NASA Langley Research Center

CFD 101: OVERVIEW

NASA LANGLEY/AMES EDL SEMINAR SERIES FOR SUMMER INTERNS

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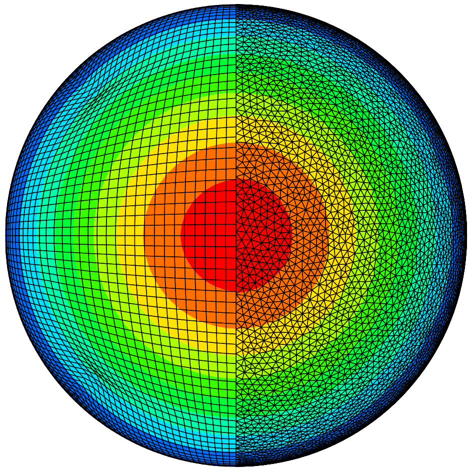
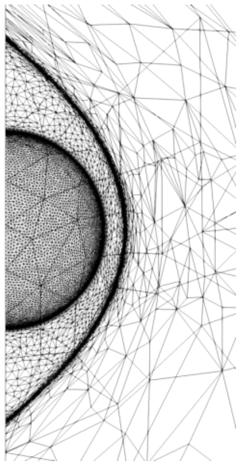
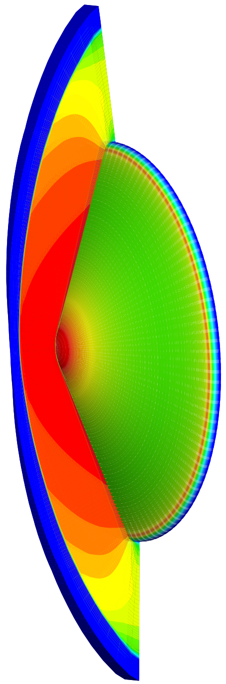
Learning Objectives

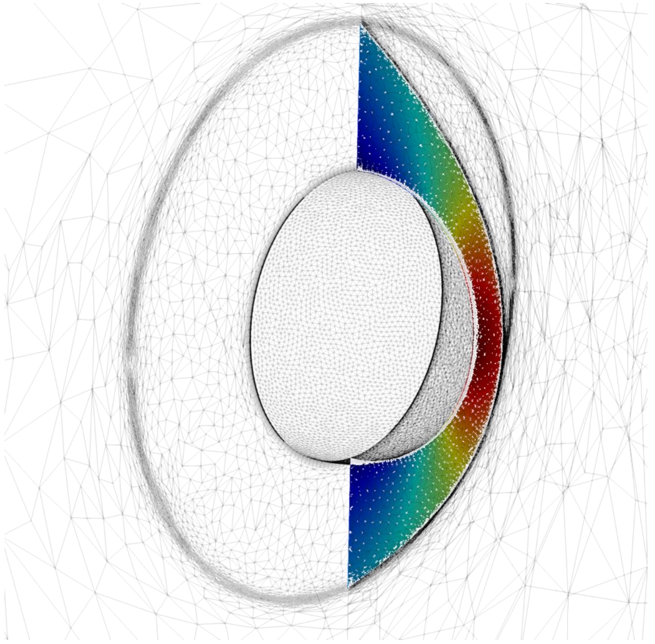
- What is CFD?
- CFD History
- CFD Ingredients
  - Partial Differential Equation
  - Mesh
  - Discretization
  - Boundary Conditions
- CFD Resources

What is CFD?

