SAND2008-7506P

Principles of compatible discretizations

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RWTH Aachen, November 12th, 2008

Chair for Computational Analysis of Technical Systems

Supported in part by

Office of Science
U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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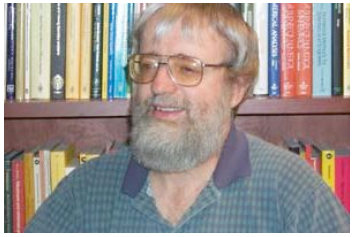
Part I

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

Collaborators

Max Gunzburger
Florida State University
Tallahassee



Misha Shashkov
Los Alamos National Laboratory

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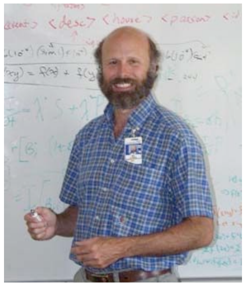
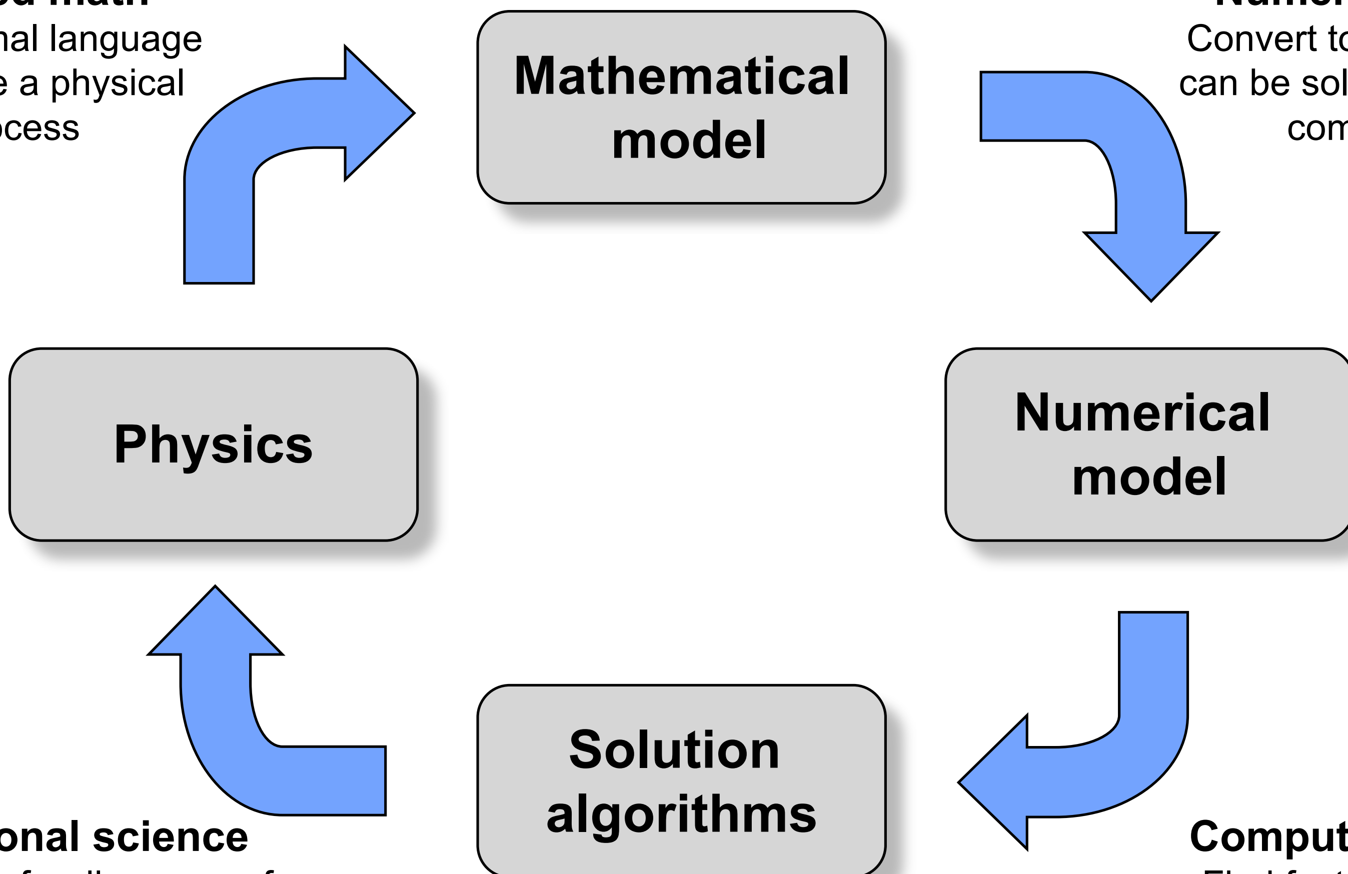
Los Alamos National Laboratory



What is this talk about?

Applied math
Use a formal language to encode a physical process

Numerical math
Convert to models that can be solved on digital computers



Computational science
Use computers for discovery of new physics, design validation, proof of concept, virtual prototyping

Computer science
Find faster and more efficient ways to solve numerical models

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 $h \to 0$?
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

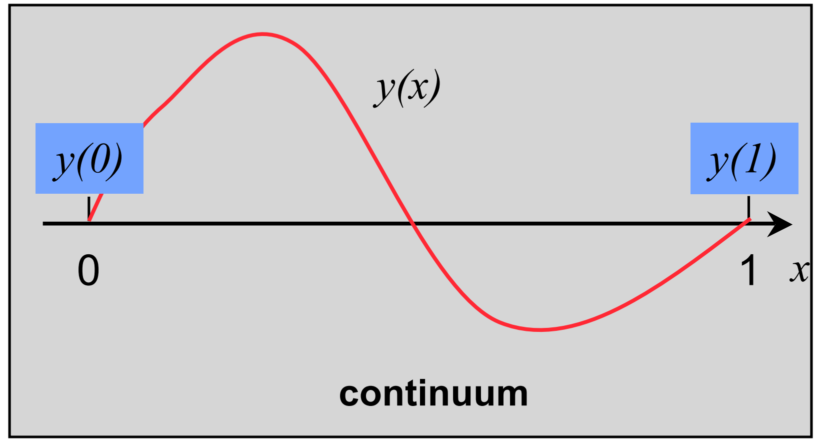
$$-ay'' + by' + cy = f \quad \text{in} \quad (0,1)$$
$$y(0) = y(1) = 0$$

