYS TO OBTAIN FINITE DIFFERENCE REPRESENTATIONS OF DERIVATIVES



- ⦿ Forward difference
- ⦿ Backward difference
- ⦿ Central difference

ON THE SELECTION OF A FINITE DIFFERENCE APPROXIMATION



- ⦿ Depends on the physics of the problem being studied
- ⦿ Any scheme that fails to represent the physics correctly will fail when you attempt to obtain a solution

Steps of Numerical Solution

- ⦿ Discretization
- ⦿ Consistency
- ⦿ Stability
- ⦿ Convergence

Discretization



- ⦿ This is the process of replacing derivatives by finite difference approximations.
- ⦿ This introduces an error due to the truncation error arising from the finite difference approximation and any errors due to treatment of BC's.
- ⦿ The size of the truncation error will depend locally on the solution. In most cases we expect the discretization error to be larger than round-off error.

Stability

A stable numerical scheme is one for which errors from any source (round-off, truncation) are not permitted to grow in the sequence of numerical procedures as the calculation proceeds from one marching step, or iteration, to the next, thus: errors grow → unstable errors decay → stable

- Stability is normally thought of as being associated with marching problems
- Stability requirements often dictate allowable step sizes
- In many cases a stability analysis can be made to define the stability requirements.

Convergence

The solution of the FDE's should approach the solution of the PDE as the mesh is refined.

Lax Equivalence Theorem (linear, initial value)

For a properly posed problem, with a consistent finite difference representation, stability is the necessary and sufficient condition for convergence.

In practice, numerical experiments must be conducted to determine if the solution appears to be converged with respect to mesh size.

Two Different Approaches

There are many difference techniques used in CFD, you will find that any technique falls into One or the other of following two different general approaches:

- Explicit approach
- Implicit approach

Explicit approach

Advantages of explicit

- Relative simple to set up and program
- This scheme is easily vectorized and a natural for massively parallel computation

Disadvantage of explicit

- Stability requirements require very small steps sizes

Implicit approach

Advantage of implicit

- Stability requirements allow a large step size

Disadvantages of implicit

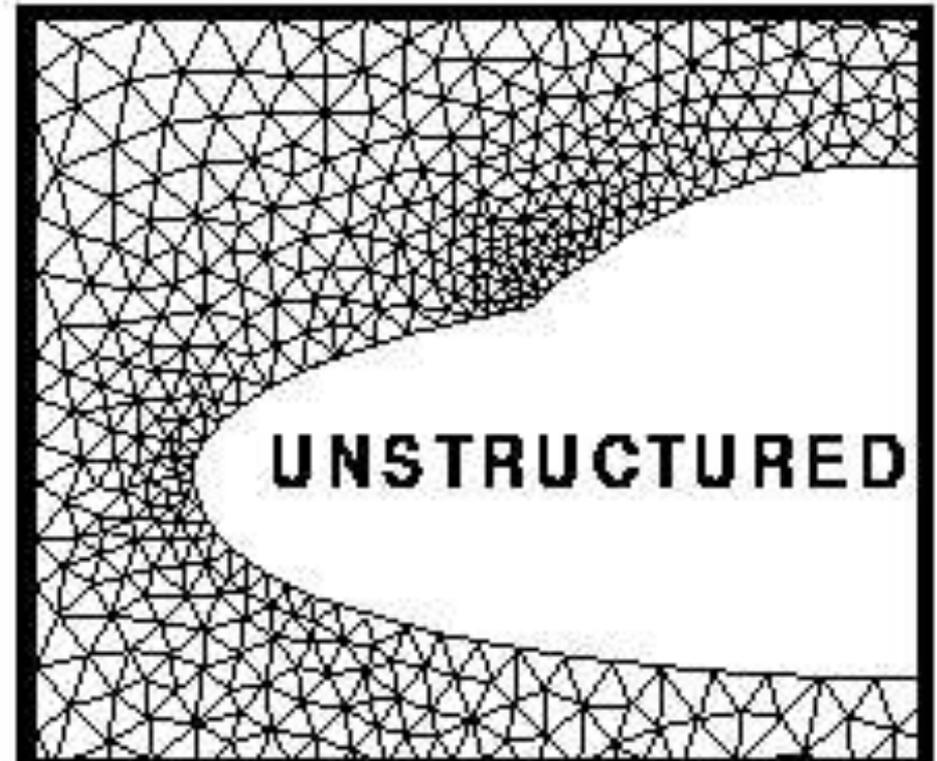
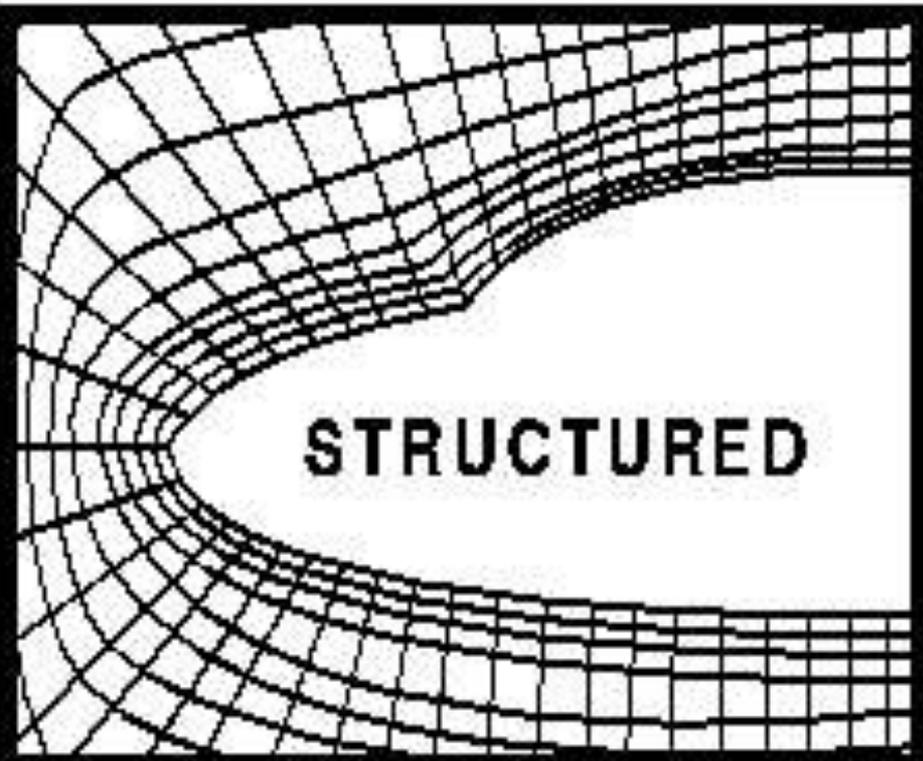
- More complicated to set up and program
- This scheme is harder to vectorize or parallelize
- Since the solution of a system of equations is required at each step, the computer time per step is much larger than in the explicit approach.

Solution schemes

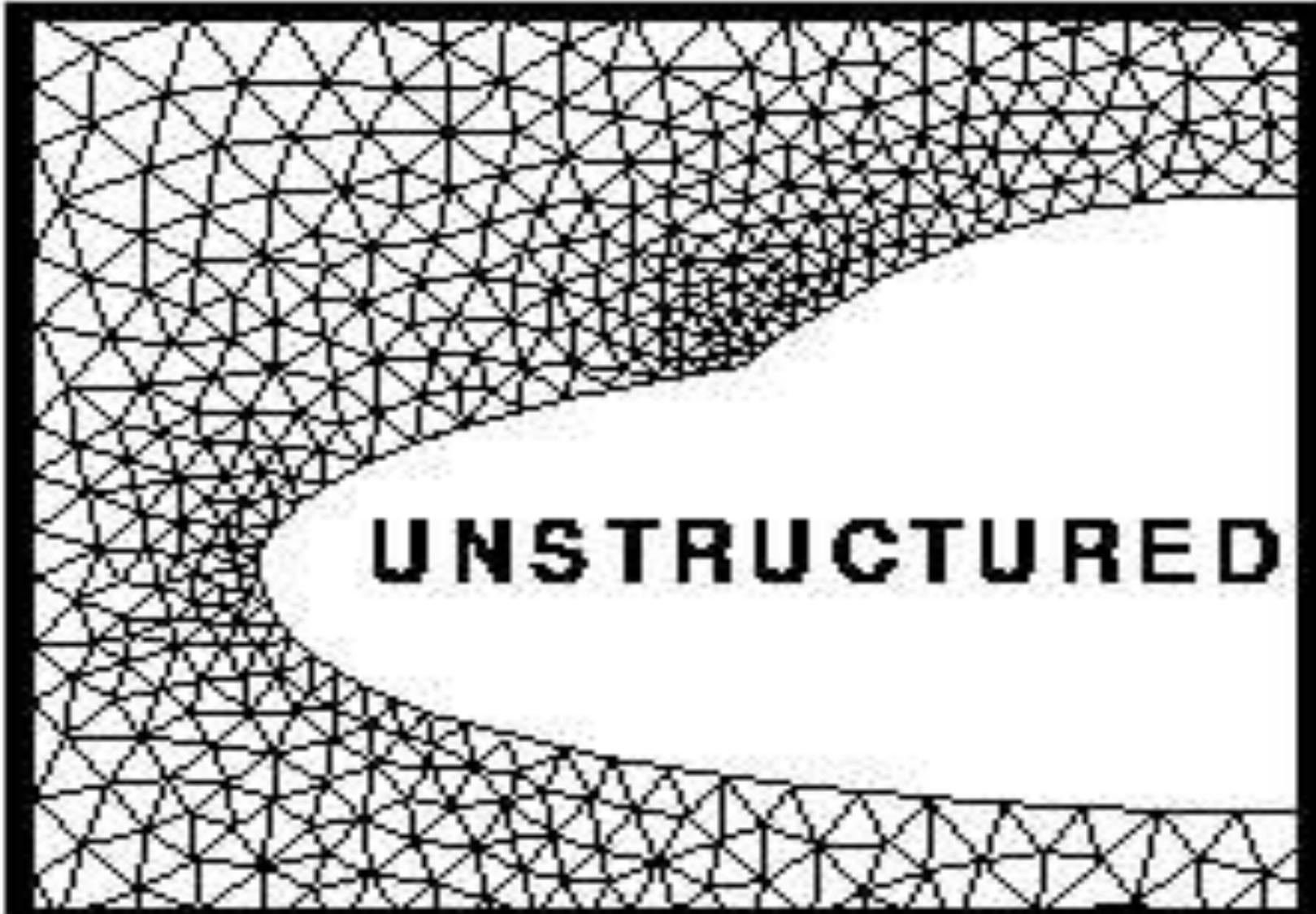
- ⦿ Because of the large number of mesh points, it is generally not practical to solve the system of equations
- ⦿ Instead, an iterative procedure is usually employed.
Initial guess for the solution is made and then each mesh point in the flow field is updated repeatedly until the values satisfy the governing equation.
- ⦿ This iterative procedure can be thought of as having a time-like quality

