



Principles of compatible discretizations

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Penn State, November 18, 2005

Supported in part by



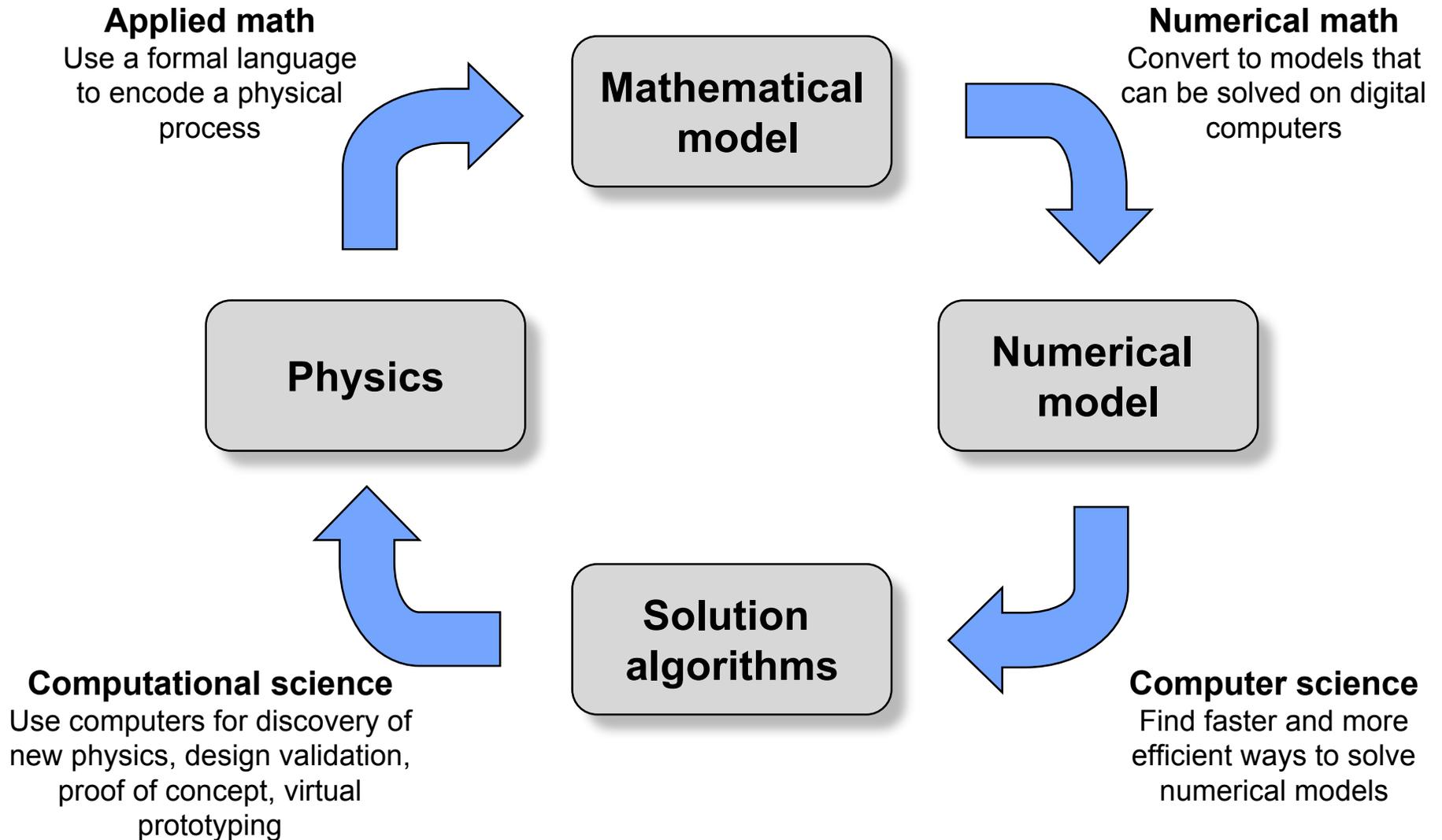


Part I

where we learn about computational modeling, discretization of PDEs, and develop two simple discrete models (with mixed success)



What is this talk about?





Focus on Numerical Math

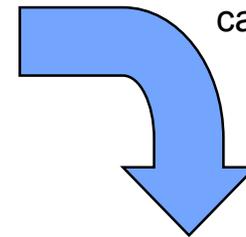
Discretization
=
Model reduction

$$\mathcal{A}u = f$$

mathematical model

Numerical math

Convert to models that can be solved on digital computers



$$\mathbf{A}_h \mathbf{u}_h = \mathbf{f}_h$$

a parameterized family of algebraic equations

1. Is the sequence of algebraic equations well-behaved?

- are all problems **uniquely** and **stably** (in h) solvable?
- do solutions **converge** to the exact solutions as $h \rightarrow 0$?

2. Are physical and discrete models compatible?

- are solutions **physically** meaningful
- do they **mimic**, e.g., **invariants**, **symmetries**, or **involutions** of actual states

3. How to make a compatible & accurate discretization?

- how to **choose** the **variables** and where to **place** them;
- how to avoid **spurious** solutions.



A toy problem

Boundary value problem

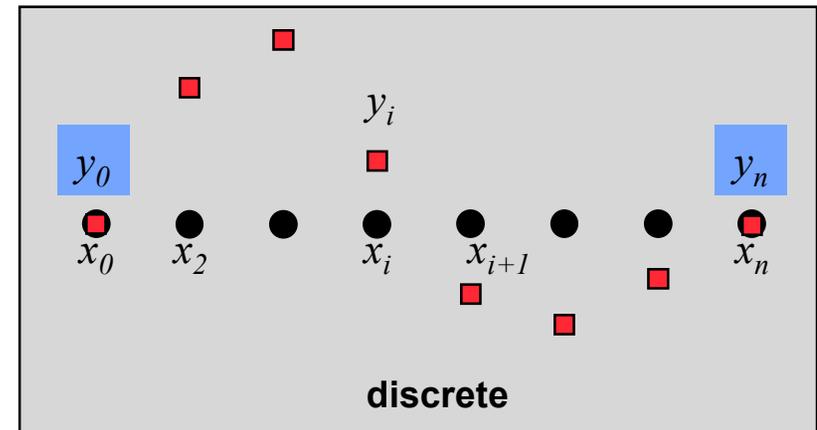
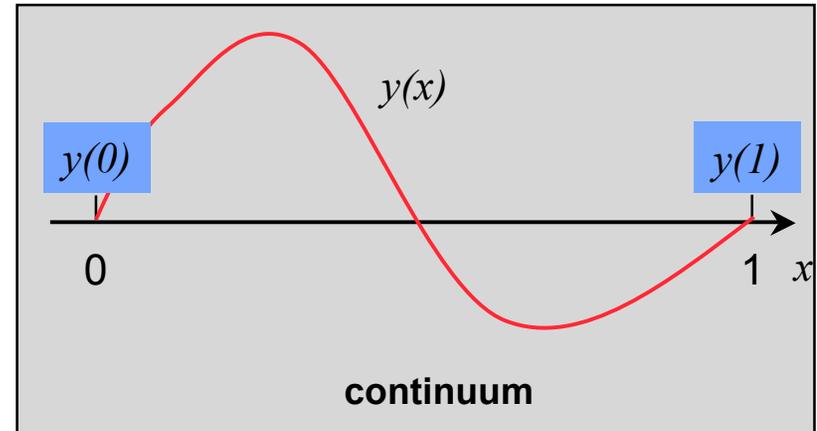
$$-ay'' + by' + cy = f \text{ in } (0,1)$$
$$y(0) = y(1) = 0$$

$$y'(x_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

$$y(x_i) \approx \frac{y_{i+1} - y_{i-1}}{2h}$$

$$-a_i \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + b_i \frac{y_{i+1} - y_{i-1}}{2h} + c_i y_i = f_i$$
$$y_0 = y_n = 0$$

Parameterized linear system



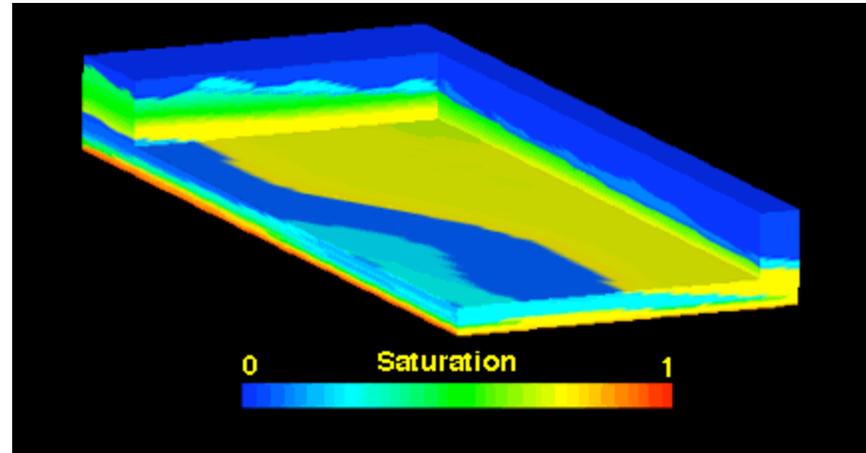


Porous Media Flow

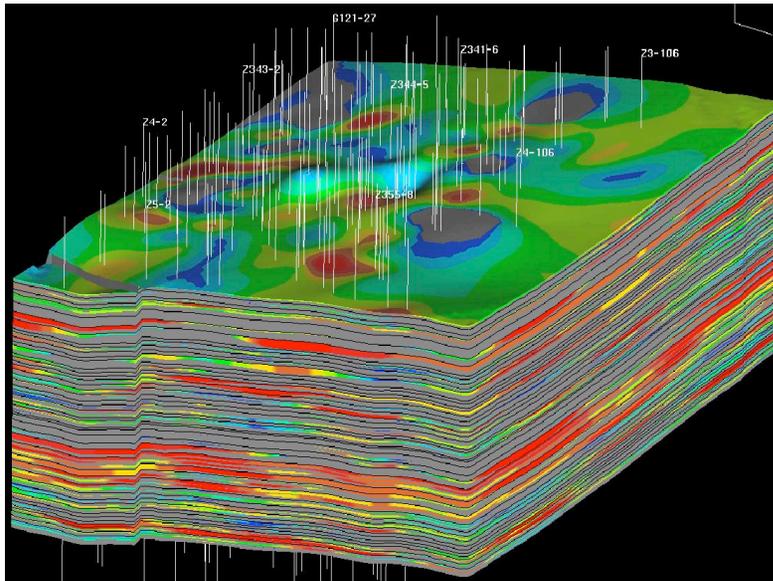
Boundary value problem

$$\begin{aligned} -\nabla \cdot \rho \nabla p &= f \text{ in } \Omega \\ p &= 0 \text{ on } \Gamma \end{aligned}$$

f - source term
 p - pressure
 ρ - permeability tensor



Steady state saturation in a site scale model of Yucca Mountain, Nevada. Model area is 1.7X4.2 square miles. Calculations like this are used for evaluating the suitability of **Yucca Mountain** as a potential repository for **high level nuclear waste**. *Courtesy LANL EES Division.*