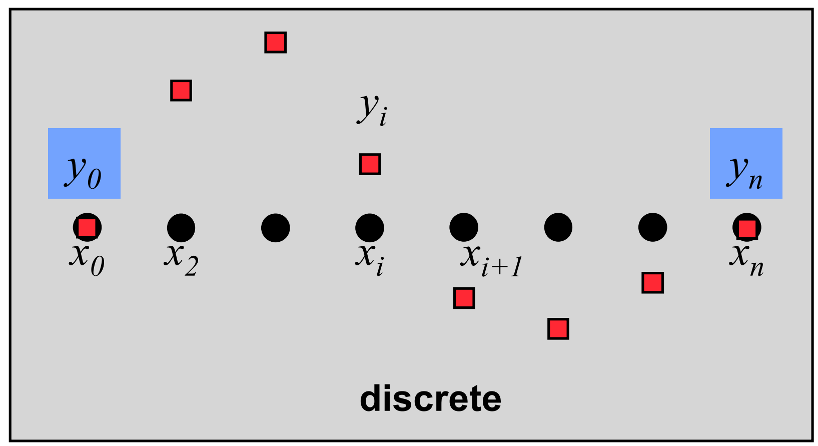
$$y''(x_i) \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

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

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

Parameterized linear system





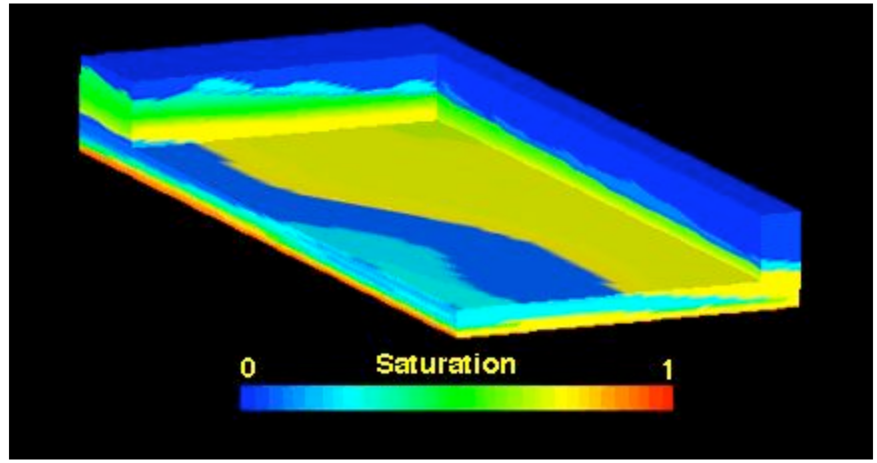
Porous Media Flow

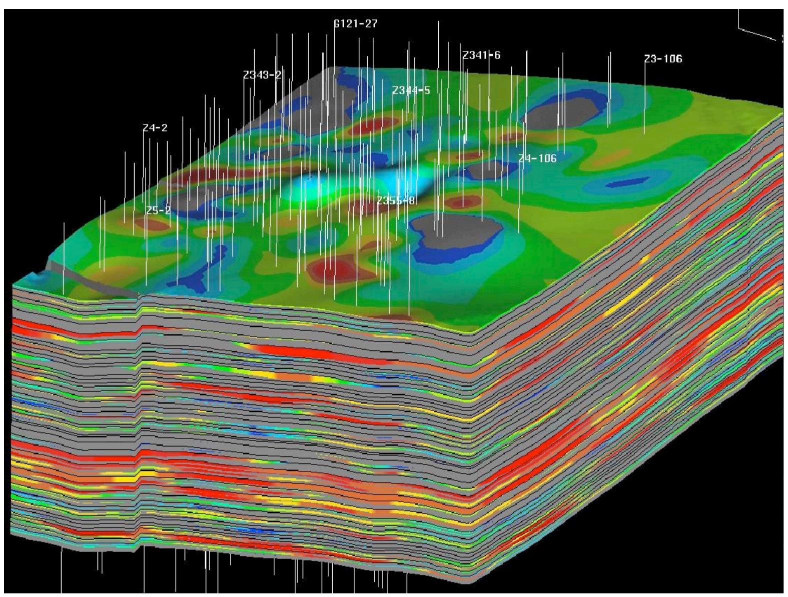
Boundary value problem

$$-\nabla \cdot \rho \nabla p = f \text{ in } \Omega$$

$$p = 0 \text{ on } \Gamma$$

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***

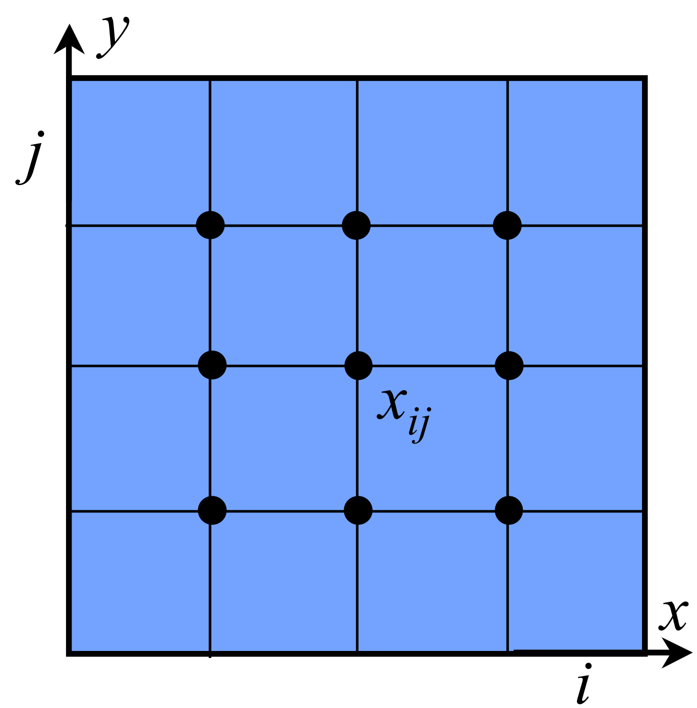
Darcy problem

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

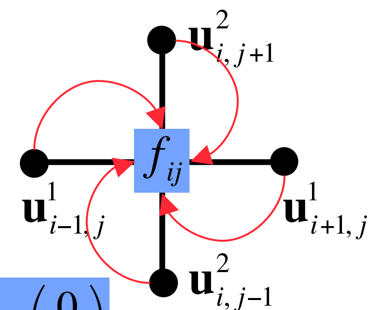
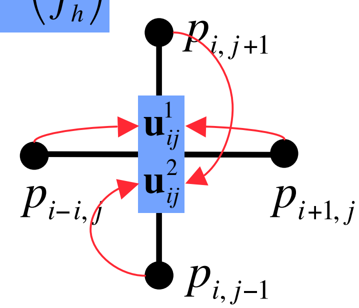
Equivalent 1st order form

