Higher-Order Discrete Calculus Methods

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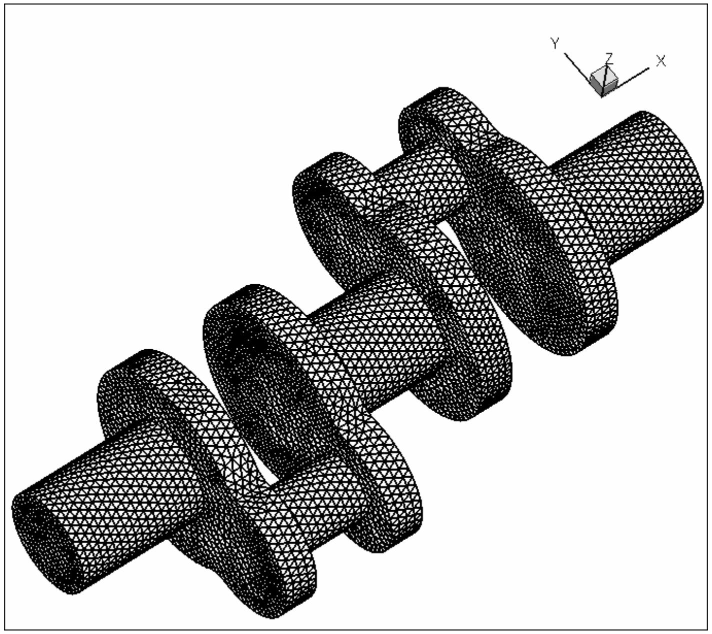
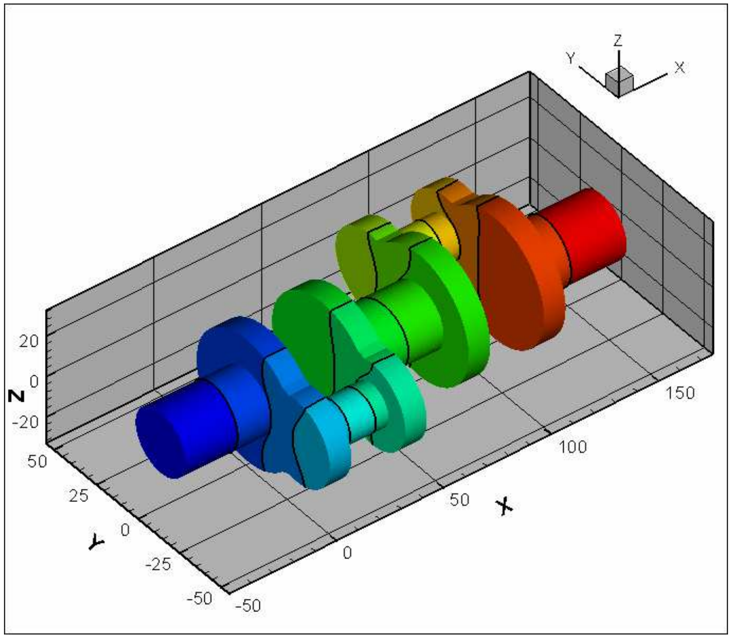
Practical, Cost-effective, Physically Accurate





Video Clip

Parallel, Moving Mesh, Complex Geometry, …

Context

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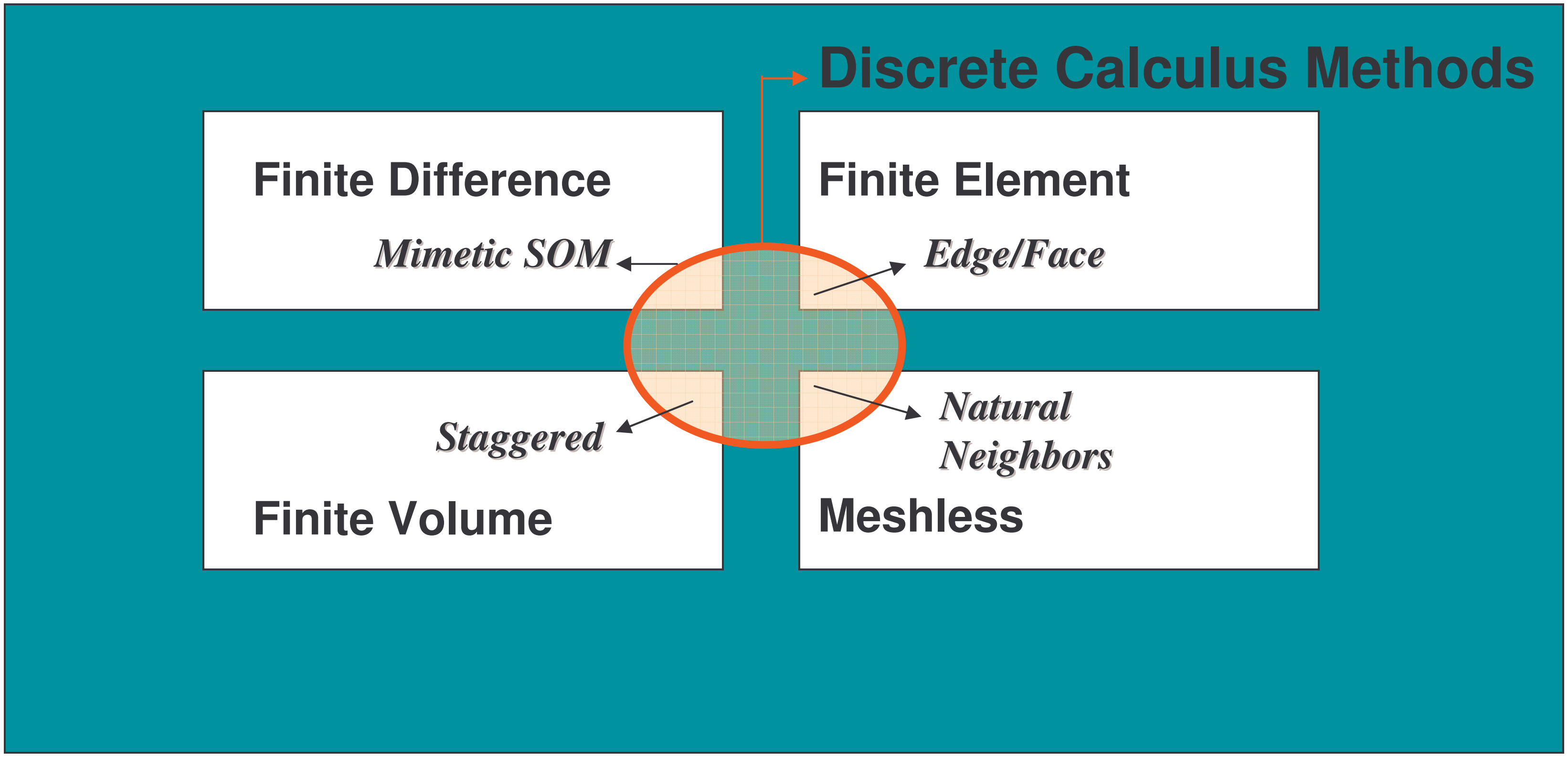