Reservoir simulation can be used to forecast the **production of oil and gas fields**, optimize reservoir development, and evaluate the distribution of remaining oil. It is an **important tool** to improve the design of wells, the efficiency of reservoirs, and enhance oil and gas recovery. *Courtesy Prof. J. Chen, SMU*



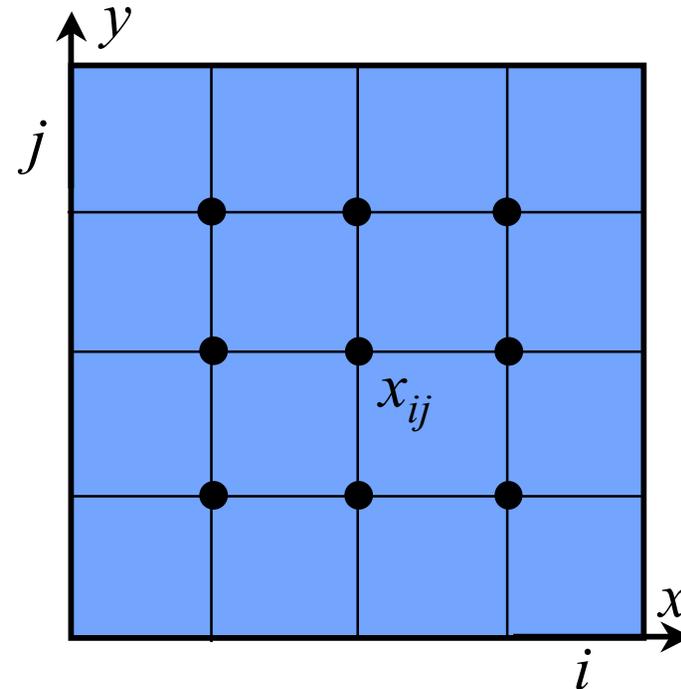
Darcy problem

In such applications, **velocity \mathbf{u}** , rather than the **pressure p** is the variable of primary interest, and direct approximation is desirable.

Equivalent 1st order form

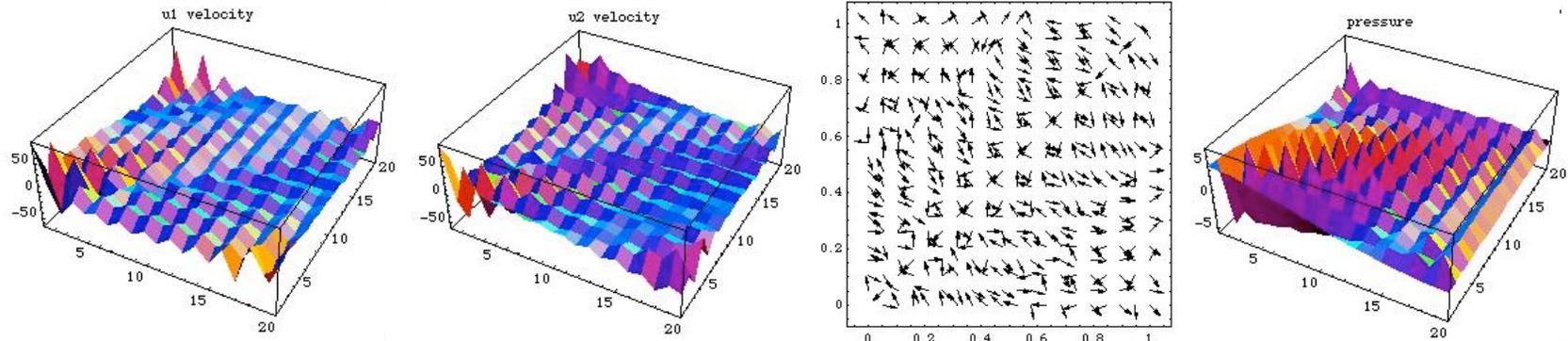
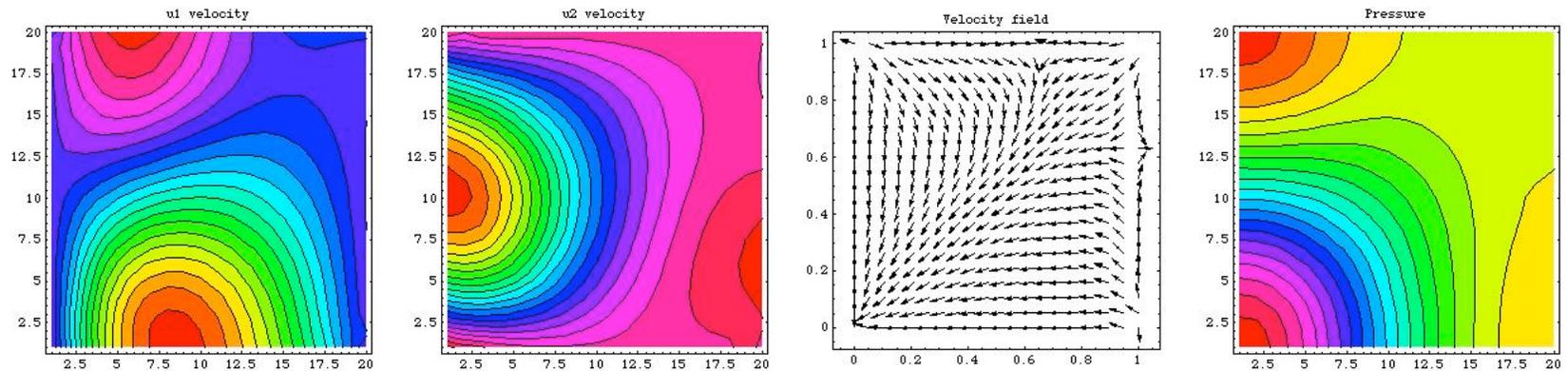
$$\begin{aligned} \nabla \cdot \rho \mathbf{u} &= f \text{ in } \Omega \\ \mathbf{u} + \nabla p &= 0 \text{ on } \Omega \\ p &= 0 \text{ on } \Gamma \end{aligned}$$

Discretized domain





Computational example



Complete DISASTER (☠ ☠ ☠)
Our discrete model is incompatible

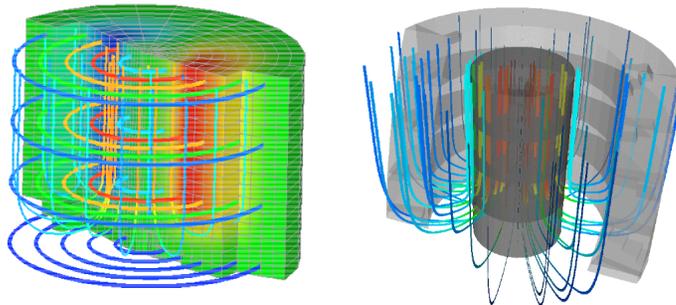


Coupled multiscale, nonlinear physics is even more challenging: Z-Pinch simulation in ALEGRA

Scales:

PULSE DURATION	10^{-9} sec
TIME SCALE	10^{-3} sec
CURRENT POWER	20×10^6 A
X-RAY POWER	10^{12} W
X-RAY ENERGY	1.9×10^6 J

C. Garasi, A. Robinson



MHD MODEL

=

Hydrodynamics + Magnetic Diffusion

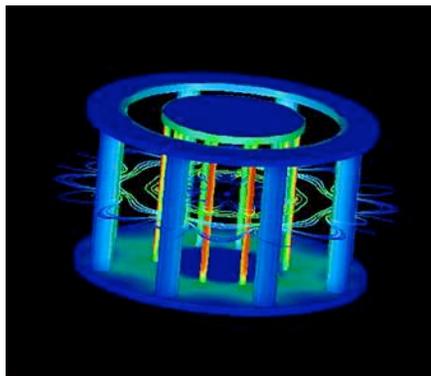
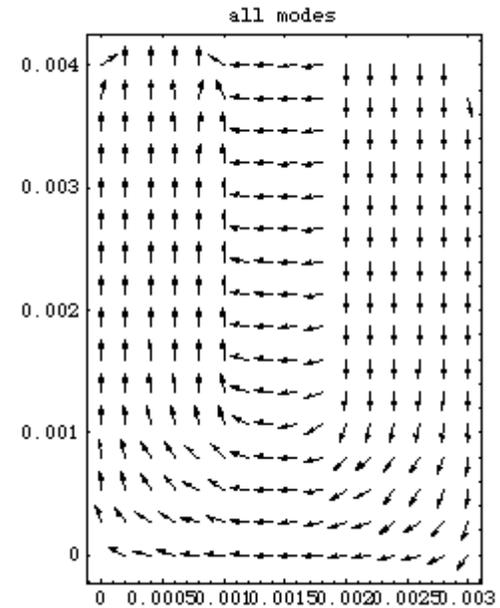
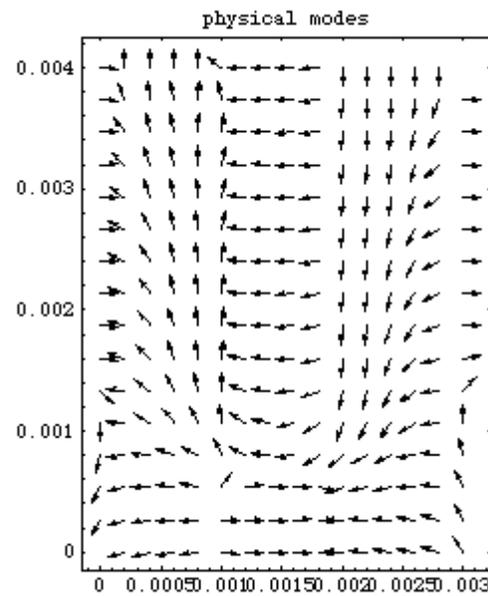
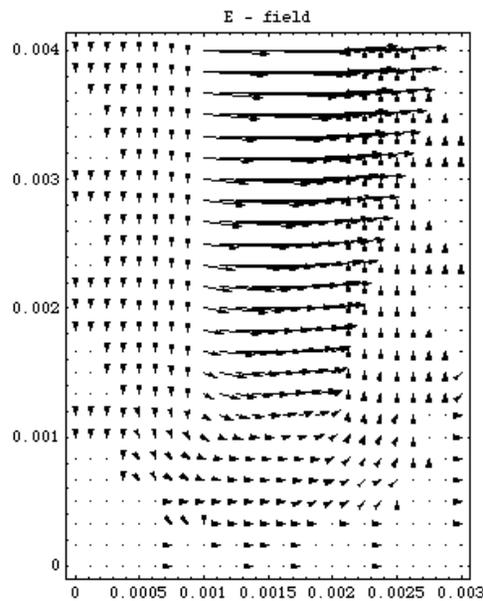


Z-machine: (Ostensibly used by Ocean's 11)