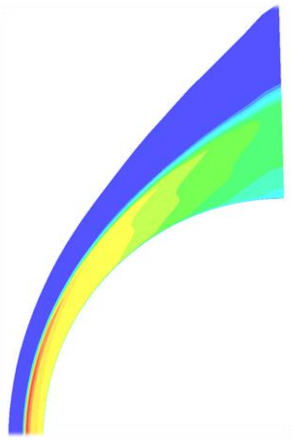


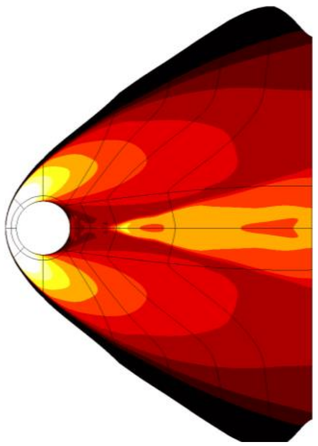


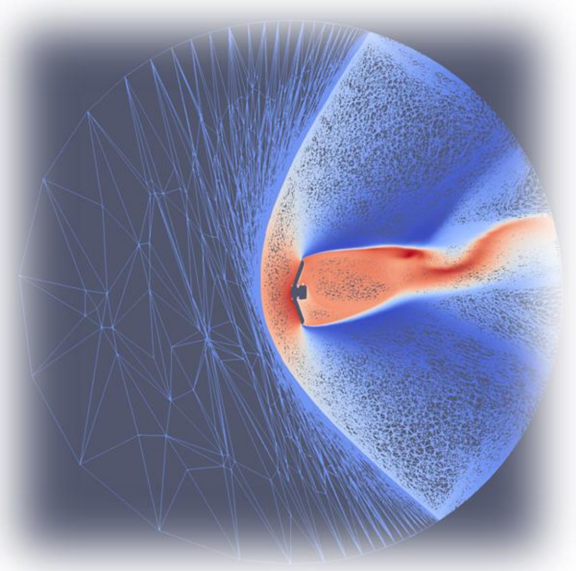




Computational Fluid Dynamics: The branch of fluid mechanics devoted to algorithms designed to simulate fluid flow.







A Brief History of CFD

1944	First CFD simulation at Los Alamos National Labs
1977	First 3D hypersonic CFD simulation
1986	First CFD simulation of a reentry vehicle configuration (X-24C-10D)
1990-2000s	Routine CFD simulation of STS and interplanetary probes
2010-present	Massively-parallel CFD reentry simulations

Ingredients of a CFD code

Partial Differential Equation

Mesh

Discretization

Boundary Conditions

Mass Conservation :

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

Momentum Conservation :

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u^2)}{\partial x}+\frac{\partial(\rho u v)}{\partial y}+\frac{\partial(\rho u w)}{\partial z}=-\frac{\partial p}{\partial x}+\frac{\partial \tau_{xx}}{\partial x}+\frac{\partial \tau_{xy}}{\partial y}+\frac{\partial \tau_{xz}}{\partial z}$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho v u)}{\partial x}+\frac{\partial(\rho v^2)}{\partial y}+\frac{\partial(\rho v w)}{\partial z}=-\frac{\partial p}{\partial y}+\frac{\partial \tau_{yx}}{\partial x}+\frac{\partial \tau_{yy}}{\partial y}+\frac{\partial \tau_{yz}}{\partial z}$$

$$\frac{\partial(\rho w)}{\partial t}+\frac{\partial(\rho w u)}{\partial x}+\frac{\partial(\rho w v)}{\partial y}+\frac{\partial(\rho w^2)}{\partial z}=-\frac{\partial p}{\partial z}+\frac{\partial \tau_{zx}}{\partial x}+\frac{\partial \tau_{zy}}{\partial y}+\frac{\partial \tau_{zz}}{\partial z}$$

Total Energy Conservation :

$$\frac{\partial \rho E}{\partial t}+\frac{\partial(\rho E+p)u}{\partial x}+\frac{\partial(\rho E+p)v}{\partial y}+\frac{\partial(\rho E+p)w}{\partial z}=\frac{\partial q_x}{\partial x}+\frac{\partial q_y}{\partial y}+\frac{\partial q_z}{\partial z}$$