DC Methods are a subset of many other classical approaches

Exact Discretization

Discretization:

Continuous PDE => Finite Dimensional Matrix Problem

This Can Be Done Exactly

Solution:

Requires Approximations/Error

- But all approximation errors occur in the constitutive equations (in material properties).
- All numerical errors appear with the modeling errors.

Discretization $\neq$ Approximation

Example

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Physical Equation (Heat Equation)

$$\frac{\partial(\rho c T)}{\partial t} = \nabla \cdot k \nabla T$$

Components of the Physical Equation

$$\frac{\partial i}{\partial t} + \nabla \cdot \mathbf{q} = 0$$ Conservation of Energy

$$\mathbf{g} = \nabla T$$ Definition of Gradient

Physics

Math

Material Approximation

$$\mathbf{q} = -k\mathbf{g}$$ Fourier's Law

$$i = \rho c T$$ Perfectly Caloric Material

The Physical (Continuous) System

Example

Exact Discretization of Physics and Calculus

$$\int_{\tilde{c}} i\,dV\,|^{n+1} - \int_{\tilde{c}} i\,dV\,|^{n} + \sum_{\tilde{f}} \int dt \int_{\tilde{f}} \mathbf{q}\cdot\mathbf{n}\,dA_{\tilde{f}} = 0 \quad \Rightarrow \quad \boxed{I_{\tilde{c}}^{n+1} - I_{\tilde{c}}^{n} + \mathbf{D}Q_{\tilde{f}} = 0}$$

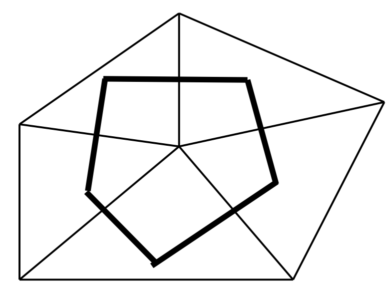
$$\int_e \mathbf{g}\cdot d\mathbf{l} = T_{n2} - T_{n1} \quad \Rightarrow \quad \boxed{g_e = \mathbf{G}T_n}$$

Numerically Exact

Numerical Approximations

$$Q_{\tilde{f}} = -M_1 g_e \quad \Rightarrow \quad \boxed{Q_{\tilde{f}} = -k\frac{A_{\tilde{f}}}{L_e} g_e}$$

$$I_{\tilde{c}} = M_2 T_n \quad \Rightarrow \quad \boxed{I_{\tilde{c}} = \rho c V_{\tilde{c}} T_n}$$



Numerically Approximate

The Numerical (Discrete) System

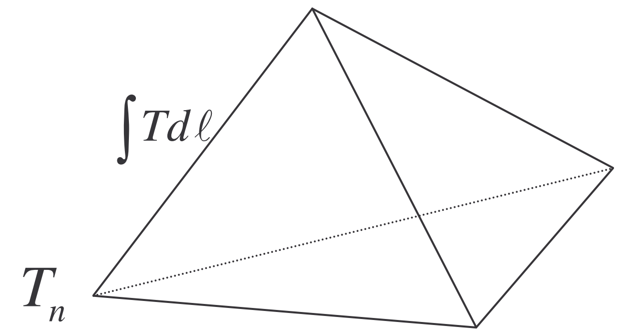
Higher Order Discrete Calculus

Higher Order Exact Gradient

$$\int_{edge} \mathbf{g}\cdot d\mathbf{l} = T_{n2} - T_{n1}$$

$$\int_{edge} (\mathbf{t}_e\cdot\mathbf{x})\mathbf{g}\cdot d\mathbf{l} = \mathbf{t}_e\cdot(\mathbf{x}_{n2}T_{n2} - \mathbf{x}_{n1}T_{n1}) - \int_{n1}^{n2} T dl$$

