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Discrete Calculus Methods and their Application to Fluid Dynamics

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Context

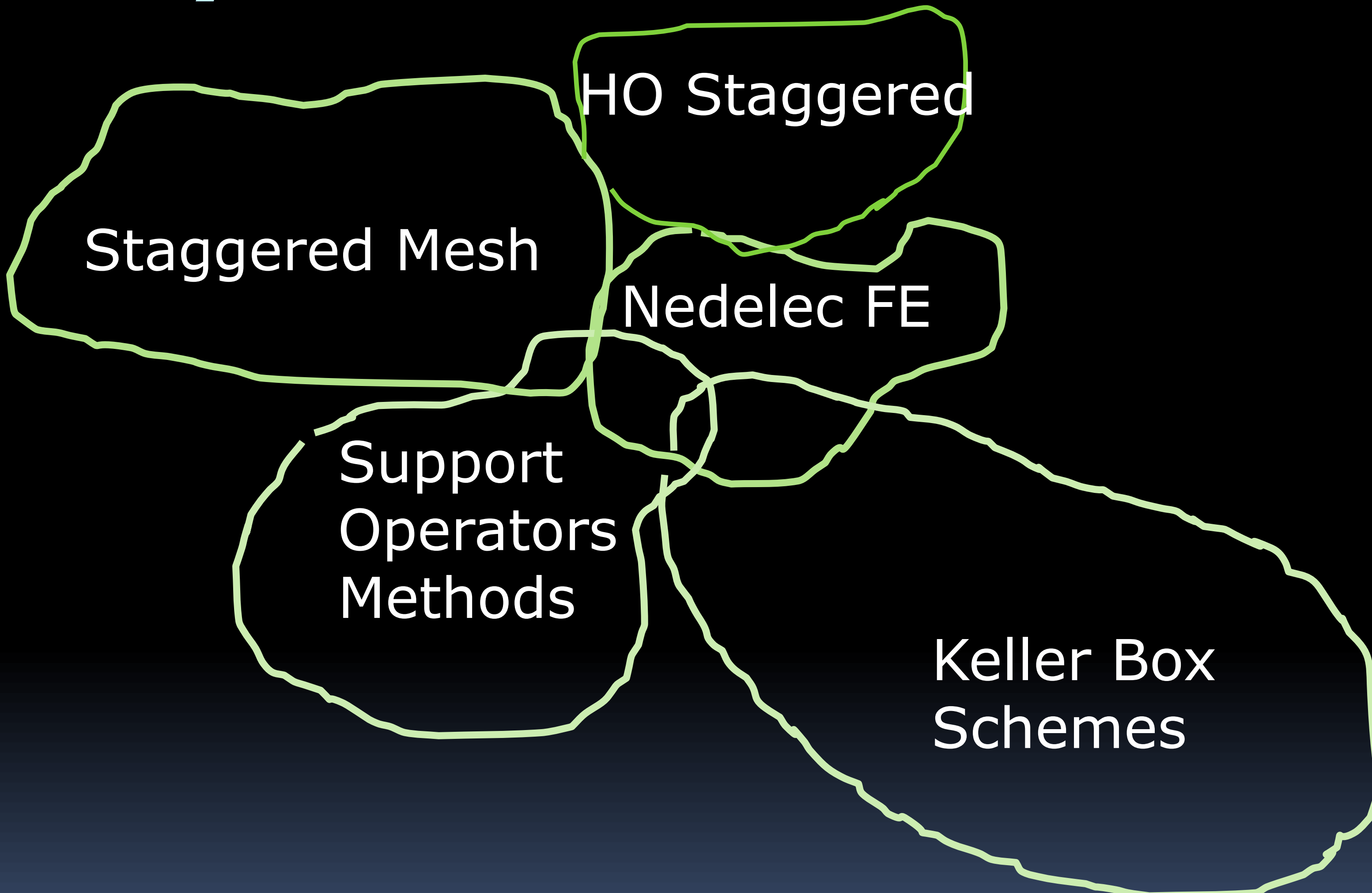
Mathematical Tools

- Order of Accuracy
- Stability
- Consistency

Physical Requirements

- Conservation
  - (mass, momentum, total energy)
- Secondary Conservation
  - (kinetic energy, vorticity, entropy)
- Unphysical Modes (pressure)
- Wave propagation (direction)
- Eigenmodes/Resonance

Many Mimetic Methods



Methods that capture physics well.

Why ?

Why do some methods capture physics well?