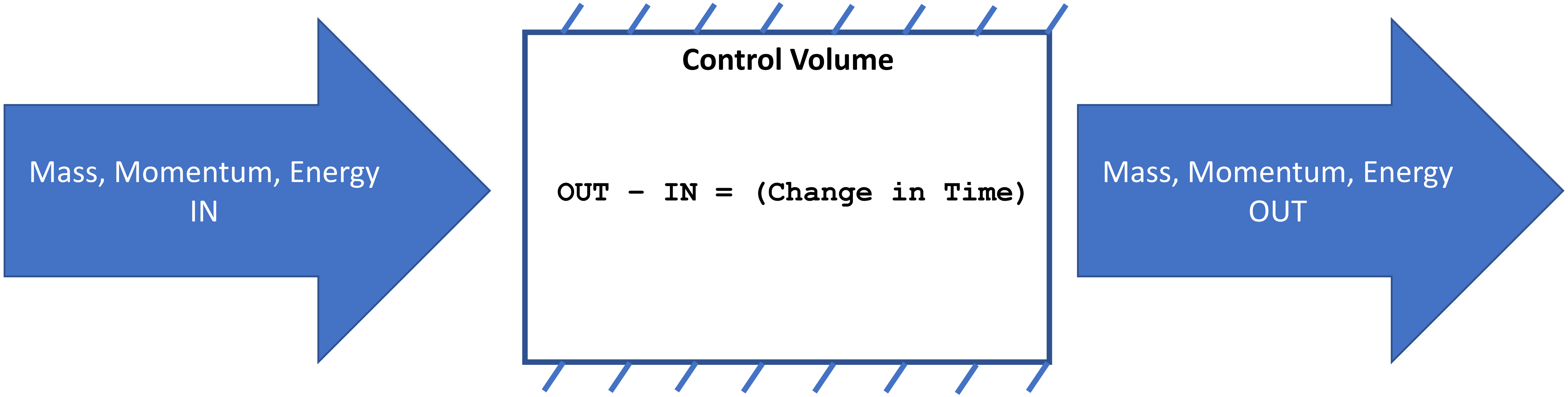
$$\frac{\partial(u\tau_{xx}+v\tau_{xy}+w\tau_{xz})}{\partial x}+\frac{\partial(u\tau_{yx}+v\tau_{yy}+w\tau_{yz})}{\partial y}+\frac{\partial(u\tau_{zx}+v\tau_{zy}+w\tau_{zz})}{\partial z}$$

The Navier-Stokes Equations

CFD Ingredient: **Partial Differential Equation**

At the core of a CFD code is a set of **conservation equations**

Conservation Equations



- Based on fundamental laws of nature
  - Mass cannot be created or destroyed (Lomonosov)
  - Momentum must be conserved (Newton's Second Law)
  - Energy cannot be created or destroyed (First Law of Thermodynamics)

Extension to Reacting Flow

Gas Mixture: Multiple "species" mass equations

Many other terms may be needed, due to ablation, shock-layer radiation, etc.

Thermodynamic nonequilibrium add an additional equation for vibrational energy carried by the gas mixture

Species Conservation :

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial (\rho_1 u)}{\partial x} + \frac{\partial (\rho_1 v)}{\partial y} + \frac{\partial (\rho_1 w)}{\partial z} = \frac{\partial D_m}{\partial x} + \frac{\partial D_m}{\partial y} + \frac{\partial D_m}{\partial z} + \omega_1$$

$$\vdots$$

$$\frac{\partial \rho_N}{\partial t} + \frac{\partial (\rho_N u)}{\partial x} + \frac{\partial (\rho_N v)}{\partial y} + \frac{\partial (\rho_N w)}{\partial z} = \frac{\partial D_m}{\partial x} + \frac{\partial D_m}{\partial y} + \frac{\partial D_m}{\partial z} + \omega_N$$

Mixture Momentum Conservation :

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho vu)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z}$$

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho wu)}{\partial x} + \frac{\partial(\rho wv)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z}$$

Total Energy Conservation :

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E + p)\, u}{\partial x} + \frac{\partial (\rho E + p)\, v}{\partial y} + \frac{\partial (\rho E + p)\, w}{\partial z} = \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}$$

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

$$+ \frac{\partial D_e}{\partial x} + \frac{\partial D_e}{\partial y} + \frac{\partial D_e}{\partial z} - Q_{rad}$$

Vibrational Energy Conservation :

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho e_v)\, u}{\partial x} + \frac{\partial (\rho e_v)\, v}{\partial y} + \frac{\partial (\rho e_v)\, w}{\partial z} = \frac{\partial q_x^v}{\partial x} + \frac{\partial q_y^v}{\partial y} + \frac{\partial q_z^v}{\partial z}$$