GRIDS

Different Types Of Grids

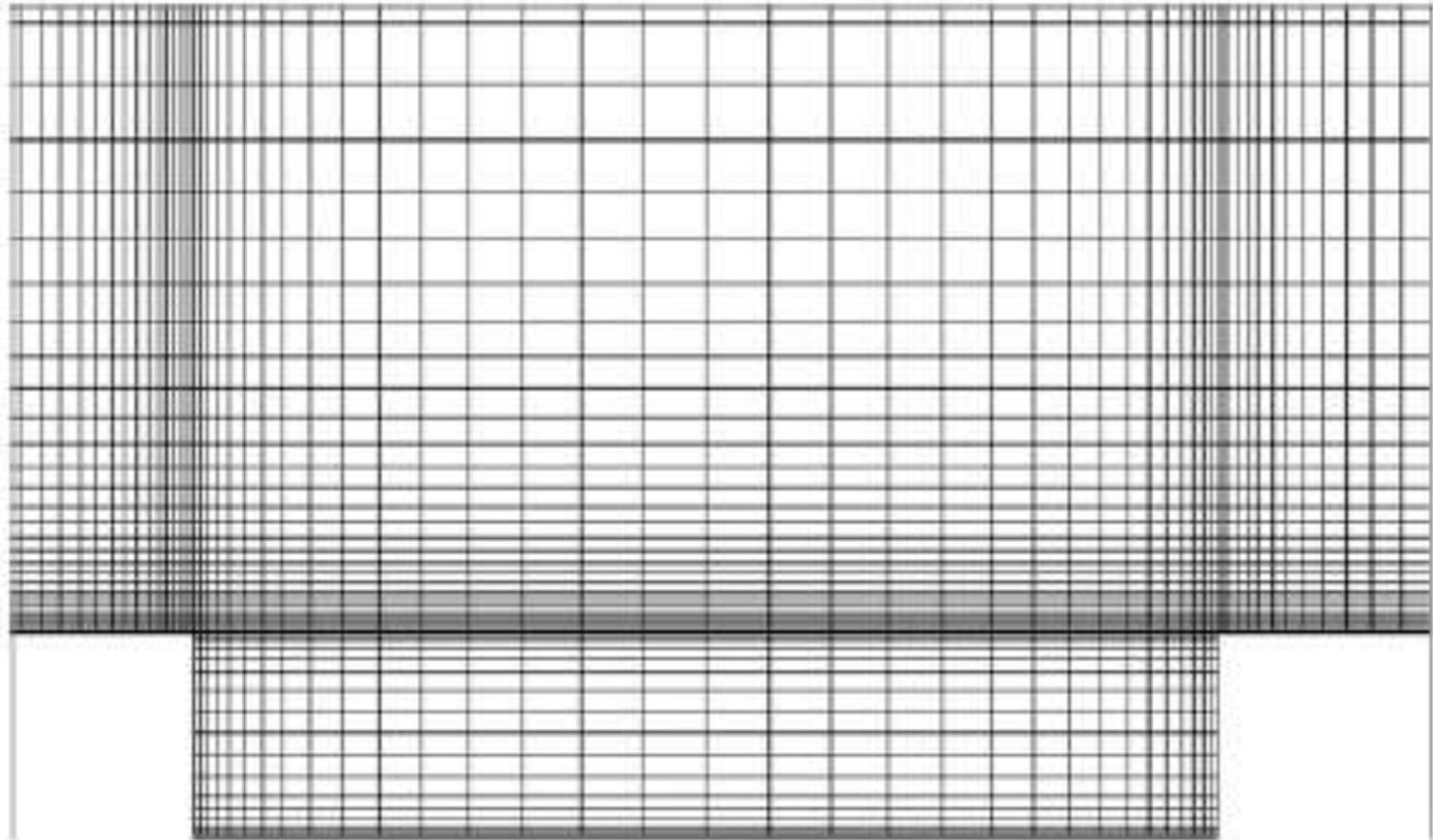


Unstructured Grid

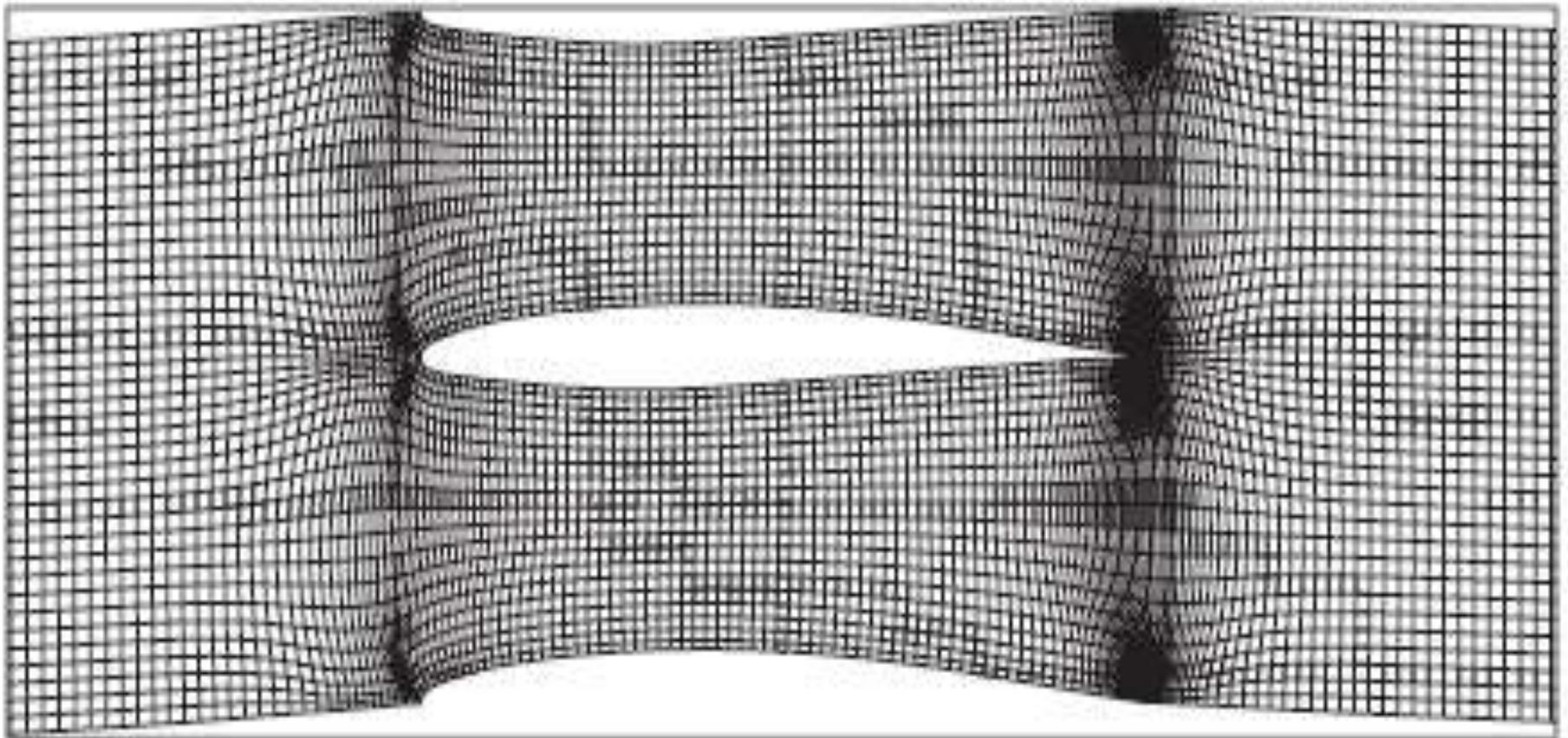


Structured Grid

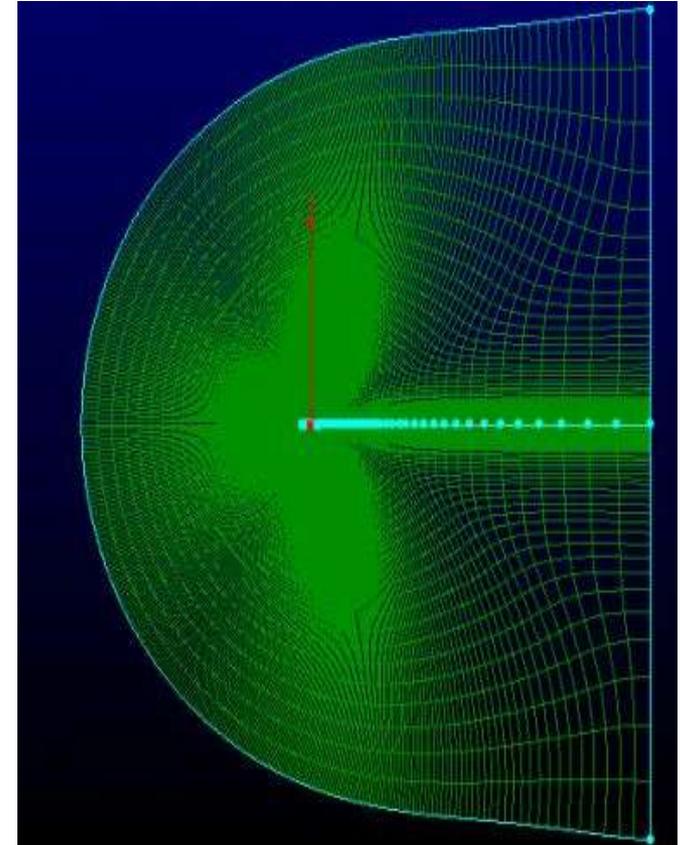
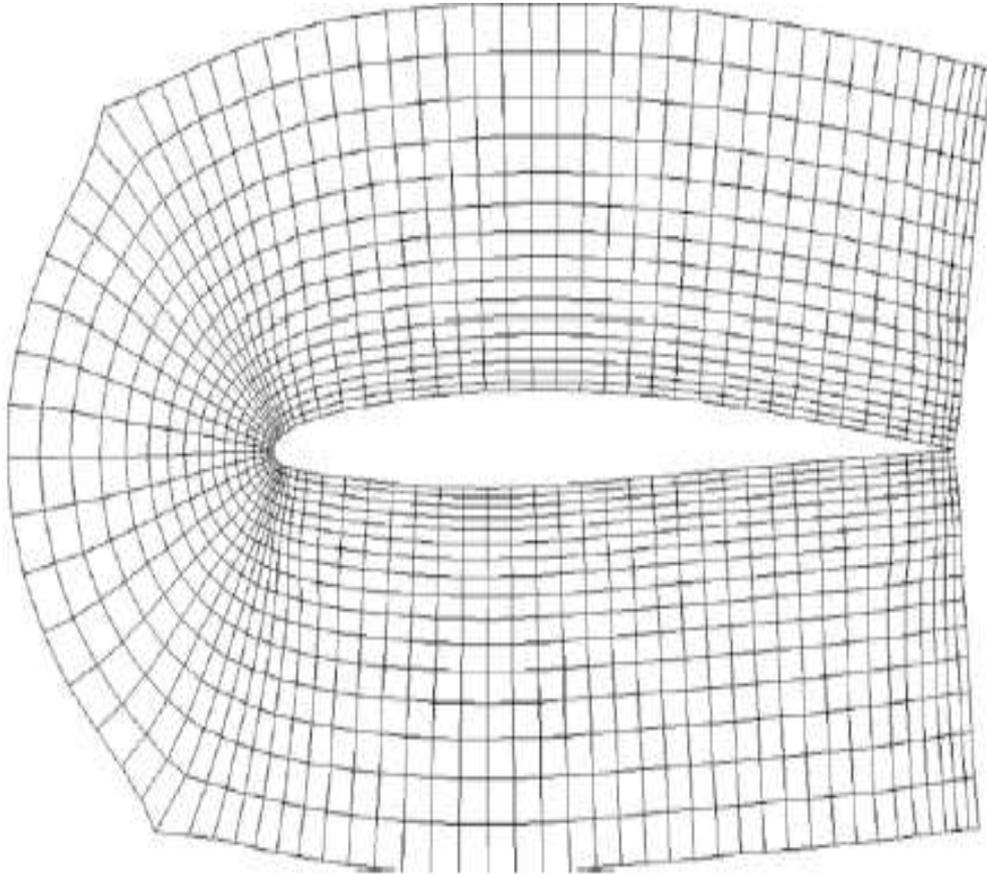
Cartesian Grids