Electric currents are used to produce an ionized gas by vaporizing a spool-of-thread sized array of 100-400 wires of diameter $\approx 10\mu\text{m}$



Magnetic diffusion

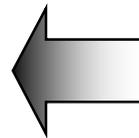
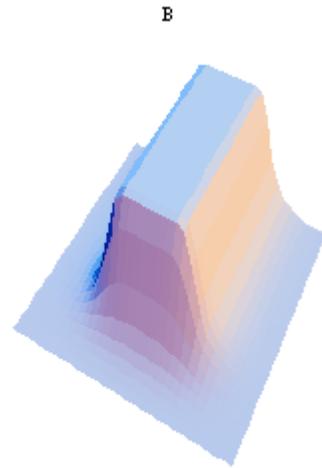
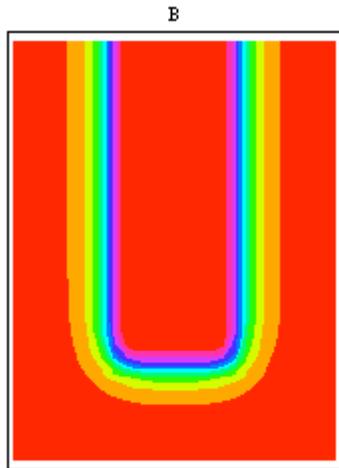


$$\nabla \times \frac{1}{\mu} \mathbf{B} = \sigma \mathbf{E} \quad \text{Ampere}$$
$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \text{Faraday}$$

Gap modeled as a heterogeneous conductor

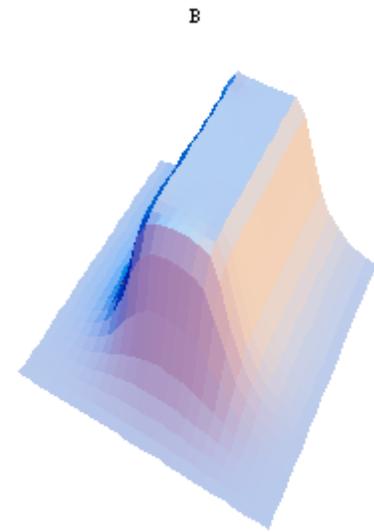
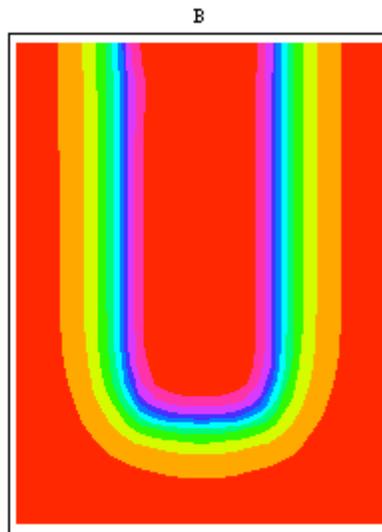
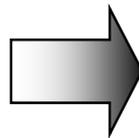


Compatible vs. Collocated: B-field



Compatible
 $\text{Ker}(\text{curl}) = \{\text{grad } p\}$

Collocated
 $\text{Ker}(\text{curl}) = \{0\}$





Part II

where we learn about duality, its role in PDE structure and what it can tell us about compatible discretizations

All you ever wanted to know about duality (but were afraid to ask)

In mathematics “duality” is used in two contexts

1. Duality pairing

The process of combining **two objects** to generate a **scalar**

$\mathbf{a}^T \mathbf{b} \rightarrow \langle \mathbf{a}, \mathbf{b} \rangle$ Vector \mathbf{a} dual to *co-vector* \mathbf{b}

$f(x) \rightarrow \langle f, x \rangle$ Function f dual to *its argument* x

$\int_{\Omega} f \rightarrow \langle f, \Omega \rangle$ Function f dual to *integration domain* Ω

$\int_{\Omega} fg \rightarrow \langle f, g \rangle$ Function f dual to *distribution* g

$\langle f | g \rangle \rightarrow \langle f, g \rangle$ Bra vector f dual to *ket vector* g

$Fd \rightarrow \langle F, d \rangle$ Force F dual to *displacement* d



Leads to the fundamental notions of adjoint and self-adjoint operators

$$\langle Af, g \rangle = \langle f, A^* g \rangle \quad A = A^*$$

$$\mathbf{b}^T \mathbf{A} \mathbf{a} = \mathbf{a}^T \mathbf{A}^T \mathbf{b}$$

$$\langle \mathbf{A} \mathbf{a}, \mathbf{b} \rangle = \langle \mathbf{a}, \mathbf{A}^T \mathbf{b} \rangle$$

Adjoint of a matrix \mathbf{A} is the **transpose**

$$\int_{\Omega} \nabla \cdot \mathbf{v} = \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{v}$$

$$\langle \nabla \cdot \mathbf{v}, \Omega \rangle = \langle \mathbf{v}, \partial\Omega \rangle$$

Adjoint of **divergence** is **boundary**

$$\int_{\Omega} u \nabla \cdot \mathbf{v} = - \int_{\Omega} \nabla u \cdot \mathbf{v}$$

$$\langle u, \nabla \cdot \mathbf{v} \rangle = \langle -\nabla u, \mathbf{v} \rangle$$