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

$$+ \frac{\partial D_v}{\partial x} + \frac{\partial D_v}{\partial y} + \frac{\partial D_v}{\partial z} + \omega_v$$

Turbulence

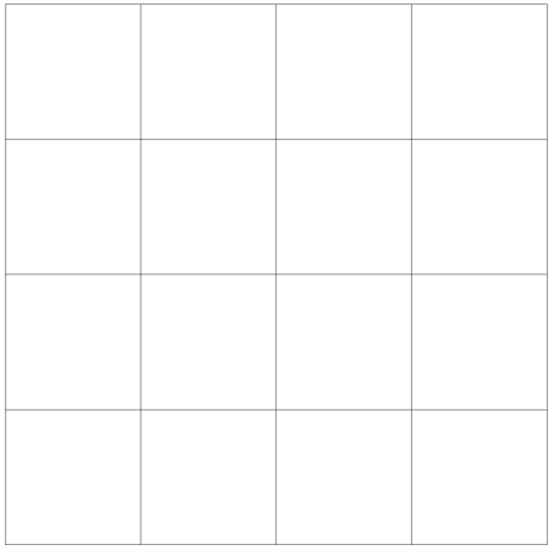
"When I meet God, I am going to ask him two questions: Why relativity? And why turbulence? I really believe he will have an answer for the first." - **Werner Heisenberg**

- Caused by chaotic motion of fluid
- Three types of methods to model turbulence
  - Reynold's Averaged Navier Stokes (RANS): Average all velocity fluctuations
  - Large Eddy-Simulation (LES): Resolve largest eddies in flow
  - Direct Numerical Simulation (DNS): Resolve all eddies
- RANS turbulence modeling is the most common and least expensive approach, but also the least accurate
- LES is an active area of research, requiring highly accurate and efficient solvers
- DNS is prohibitively expensive for almost all EDL applications

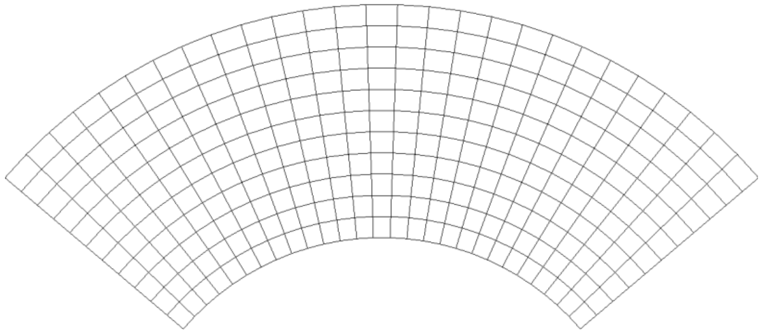
CFD Ingredient: Mesh

- Need to represent the solution discretely
- Mesh is used to define the geometry and the domain where we need the solution
- Meshing techniques will be coved in a follow-on presentation