They use exact discretization

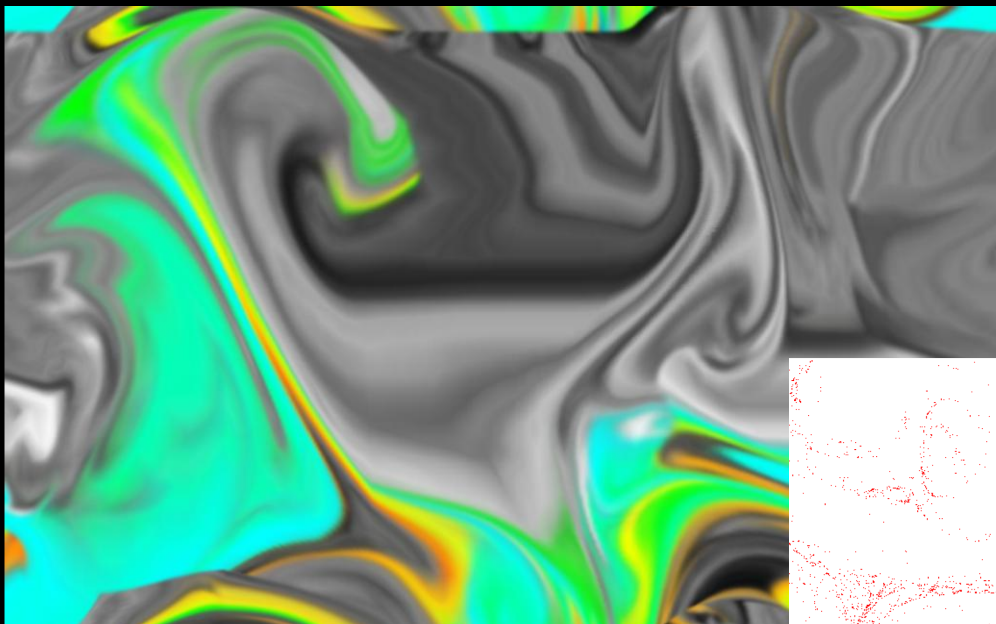
What do they have in common?

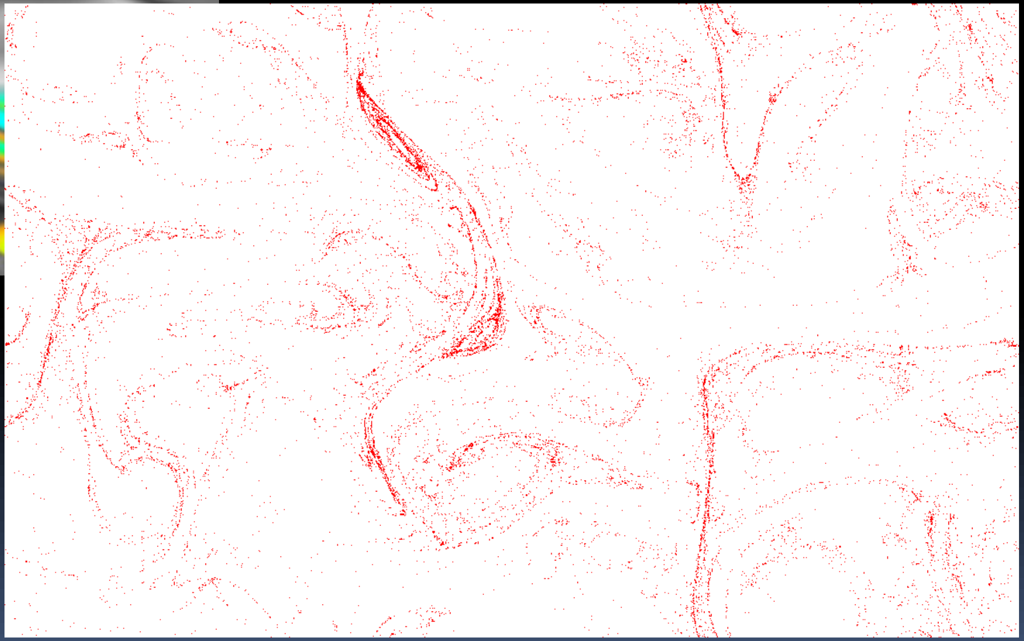
All are Discrete Calculus Methods

Can you make a numerical method so that is mimetic from its design?

Yes (I think)

Discretization





Take a continuous problem to a finite dimensional one.

Discrete Calculus: Part 1

Exact Discretization

$$\frac{\partial a}{\partial t} + \nabla \cdot \mathbf{b} = 0 \quad \Longrightarrow \quad \begin{bmatrix} \mathbf{A} & \mathbf{B} \end{bmatrix} \begin{pmatrix} \vec{\mathbf{a}} \\ \vec{\mathbf{b}} \end{pmatrix} = \vec{\mathbf{r}}$$

Infinite Dimensional **Finite Dimensional**

Partial Differential Eqn. **Matrix Problem**

Basic unknowns are integral quantities.
Collect infinite data into finite groups.