Adjoint of **divergence** is **-gradient**

$$\int_{\Omega} -\Delta u v = \int_{\Omega} -\Delta v u$$

$$\langle -\Delta u, v \rangle = \langle u, -\Delta v \rangle$$

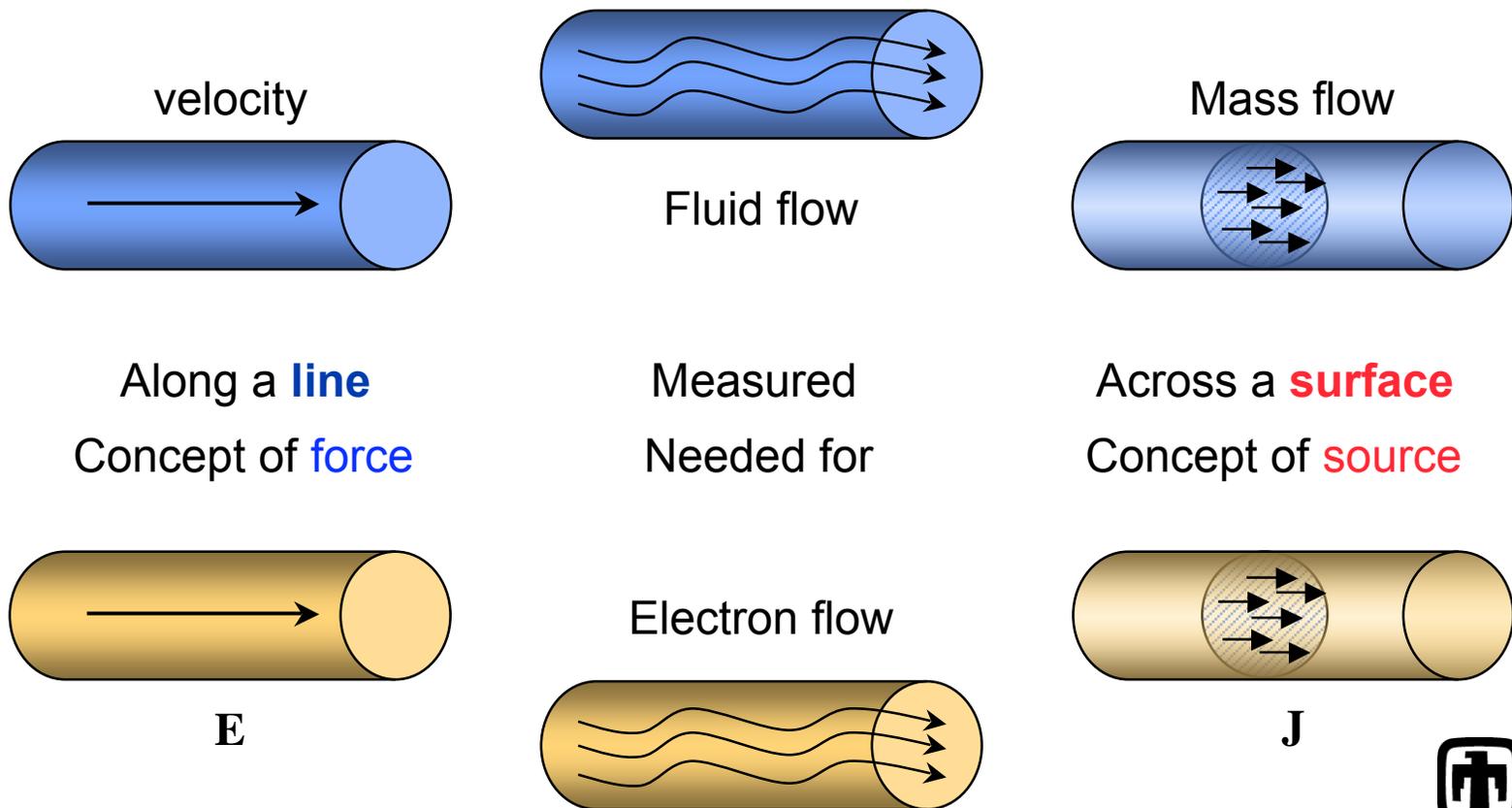
Laplacian is **self-adjoint**



A second duality concept

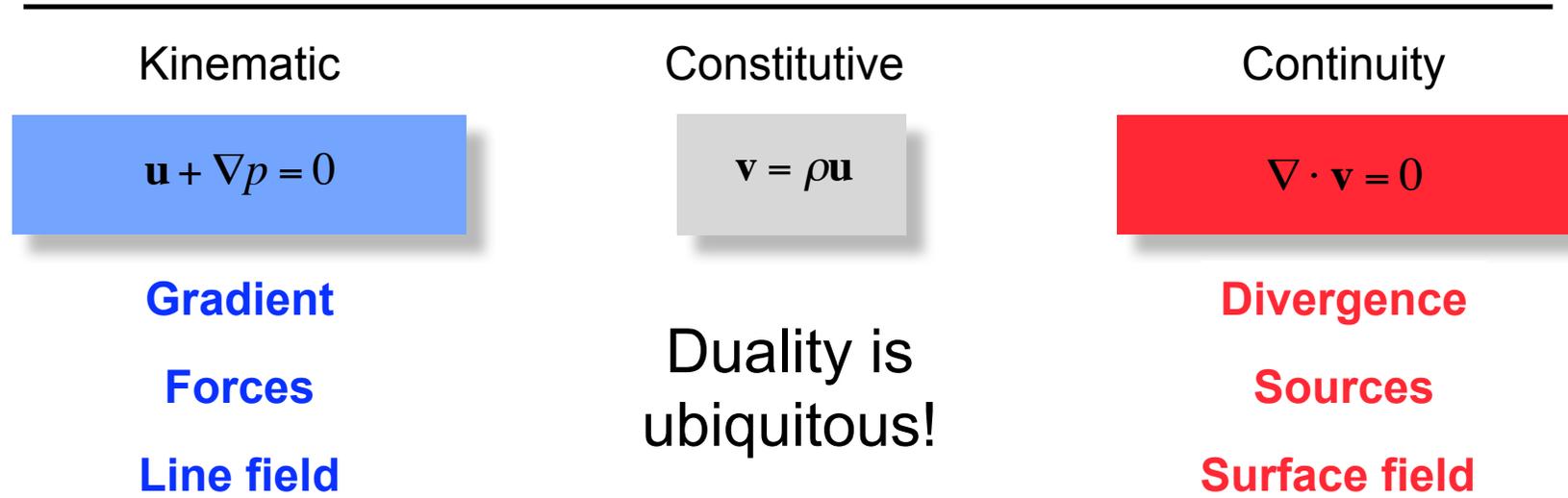
2. Duality of representations

The process of using complementary descriptions of the same process

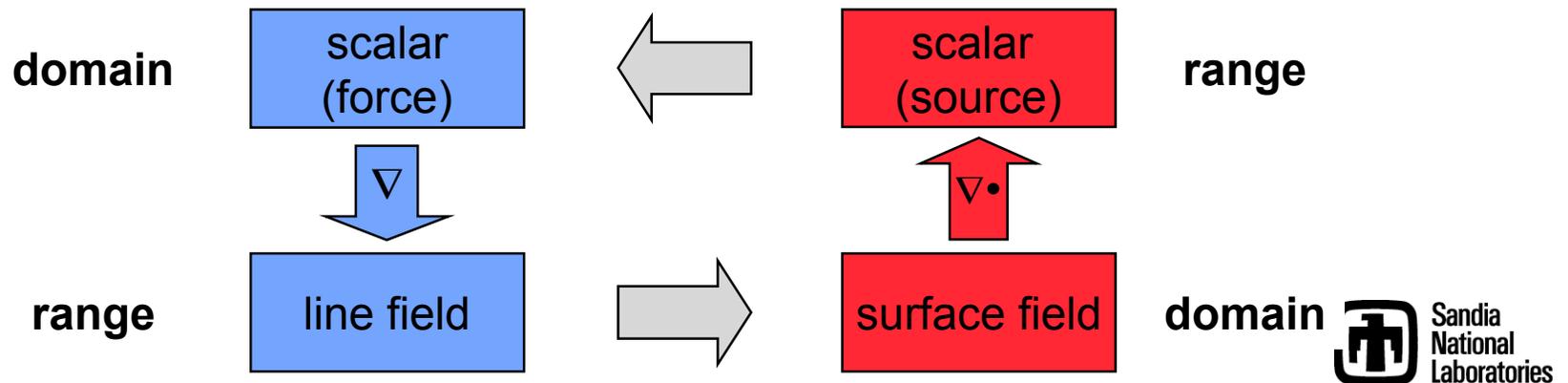




Darcy problem deconstructed



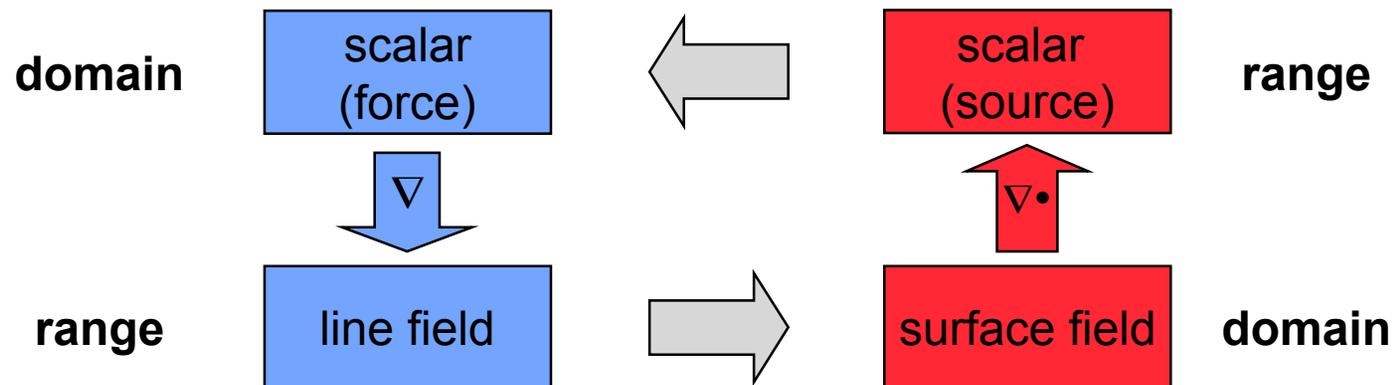
Duality structure can be encoded by the following diagram





Compatible discretizations

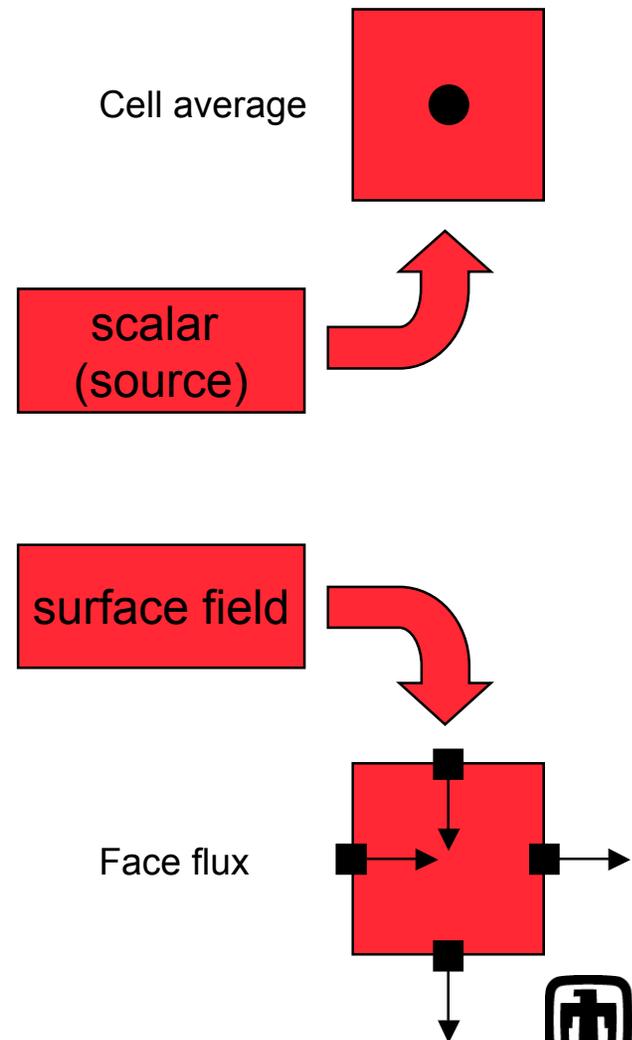
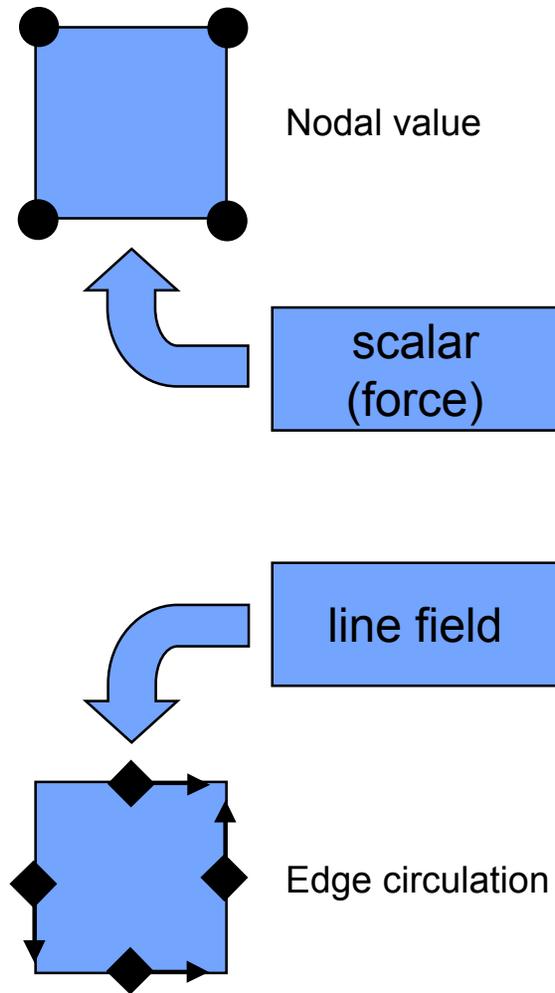
A compatible discretization should mimic the duality structure of the PDE



We need to build a discrete analogue of this diagram!