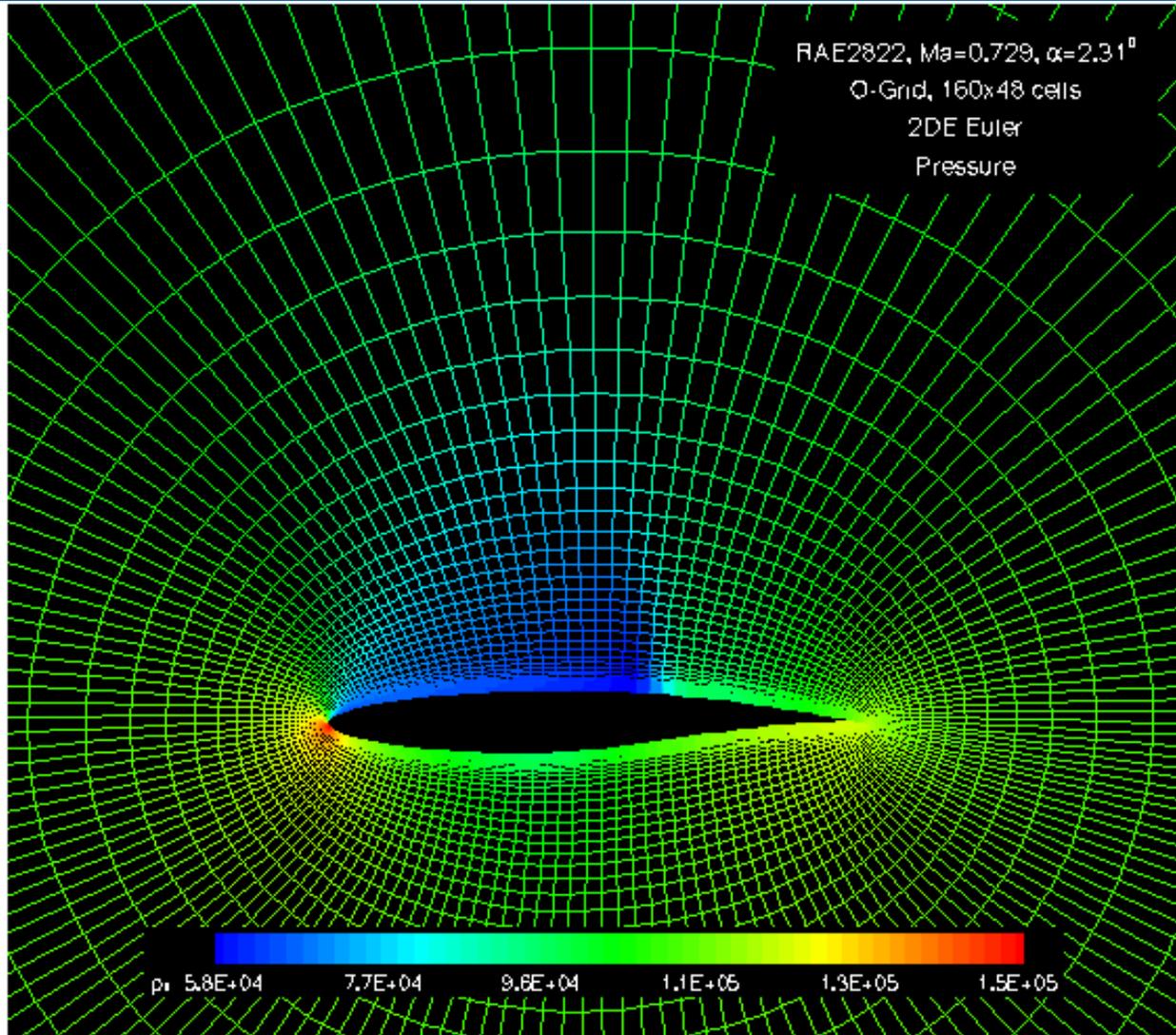
H Type



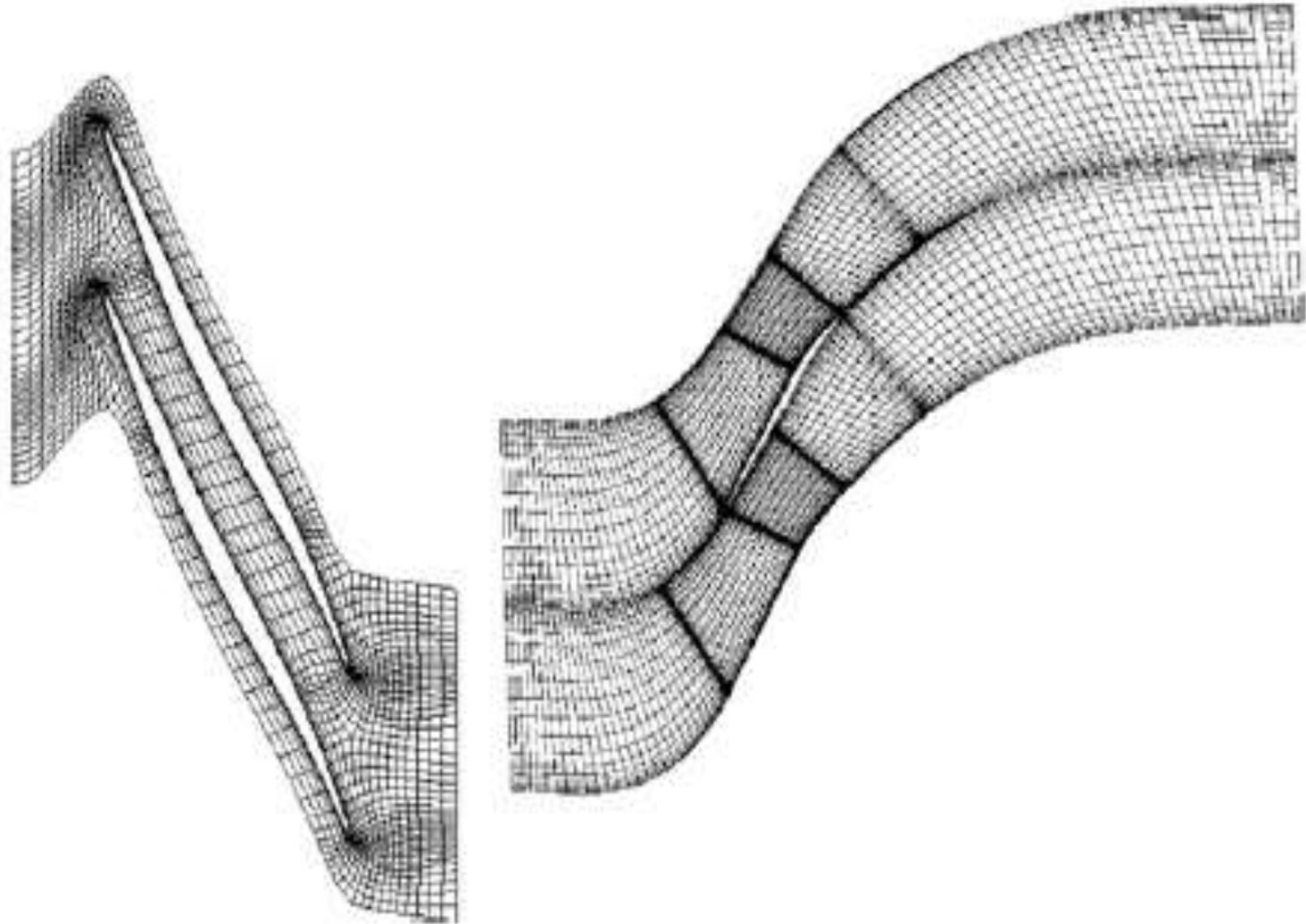
C Type



O Type

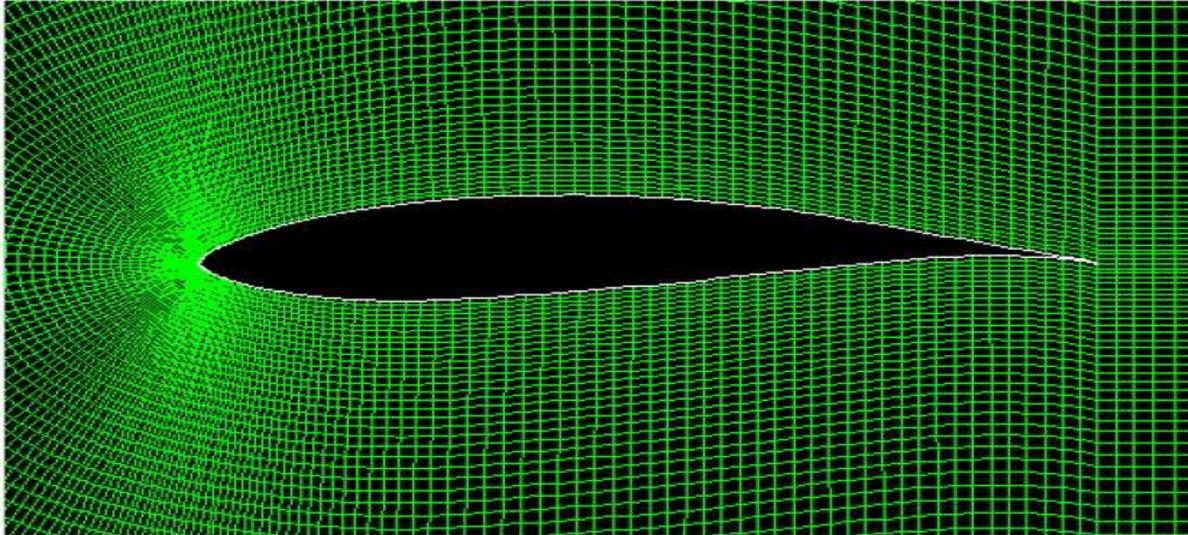


I Type

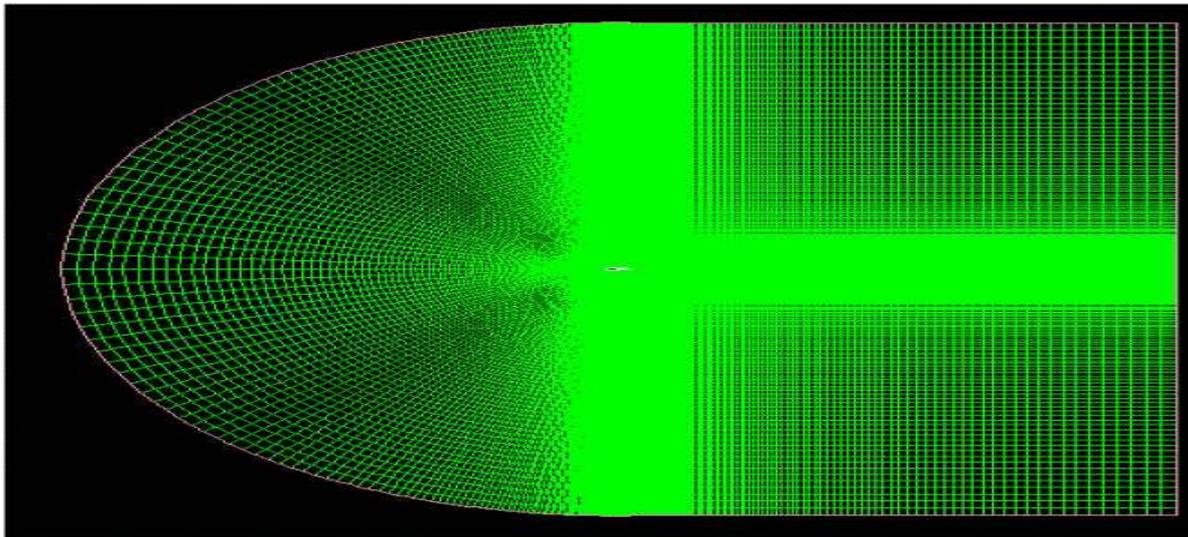


C-H Grid

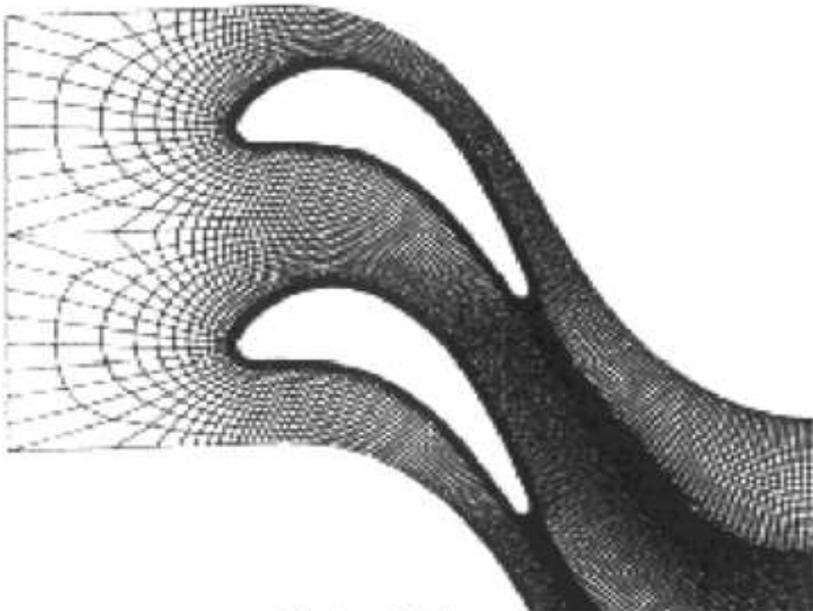
a)



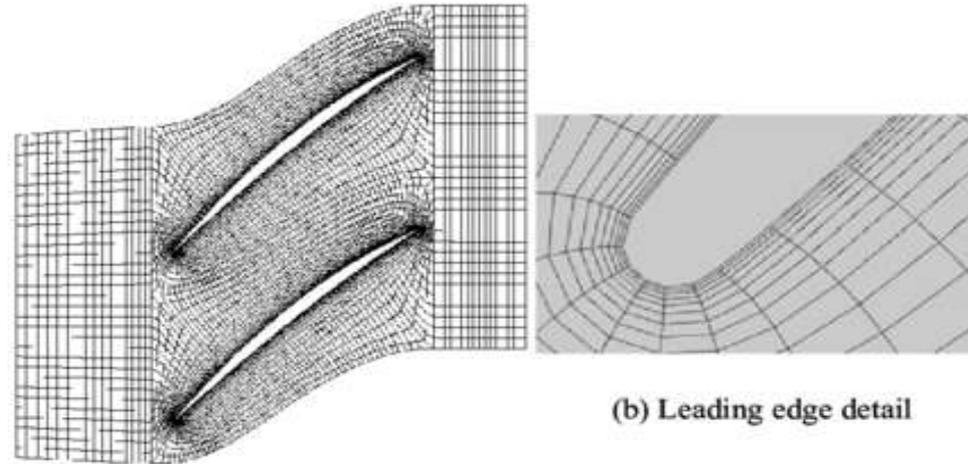
b)



H-O-H Type



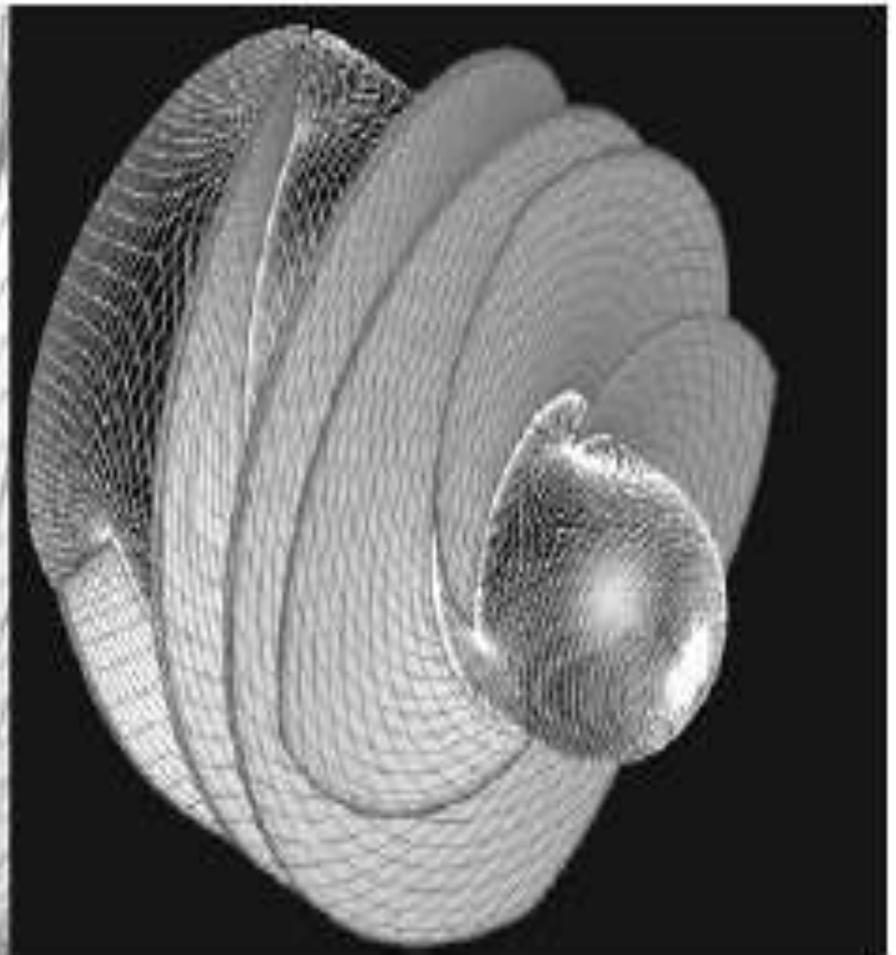
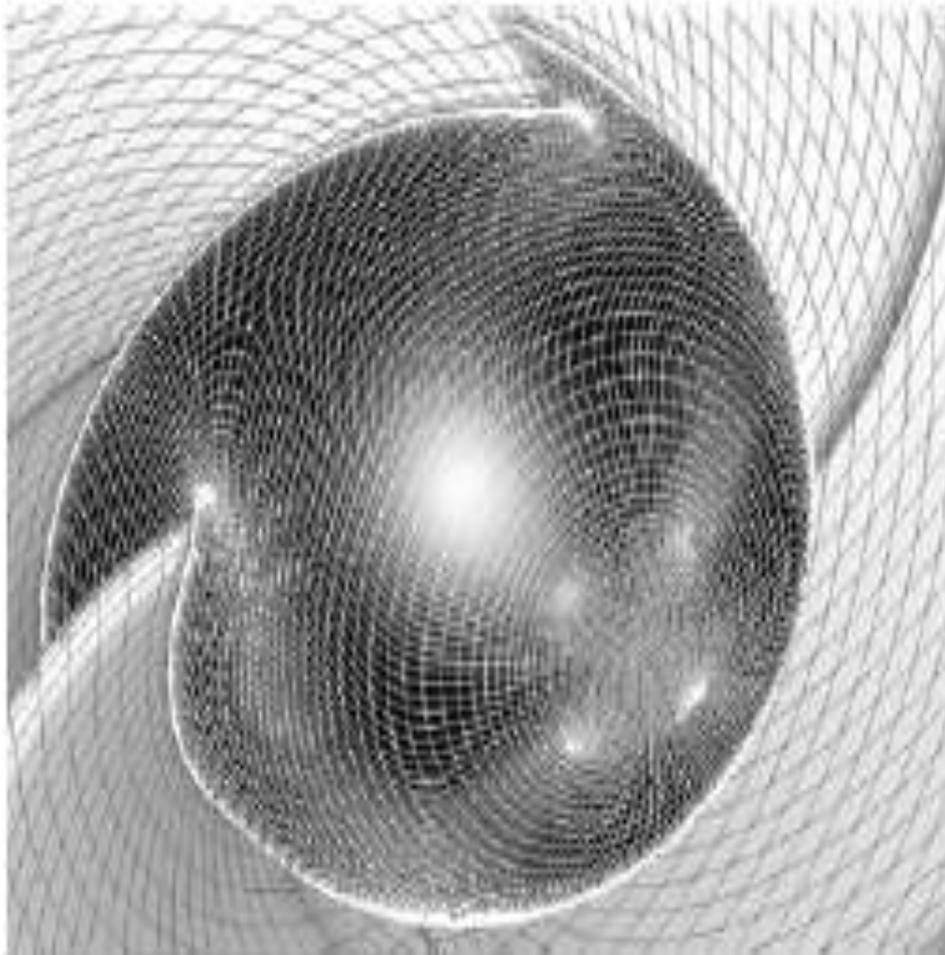
Blade to blade mesh