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

Discretized domain



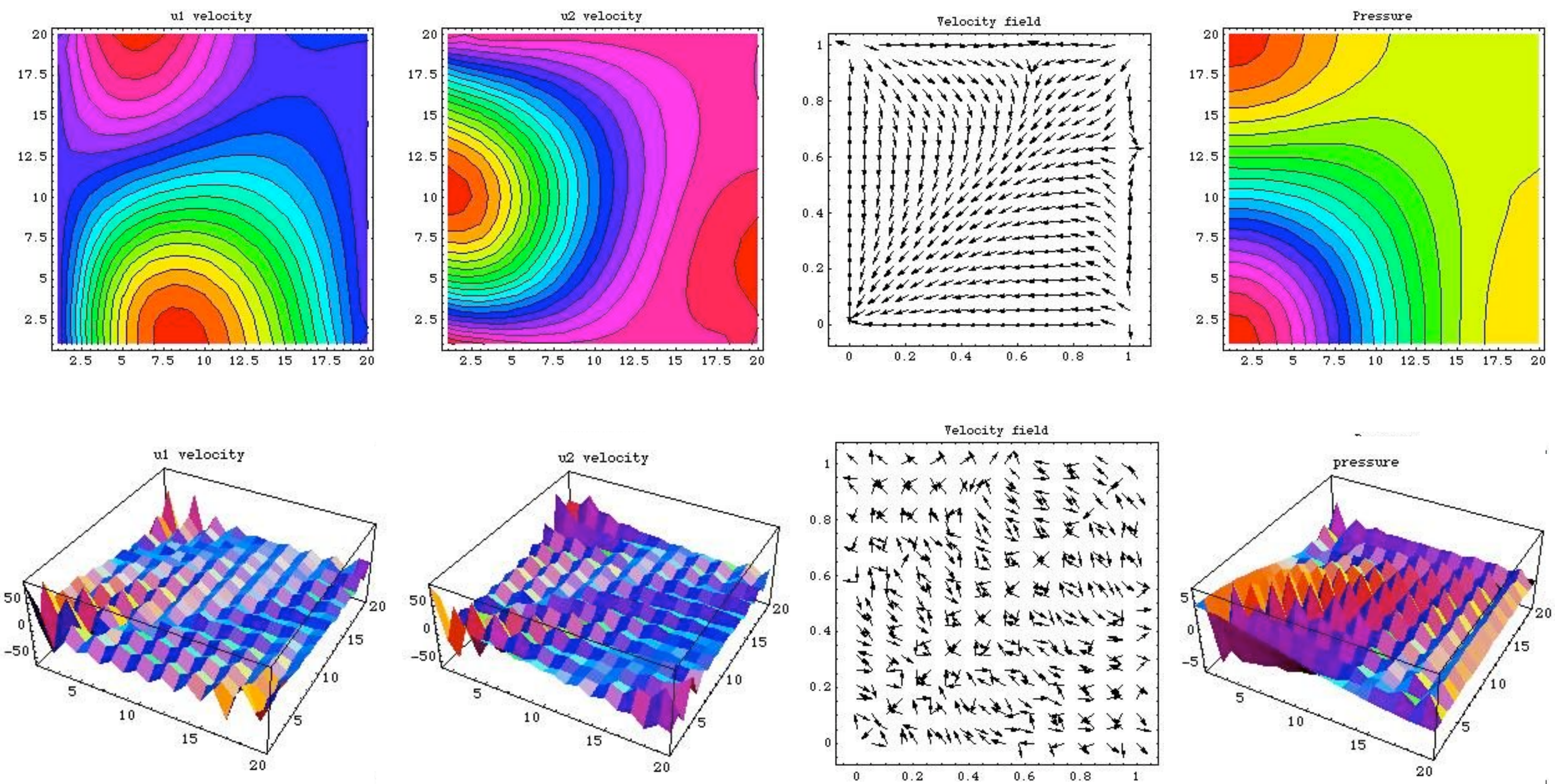
PDE→Parameterized Linear System

Continuum	Discrete	Stencil
$\nabla \cdot \rho \mathbf{u} \equiv \mathbf{u}_x^1 + \mathbf{u}_y^2 = f$	$\dfrac{\mathbf{u}_{i+1,j}^1 - \mathbf{u}_{i-1,j}^1}{2h} + \dfrac{\mathbf{u}_{i,j+1}^2 - \mathbf{u}_{i,j-1}^2}{2h} = f_{ij}$	
$\left.\begin{matrix} \mathbf{u} + \nabla p = 0 \\ \nabla \cdot \mathbf{u} = f \end{matrix}\right\} \rightarrow$	$\left\{\begin{matrix} A_h \mathbf{u}_h + B_h^T p_h = 0 \\ B_h \mathbf{u}_h = f_h \end{matrix}\right. \rightarrow$	$\begin{pmatrix} A_h & B_h^T \\ B_h & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u}_h \\ p_h \end{pmatrix} = \begin{pmatrix} 0 \\ f_h \end{pmatrix}$
$\mathbf{u}^1 + p_x = 0$ $\mathbf{u}^2 + p_y = 0$	$\mathbf{u}_{ij}^1 + \dfrac{p_{i+1,j} - p_{i-1,j}}{2h} = 0$ $\mathbf{u}_{ij}^2 + \dfrac{p_{i,j+1} - p_{i,j-1}}{2h} = 0$	

Collocated discretization: variables share **same grid location**

Divergence and **gradient** discretized by the **same stencil**

Computational example



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

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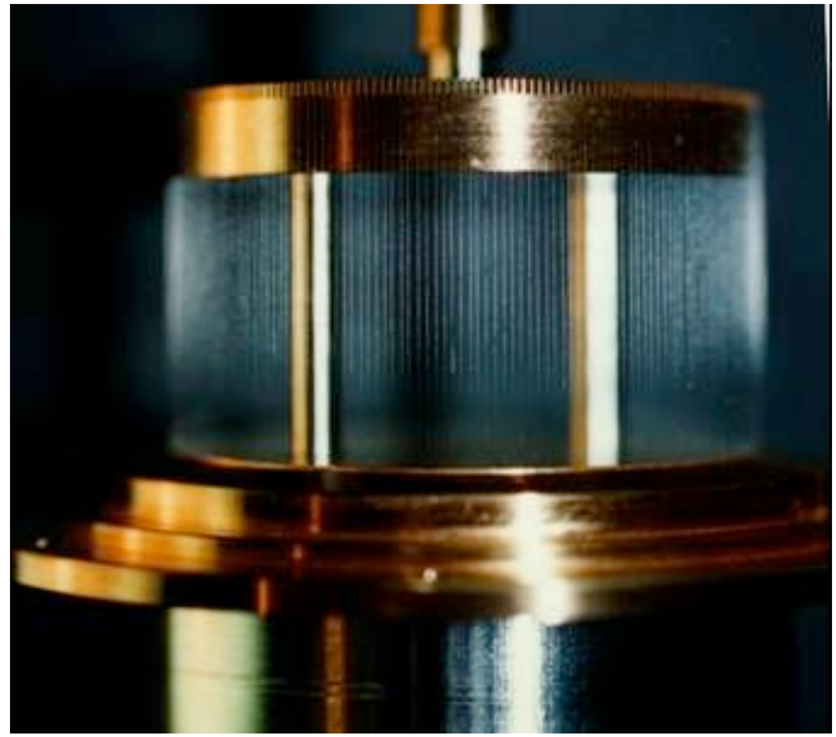
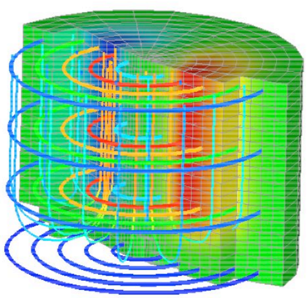
Coupled multiscale, nonlinear physics is even more challenging: Z-Pinch simulation in ALEGRA