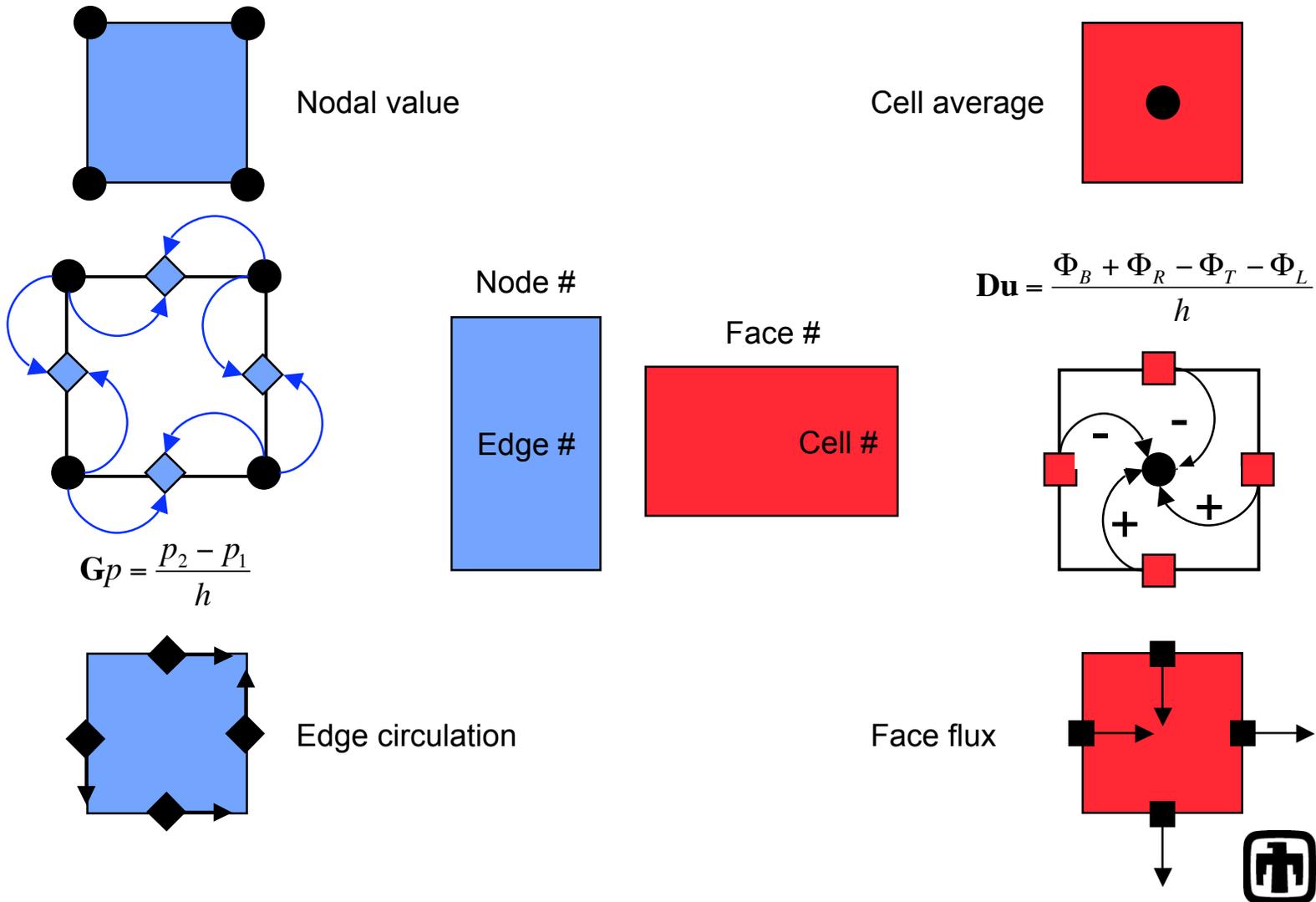


1. Compatible representations



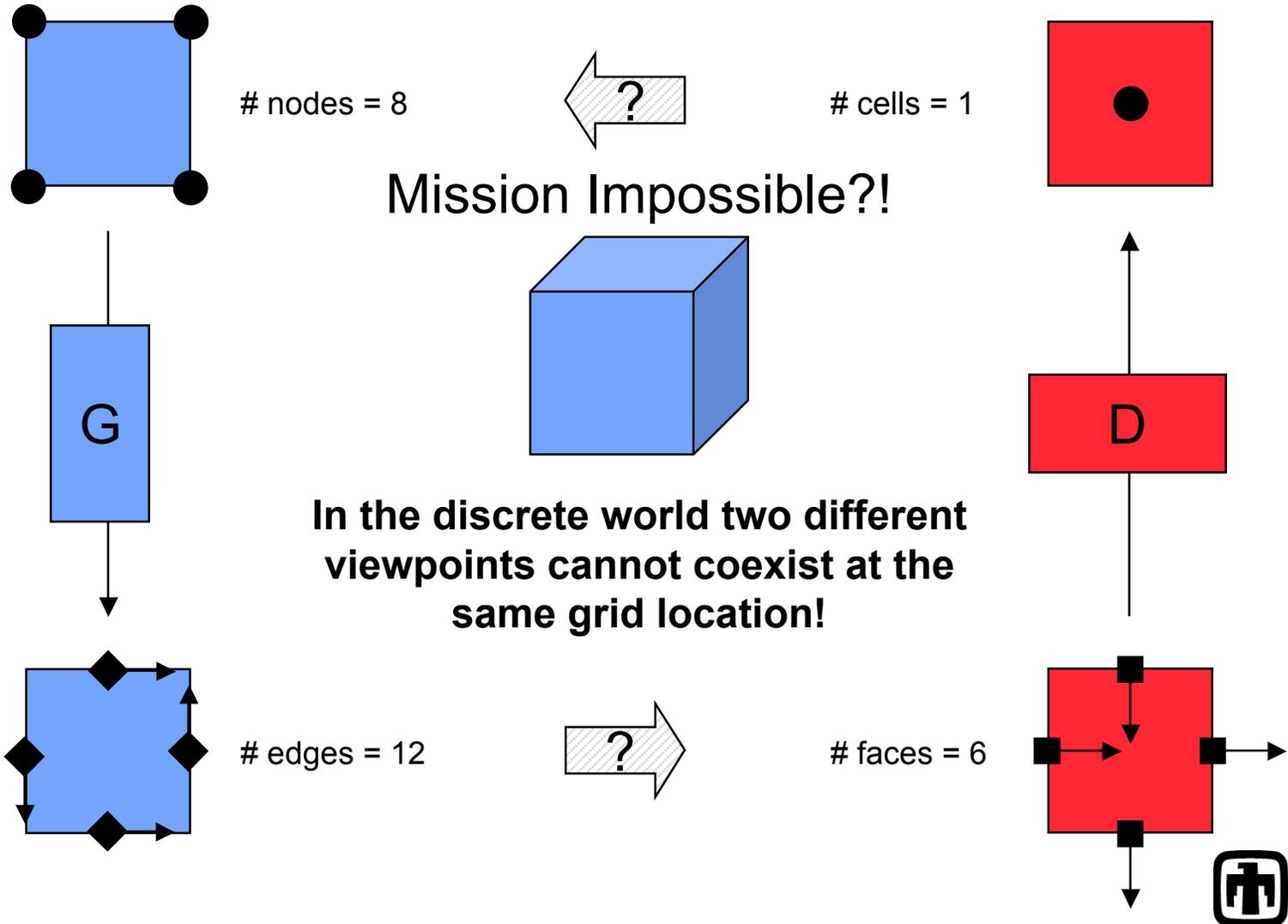


2. Compatible discrete operators



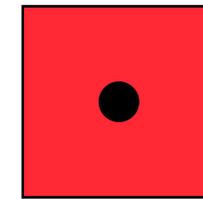
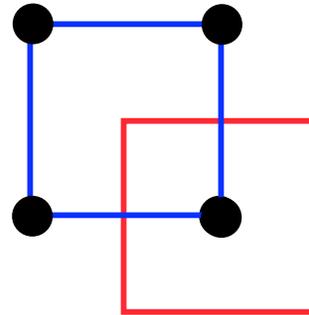
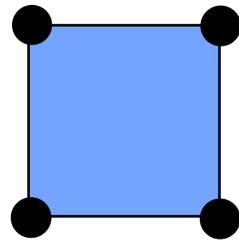


3. Putting it together

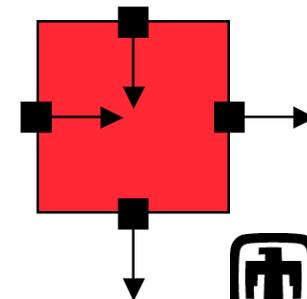
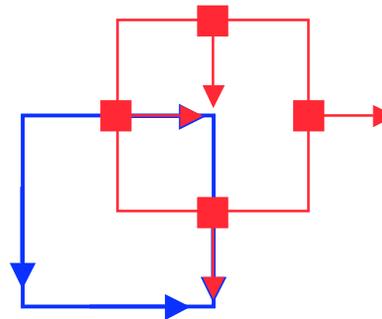
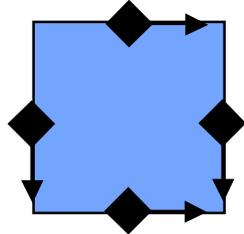




Solution #1 Primal-Dual Grid Complex



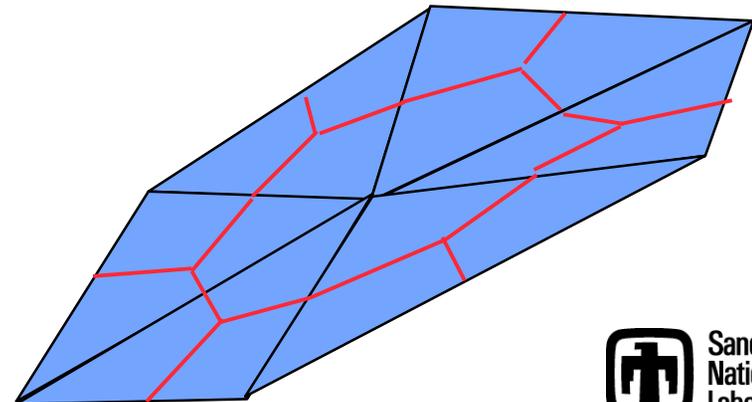
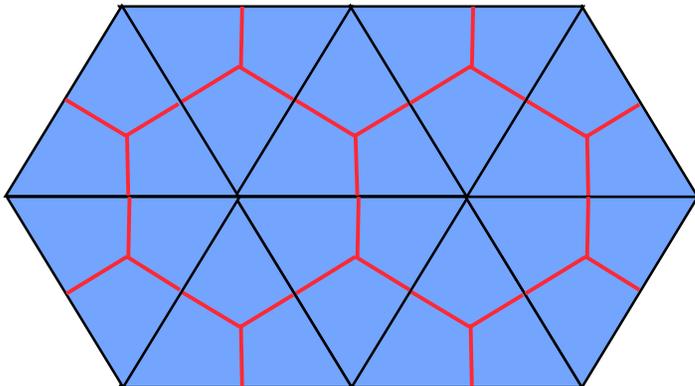
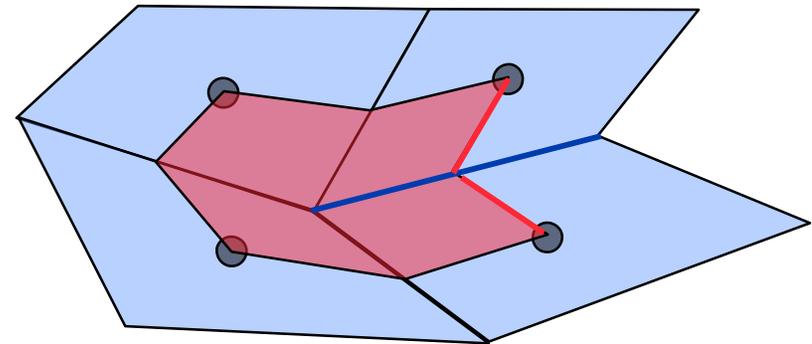
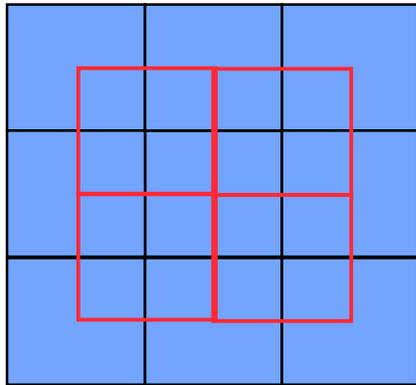
Staggered grid discretizations
Covolume (Delaunay-Voronoi)
Box Integration Method