Discrete Calculus: Part 2

Solution <u>requires</u> Approximation

$$\begin{bmatrix} A & B \end{bmatrix}\begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix} = \vec{r} \quad \Rightarrow \quad \begin{bmatrix} A & B \\ C & D \end{bmatrix}\begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix} = \begin{pmatrix} \vec{r} \\ 0 \end{pmatrix}$$

Underdetermined **Unique Square**

Relate discrete unknowns to each other.
This relation is a material law.
Also related to an dual mesh interpolation.
Also related to inner products

Implications

Exact Discretization means that:

- Calculus is exact.
- Physics is exact.
- Method is mimetic.

Discrete Solution Requires:

- Approximation of material laws.
- Interpolation between meshes.
- Assumptions about the solution.

Example: Heat Equation

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T$$

$$\frac{\partial(\rho C T)}{\partial t} = -\nabla \cdot \vec{\mathbf{q}}$$ Conservation of Energy

$$\vec{\mathbf{q}} = -k \nabla T$$ Fourier's Heat Flux Law

Figure out what should NOT be approximated and what is already an approximation (Tonti).

Heat Eqn: Fully Separated

Heat Equation

$\frac{\partial i}{\partial t} = -\nabla \cdot \mathbf{q}$	Conservation of Energy (Physics)
$i \approx \rho C T$	Perfectly Caloric Material (Mat.)
$\mathbf{q} \approx -k\mathbf{g}$	Fourier's Heat Flux Law (Mat.)
$\mathbf{g} = \nabla T$	Def. of Gradient (Math)

- **Discretize Physics and Math - exactly.**
- **Approximate Material laws - using interpolation.**

Exact Discretization

$$I_{\tilde{c}}^{n+1} - I_{\tilde{c}}^{n} = -\sum_{faces} \bar{Q}_{\tilde{f}}^{out}$$

Gauss' Theorem (with time)
Like FV: Not very original.

$$I_{\tilde{c}}^{n+1} = \int_{\Omega_{\tilde{c}}^{n+1}} i dV \qquad \bar{Q}_{\tilde{f}}^{out} = \int_{t^n}^{t^{n+1}} dt \int_{\partial\Omega_{\tilde{f}}} \mathbf{q} \cdot \mathbf{n}^{out} dA$$

$$g_e^{n+1} = \int_{v_1}^{v_2} \mathbf{g} \cdot d\mathbf{l} \,\Big|^{n+1} = \int_{v_1}^{v_2} \nabla T \cdot d\mathbf{l} \,\Big|^{n+1} = T_{v_2}^{n+1} - T_{v_1}^{n+1}$$

Math: still exact

Exact Discrete System

$$\frac{\partial i}{\partial t} = -\nabla \cdot \mathbf{q}$$

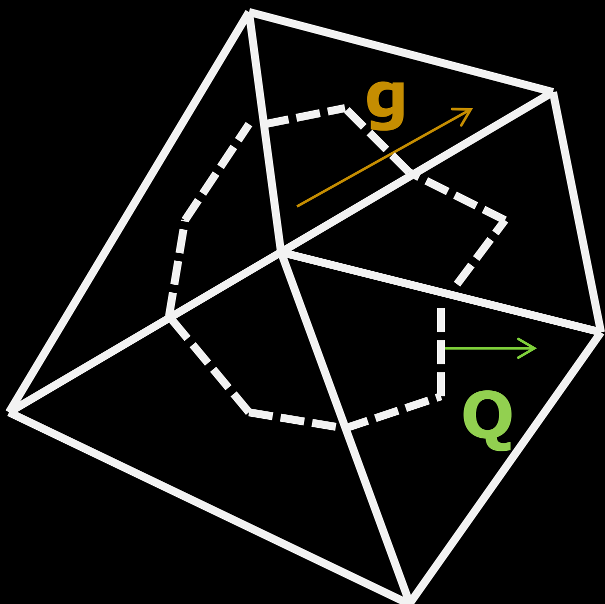
$$\mathbf{g} = \nabla T$$

$$\Rightarrow \begin{bmatrix} \mathbf{I} & \mathbf{D} & 0 & 0 \\ 0 & 0 & \mathbf{I} & -\mathbf{G} \end{bmatrix} \begin{pmatrix} I_{\tilde{c}}^{n+1} \\ \overline{Q}_{\tilde{f}} \\ g_e^{n+1} \\ T_v^{n+1} \end{pmatrix} = \begin{pmatrix} I_{\tilde{c}}^{n} \\ 0 \end{pmatrix}$$

- **Exact**
- **Over-determined**
- **Uncoupled**
- **Unknowns on different meshes**

Step 3

Vertex Centered Mimetic



- (C1) Vertex Centered
- (C2) Median dual mesh

$$I_{\tilde{c}}^{n+1} \approx M_{\tilde{c}} C_{\tilde{c}} T_v$$

$$i \approx \rho C T$$

$$\mathbf{q} \approx -k\mathbf{g}$$

$$\overline{Q}_{\tilde{f}} \approx -\frac{k\Delta t}{2}\left(\mathbf{B}^{n+1} g_e^{n+1} + \mathbf{B}^n g_e^n\right)$$