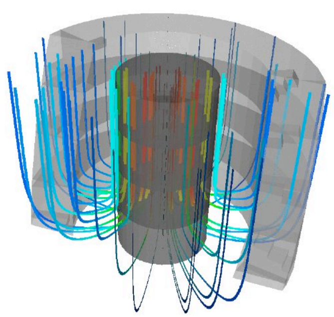


Scales:

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



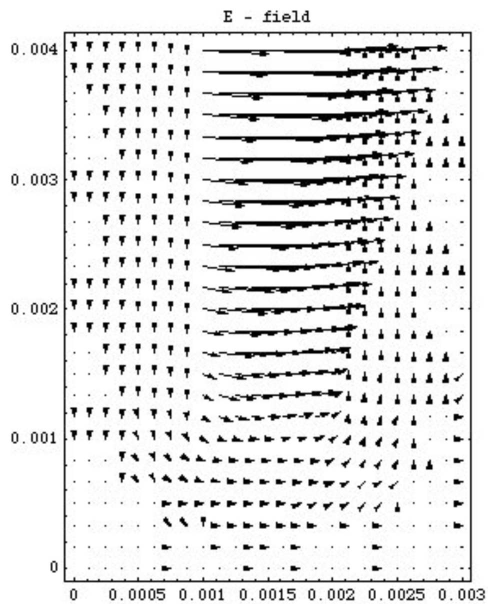


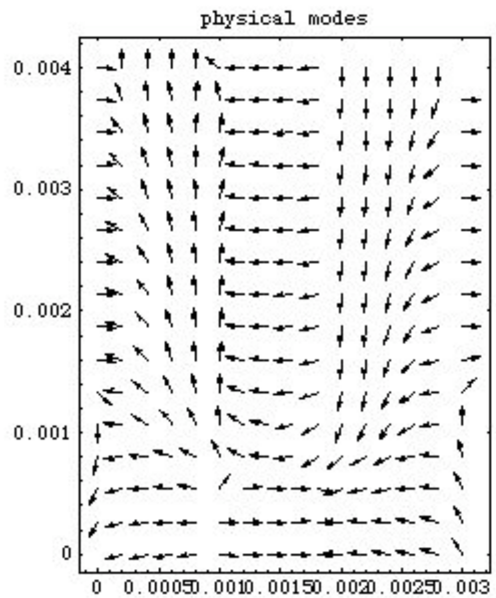
MHD MODEL
=
Hydrodynamics + Magnetic Diffusion

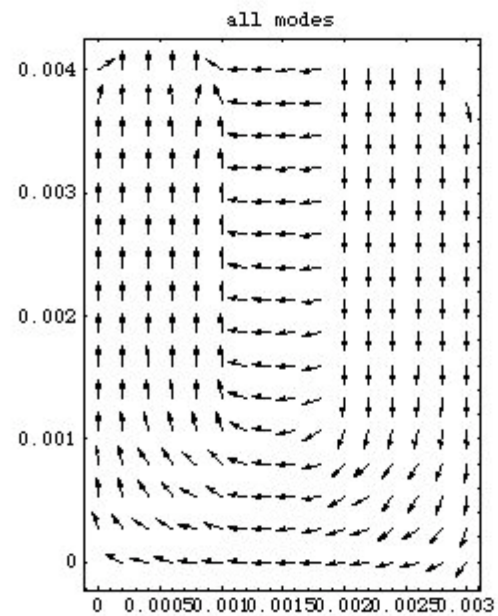
Z-machine: (Ostensibly used by Ocean's 11)

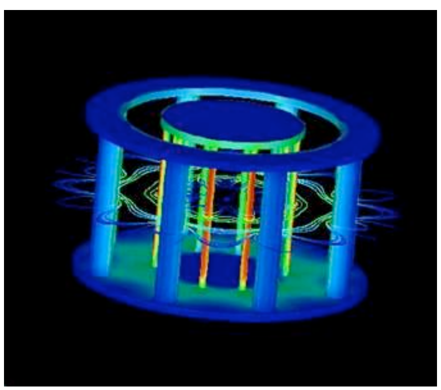
Electric currents are used to produce an ionized gas by vaporizing a spool-of-thread sized array of 100-400 wires of diameter ≈ 10µm

Magnetic diffusion







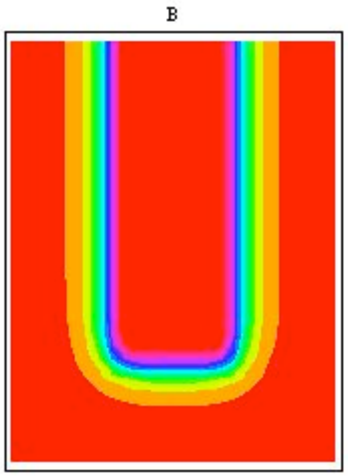


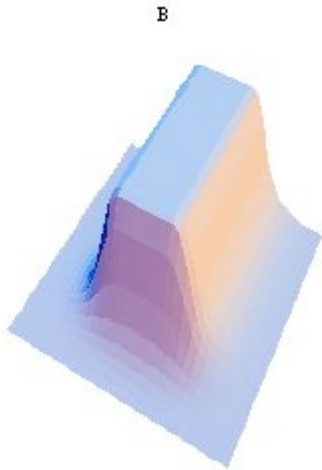
$$\nabla \times \frac{1}{\mu}\mathbf{B} = \sigma\mathbf{E} \quad \text{Ampere}$$