$$\int_{face} \mathbf{n}\times\mathbf{g}\,dA = \sum_{edges} \mathbf{t}_e \int T dl$$



$$\Rightarrow \begin{bmatrix} \int_{edge} \mathbf{g}\cdot d\mathbf{l} \\ \int_{edge} (\mathbf{t}_e\cdot\mathbf{x})\mathbf{g}\cdot d\mathbf{l} \\ \int_{face} \mathbf{n}\times\mathbf{g}\,dA \end{bmatrix} = \mathbf{G}^{[2]} \begin{bmatrix} T_n \\ \int_e T dl \end{bmatrix}$$

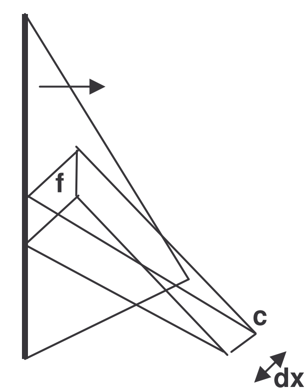
Applicable to Any Polyhedron

Same Mesh – More Unknowns

Higher Order Exact Divergence

- Need one equation for each edge.
- Integrate over the very thin CVs surrounding the dual faces.
- Take the 'thin' limit carefully – so thin elements align.

$$\int_{\tilde{f}} \frac{\partial(\mathbf{q}\cdot\mathbf{n}_{\tilde{f}})}{\partial n_{\tilde{f}}} dA + \sum_{\substack{edge \\ faces}} \mathbf{n}_{fc} \cdot \int_{\tilde{e}} \mathbf{q}\, dl = 0$$



or

$$\sum_{\substack{edge \\ cells}} \int_{\tilde{f}_\perp} \nabla \cdot \mathbf{q}\, dA_\perp + \sum_{\substack{edge \\ faces}} \int_{l_\perp} [\mathbf{q}]_f \bullet \mathbf{n}_f\, dl_\perp = 0$$

Reconstruction

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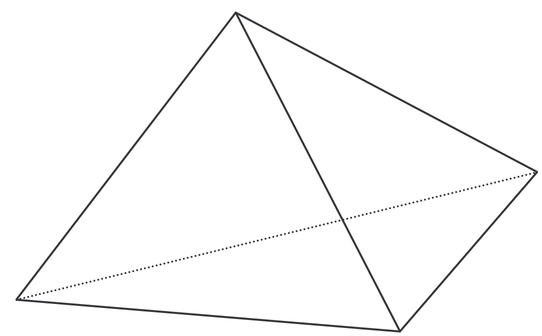
Have

$$\begin{bmatrix} \int_e \mathbf{g} \bullet d\mathbf{l} \\ \int_e \mathbf{x}\mathbf{g} \cdot d\mathbf{l} \\ \int_f \mathbf{n} \times \mathbf{g}\, dA \end{bmatrix}$$