Approximation Part

Solvable Vertex System

$$\begin{bmatrix} \mathbf{I} & \mathbf{D} & 0 & 0 \\ \mathbf{I} & 0 & 0 & -\mathbf{M}_C \\ 0 & 0 & \mathbf{I} & -\mathbf{G} \\ 0 & \mathbf{I} & \frac{k\Delta t}{2}\mathbf{B}^{n+1} & 0 \end{bmatrix} \begin{pmatrix} I_{\tilde{c}}^{n+1} \\ \bar{Q}_{\tilde{f}} \\ g_e^{n+1} \\ T_v^{n+1} \end{pmatrix} = \begin{pmatrix} I_{\tilde{v}}^{n} \\ 0 \\ 0 \\ \frac{k\Delta t}{2}\mathbf{B}^n g_e^n \end{pmatrix}$$

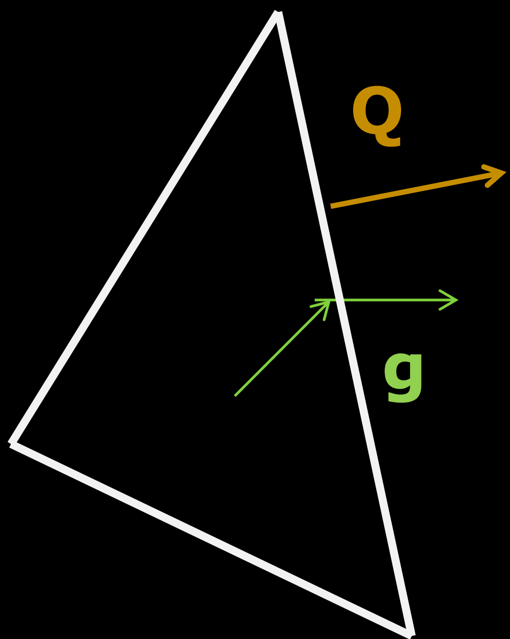
$$\mathbf{M}_C T_v^{n+1} - I_{\tilde{c}}^{n} = \mathbf{D}(\tfrac{\Delta t k}{2}\mathbf{B}^{n+1})\mathbf{G}T_v^{n+1} + \mathbf{D}(\tfrac{\Delta t k}{2}\mathbf{B}^{n})\mathbf{G}T_v^{n}$$

- **Single unknown (T at vertices).**
- **Looks like no dual mesh was used.**
- **B is Hodge * operator.**

Other Possibilities

- **Mesh: Use polygons as the primary mesh.**
  (quad/hex meshes, particle methods, SOM)
- **Approx: Use other basis functions for interpolation.**
  (Rational polynomials, Natural Neighbors, Fourier)
- **Exact: Use different exact discretizations**
  (FE, Keller/Priessman Box Schemes)

Cell Centered Mimetic



- Cell Centered
- Median dual mesh
- Raviart-Thomas for Q

$$I_c^{n+1} \approx M_c C_c T_{\tilde{c}}$$

$$i \approx \rho C T$$

$$\mathbf{q} \approx -k\mathbf{g}$$

$$\frac{\Delta t}{2}\left(g_{\tilde{e}}^{n+1} + g_{\tilde{e}}^{n}\right) \approx -\mathbf{A}_{1/k_c}^{n+1}\overline{Q}_f$$