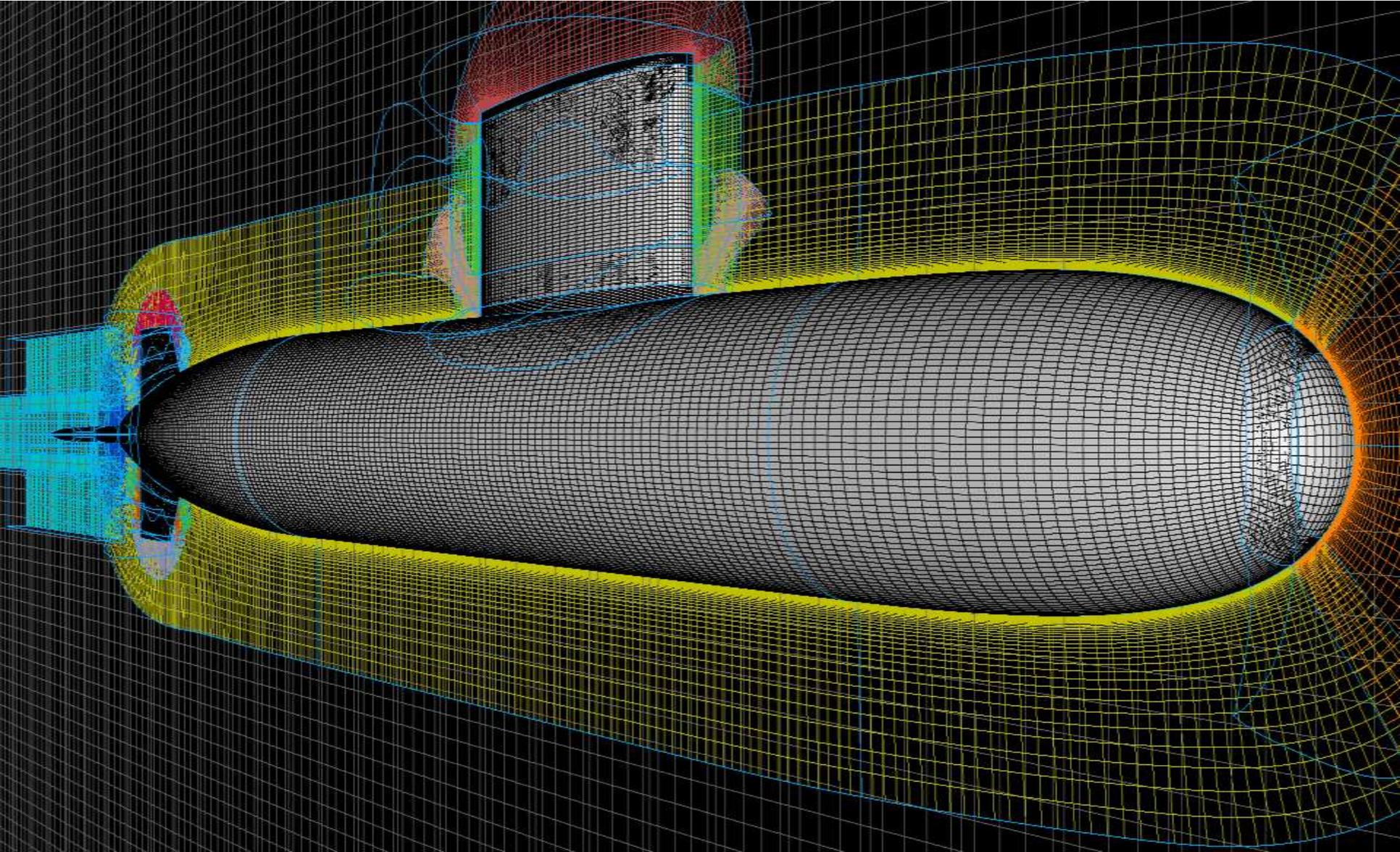
(a) Blade to blade mesh

(b) Leading edge detail

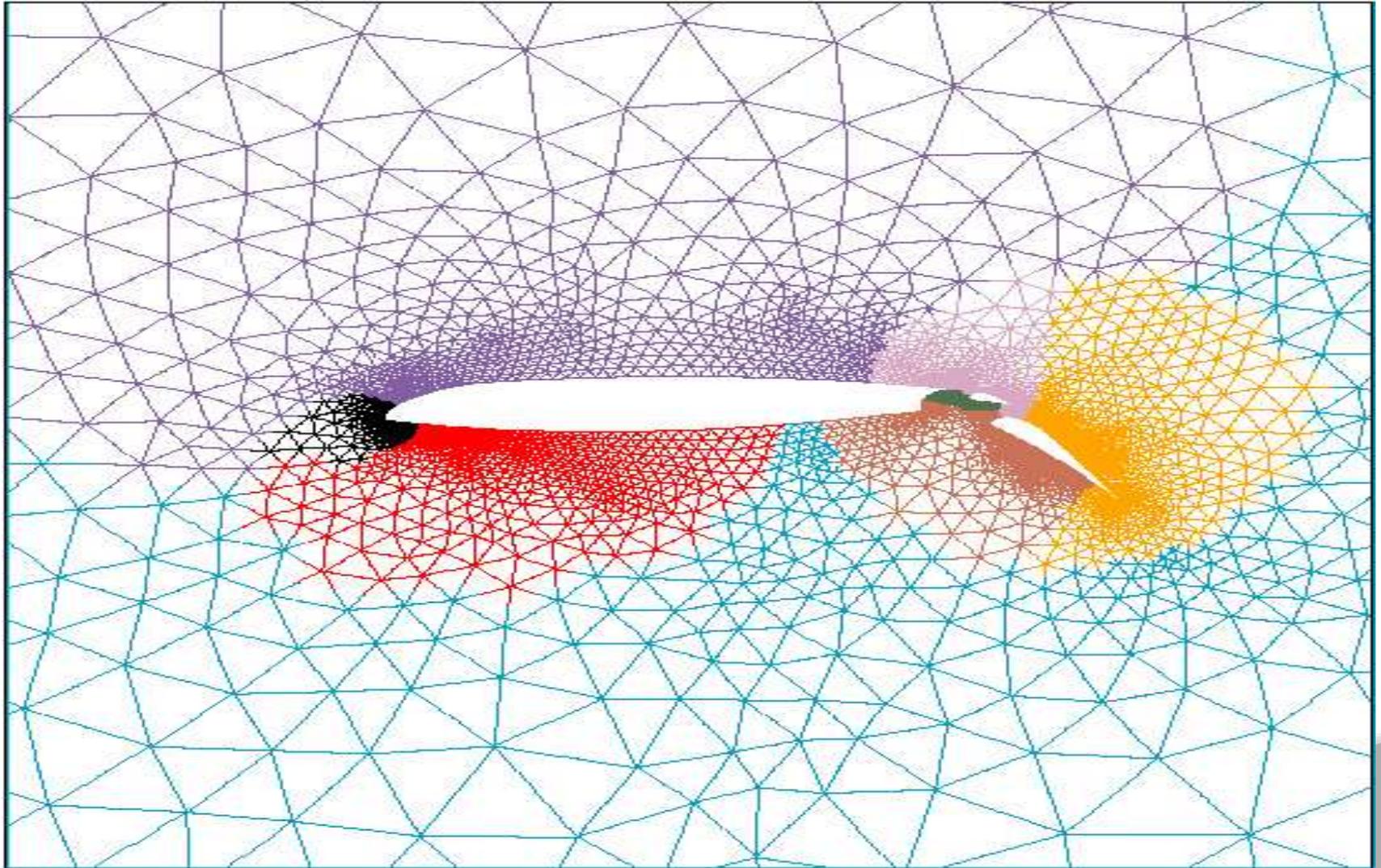
Butterfly Grid



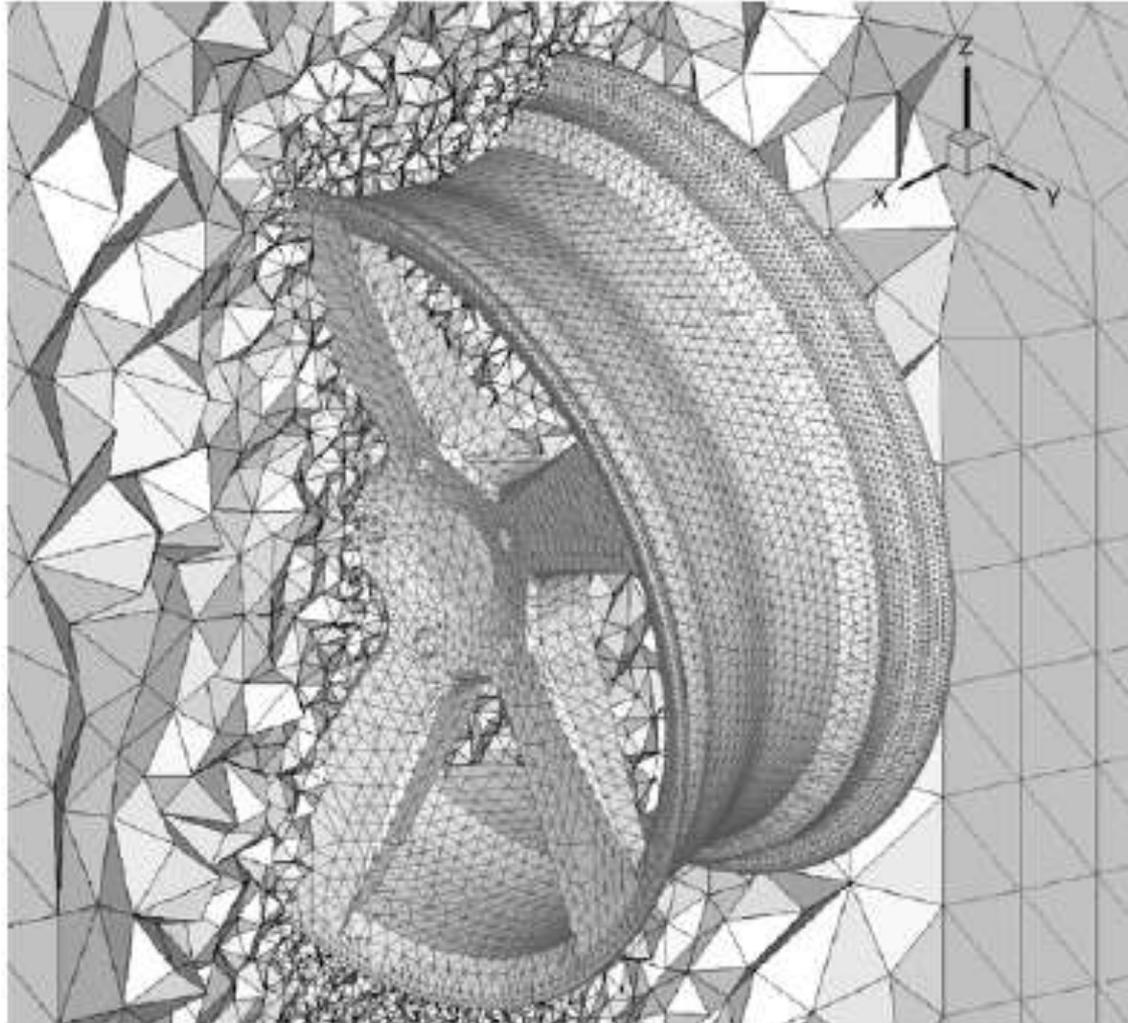
Overset Grid



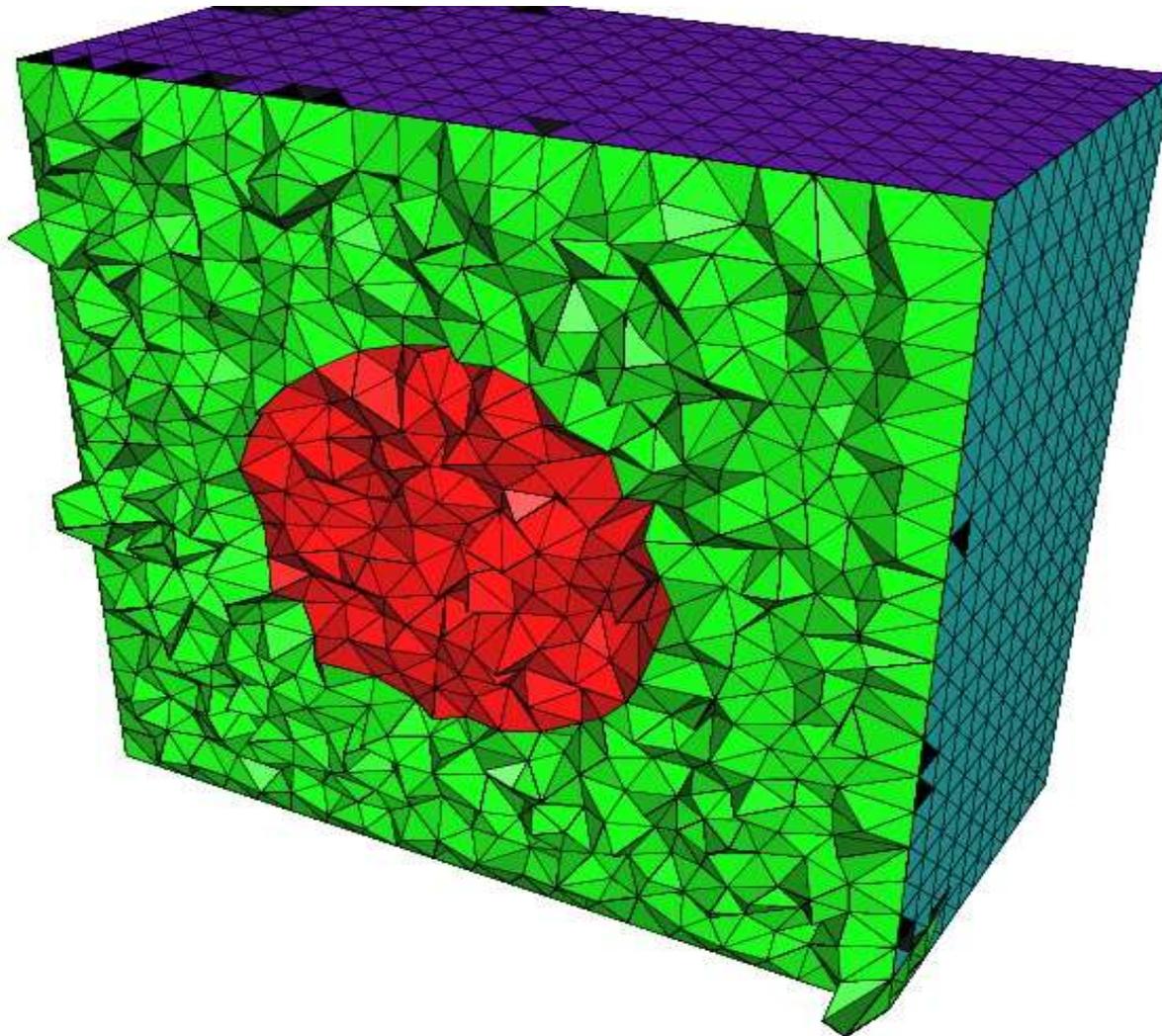
Unstructured grid



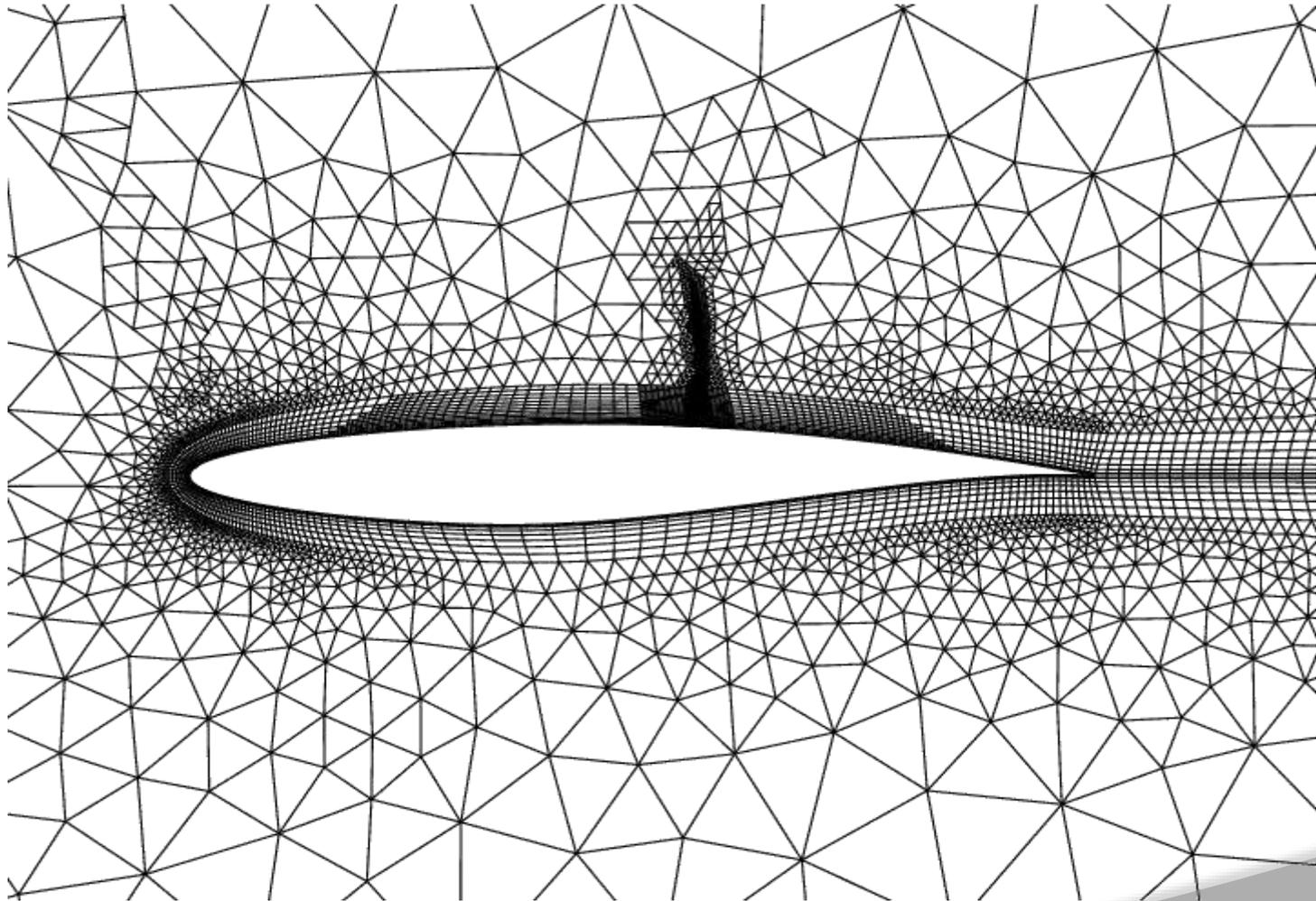
Tetrahedra grid



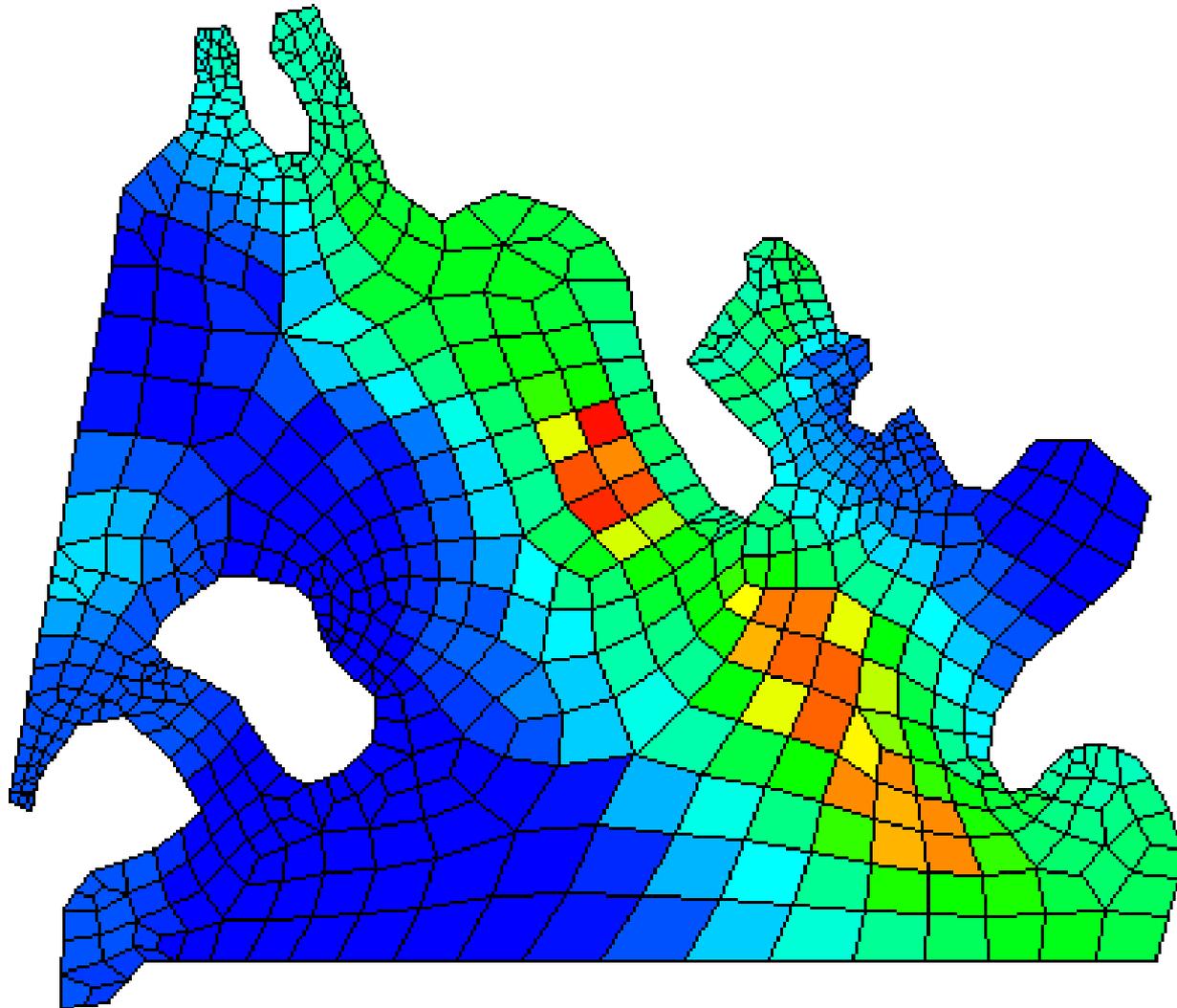
Tetrahedra grid



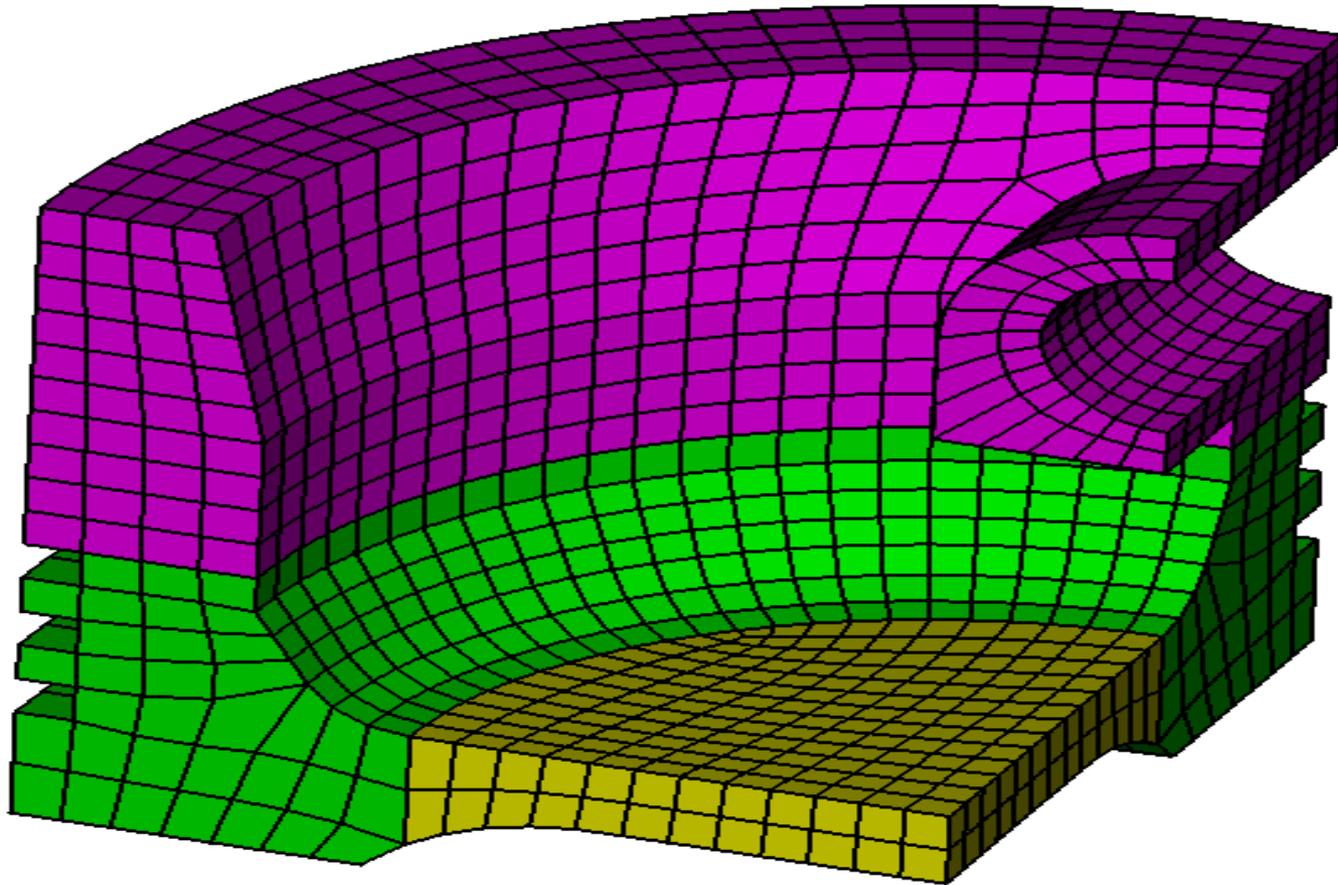
Hybrid Grid



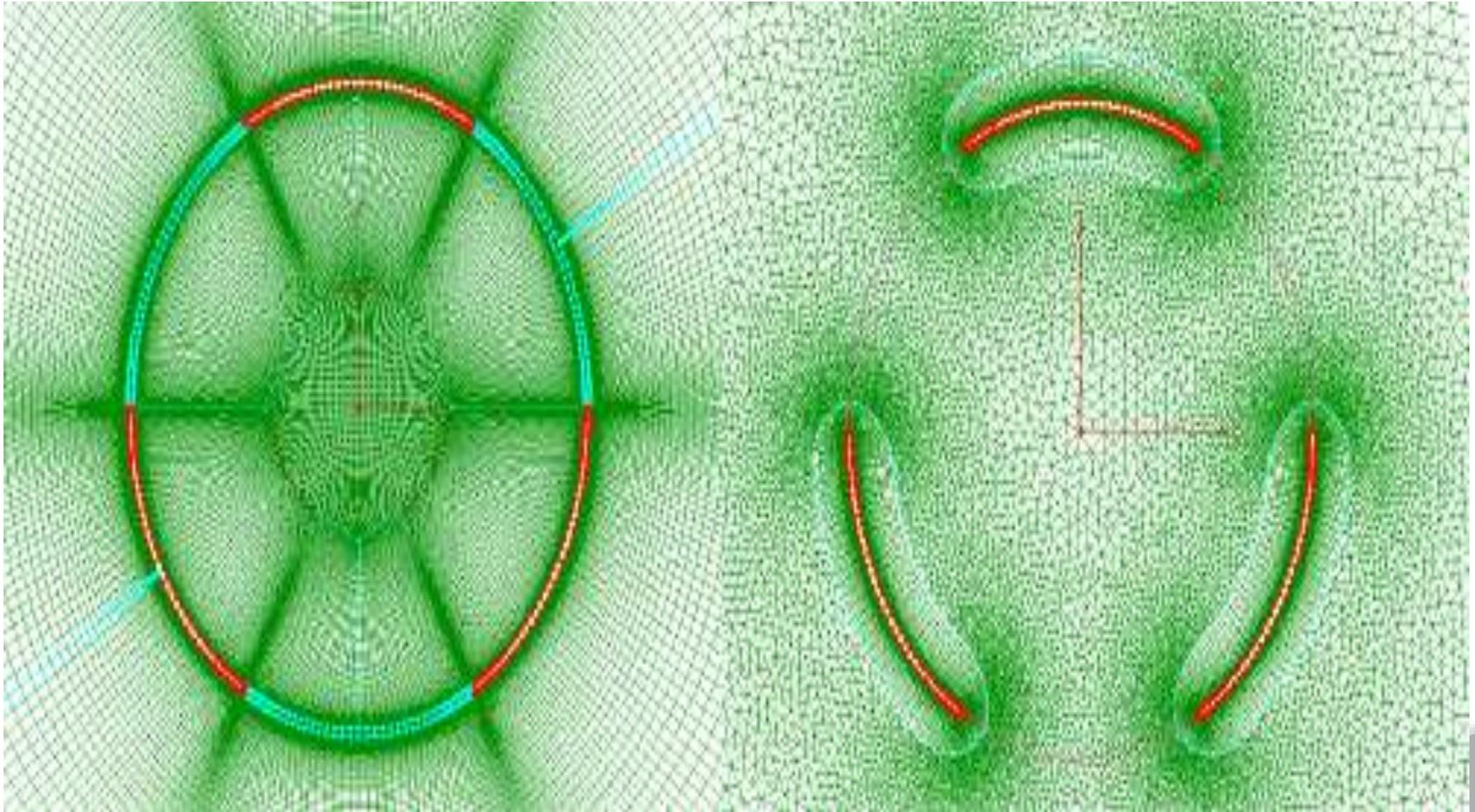
Quadrilateral Grid



Hexahedral Cells



Structured and Hybrid Grids



CFD TECHNIQUES

UNIT - IV

CLOs	Course Learning Outcome
CLO15	Discuss the aspects of numerical dissipation and numerical dispersion and explain the applications of each in CFD techniques.
CLO16	Explain the technique of pressure correction method with the need of staggered grid and its philosophy.
CLO17	Explain the numerical procedures for analysis like SIMPLE, SIMPLER SIMPLEC and PISO algorithms and differentiate with regular CFD techniques.

LAX–WENDROFF TECHNIQUE



- ⦿ The Lax–Wendroff method, named after Peter Lax and Burton Wendroff, is a numerical method for the solution of hyperbolic partial differential equations, based on finite differences.
- ⦿ It is second-order accurate in both space and time. This method is an example of explicit time integration where the function that defines governing equation is evaluated at the current time.

Suppose one has an equation of the following form:

- ⦿ Where x and t are independent variables, and the initial state, $u(x, 0)$ is given.
- ⦿ The first step in the Lax–Wendroff method calculates values for $u(x, t)$ at half time steps, $t_{n+1/2}$ and half grid points, $x_{i+1/2}$. In the second step values at t_{n+1} are calculated using the data for t_n and $t_{n+1/2}$.

LAX–WENDROFF TECHNIQUE

⊙ **First (Lax) steps:**

$$u_{i+1/2}^{n+1/2} = \frac{1}{2}(u_{i+1}^n + u_i^n) - \frac{\Delta t}{2\Delta x}(f(u_{i+1}^n) - f(u_i^n)),$$

$$u_{i-1/2}^{n+1/2} = \frac{1}{2}(u_i^n + u_{i-1}^n) - \frac{\Delta t}{2\Delta x}(f(u_i^n) - f(u_{i-1}^n)).$$

⊙ **Second step:**

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{\Delta x} \left[f(u_{i+1/2}^{n+1/2}) - f(u_{i-1/2}^{n+1/2}) \right].$$

MAC-CORMACKS TECHNIQUE

- ⦿ In computational fluid dynamics, the MacCormack method is a widely used discretization scheme for the numerical solution of hyperbolic partial differential equations.