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

Gap modeled as a heterogeneous conductor

Compatible vs. Collocated: B-field



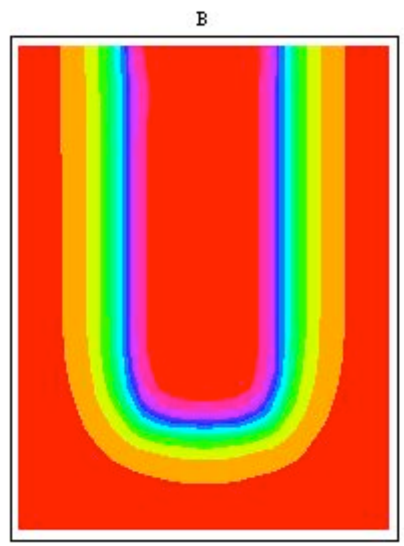


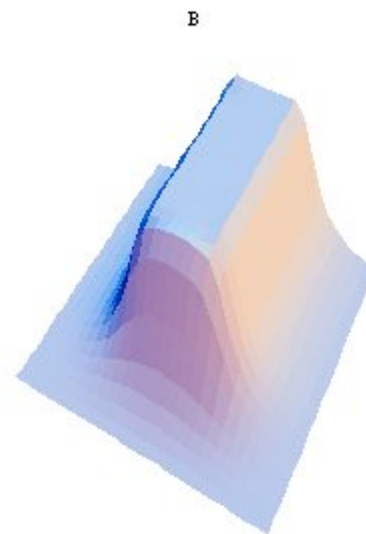
Compatible

Ker(curl)={grad p}

Collocated

Ker(curl)={0}





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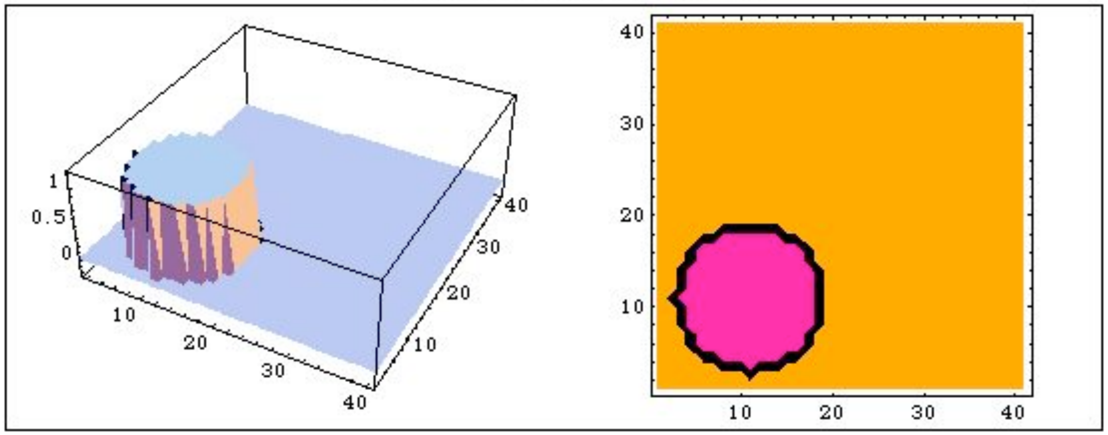
Incompatibility arises in other contexts as well, which are not discussed here!

Courant Number = 0.012, Pe=Infinity



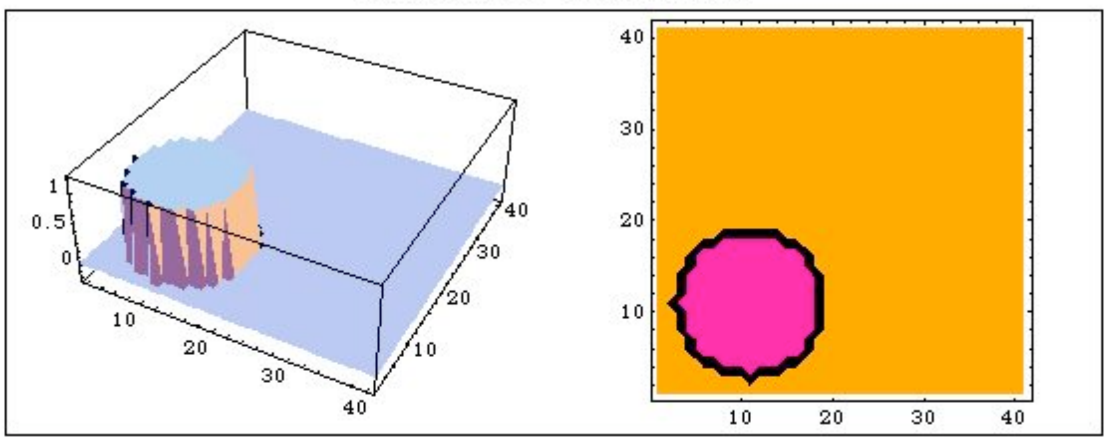
Galerkin

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.

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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**

$\mathbf{a}^T\mathbf{b} \to \langle \mathbf{a},\mathbf{b} \rangle$	Vector **a** dual to *co-vector* **b**
$f(x) \to \langle f, x \rangle$	Function f dual to *its argument* x
$\int_\Omega f \to \langle f, \Omega \rangle$	Function f dual to *integration domain* Ω
$\int_\Omega fg \to \langle f, g \rangle$	Function f dual to *distribution* g
$\langle f \mid g \rangle \to \langle f, g \rangle$	Bra vector f dual to *ket vector* g
$Fd \to \langle F, d \rangle$	Force F dual to *displacement* d

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

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

$\mathbf{b}^T \mathbf{A} \mathbf{a} = \mathbf{a}^T \mathbf{A}^T \mathbf{b}$	$\langle \mathbf{A}\mathbf{a}, \mathbf{b} \rangle = \langle \mathbf{a}, \mathbf{A}^T \mathbf{b} \rangle$	Adjoint of a matrix **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**