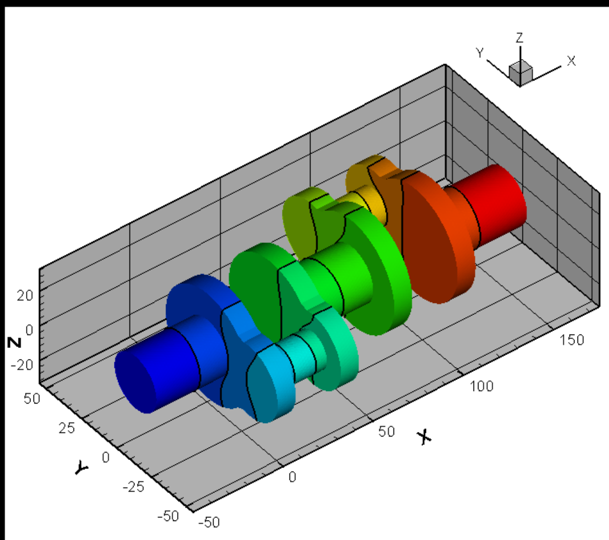
Cell System

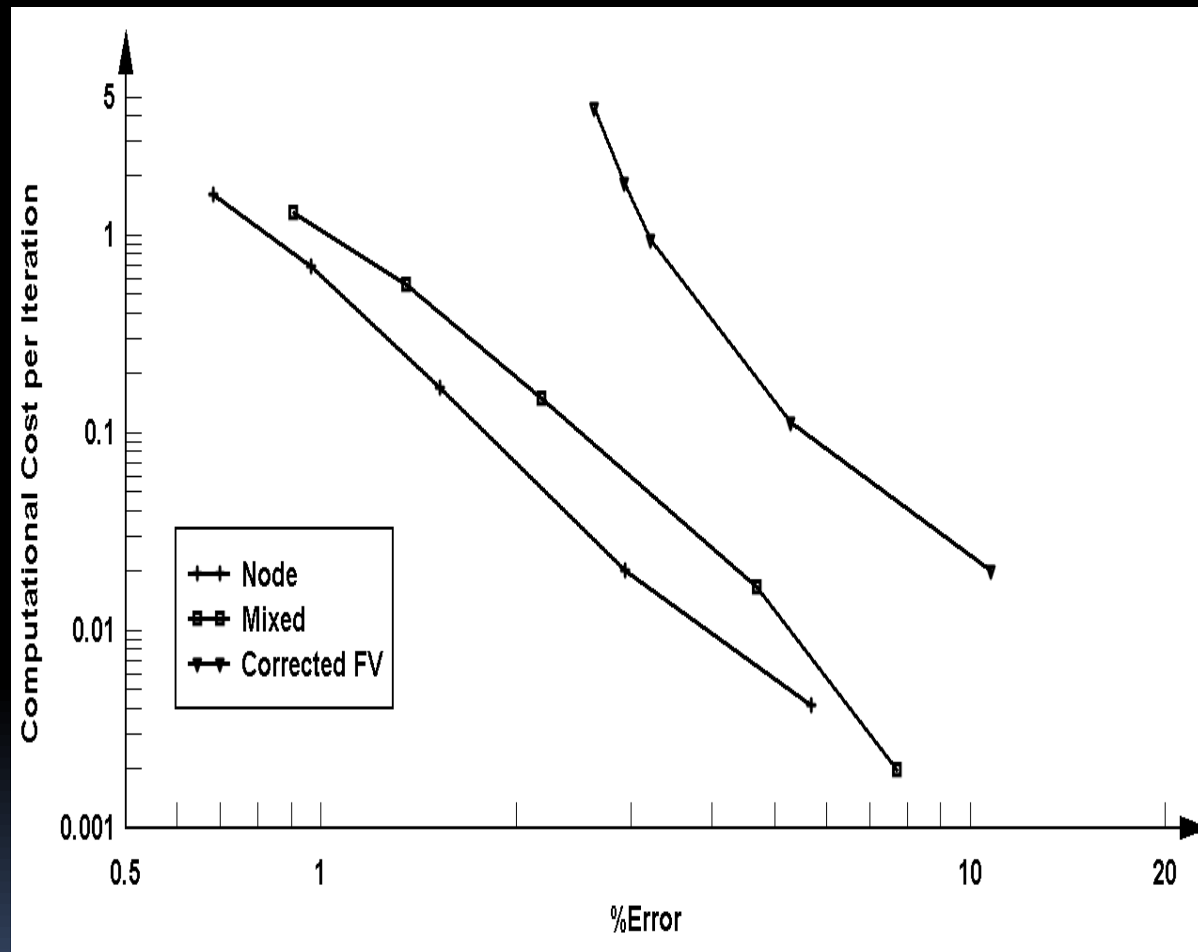
$$\begin{bmatrix} \mathbf{I} & \mathbf{D} & 0 & 0 \\ \mathbf{I} & 0 & 0 & -\mathbf{M}_C \\ 0 & 0 & \mathbf{I} & -\mathbf{G} \\ 0 & \mathbf{A}_{1/k_c}^{n+1} & -\frac{\Delta t}{2}\mathbf{I} & 0 \end{bmatrix} \begin{pmatrix} I_c^{n+1} \\ \bar{Q}_f \\ g_{\tilde{e}}^{n+1} \\ T_{\tilde{c}}^{n+1} \end{pmatrix} = \begin{pmatrix} I_c^n \\ 0 \\ 0 \\ \frac{\Delta t}{2} g_{\tilde{e}}^n \end{pmatrix}$$

$$\boxed{\begin{bmatrix} \mathbf{M}_C & \mathbf{D} \\ -\mathbf{G} & -\frac{2}{\Delta t}\mathbf{A}_{1/k_c}^{n+1} \end{bmatrix} \begin{pmatrix} T_{\tilde{c}}^{n+1} \\ \bar{Q}_f \end{pmatrix} = \begin{pmatrix} I_c^n \\ g_{\tilde{e}}^n \end{pmatrix}}$$