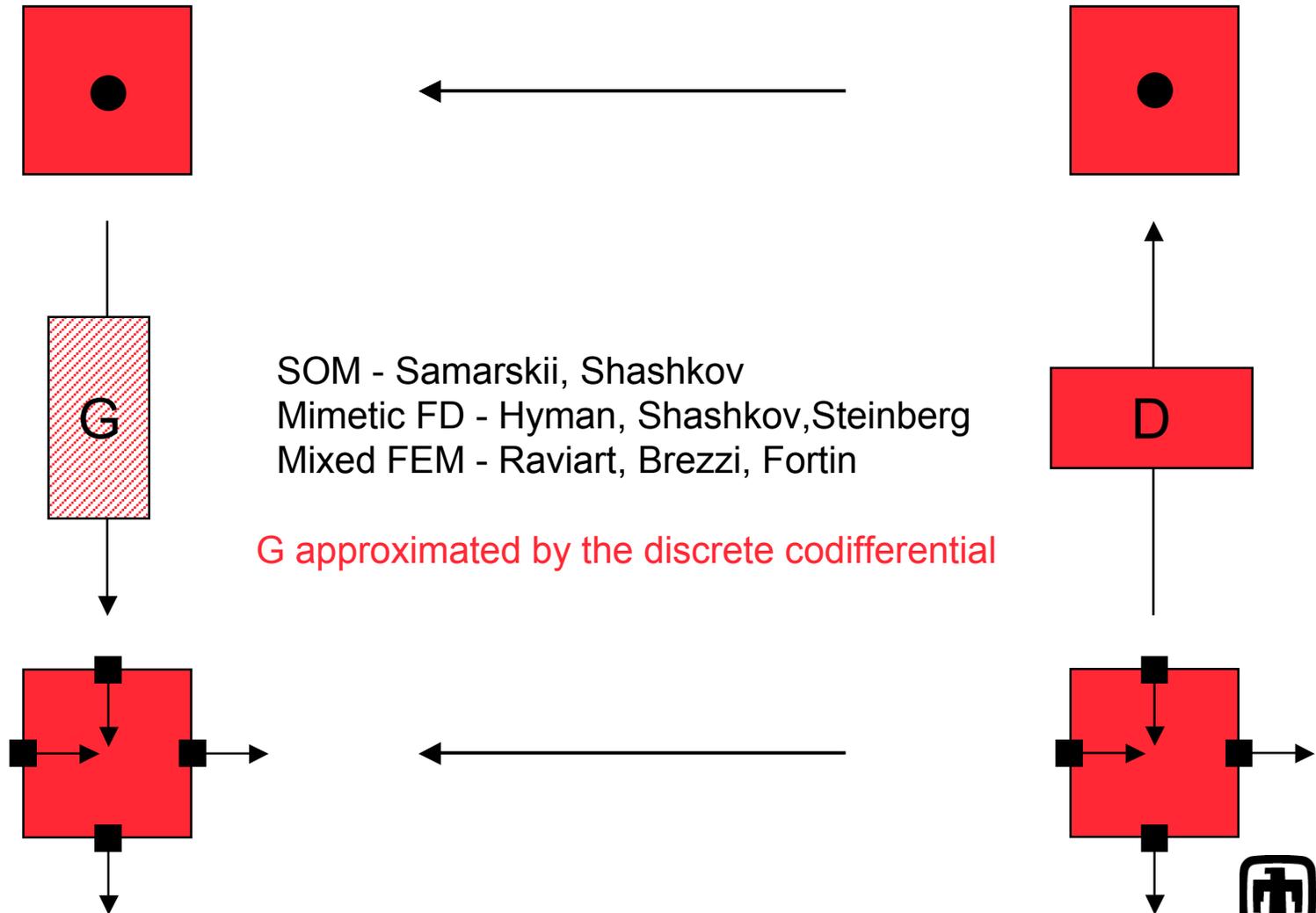
Not always feasible

Topologically dual grids hard to maintain for unstructured meshes such as arising in ALE computations





Solution #2: cheat cleverly





So what went wrong earlier?



1. We used the same discrete representation for **all (!)** fields which was **incompatible** with their physical **meaning** and their **places** in the **domain** and the **range** of the gradient and divergence operators





The loss of coexistence

In the continuum world line and surface fields **can coexist** at the same point in space:

⇒ Only one vector field can be used in the model

⇒ The other can be eliminated:

$$\begin{array}{l} \nabla \cdot \mathbf{v} = 0 \\ \mathbf{u} + \nabla p = 0 \\ \mathbf{v} - \rho \mathbf{u} = 0 \end{array} \quad \longrightarrow \quad \mathbf{v} = \rho \mathbf{u} \quad \longrightarrow \quad \begin{array}{l} \nabla \cdot \rho \mathbf{u} = 0 \\ \mathbf{u} + \nabla p = 0 \end{array}$$

Unfortunately, in the discrete world line and surface fields **cannot coexist** at the same grid location

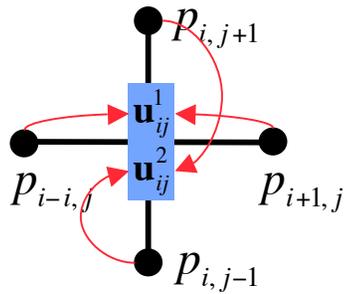
⇒ Either both types must be retained (requires primal-dual grid)

⇒ Or one of the operators must be modified



Collocated discrete operators can't work properly!

Discrete gradient



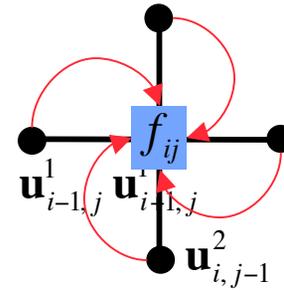
node → node

Adjoint of discrete divergence not boundary

$$\int_{\Omega} \nabla \cdot \mathbf{v} = \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{v}$$

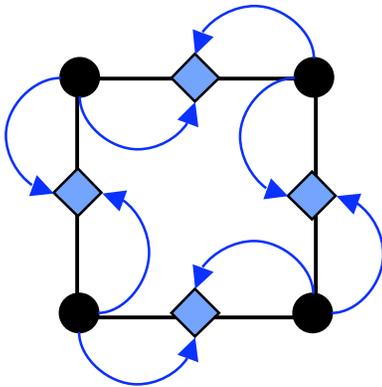
Non-conservative method

Discrete divergence



node → node

node → edge

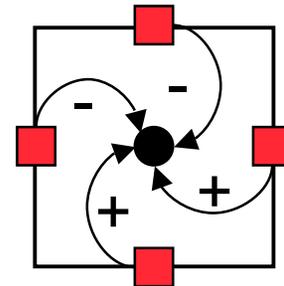


Adjoint of discrete divergence is boundary

$$\int_{\Omega} \nabla \cdot \mathbf{v} = \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{v}$$

Conservative method

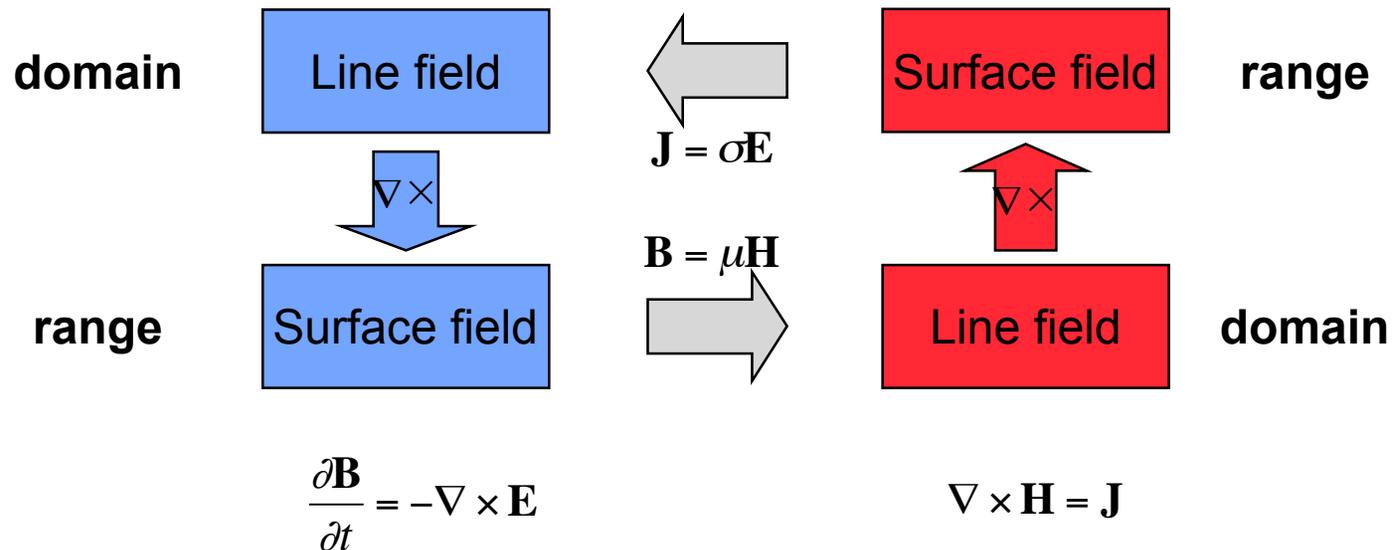
face → center





Is this stuff useful in other cases?

Many other important models have identical duality structure



E & J provide dual description of electric phenomena
B & H provide dual description of magnetic phenomena
Curl is self-adjoint.



Part III

The afternoon talk:

- The formal math behind compatible discretizations
- A fresh look at least-squares principles

Bonus

The origin of "mimetic" revealed!!

Eds. D. Arnold, M. Shashkov

<http://www.ima.umn.edu/talks/workshops/5-11-15.2004>



A heads up: what is a derivative?

1-dimension: it is a velocity

n-dimensions: two possible viewpoints

“Vector calculus”

Based on the idea of **approximation** of a mapping by a linear function

– **Derivative = differential** (slope) of the linear map

$$F(x) = F(x_0) + dF(x_0)(x - x_0) + o(x^2)$$

– Coordinate & metric **dependent**.

“Exterior calculus”

Based on the idea of **duality** between sections of Λ^r bundles and r -manifolds

– **Derivative = adjoint** of the boundary operator

$$\langle dF, \Omega \rangle = \langle F, \partial\Omega \rangle$$

– Coordinate & metric **independent**.



Differential geometry

Compatible discretization:

algebraic equations that describe “actual” physical systems.