Need

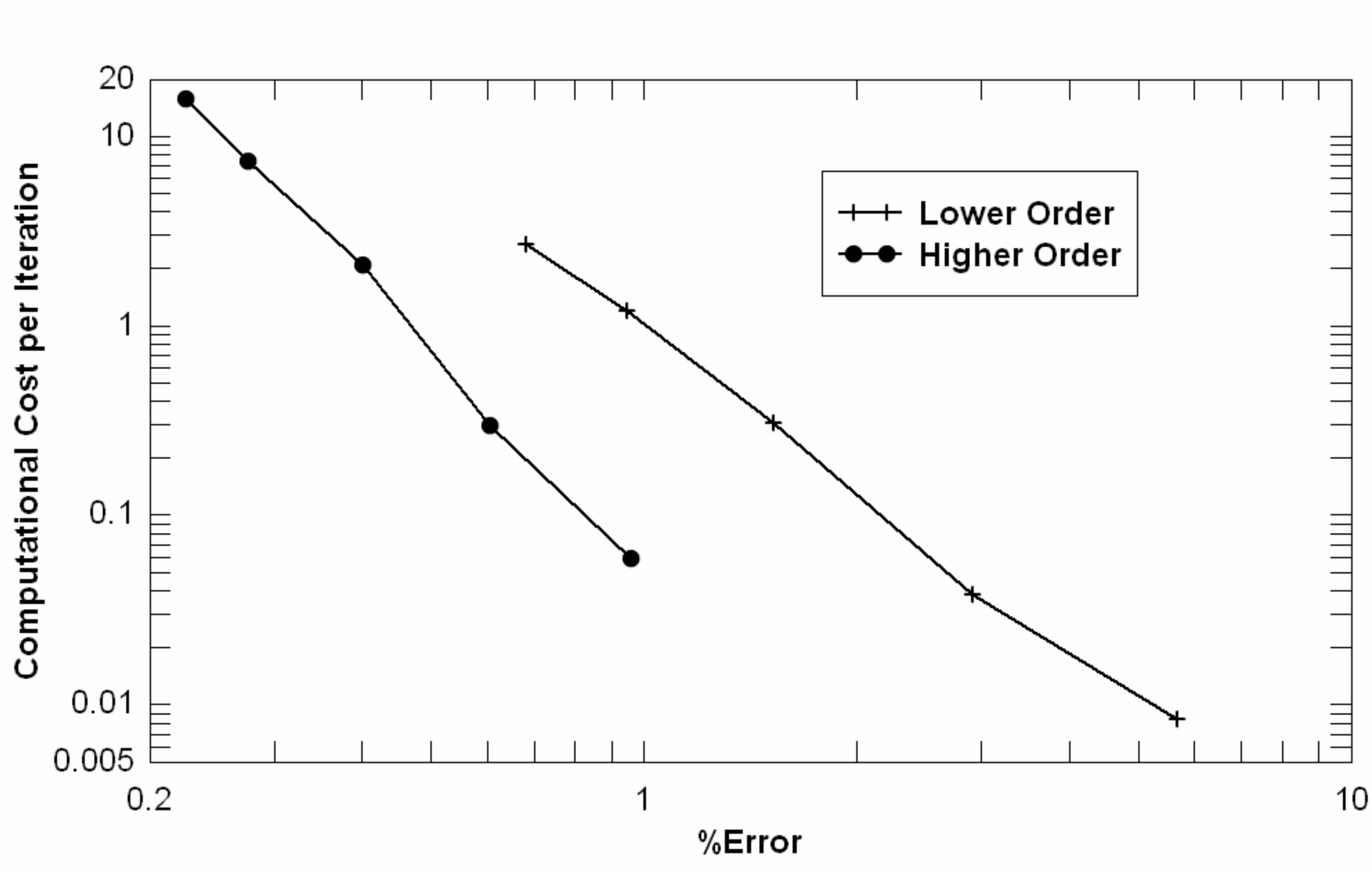
$$\begin{bmatrix} \int_{\tilde{f}} \mathbf{q} \cdot \mathbf{n}_{\tilde{f}}\, dA \\ \int_{\tilde{f}} \frac{\partial(\mathbf{q} \cdot \mathbf{n}_{\tilde{f}})}{\partial n_{\tilde{f}}}\, dA \\ \int_{\tilde{e}} \mathbf{q} \times d\mathbf{l} \end{bmatrix}$$

Assume q=-kg is linear on primary mesh cells.



Basis Functions not Required

Results



Good Cost/Accuracy for 'Smooth' Solutions

Conclusions

- **Exact discretization** of PDEs is possible and **strongly** encouraged.

- Excellent numerical/mathematical properties are NOT restricted to FE methods.

- Applicable to ANY polygon mesh (including meshless), no explicit basis functions, no need to build matrices.

JCP Publications

- Subramanian, V., and Perot, J. B. *Higher Order Mimetic Methods for Unstructured Meshes*, J. Comput. Phys., **219**, 68-85, 2006
- Perot, J. B., and Subramanian, V. *Discrete Calculus Methods for Diffusion*, J. Comput. Phys., **224** (1), 59-81, 2007.
- Subramanian, V., and Perot, J. B. *A Discrete Calculus Analysis of the Keller-Box Scheme and a Generalization of the Method to Arbitrary Meshes*, Accepted to J. Comput. Phys., 2007.

Discrete Calculus Operators

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Gradient Operator	**G**	$\left(T_{\tilde{n}2} - T_{\tilde{n}1} \Rightarrow \mathbf{G}T_{\tilde{n}}\right)$	$\mathbf{G} = -\mathbf{D}^T$
Divergence Operator	**D**	$\left(\sum_f Q_f \Rightarrow \mathbf{D}Q_f\right)$	
Curl Operator	**C**	$\left(\sum_e s_e \Rightarrow \mathbf{C}s_e\right)$	$\mathbf{C} = \mathbf{R}^T$
Rotation Operator	**R**	$\left(\sum_f U_f \Rightarrow \mathbf{R}U_f\right)$	

$\nabla\phi = 0 \Rightarrow \phi = \text{constant}$	$\nabla \bullet \nabla \times (\ \ ) = 0$	$\nabla \times \nabla (\ \ ) = 0$
$\mathbf{G}T_{\tilde{n}} = 0 \Rightarrow \{T_{\tilde{n}}\} = \{c\}$	$\mathbf{DC} = 0$	$\mathbf{CG} = 0$

Discrete Calculus Operators *mimic* Continuous Operators

The Discrete Calculus Approach

Physics		Numerics	
$\frac{\partial i}{\partial t} + \nabla \bullet \mathbf{q} = 0$ $\mathbf{g} = \nabla T$	***Physically Exact***	$I_c^{n+1} - I_c^n + \mathbf{D}Q_f = 0$ $g_{\tilde{e}} = \tilde{G} T_{\tilde{n}}$	***Numerically Exact***
$\mathbf{q} = -k\mathbf{g}$ $i = \rho c T$	***Physically Approximate***	$Q_f = -k \frac{g_{\tilde{e}}}{L_{\tilde{e}}} A_f$ $I_c = \rho c V_c T_{\tilde{n}}$	***Numerically Approximate***
$\frac{\partial(\rho c T)}{\partial t} = \nabla \bullet k \nabla T$		$\frac{\partial(\rho c V_c \mathrm{I}\, T_{\tilde{n}})}{\partial t} = \mathbf{D}\left(-k \frac{A_f}{L}\right)\mathbf{G} T_{\tilde{n}}$	