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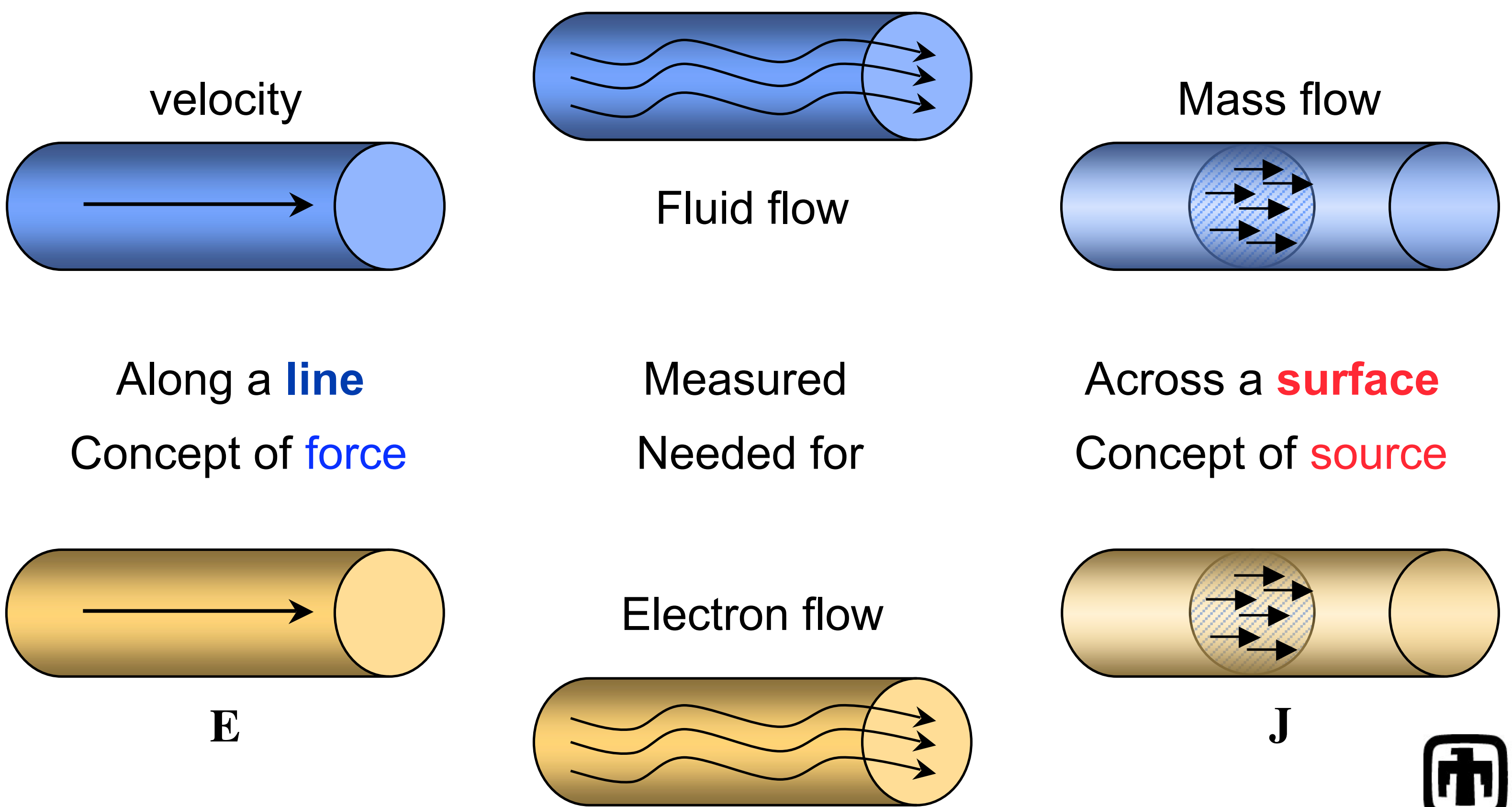
A second duality concept

2. Duality of representations

The process of using complementary descriptions of the same process



Darcy problem deconstructed

Kinematic	Constitutive	Continuity
$\mathbf{u} + \nabla p = 0$	$\mathbf{v} = \rho \mathbf{u}$	$\nabla \cdot \mathbf{v} = 0$

Gradient

Forces

Line field

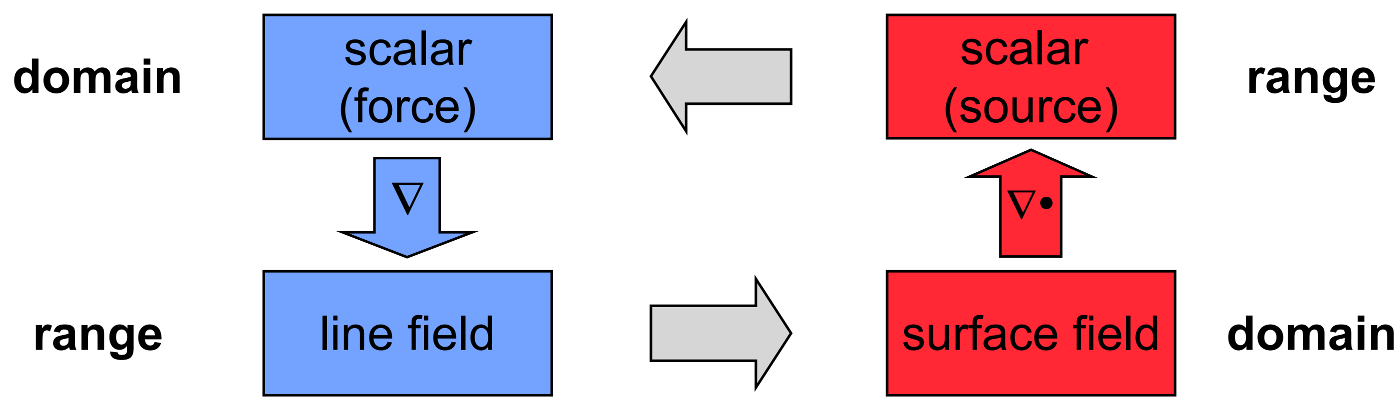
Duality is ubiquitous!