- ⦿ This second-order finite difference method was introduced by Robert W. MacCormack in 1969. The MacCormack method is elegant and easy to understand and program.

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0.$$

- ⦿ The application of MacCormack method to the above equation proceeds in two steps; a predictor step which is followed by a corrector step.

Predictor step

- ⦿ In the predictor step, a "provisional" value of u_i at time level $n+1$ (denoted by $\overline{u_i^{n+1}}$) is estimated as follows

$$\overline{u_i^{n+1}} = u_i^n - a \frac{\Delta t}{\Delta x} (u_{i+1}^n - u_i^n)$$

- ⦿ It may be noted that the above equation is obtained by replacing the spatial and temporal derivatives in the previous first order hyperbolic equation using forward differences.

Corrector step

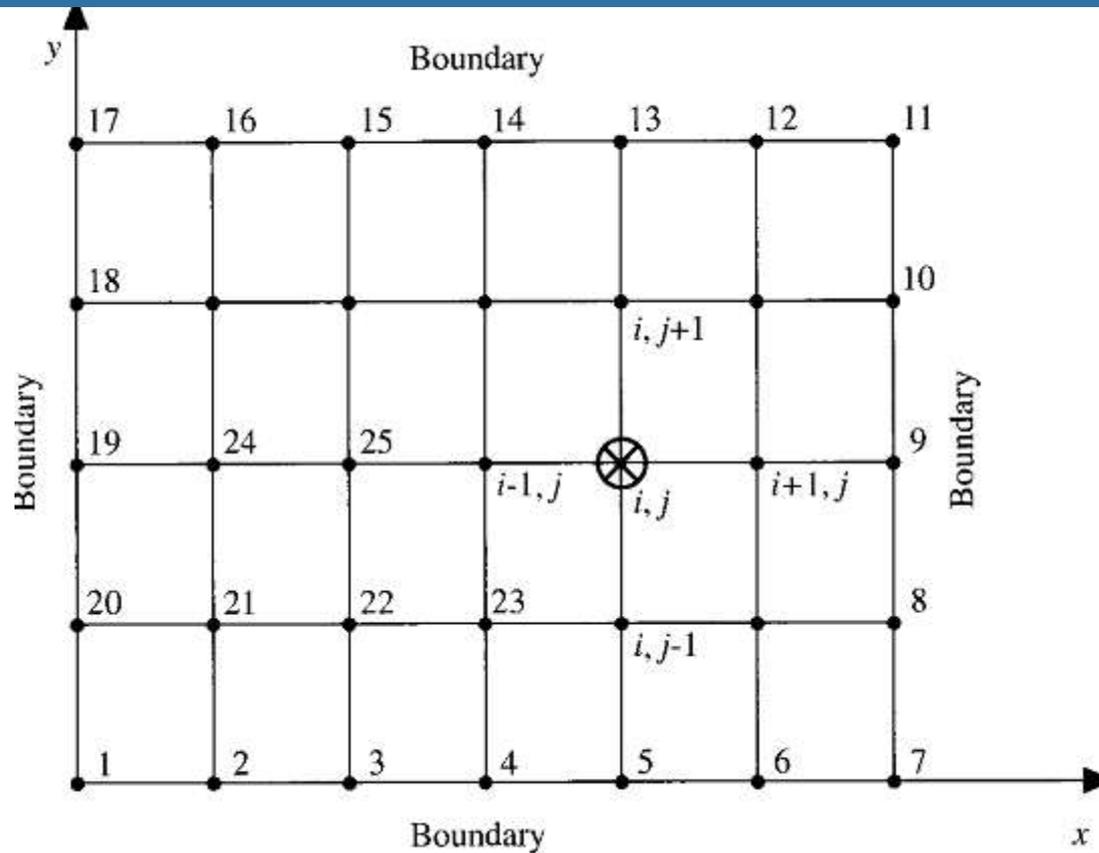
- ⦿ In the corrector step, the predicted value is corrected according to the equation

$$u_i^{n+1} = u_i^{n+1/2} - a \frac{\Delta t}{2\Delta x} (u_i^{n+1} - u_{i-1}^{n+1})$$

- ⦿ Note that the corrector step uses backward finite difference approximations for spatial derivative. Note also that the time-step used in the corrector step is in contrast to the used in the predictor step.
- ⦿ Replacing the Δt term by the temporal average to obtain the corrector step as $u_i^{n+1/2}$

$$u_i^{n+1} = \frac{u_i^n + u_i^{n+1}}{2} - a \frac{\Delta t}{2\Delta x} (u_i^{n+1} - u_{i-1}^{n+1})$$

RELAXATION TECHNIQUE



$$\Phi_{i,j}^{n+1} = \frac{(\Delta x)^2 (\Delta y)^2}{2(\Delta y)^2 + 2(\Delta x)^2} \left[\frac{\Phi_{i+1,j}^n + \Phi_{i-1,j}^n}{(\Delta x)^2} + \frac{\Phi_{i,j+1}^n + \Phi_{i,j-1}^n}{(\Delta y)^2} \right]$$

ALTERNATING-DIRECTION-IMPLICIT (ADI) TECHNIQUE



In numerical analysis, the Alternating Direction Implicit (ADI) method is a finite difference method for solving parabolic, hyperbolic and elliptic partial differential equations.

It is most notably used to solve the problem of heat conduction or solving the diffusion equation in two or more dimensions.

It is an example of an operator splitting method

ALTERNATING-DIRECTION-IMPLICIT (ADI) TECHNIQUE

- Consider the linear diffusion equation in two dimensions,

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = (u_{xx} + u_{yy}) = \Delta u$$

- The implicit Crank–Nicolson method produces the following finite difference equation:

$$\frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t} = \frac{1}{2} (\delta_x^2 + \delta_y^2) (u_{ij}^{n+1} + u_{ij}^n)$$