Continuous vs. Discrete System

Discrete Calculus Methods

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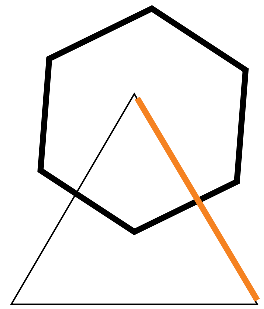
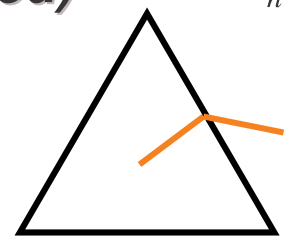
Node-Based Method

T_n



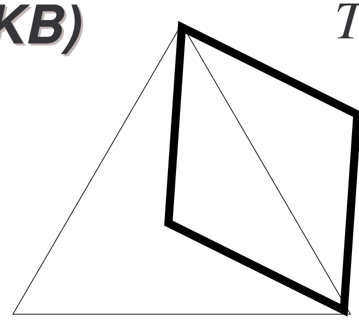
Cell-Based Method (Mixed)

$T_{\tilde{n}}, Q_f$



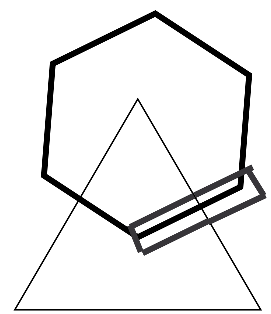
Face-Based Method (KB)

T_f, Q_f



Higher Order Method

T_n, T_e

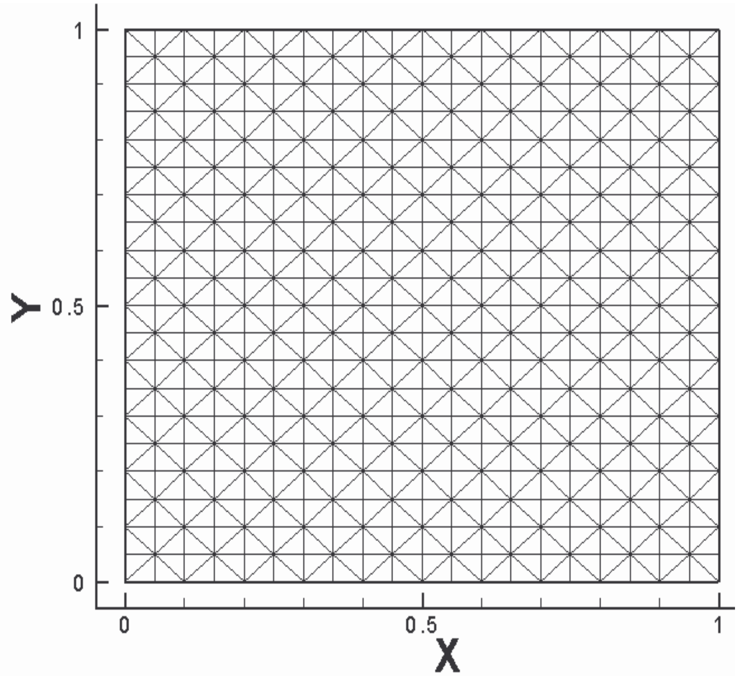


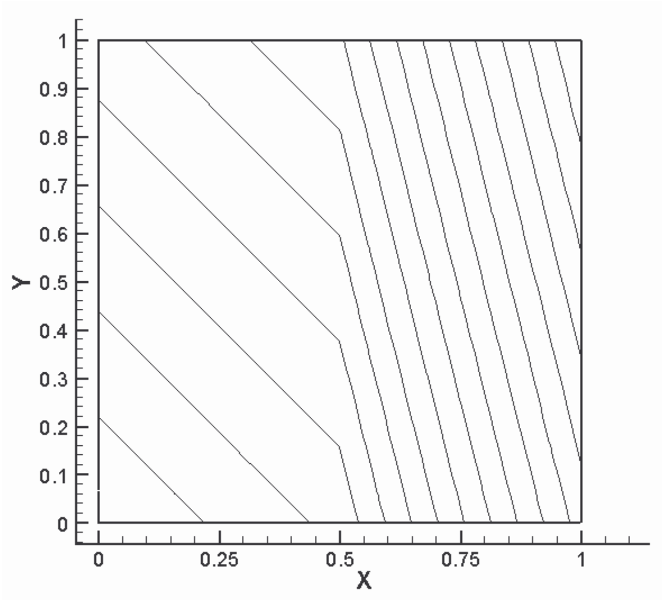
DC Approach is a methodology – not a particular method!