- **Symmetric system of unknowns**
- **Not reducible**

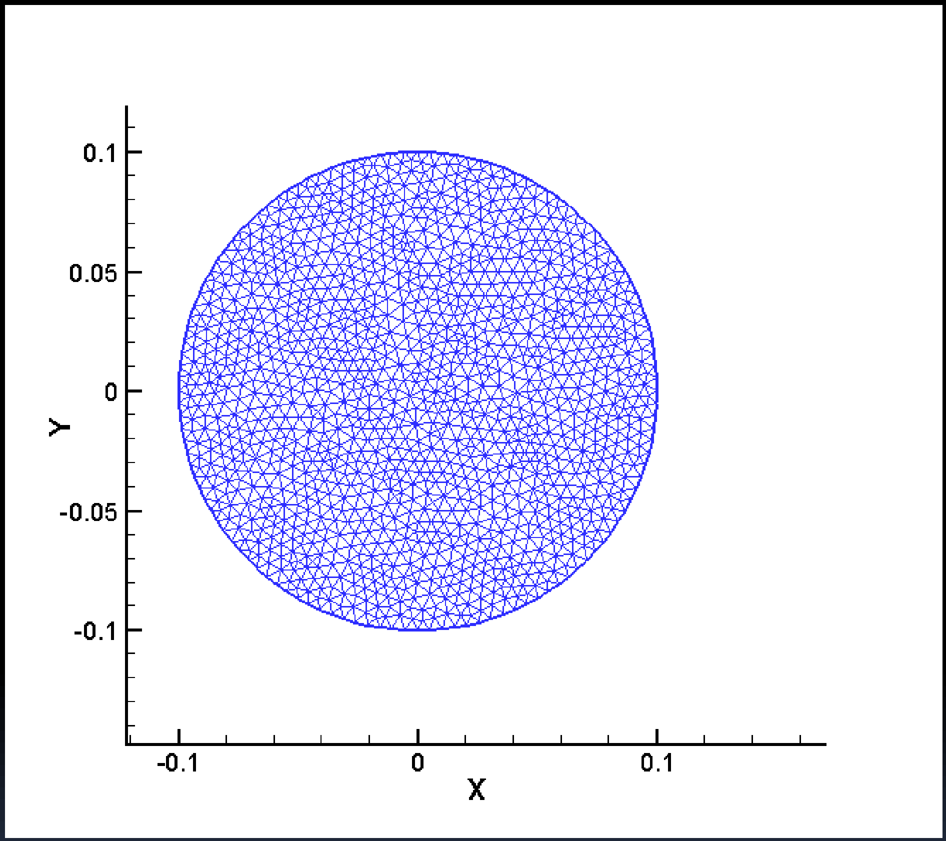
Comparison



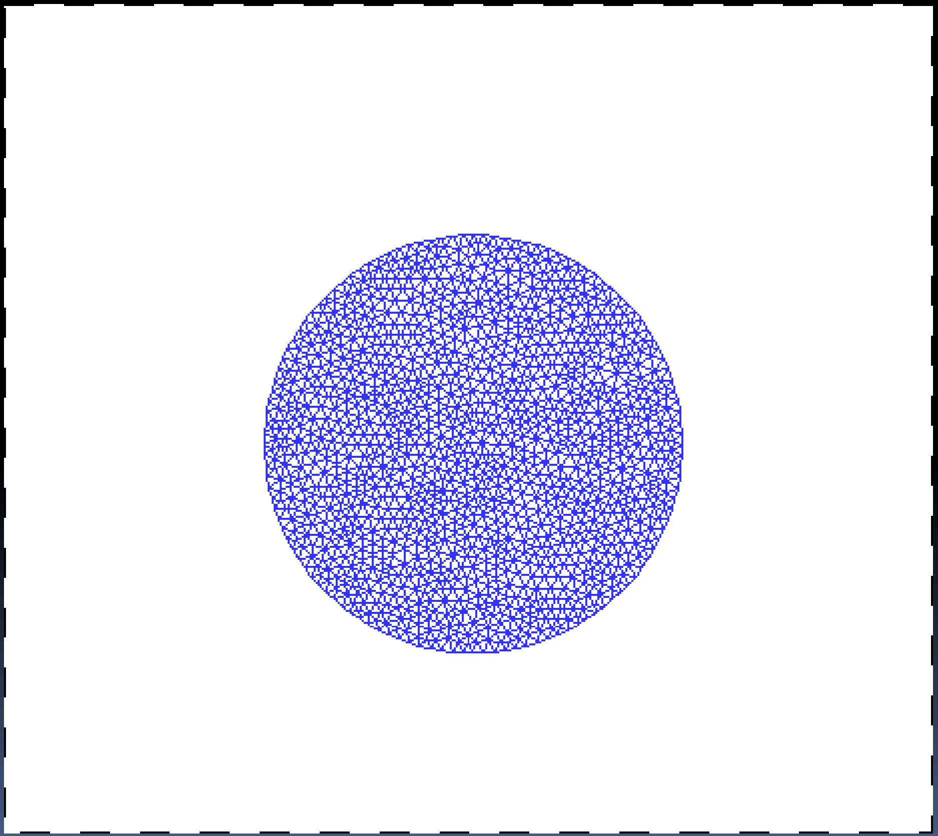


Mimetic 10x more accurate or $1/10^{th}$ cost.