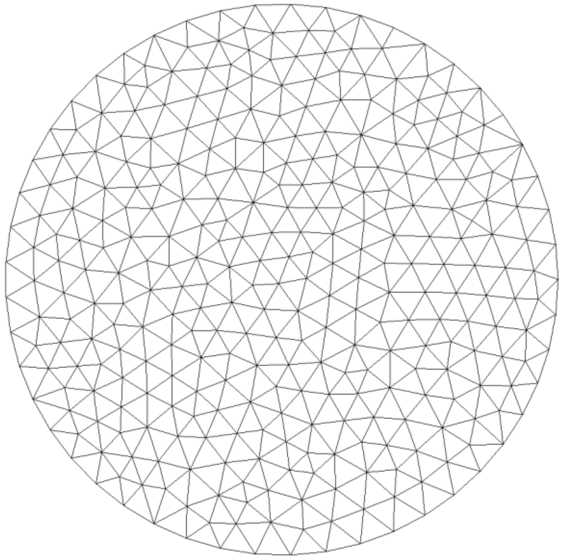
Mesh Types



Cartesian Mesh



Structured Mesh



Unstructured Mesh

CFD Ingredient: Discretization

Differential Form

Directly approximate the derivatives

Integral Form

Integrate the PDE and then solve

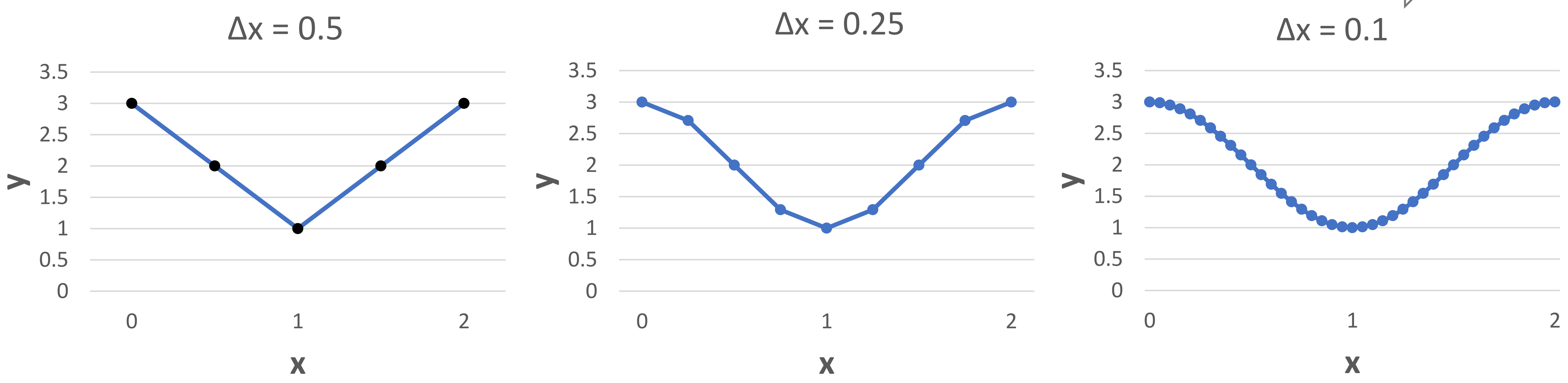
Sidebar: What is Discretization?

- Discretization is the process of representing a continuous function as discrete data.