Physical Accuracy

Discontinuous Diffusion: Heat Flow at an Angle

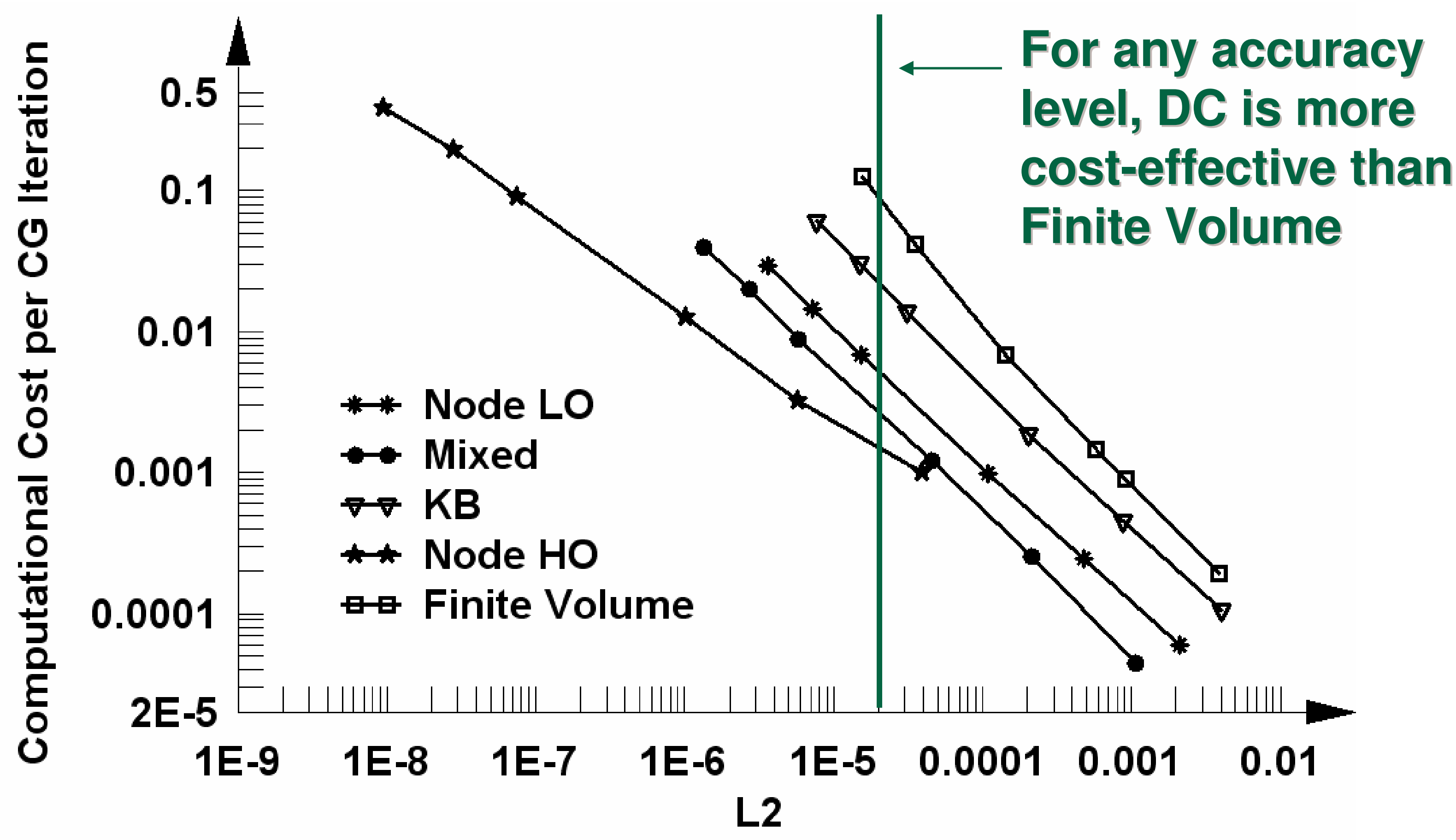
$$k = \begin{cases} 4 & 0 < x < 0.5 \\ 1 & 0.5 < x < 1 \end{cases} \qquad T_{exact} = \begin{cases} 1 + x + y & 0 \le x \le 0.5 \\ 4x + y - 0.5 & 0.5 \le x \le 1 \end{cases}$$