Fluid Example - Droplets

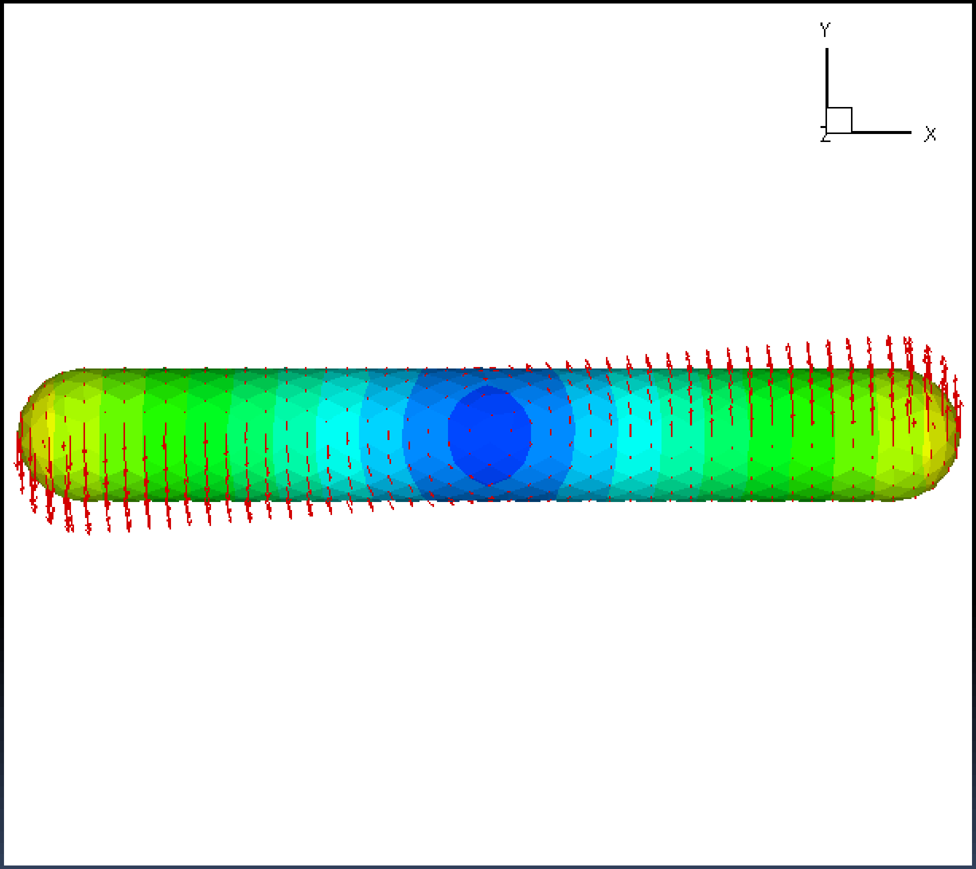


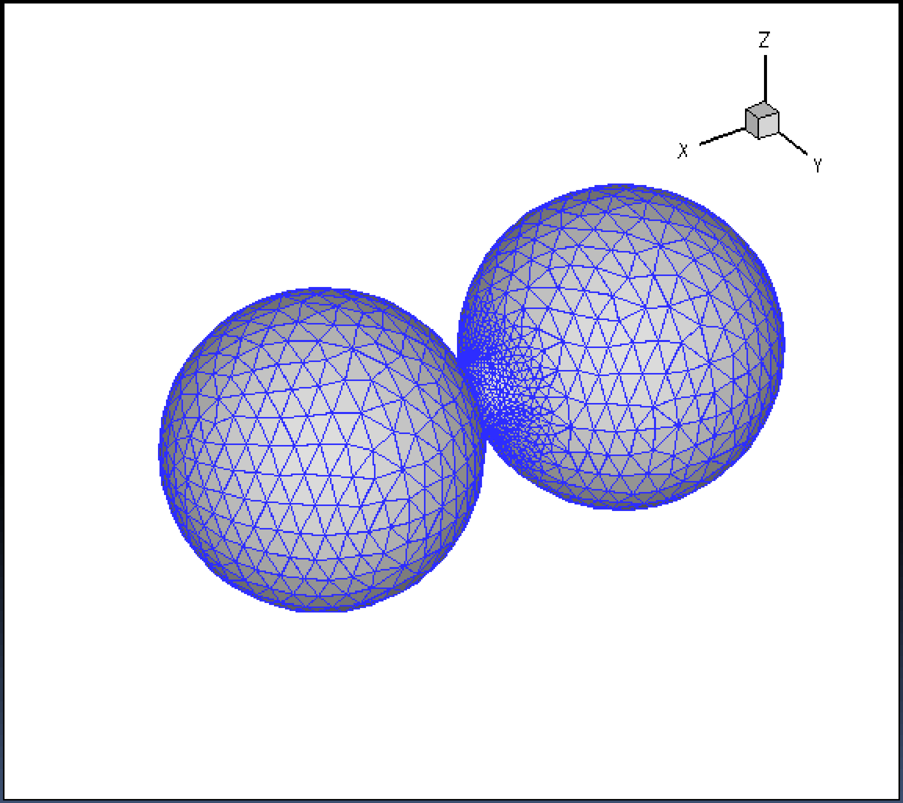
- Moving Mesh
- Unstructured
- Surface Tension