Divergence

Sources

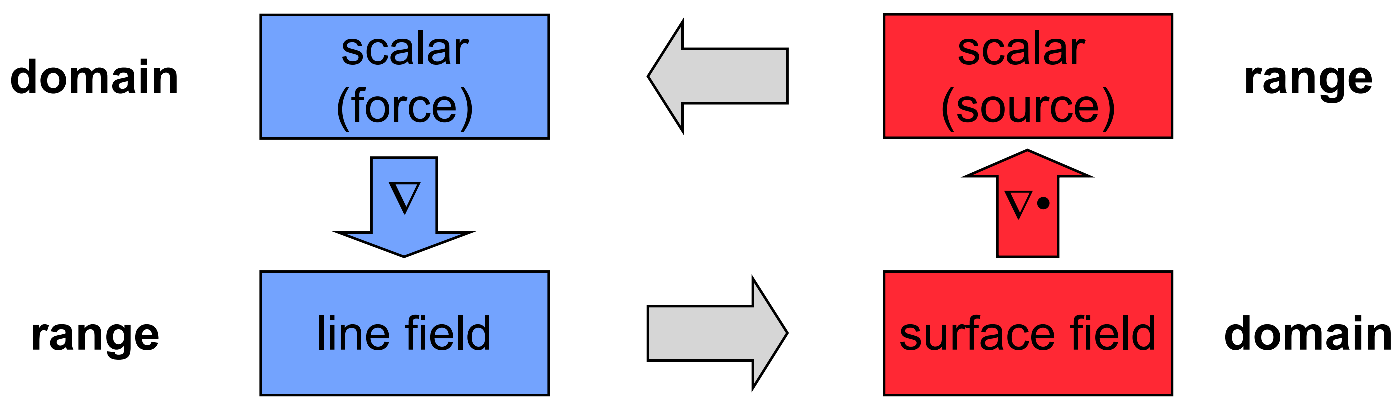
Surface field

Duality structure can be encoded by the following diagram



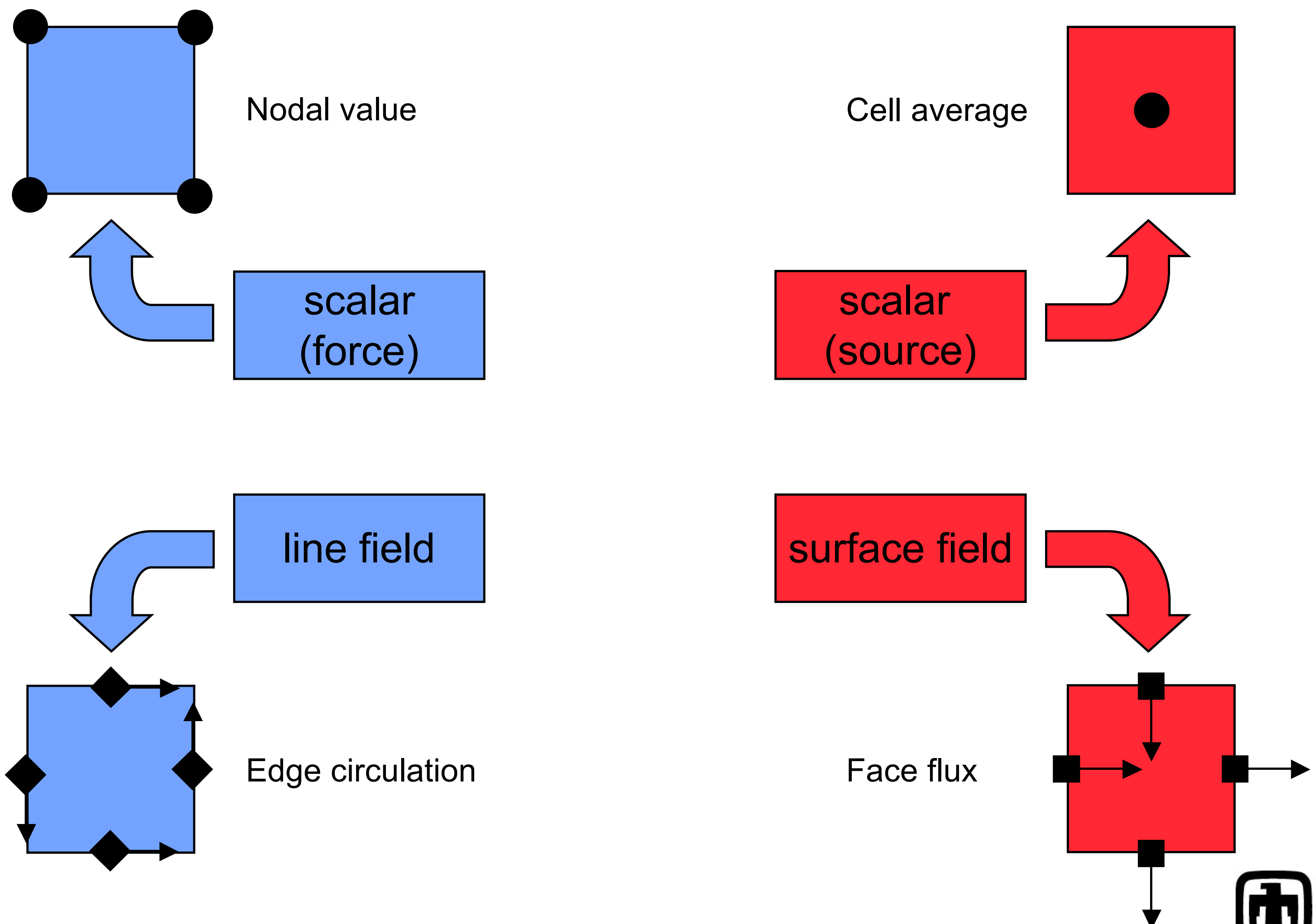
Compatible discretizations

A compatible discretization should mimic the duality structure of the PDE

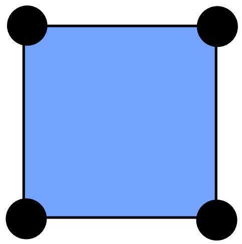


We need to build a discrete analogue of this diagram!

1. Compatible representations

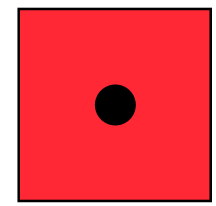


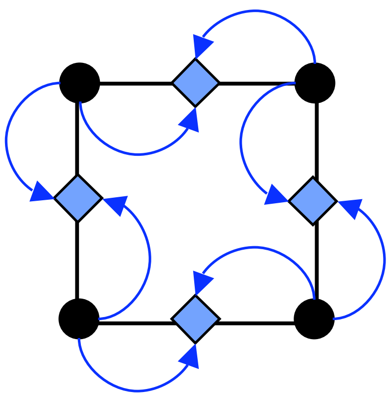
2. Compatible discrete operators



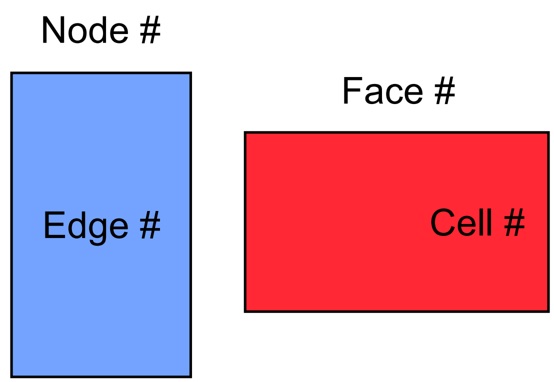
Nodal value

Cell average

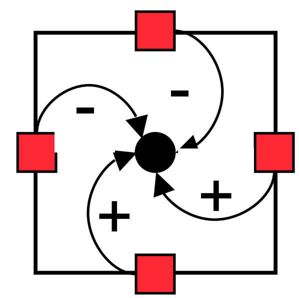


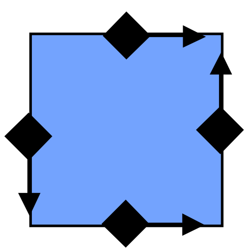


$$\mathbf{G}p = \frac{p_2 - p_1}{h}$$



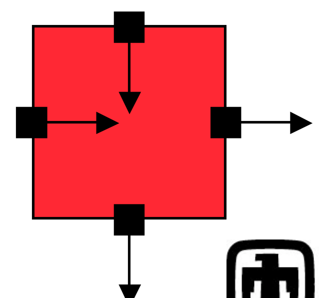
$$\mathbf{Du} = \frac{\Phi_B + \Phi_R - \Phi_T - \Phi_L}{h}$$