Requires to discover structure and invariants of physical systems and then copy them to a discrete system

- Fields are observed **indirectly** by measuring **global** quantities (flux, circulation, etc)
- Physical laws are **relationships** between **global** quantities (conservation, equilibrium)

Differential forms provide the tools to **encode** such relationships

- **Integration:** an abstraction of the *measurement* process
- **Differentiation:** equality of *mixed partials* gives rise to *local invariants*
- **Poincare Lemma:** expresses *local geometric* relations
- **Stokes Theorem:** expresses *global relations* (differentiation + integration)



Algebraic topology

Algebraic topology provides the tools to **copy** the structure

1. System states are **differential forms** reduced to **co-chains**
2. Exterior **differentiation** approximated by the **co-boundary** operator
3. **Dual** operators defined using **Hodge** * operator

Branin (1966), Dodzuik (1976), Hyman & Scovel (1988-92), Mattiussi (1997), Teixeira (2001)

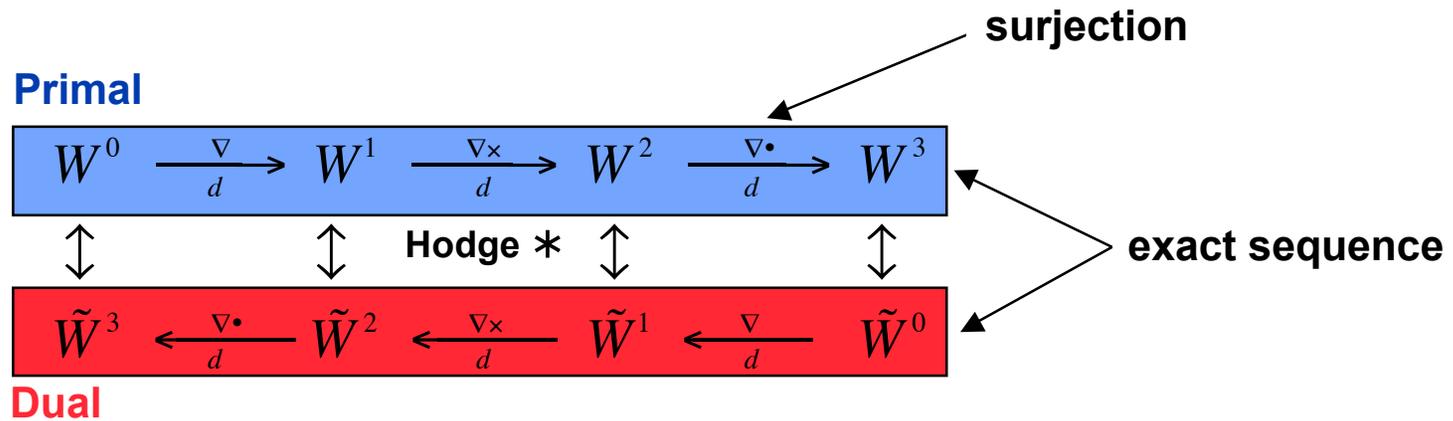
Mimetic and co-volume methods fit this reduction model

- **Vector fields** represented by their integrals (fluxes or circulations)
- **Differential operators** defined via Stokes Theorem (coordinate-invariant)
- **Primal and dual** equations/operators (B and B^T) and an inner product (A)



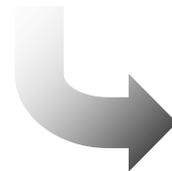
The Formal Math: Differential Complexes

De Rham Cohomology



Exactness: $dd = 0$

Poincare Lemma $d\omega^k = 0 \Rightarrow \omega^k = d\omega^{k-1}$



Existence of potentials:

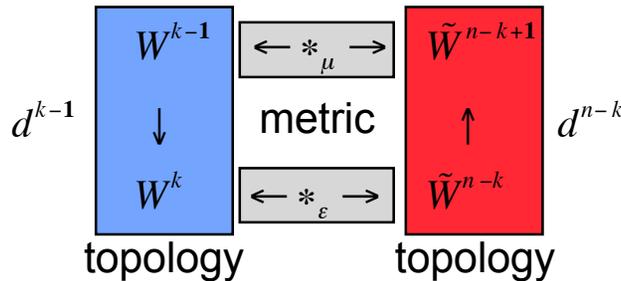
$$\begin{aligned} \nabla \psi = 0 &\Rightarrow \psi = Const \\ \nabla \times \mathbf{E} = 0 &\Rightarrow \mathbf{E} = \nabla \varphi \\ \nabla \cdot \mathbf{B} = 0 &\Rightarrow \mathbf{B} = \nabla \times \mathbf{A} \end{aligned}$$



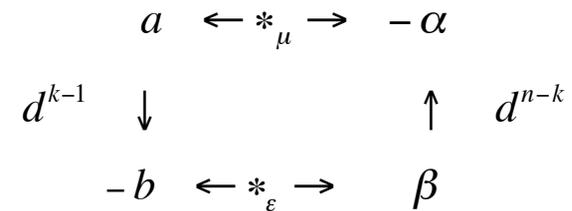
Tonti (1974), Bossavit (1989), Hiptmair (2000)

Factorization Diagrams

Factorization diagram



“All” 2nd order PDE’s



We used
k=1

Primal	Hodge operator		Dual
0-form ϕ	\leftarrow	$\psi = * \phi$	\rightarrow 3-form
$d^0 \rightarrow$	∇		$\nabla \cdot$ $\leftarrow d^2$
1-form $-u$	\leftarrow	$q = * u$	\rightarrow 2-form

Equilibrium

$$-u = \nabla \phi \quad \& \quad \nabla \cdot q = -\gamma \psi$$

$$\phi \in W^0 \quad \psi \in \tilde{W}^3$$

Constitutive

$$\psi = * \phi \quad \& \quad q = * u$$

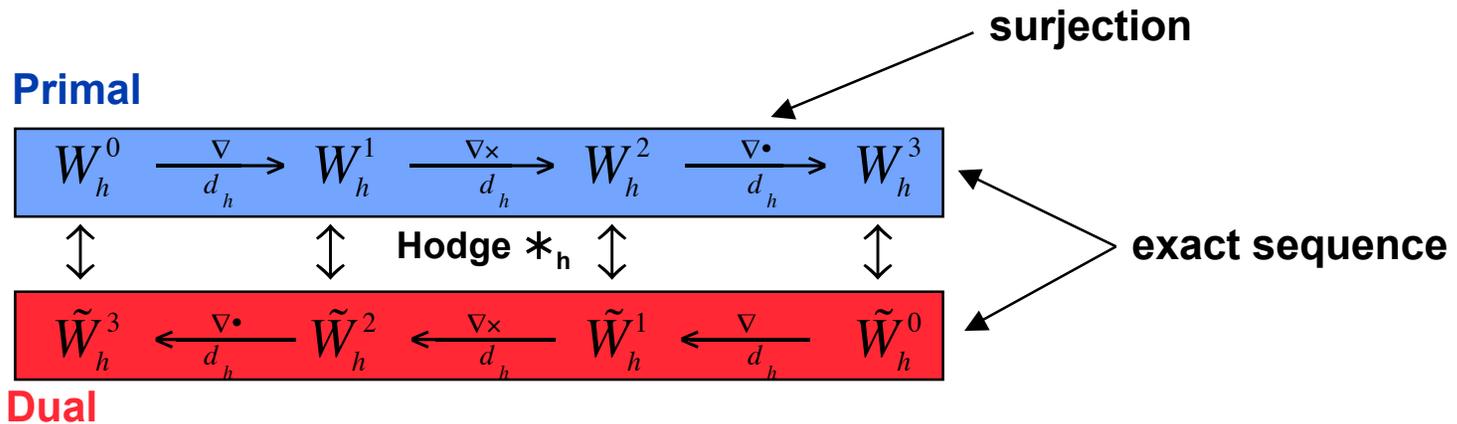
$$u \in W^1 \quad q \in \tilde{W}^2$$

Note that $q \in W^2 \Rightarrow d^1 q$ (i.e. $\nabla \times q$) not meaningful!



Discrete Differential Complexes

Discrete De Rham complex



Discrete Exactness: $d_h d_h = 0$

Poincare Lemma $d_h \omega_h^k = 0 \Rightarrow \omega_h^k = d_h \omega_h^{k-1}$



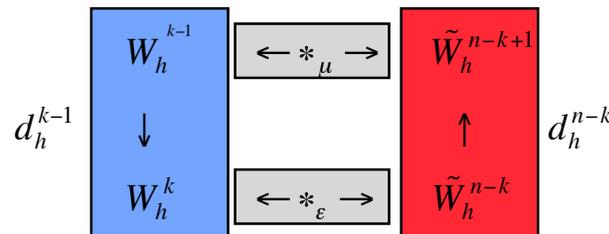
Existence of potentials:

$$\begin{aligned}
 G \psi_h = 0 &\Rightarrow \psi_h = Const \\
 C \mathbf{E}_h = 0 &\Rightarrow \mathbf{E}_h = G \varphi_h \\
 D \mathbf{B}_h = 0 &\Rightarrow \mathbf{B}_h = C \mathbf{A}_h
 \end{aligned}$$



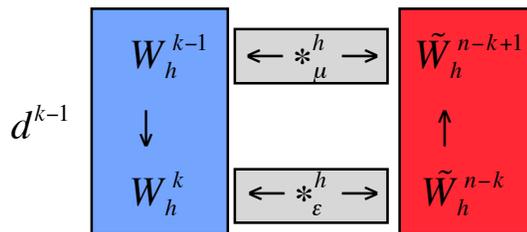
Where are the Compatible Methods?

Discrete Factorization diagram



Tonti (1974)
 Bossavit (1989)
 Mattiussi (1997)
 Teixeira (1999)
 Hiptmair (2000)

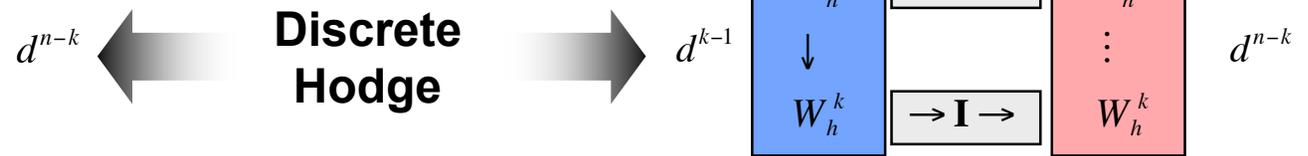
Primal-dual



Typical: co-volume, FV

- Use **topologically dual** grids
- **2 equilibrium** relations → exact
- **2 constitutive** relations → exact

Elimination



Typical: FEM, Mimetic FD

- Use **single grid**
- **1 equilibrium** relation → exact
- **2 constitutive** relation → exact

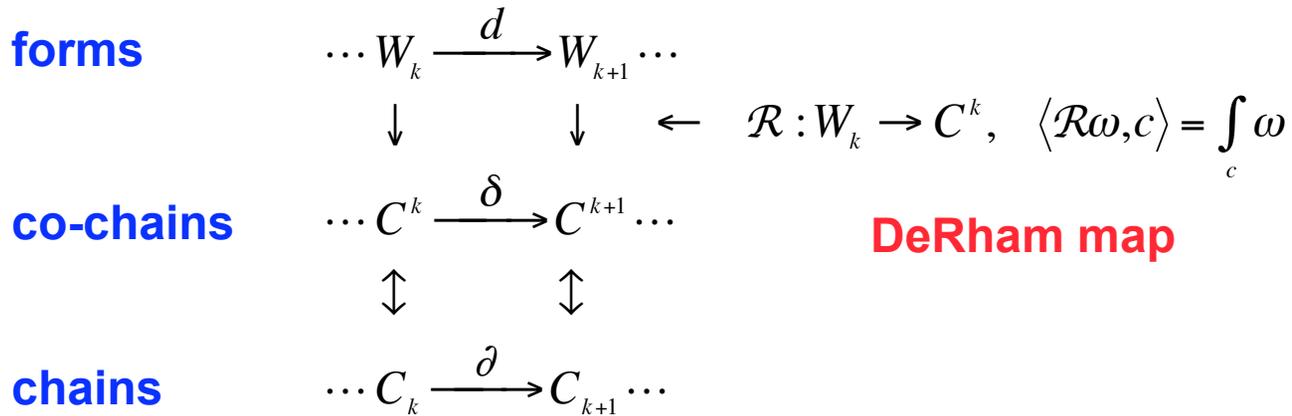
Discrete
Hodge



Algebraic Topology Approach

1. System reduction

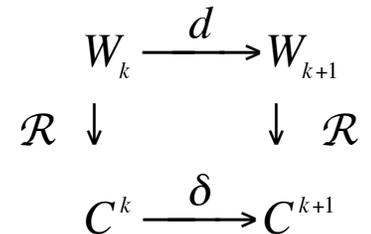
3 exact sequences: $(W_0, W_1, W_2, W_3), (C_0, C_1, C_2, C_3), (C^0, C^1, C^2, C^3)$