- The idea behind the ADI method is to split the finite difference equations into two, one with the x -derivative taken implicitly and the next with the y -derivative taken implicitly,

$$\frac{u_{ij}^{n+1/2} - u_{ij}^n}{\Delta t/2} = (\delta_x^2 u_{ij}^{n+1/2} + \delta_y^2 u_{ij}^n)$$

$$\frac{u_{ij}^{n+1} - u_{ij}^{n+1/2}}{\Delta t/2} = (\delta_x^2 u_{ij}^{n+1/2} + \delta_y^2 u_{ij}^{n+1}).$$

- Pressure-correction method is a class of methods used in computational fluid dynamics for numerically solving the Navier-Stokes equations normally for incompressible flows.

$$\rho \left(\underbrace{\frac{\partial \mathbf{v}}{\partial t}}_{\text{Unsteady acceleration}} + \underbrace{(\mathbf{v} \cdot \nabla) \mathbf{v}}_{\text{Convective acceleration}} \right) = \underbrace{-\nabla p}_{\text{Pressure gradient}} + \underbrace{\mu \nabla^2 \mathbf{v}}_{\text{Viscosity}} + \underbrace{\mathbf{f}}_{\text{Other forces}}$$

- The equations solved in this approach arise from the implicit time integration of the incompressible Navier–Stokes equations.

Numerical Procedures



- SIMPLE
- SIMPLER
- SIMPLEC and
- PISO

SIMPLE algorithm



- In computational fluid dynamics (CFD), SIMPLE algorithm is a widely used numerical procedure to solve the Navier-Stokes equations.
- SIMPLE is an acronym for Semi-Implicit Method for Pressure Linked Equations.

SIMPLEC ALGORITHM

- ⦿ Specify the boundary conditions and guess the initial values.
- ⦿ Determine the velocity and pressure gradients.
- ⦿ Calculate the pseudo velocities.
- ⦿ Solve for the pressure equation and get the p .
- ⦿ Set $p^*=p$.
- ⦿ Using p^* solve the discretized momentum equation and get u^* and v^* .
- ⦿ Solve the pressure correction equation.
- ⦿ Get the pressure correction term and evaluate the corrected velocities and get p , u , v , Φ^* .
- ⦿ Solve all other discretized transport equations.
- ⦿ If Φ shows convergence, then STOP and if not, then set $p^*=p$, $u^*=u$, $v^*=v$, $\Phi^*=\Phi$ and start the iteration again.

PISO ALGORITHM

Set the boundary conditions

- ⦿ Solve the discretized momentum equation to compute an intermediate velocity field.
- ⦿ Compute the mass fluxes at the cells faces.
- ⦿ Solve the pressure equation.
- ⦿ Correct the mass fluxes at the cell faces.
- ⦿ Correct the velocities on the basis of the new pressure field.
- ⦿ Update the boundary conditions.
- ⦿ Repeat from 3 for the prescribed number of times.
- ⦿ Increase the time step and repeat from 1.