Linearly Complete as well as Physically Realistic

Cost of DC Methods



More Cost-Effective than Traditional Methods

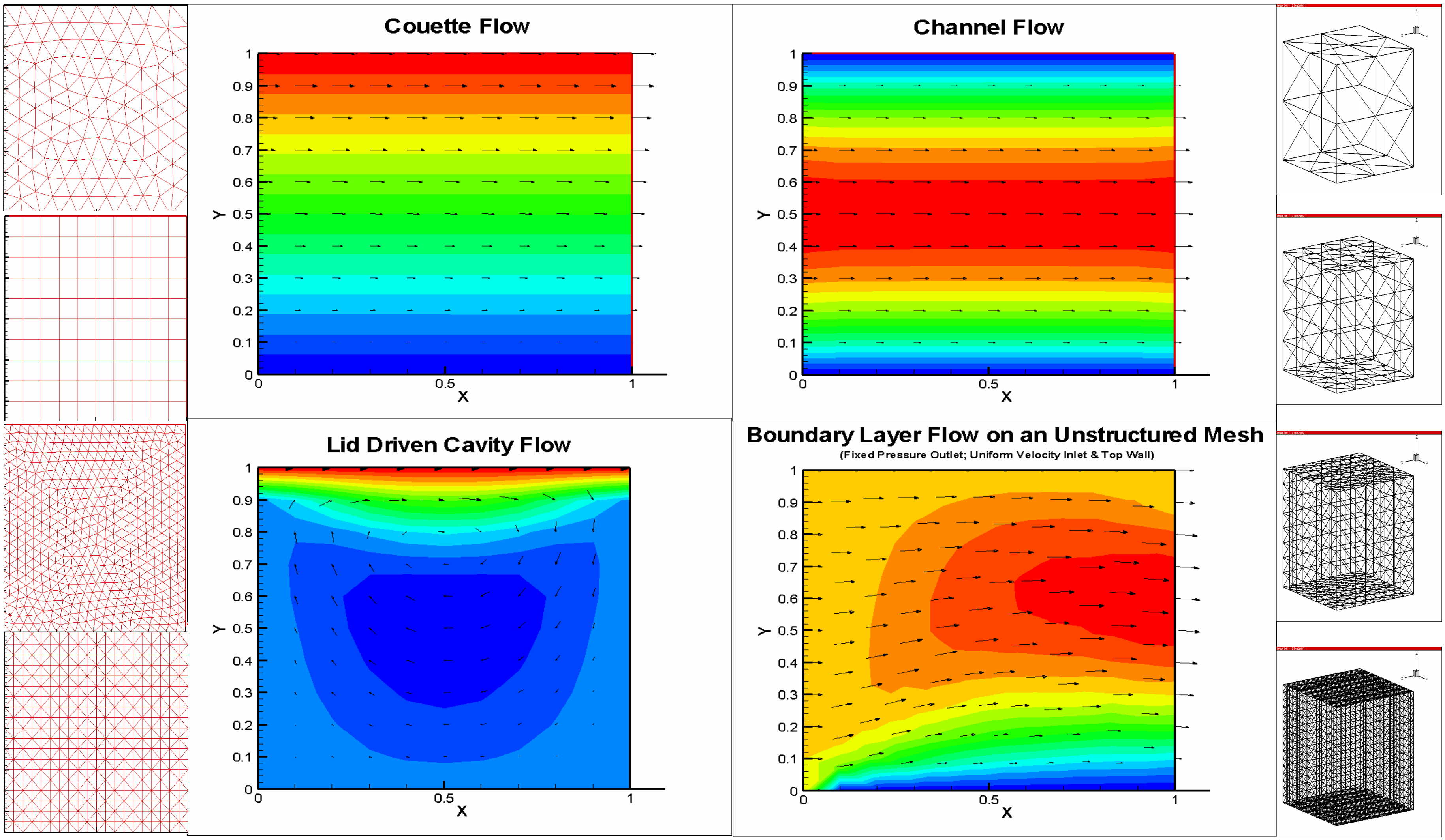
Implications

Exact Discretization:

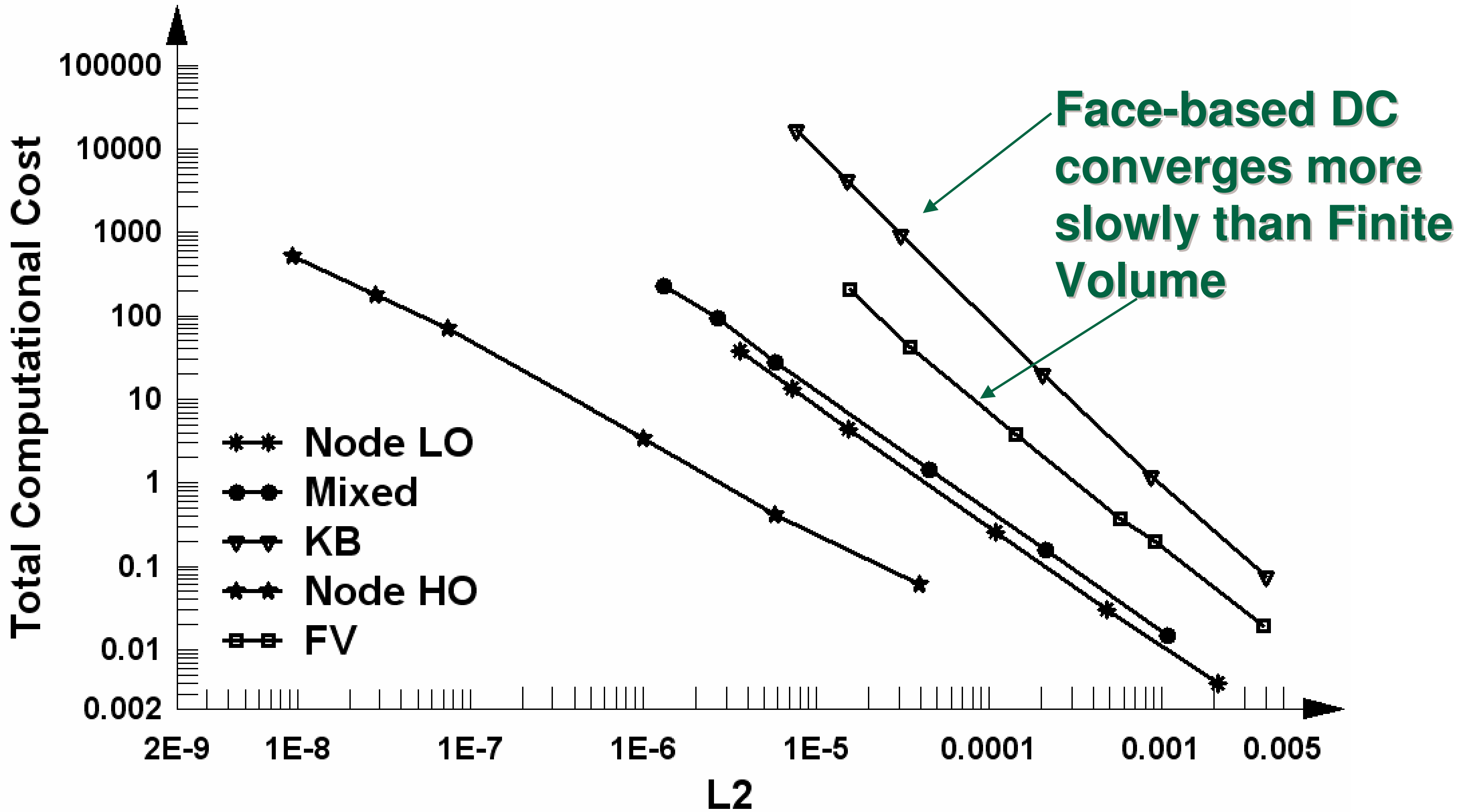
- Discrete Operators (Div, Grad, Curl)
  behave just like the continuous operators.
- Mimetic.
- Discrete de Rham Complex (algebraic topology).
- $\nabla \times \nabla(\ ) = 0$, etc
- Physics is always captured
  (conservation, wave propagation, max principal, …).
- No spurious modes.
- No surprises.

