Discrete Calculus Methods and their Application to Fluid Dynamics

Blair Perot

Theoretical and Computational Fluid Dynamics Laboratory

October 6, 2011
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 it is mimetic from its design? Yes (I think).
Discretization

Take a continuous problem to a finite dimensional one.
Discrete Calculus: Part 1

Exact Discretization

\[ \frac{\partial a}{\partial t} + \nabla \cdot b = 0 \]

\[ [A \ B] \begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix} = \vec{r} \]

Infinite Dimensional

Finite Dimensional

Partial Differential Eqn.

Matrix Problem

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

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

Conservation of Energy

\[ \frac{\partial (\rho C T)}{\partial t} = -\nabla \cdot \vec{q} \]

Fourier’s Heat Flux Law

\[ \vec{q} = -k \nabla T \]

Figure out what should NOT be approximated and what is already an approximation (Tonti).
Heat Eqn: Fully Separated

Heat Equation

\[
\frac{\partial i}{\partial t} = -\nabla \cdot q
\]

Conservation of Energy (Physics)

\[i \approx \rho C T\]

Perfectly Caloric Material (Mat.)

\[q \approx -k g\]

Fourier’s Heat Flux Law (Mat.)

\[g = \nabla T\]

Def. of Gradient (Math)

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

\[ I_{\tilde{c}}^{n+1} - I_{\tilde{c}}^n = - \sum_{\text{faces}} Q_{\tilde{f}}^{\text{out}} \]

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

\[ I_{\tilde{c}}^{n+1} = \int_{\Omega_{\tilde{c}}^{n+1}} idV \]
\[ Q_{\tilde{f}}^{\text{out}} = \int_{t^n}^{t^{n+1}} dt \int_{\partial \Omega_{\tilde{f}}} q \cdot n^{\text{out}} dA \]

\[ g_e^{n+1} = \int_{v_1}^{v_2} g \cdot dl |^{n+1} = \int_{v_1}^{v_2} \nabla T \cdot dl |^{n+1} = T_{v_2}^{n+1} - T_{v_1}^{n+1} \]

Math: still exact
Exact Discrete System

\[ \frac{\partial i}{\partial t} = -\nabla \cdot q \]

\[ g = \nabla T \]

\[ \begin{bmatrix} I & D & 0 & 0 \\ 0 & 0 & I & -G \end{bmatrix} \begin{pmatrix} I_{n+1}^n \\ \overline{Q}_f \tilde{c} \\ g_{n+1} \\ T_{n+1}^n \end{pmatrix} = \begin{pmatrix} I_{\tilde{c}}^n \\ 0 \end{pmatrix} \]

- Exact
- Over-determined
- Uncoupled
- Unknowns on different meshes
Vertex Centered Mimetic

(C1) Vertex Centered
(C2) Median dual mesh

\[ i \approx \rho CT \]
\[ q \approx -kg \]
\[ \nabla Q \approx -\frac{k\Delta t}{2} \left( B^{n+1} g^{n+1} + B^n g^n \right) \]

Approximation Part
Solvable Vertex System

\[
\begin{bmatrix}
I & D & 0 & 0 \\
I & 0 & 0 & -M_c \\
0 & 0 & I & -G \\
0 & I & \frac{k \Delta t}{2}B^{n+1} & 0 \\
\end{bmatrix}
\begin{bmatrix}
I^{n+1} \\
\tilde{c} \\
\tilde{Q}_f \\
g^{n+1} \\
T^{n+1}_v \\
\end{bmatrix}
=
\begin{bmatrix}
I^n \\
\tilde{v} \\
0 \\
0 \\
0 \\
\end{bmatrix}
\begin{bmatrix}
\frac{k \Delta t}{2}B^n \\
g^n_e \\
\end{bmatrix}
\]

\[
M_CT_v^{n+1} - I^{n+1}_{\tilde{c}} = D\left(\frac{\Delta t k}{2}B^{n+1}\right)GT_v^{n+1} + D\left(\frac{\Delta t k}{2}B^n\right)GT_v^n
\]

- 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 $Q$

$i \approx \rho C T$

$q \approx -k g$

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

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

\[
\begin{bmatrix}
I & D & 0 & 0 \\
I & 0 & 0 & -M_C \\
0 & 0 & I & -G \\
0 & A^{n+1}_{1/k_c} & -\frac{\Delta t}{2}I & 0 \\
\end{bmatrix}
\begin{bmatrix}
I_{c}^{n+1} \\
\bar{Q}_f \\
g_{\tilde{\varepsilon}}^{n+1} \\
T_{\tilde{\varepsilon}}^{n+1} \\
\end{bmatrix}
= 
\begin{bmatrix}
I_{c}^{n} \\
0 \\
0 \\
\frac{\Delta t}{2}g_{\tilde{\varepsilon}}^{n} \\
\end{bmatrix}
\]

• Symmetric system of unknowns
• Not reducible
Comparison

Mimetic 10x more accurate or \( \frac{1}{10} \text{th} \) 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