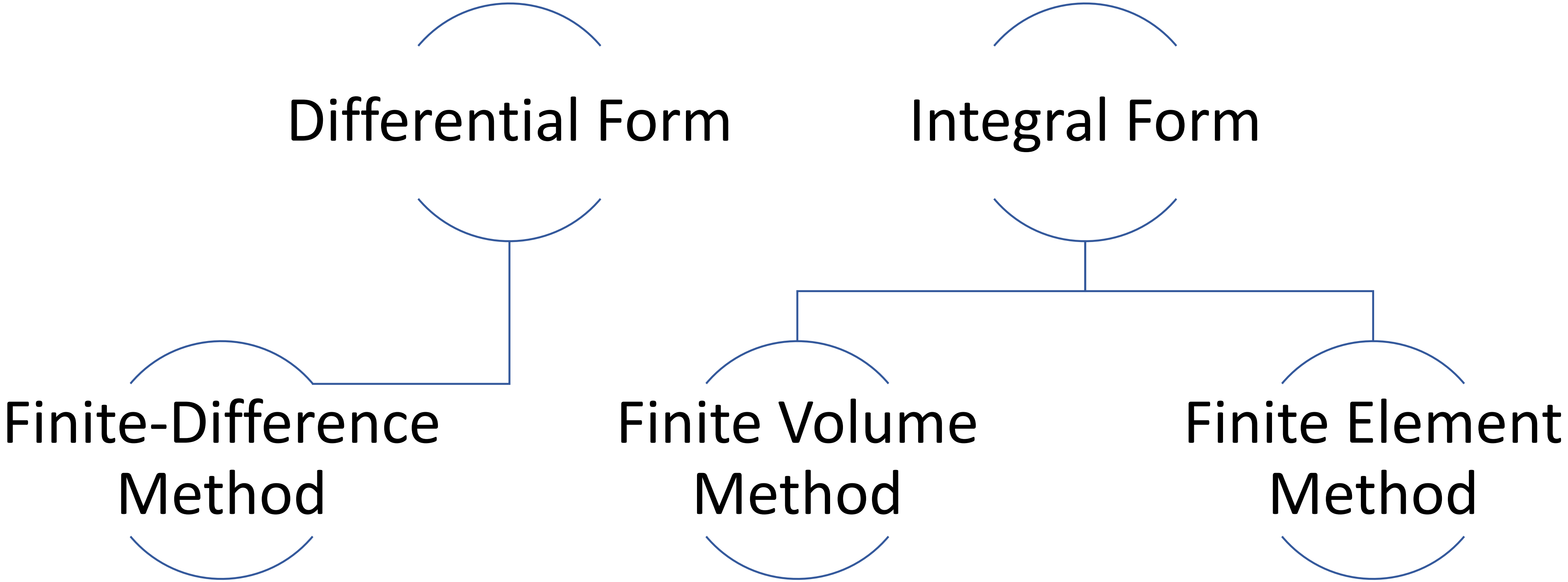
Example Function

$$y = cos(\pi x) + 2$$

Adding points better represents the continuous function



Spatial Discretization Types



Spatial Discretization: Finite Difference Method

Finite-Difference Derivative Approximation

$$\frac{\partial y}{\partial x} = \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

- Solve equations in differential form
- Derivatives in the equations approximated directly using finite-difference formulas
- Pros: Simple to implement and can be made highly accurate
- Cons: Care must be taken to ensure this method maintains conservation
- This approach is less common in current NASA EDL CFD codes, but still used
  - The OVERFLOW CFD code uses this method

Spatial Discretization: Finite Volume Method

Divergence Formula

$$\iiint_V \frac{\partial \mathbf{F}}{\partial \mathbf{x}}\, dV = \iint_S \mathbf{F} \cdot \mathbf{n}\, dS$$

- Solve equations in integral form
- Integrate the PDE and represent the solution as average of “control volumes”
- Convert control volume integrals to surface integrals via the divergence formula
- Pros: simple to implement and ensures conservation by design
- Cons: difficult to achieve high accuracy on arbitrary meshes
- The most common algorithm used by NASA EDL CFD codes
  - The DPLR, LAURA, US3D, and FUN3D codes use this algorithm

Spatial Discretization: Finite Element Method

Integration by Parts

$$\int u\,dv = uv - \int v\,du$$

- Solve equations in integral form
- Integrate the PDE by parts and represent the solution via a "basis function"
- The solution is essentially a curve fit on each element in the mesh
- Pros: Highly accurate
- Cons: Relatively complex and can be computationally expensive
- This method is commonly used for turbulence modeling research requiring high accuracy (LES/DNS simulations)

Temporal Discretization

- This is the part responsible for evolving the solution
- The CFD solver iterates until enough time history/statistics have accumulated
- Explicit vs Implicit
  - Explicit = simple, but restricted to small timesteps
  - Implicit = larger timesteps, but requires solving a linear system
- Steady State – no time dependence

$$\frac{\partial x}{\partial t} + \mathbf{R}(x) = 0$$

Implicit Methods

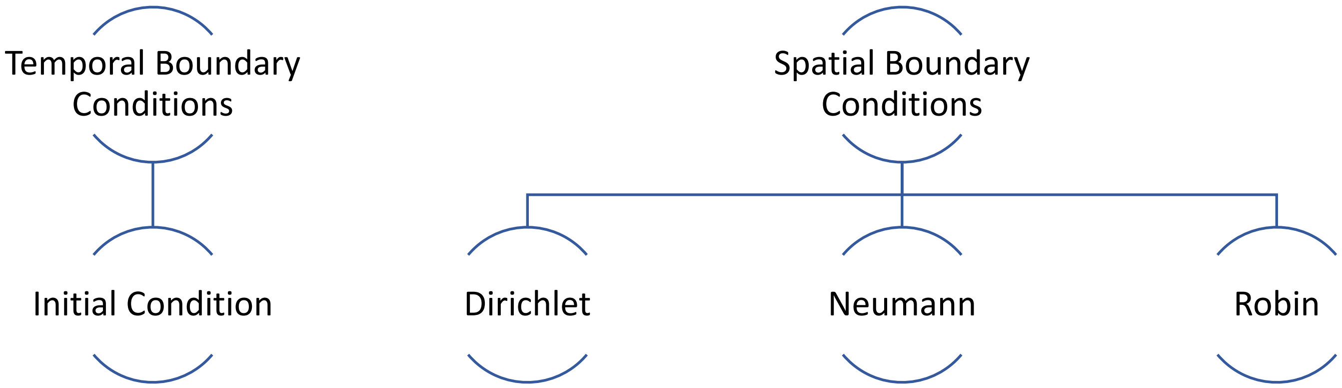
$$\frac{x^{n+1} - x^n}{\Delta t} + \mathbf{R}(x^{n+1}) = 0$$