SIMPLER ALGORITHM



- ⦿ Guess velocity field
- ⦿ Compute momentum coefficients and store.
- ⦿ Compute pressure coefficients and store.
- ⦿ Solve pressure equation and obtain pressure
- ⦿ Solve momentum equations using stored momentum
- ⦿ coefficients and just-computed pressure. Find u^* and v^*
- ⦿ Find b term in pressure-correction equation using u^*

FINITE VOLUME METHODS

UNIT - V

CLOs	Course Learning Outcome
CLO18	Discuss the concepts of finite volume method and explain the difference from finite difference method for solving different flow field.
CLO19	Demonstrate the need of finite volume discretization and its general formulation of a numerical scheme in finite volume method.
CLO20	Understand the principle of two dimensional finite volume methods in solving flow fields with finite control volume.

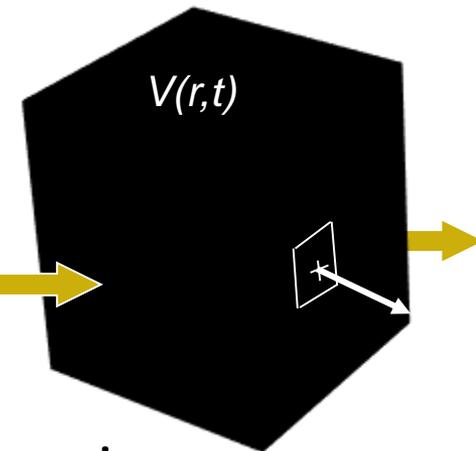
Finite-Volume Formulation

Review of the Integral Equation

The integral equation for the conservation statement is:

$$\frac{d}{dt} \int_{V(\vec{r},t)} Q dV + \oint_{S(\vec{r},t)} [(\vec{v} - \vec{g})Q - \mathbf{D}] \cdot \hat{n} dS = \int_{V(\vec{r},t)} P dV$$

- Equation applies for a control volume.
- Control surface bounds the control volume.
- Q is conserved quantity representing the flow.
- Flow can be through the control surface.
- Control volume and control surface can vary shape in time and space.
- Flow can be time-varying (unsteady).



Objective of the F-V Formulation



Represent the integral equation as an ordinary differential equation (then eventually an algebraic equation) amenable to a solution using computational (numerical) methods.

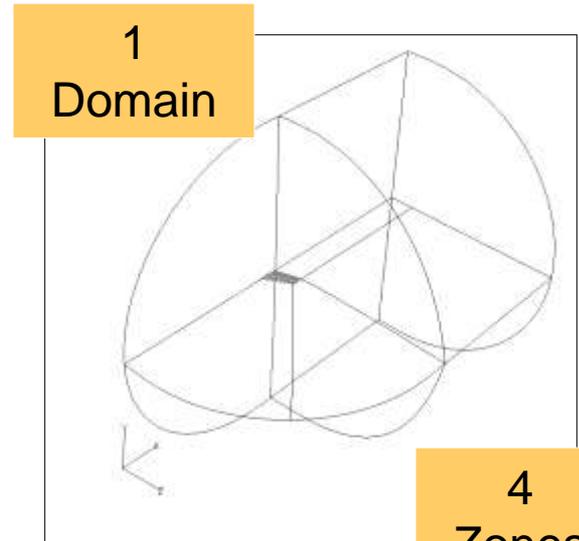
Thus, we need to approximate the *volume integrals* and the *surface integrals* to form algebraic expressions.

Prior to discussing these approximations, let's examine the control volumes on which the integrals will be approximated...

Domain, Zone, Grid, and Cell

The control volumes exists at several levels:

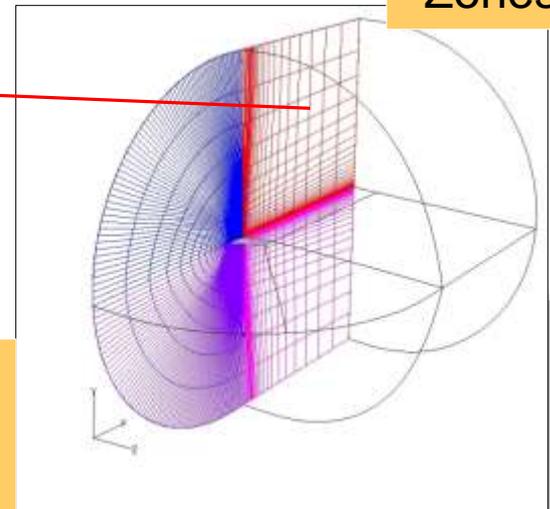
1. Flow Domain, *Extent of CFD analysis*
2. Zone, *Divide domain for convenience, if needed*
3. Grid, *Divides the zone into cells*
4. Cell, *Smallest control volume, but “finite”*



Let's Examine
a hexahedral
cell

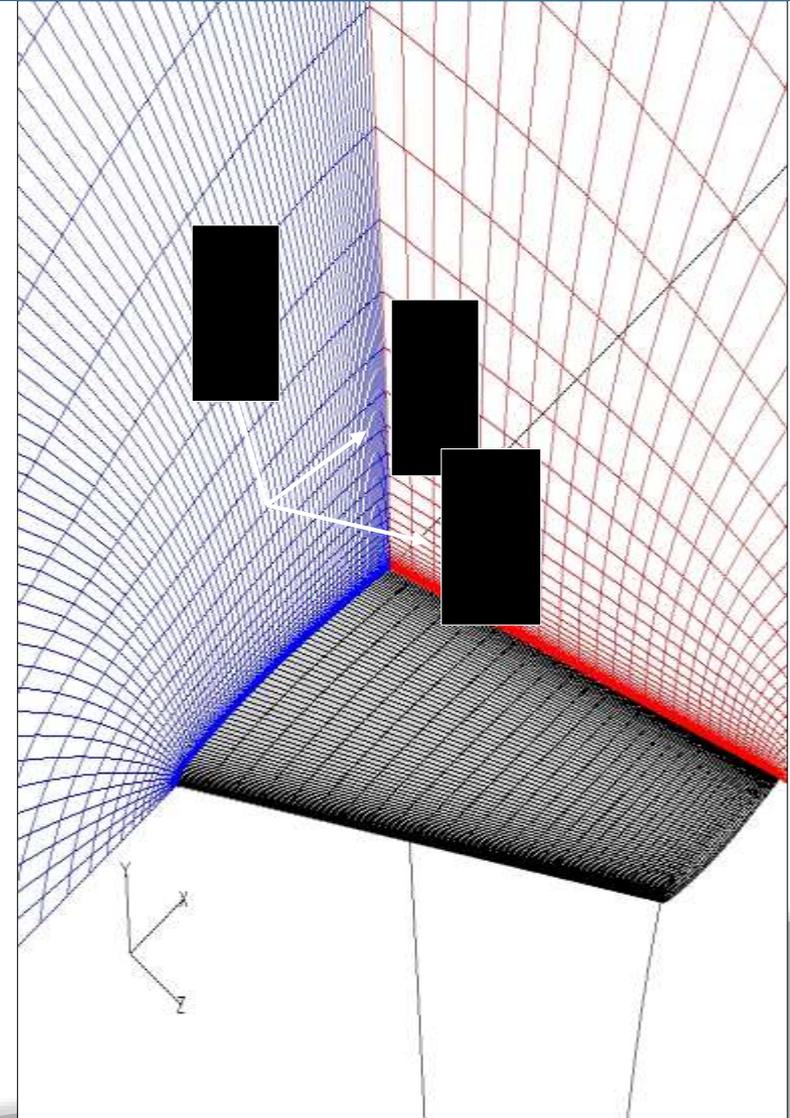
Each control volume is “air-tight”

Grid in each zone
with 1000s of
cells



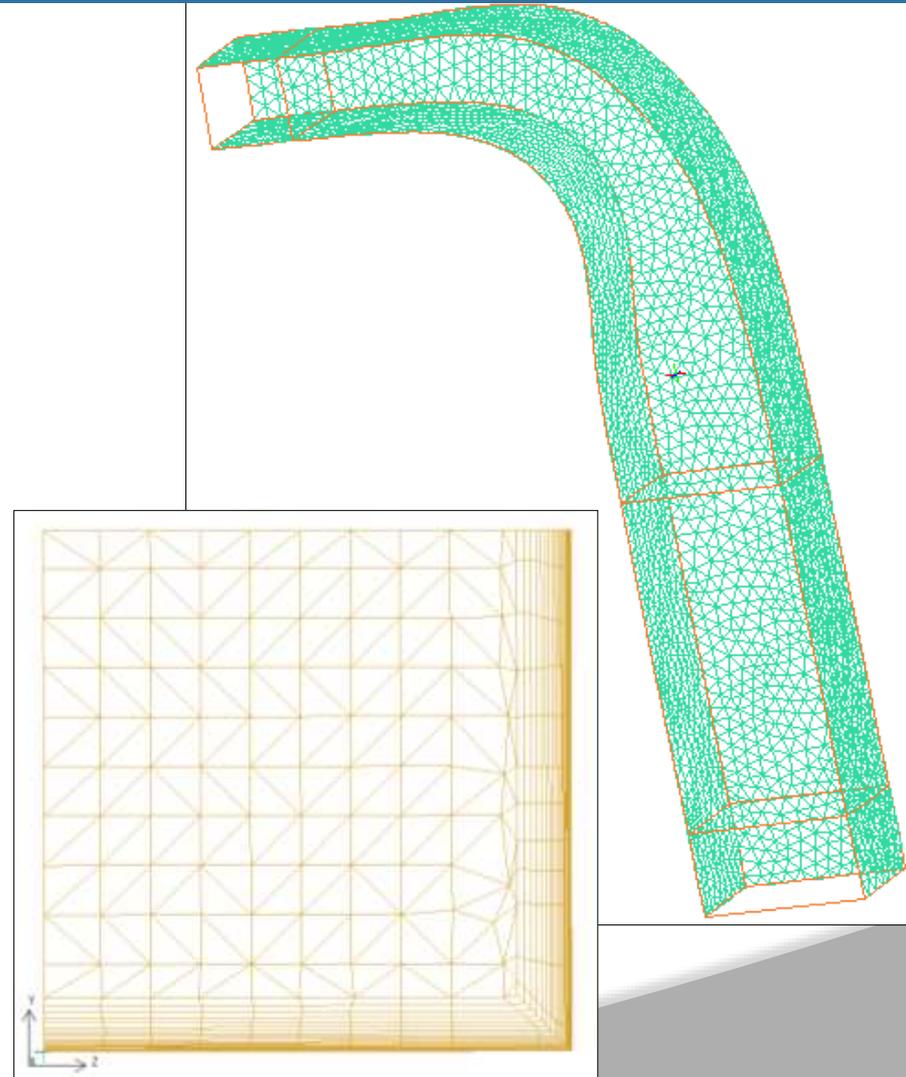
Structured Grid Example

Grid is “body-fitted” to the follow the shape of the body (wing).
 Grid points (vertices) are arranged in an array structure with indices (i,j,k) .
 Transformation between physical space (x,y,z) and a Cartesian computational space with coordinates directions (ξ, η, ζ) .
 Grid points are clustered to the wing to provide resolution of the boundary layer.
 Cells are hexahedral (6 quadrilateral sides).



Unstructured Grid Example

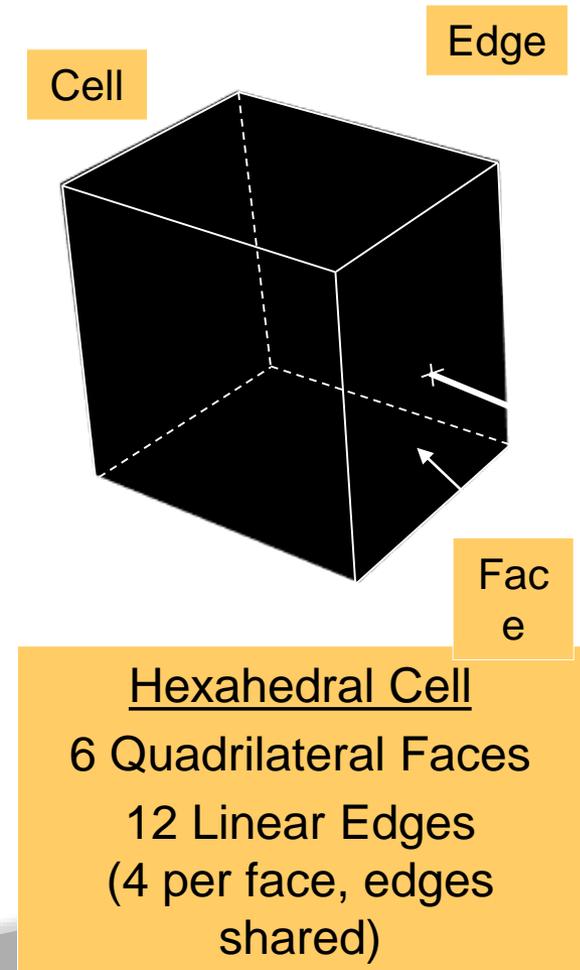
Grid is “body-fitted” to the follow the shape of the body (duct).
Grid points (vertices) are do not have any set structure.
No transformation from physical space (x,y,z) and a computational Space. Specify and store geometric and connectivity information.
Grid points are clustered to the duct surfaces to provide resolution of the boundary layer.
Cells are tetrahedral (4 triangular sides).



Anatomy of a Finite-Volume Cell

Finite-Volume Cell:

- Cell can take on a generalized shape.
- Cell contains a finite (positive) volume.
- Integral equation will be approximated on the cell to form an algebraic relation.
- Size of cell indicates the level of computational resolution of the CFD analysis.
- Control surface is *faceted* into a finite number of faces.
- Faces can take on a variety of shapes.
- Face is bounded by edges.
- Edges are usually straight lines.