Fundamental property: $\mathcal{R}d = \delta\mathcal{R}$

$$\langle \delta\mathcal{R}\omega, c \rangle = \langle \mathcal{R}\omega, \partial c \rangle = \int_{\partial c} \omega = \int_c d\omega = \langle \mathcal{R}d\omega, c \rangle$$

Commuting Diagram I



$\{G, D, C\} \leftarrow \delta \text{ approximates } d \rightarrow \{\text{grad, curl, div}\}$



Algebraic Topology Approach

2. Inner products and dual operators

Inner product $W_k \times W_k$

$$*: W_k \rightarrow W_{n-k} \quad (\omega, \varphi)_W = \int_{\Omega} \omega \wedge * \varphi$$

Inner product $C^k \times C^k$

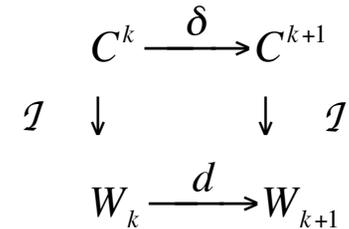
$$\mathcal{I}: C^k \rightarrow W_k \quad (a, b)_c = (\mathcal{I}a, \mathcal{I}b) = \int_{\Omega} \mathcal{I}a \wedge * \mathcal{I}b = \mathbf{a}^T \mathbf{M} \mathbf{b}$$

Dual operators

$$(\delta a, b)_c = (a, \delta^* b) \quad \rightarrow \quad \mathbf{G}^*, \mathbf{C}^*, \mathbf{D}^*$$

$\mathbf{C}^* \mathbf{G}^* = \mathbf{D}^* \mathbf{C}^* = 0$ requires $d\mathcal{I} = \mathcal{I}\delta$

Commuting Diagram II





Algebraic Topology Framework: Summary

1. Structures:

(W_0, W_1, W_2, W_3)	Forms
(C_0, C_1, C_2, C_3)	Chains
(C^0, C^1, C^2, C^3)	Co-chains

2. De Rham map

$$\mathcal{R} : W_k \rightarrow C^k \quad \mathcal{R}d = \delta\mathcal{R}$$

3. Interpolation operator

$$\mathcal{I} : C^k \rightarrow W_k \quad d\mathcal{I} = \mathcal{I}\delta$$

4. Inner product

$$(a, b)_c = (\mathcal{I}a, \mathcal{I}b) \quad \mathbf{M}$$

5. Primal and dual operators

$$\{G, C, D\} \text{ \& \} \{G^*, C^*, D^*\}$$

Geometric compatibility

$W_k \xrightarrow{d} W_{k+1}$	
$\mathcal{R} \downarrow$	$\downarrow \mathcal{R}$
$C^k \xrightarrow{\delta} C^{k+1}$	CDP 1
$C^k \xrightarrow{\delta} C^{k+1}$	
$\mathcal{I} \downarrow$	$\downarrow \mathcal{I}$
$W_k \xrightarrow{d} W_{k+1}$	CDP 2



What does geometric compatibility buy you?

$$\begin{aligned} \text{Co-cycles of } (W_0, W_1, W_2, W_3) &\xrightarrow{\mathcal{R}} \text{co-cycles of } (C^0, C^1, C^2, C^3) \\ d\omega = 0 &\Rightarrow \delta\mathcal{R}\omega = 0 \end{aligned}$$

Discrete Poincare lemma (existence of potentials in contractible domains)

$$d\omega_k = 0 \Rightarrow \omega_k = d\omega_{k+1} \qquad \delta c^k = 0 \Rightarrow c^k = \delta c^{k+1}$$

Discrete Stokes Theorem

$$\langle d\omega_{k-1}, c_k \rangle = \langle \omega_{k-1}, \partial c_k \rangle \qquad \langle \delta c^{k-1}, c_k \rangle = \langle c^{k-1}, \partial c_k \rangle$$

Discrete “Vector Calculus”

$$dd = 0 \qquad \delta\delta = 0 \rightarrow CG = DC = 0; C^*G^* = D^*C^* = 0$$

Any feature of the continuum system that is implied by differential forms calculus is inherited by the discrete model

Called *mimetic* property by Hyman and Scovel (1988)



Conclusions

- Discretization is a **model reduction**
- Careless discretization causes **unphysical behavior**
- Compatible discretizations **mimic** continuum structures
- Differential geometry provides the **tools to encode** this structure
- Algebraic topology provides the **tools to copy** the structure to discrete models
- Cheating is possible but requires “**stabilization**”, some or all conservative properties are lost.

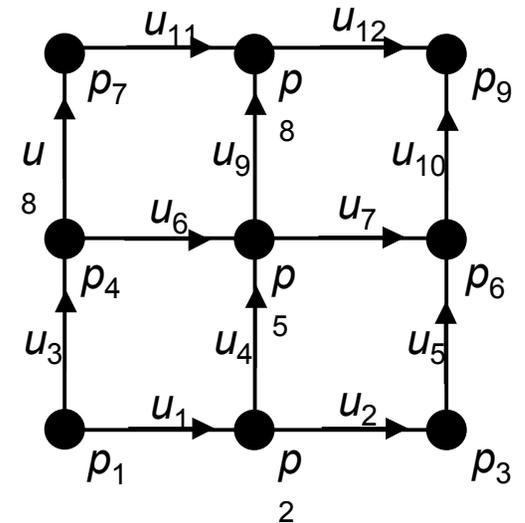


Network Equations

Equilibrium conditions

Force	← concept →	source
$u_1 = p_2 - p_1$	Constitutive equation	$-v_1 - v_3 = 0$ $+v_1 - v_2 - v_4 = 0$ $+v_2 - v_5 = 0$ $+v_3 - v_6 - v_8 = 0$ $+v_4 + v_6 - v_7 - v_9 = 0$ $+v_7 + v_5 - v_{10} = 0$ $+v_8 - v_{11} = 0$ $+v_9 + v_{11} - v_{12} = 0$ $+v_{10} + v_{12} = 0$
$u_2 = p_3 - p_2$		
$u_3 = p_4 - p_1$		
$u_4 = p_5 - p_2$		
$u_5 = p_6 - p_3$		
$u_6 = p_5 - p_4$		
$u_7 = p_6 - p_5$		
$u_8 = p_7 - p_4$		
$u_9 = p_8 - p_5$		
$u_{10} = p_9 - p_6$		
$u_{11} = p_8 - p_7$		
$u_{12} = p_9 - p_8$		

$$v_i = \rho_i u_i$$



$p \rightarrow$ "pressure"

$u \rightarrow$ "velocity"

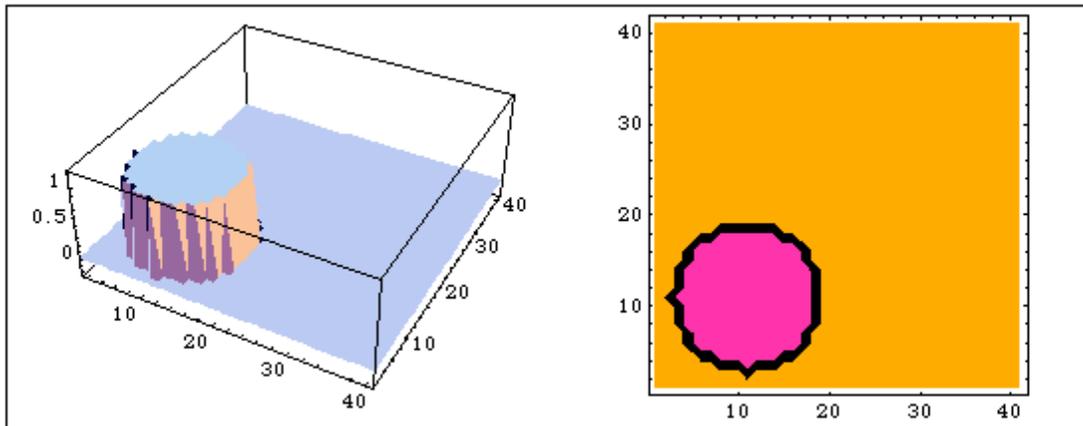
$\rho \rightarrow$ "density"

$v \rightarrow$ "flow"



Further examples of incompatibility

Courant Number = 0.012, Pe=Infinity



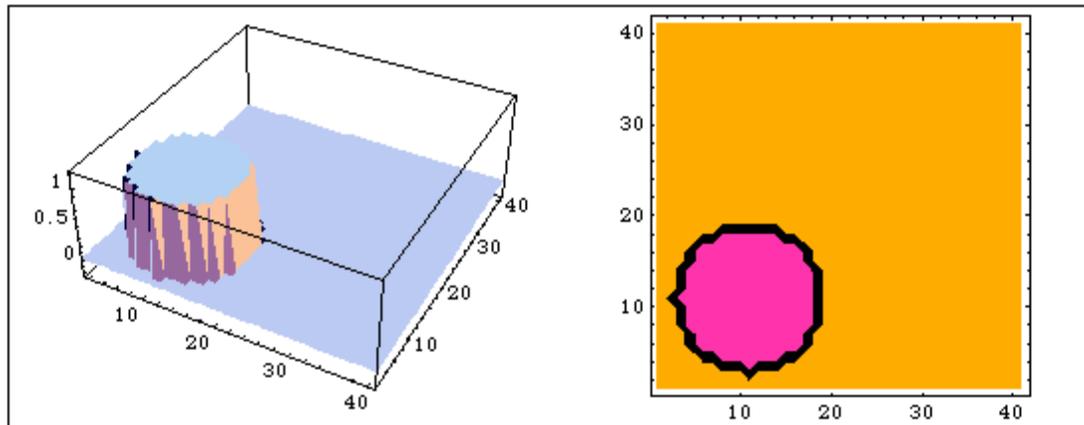
Galerkin

Advection of a scalar quantity

$$\nabla \cdot (\mathbf{a}\psi) = f$$

An extremely simplified case of a transport problem

Courant Number = 0.012, Pe=11.517



Adjoint Stabilized Galerkin

Seemingly reasonable fixes can make things even worse.