Explicit Methods

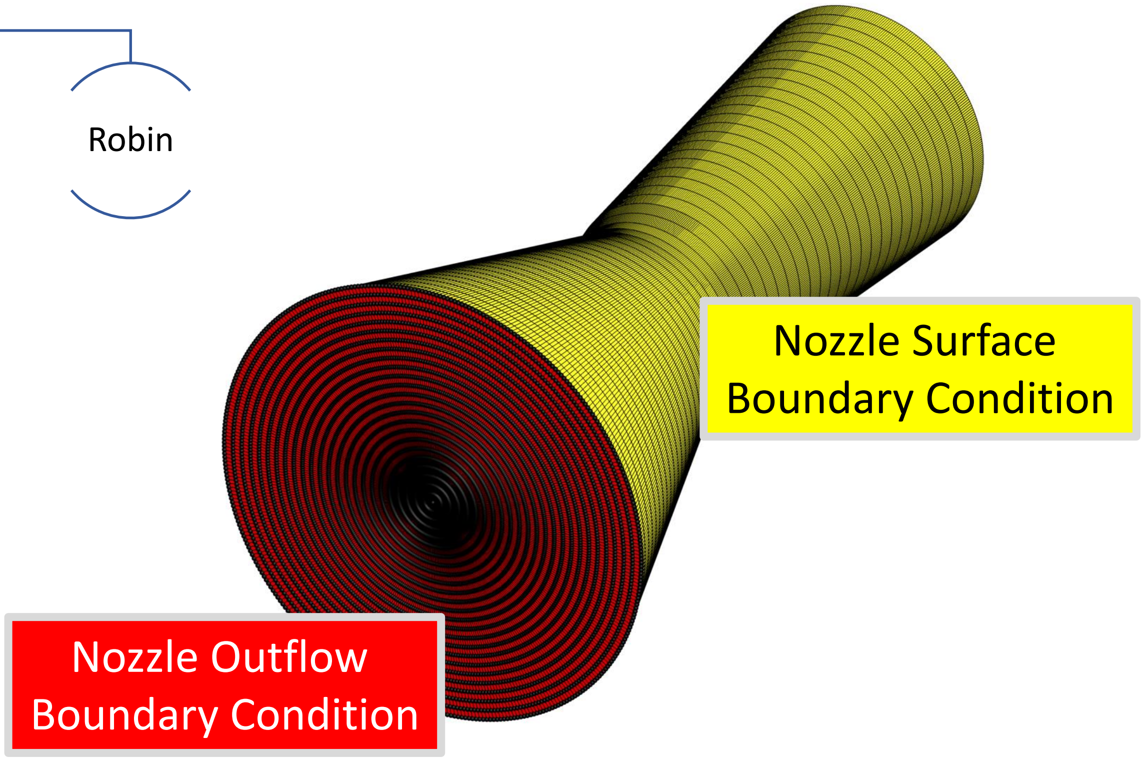
$$\frac{x^{n+1} - x^n}{\Delta t} + \mathbf{R}(x^n) = 0$$

A key distinction is the state applied to the spatial discretization

Boundary Conditions



Example Nozzle Mesh



- The final piece needed to define a CFD simulation
- These are defined by the user and associated with parts of the mesh

CFD Resources

- This has barely scratched the surface of CFD, but there are many great resources available on this subject:
  - Anderson, John D. *Computational Fluid Dynamics: the Basics with Applications*.
  - Anderson, Dale A., et al. *Computational Fluid Mechanics and Heat Transfer*.
  - Press, William H., et al. *Numerical Recipes: the Art of Scientific Computing*.
  - ”I Do Like CFD”- http://www.cfdbooks.com