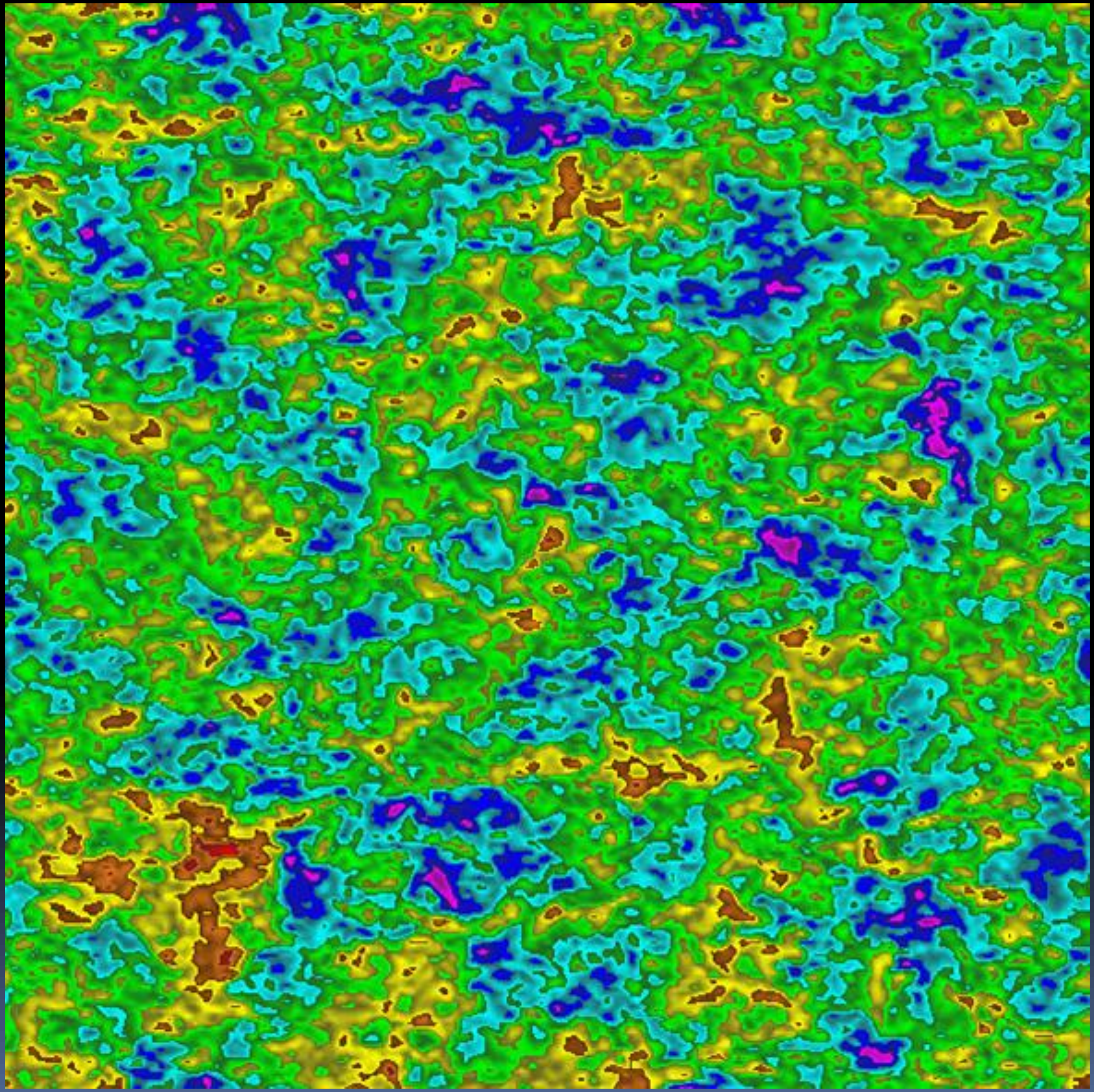
Example – 3D Droplets

- Moving Mesh
- Large distortions
- Complex BCs





DNS



Summary

- **Exact discretization (or 2 step construction) leads to mimetic methods.**
- **Place numerical approximations with the physical approximation.**
- **Discrete Calculus analysis is accessible to all computational scientist. (Gauss' Theorem).**
- **Discrete Calculus Methods are not a type of numerical method. The approach can produce some FV, FE, FD, and other methods.**

www.ecs.umass.edu/mie/tcfd/Publications.html