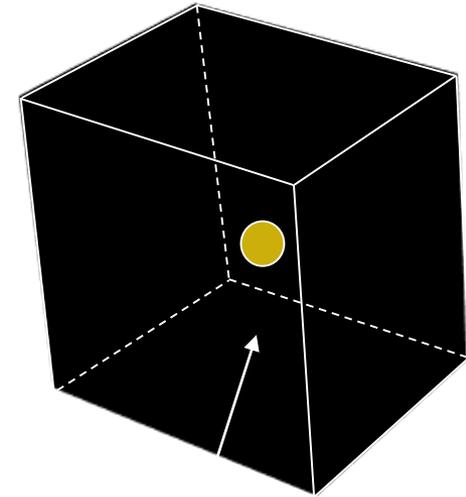


Volume Integral Approximation

Approximation: Q is uniform within the finite-volume:

$$\int_{V(\vec{r},t)} Q dV \approx V Q = \hat{Q}$$

$$\int_{V(\vec{r},t)} P dV \approx V P = \hat{P}$$



The position of the solution point in the cell is not yet defined.

$$V_i Q_i = \hat{Q}_i$$

$$V_i P_i = \hat{P}_i$$

Cell i
(i is an index for the cell)

Surface Integral Approximation

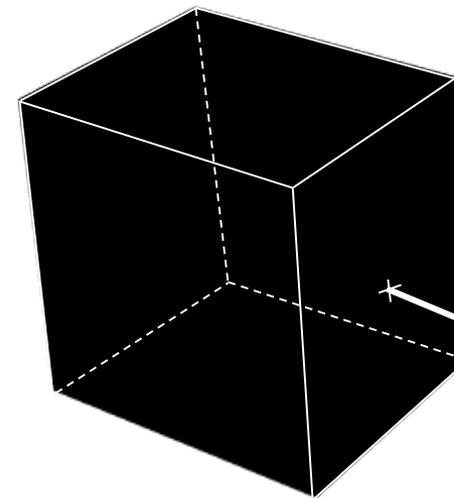
Approximation: The flux is uniform over the surface of each face of the cell:

$$\oint_{S(\vec{r},t)} [(\vec{v} - \vec{g})Q - \mathbf{D}] \cdot \hat{n} dS \approx \sum_{f=1}^{nf} \hat{F}_f = \hat{F}$$

where the flux on the face is define as

$$\hat{F}_f = [(\vec{v} - \vec{g})Q - \mathbf{D}]_f \cdot (\hat{n} dS)_f$$

Computing the flux on the face is one of the most difficult and computationally intensive operations of a CFD code.



Area
normal
vector for
face f

$(\hat{n} dS)_f$
 \hat{F}_f

Face f
(f is an index for the
face)

Resulting Equation

Start with the integral equation,

$$\frac{d}{dt} \int_{V(\vec{r},t)} Q dV + \oint_{S(\vec{r},t)} [(\vec{v} - \vec{g})Q - \mathbf{D}] \cdot \hat{n} dS = \int_{V(\vec{r},t)} P dV$$

and substitute in the volume and surface integral approximations to yield:

$$\frac{d\hat{Q}}{dt} = \hat{P} - \hat{F}$$

This equation is a first-order, non-linear, ordinary differential equation for which various numerical methods exist for its solution.

Other Cell Shapes

A *structured grid* can only contain finite-volume cells with a *hexahedral* shape. *Unstructured grids* allow greater freedom for cell shapes. Possibilities include:

- Generalized Cell (*X quadrilateral faces, Y triangular faces*)
- Prismatic Cell (*3 quadrilateral faces, 2 triangular faces*)
- Pyramidal Cell (*1 quadrilateral face, 4 triangular faces*)
- Tetrahedral Cell (*4 triangular faces*)

To keep cell geometry simple, quadrilateral or triangular faces with straight-line edges are generally used. The geometry and the normal area vector of a triangle is uniquely known, and so, quadrilaterals are usually divided into triangles to compute their geometric properties.

Location of the Solution in the Cell



The location of the flow solution and geometry of the finite volume cell with respect to the grid can be of two types:

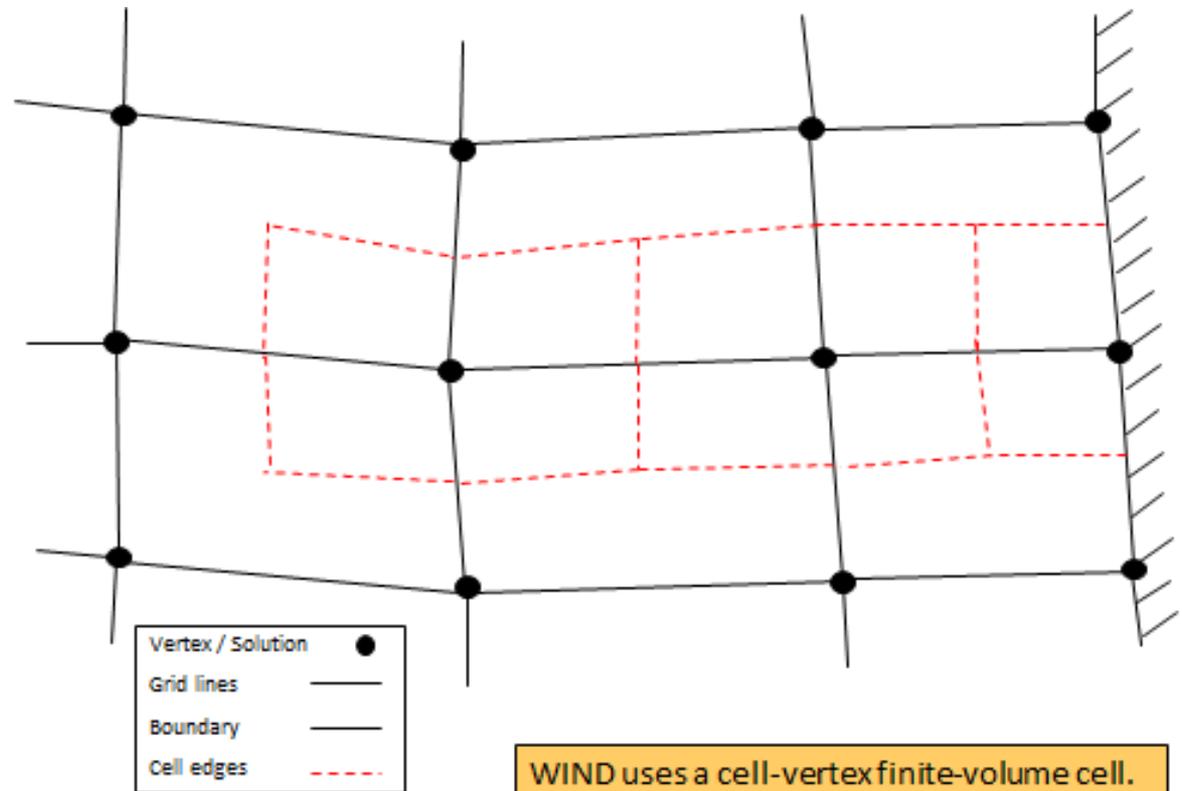
Cell-Vertex (Node-Centered) Cell. The flow solution is located at the vertices of the grid. The finite-volume cell is formed about the vertex.

Cell-Centered Cell. The flow solution is located at the centroid of the cell volume defined by the grid lines (primary grid).

Each approach has its advantages and disadvantages, but if things are done right, both approaches do well.

Cell-Vertex Cell

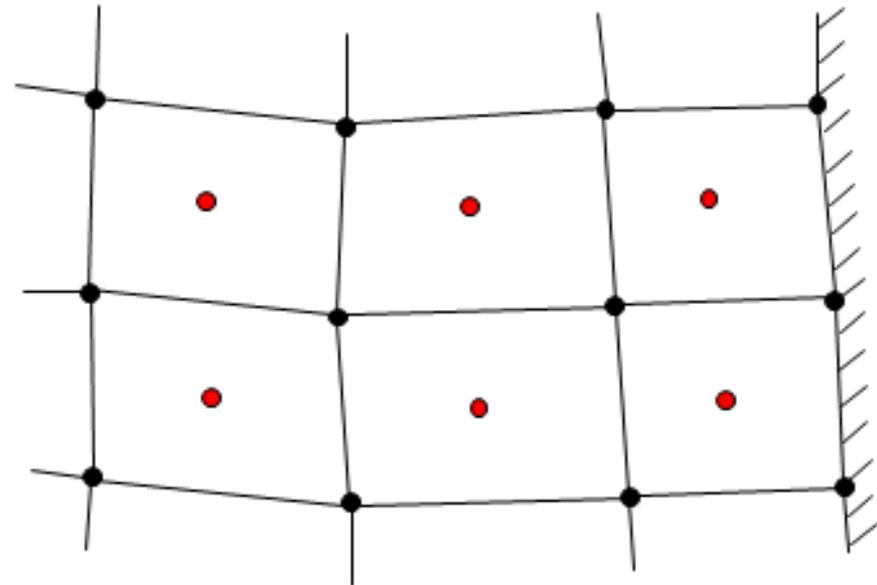
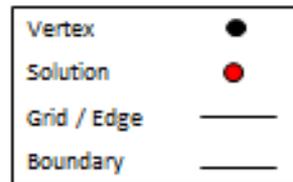
- Solution located at vertices.
- Cell formed about vertex.
- Half-cell at the boundary.
- Solution point at boundary.



WIND uses a cell-vertex finite-volume cell.

Cell-Centered Cell

- Solution located at centroid.
- Grid forms the cell.
- Full cell at the boundary.
- Flux at boundary.



Simplified Cell Shapes



Often assumptions can be applied to simplify the geometry of the flow domain, grid, and cells from a three-dimensional geometry:

Quasi-three dimensional cell. Grid is planar (x,y) with the z -coordinate varying to indicate variable depth of the cell.

Planar axisymmetric cell. Grid is planar (x,y) with y indicating the distance from an axis-of-symmetry. Angle of axisymmetric wedge indicates depth.

Planar two-dimensional cell. Grid is planar (x,y) with the z -coordinate indicating the fixed depth of the cell.

Quasi-one-dimensional cell. Grid is one-dimensional (x) with the cross-sectional area variable and specified along x .

One-dimensional cell. Grid is one-dimensional (x) with the cross-sectional area constant along x .

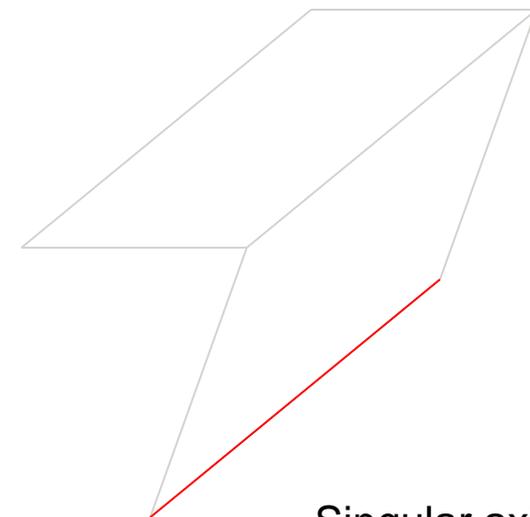
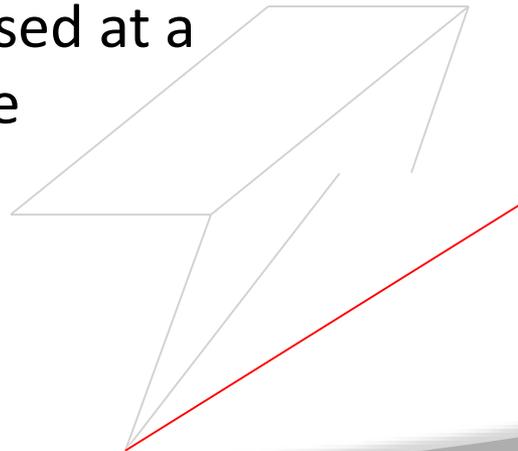
Degenerate Cell Shapes

Degenerate cell shapes are sometimes used to build in flexibility:

Wedged-shaped cell. The hexahedral has one face on the boundary that has collapsed to a line that is a singular axis. Since face as zero area, the flux is zero, so all is fine with the numerical methods. Special boundary condition is usually applied to handle these.

Sharp Nose Cell. The hexahedral has one edge that has collapsed to a point. This type of cell is used at a sharp nose (i.e. nose of a cone).

Nose



Singular axis

Degenerate Cell Shapes

The strength of the FVM is its direct connection to the physical flow properties.

Indeed, the basis of the method relies on the direct discretization of the integral form of the conservation law.

Integral form is the most general expression of a conservation law, as it does not require the fluxes to be continuous (property which is not satisfied for instance along shock waves or along free Surfaces).

This is why we can state that the FVM is close to the physics of the flow system.

Degenerate Cell Shapes

The FVM requires setting up the following steps:

Subdivide the mesh, obtained from the space discretization, into finite (small) volumes, one Control volume being associated to each mesh point.

Apply the integral conservation law to each of these finite volumes.

Definition of the Finite Volume Discretization

- ⦿ The integral conservation law is applied to each control volume Ω_J associated to mesh point J defining hereby the discretized equation for the unknowns U_J attached to that same vertex or cell. The advantage of this method, especially in absence of sources terms, is that the fluxes are calculated only on two-dimensional surfaces instead of in the three-dimensional space.
- ⦿ Equation is replaced by its discrete form, where the volume integrals are expressed as the averaged values over the cell and where the surface integral is replaced by a sum over all the bounding faces of the considered volume Ω_J

General Formulation of a Numerical Scheme



A general and important interpretation of any numerical, conservative scheme is obtained directly from the integral conservation laws.

The formulation that follows is valid for all possible cases, with structured grids or unstructured grids, either cell-centred or cell-vertices

Alternative formulation of the conservative condition

Extending the subdivisions of equation to an arbitrary number of cells, $J = 1-N$, and summing over all the cells it is seen, after cancellation of the contributions from all the internal cell faces, that the sum will contain only contributions from the fluxes along the parts of the cells belonging to the boundaries of the domain and from the sources.

Therefore, the conservative condition can be expressed as a requirement on the transient time evolution of the scheme.

Note that for stationary sources and boundary fluxes, the right-hand side of this equation vanishes at convergence.

Defining $\Delta U_J / \Delta t$ as the average value of $\partial U / \partial t$ over the cell Ω_J , conservation of the scheme requires that, at each time step, the following condition is to be satisfied.