Methods that capture physics well

Incompressible Navier-Stokes Tests



Total cost for a desired accuracy level

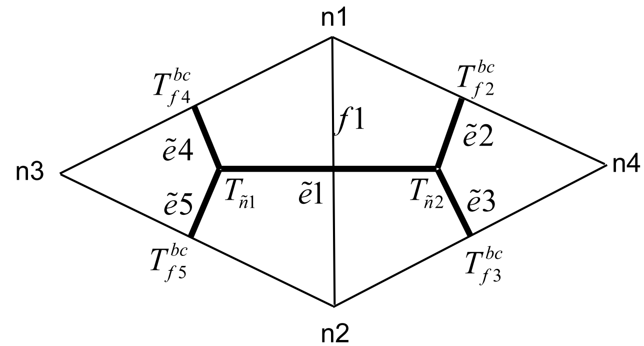


High Matrix Condition Numbers Adversely Impacts the Cost

Discrete Calculus Operators

Discrete Gradient Operator $(\tilde{n} \to \tilde{e})$

$$
\begin{aligned}
g_{\tilde{e}1} &= T_{\tilde{n}2} - T_{\tilde{n}1} \\
g_{\tilde{e}2} &= -T_{\tilde{n}2} + T_{f2}^{bc} \\
g_{\tilde{e}3} &= -T_{\tilde{n}2} + T_{f3}^{bc} \\
g_{\tilde{e}4} &= -T_{\tilde{n}1} + T_{f4}^{bc} \\
g_{\tilde{e}5} &= -T_{\tilde{n}1} + T_{f5}^{bc}
\end{aligned}
\quad \Rightarrow \quad
\tilde{G} = \begin{bmatrix} -1 & 1 \\ 0 & -1 \\ 0 & -1 \\ -1 & 0 \\ -1 & 0 \end{bmatrix}
$$



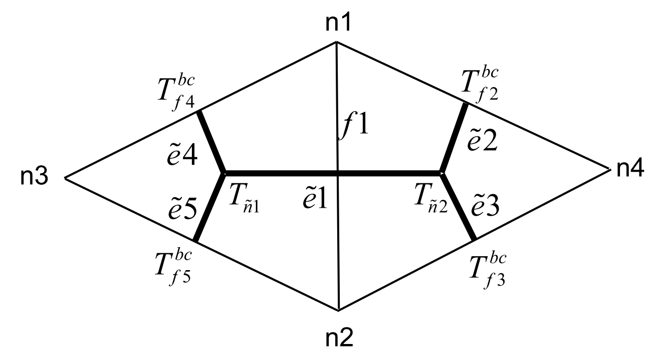
Discrete Divergence Operator $(f \to c)$

$$
\begin{aligned}
DQ_f\big|_{c1} &= Q_{f1} + Q_{f4} + Q_{f5} \\
DQ_f\big|_{c2} &= -Q_{f1} + Q_{f2} + Q_{f3}
\end{aligned}
\quad \Rightarrow \quad
D = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ -1 & 1 & 1 & 0 & 0 \end{bmatrix}
$$

$$\boxed{\tilde{G} = -D^T}$$

More Discrete Calculus Operators

Discrete Curl Operator $\left(e \to f\right)$



$$C = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & -1 & 0 \end{bmatrix}$$

Discrete Rotation Operator $\left(\tilde{e} \to \tilde{f}\right)$

$$\tilde{C} = \begin{bmatrix} 1 & 1 & 0 & -1 & 0 \\ -1 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & -1 & 1 & 0 & 0 \end{bmatrix}$$

$$C = \tilde{C}^T$$