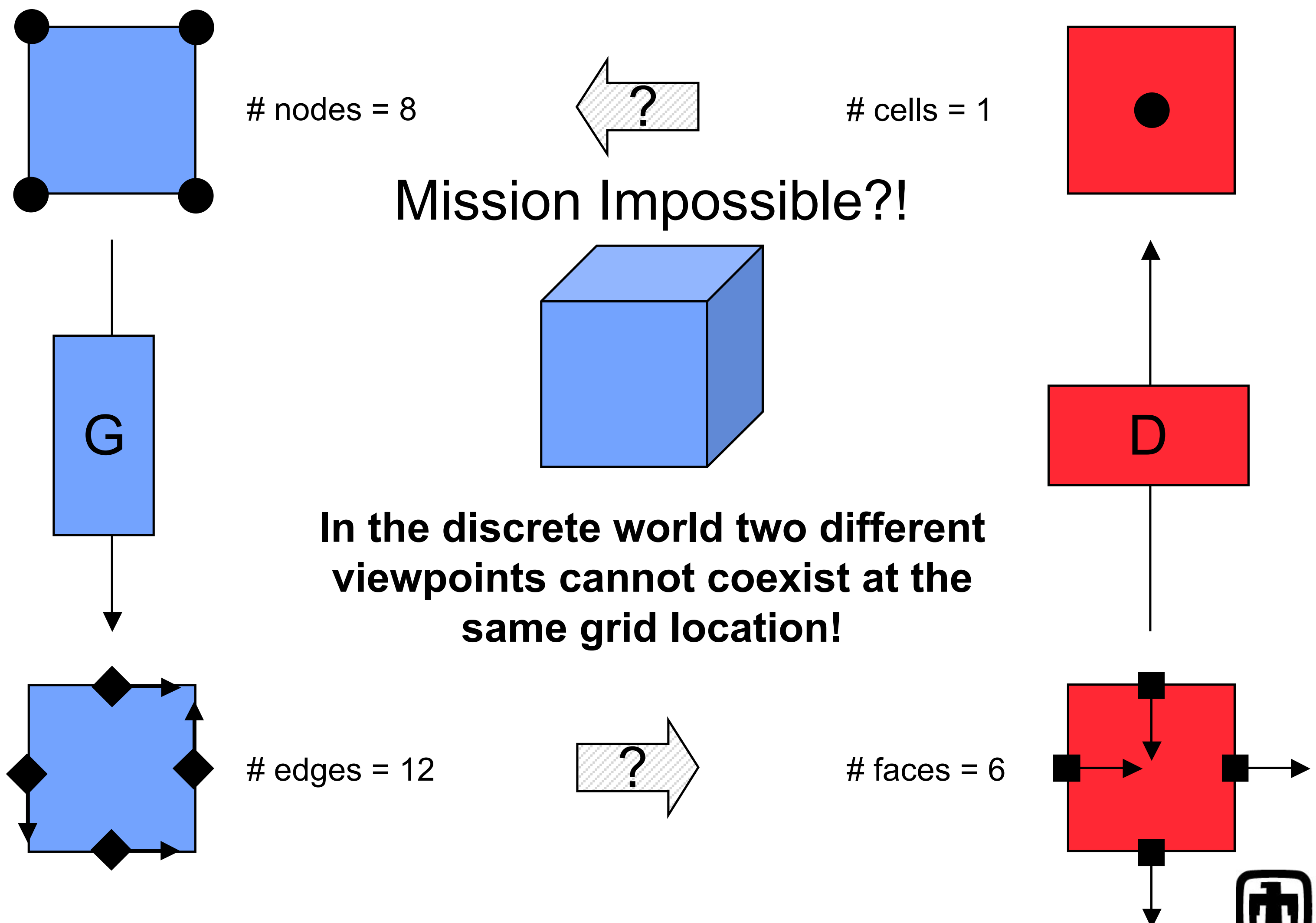


Edge circulation

Face flux

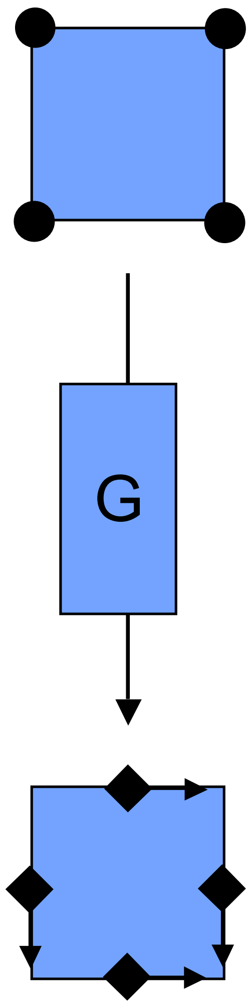


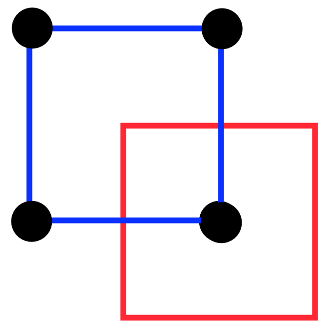
3. Putting it together



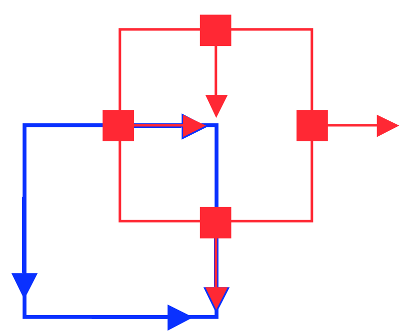
In the discrete world two different viewpoints cannot coexist at the same grid location!

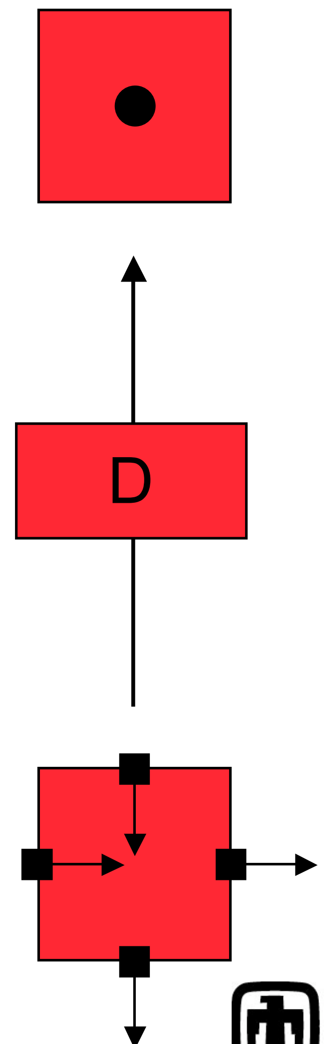
Solution #1 Primal-Dual Grid Complex





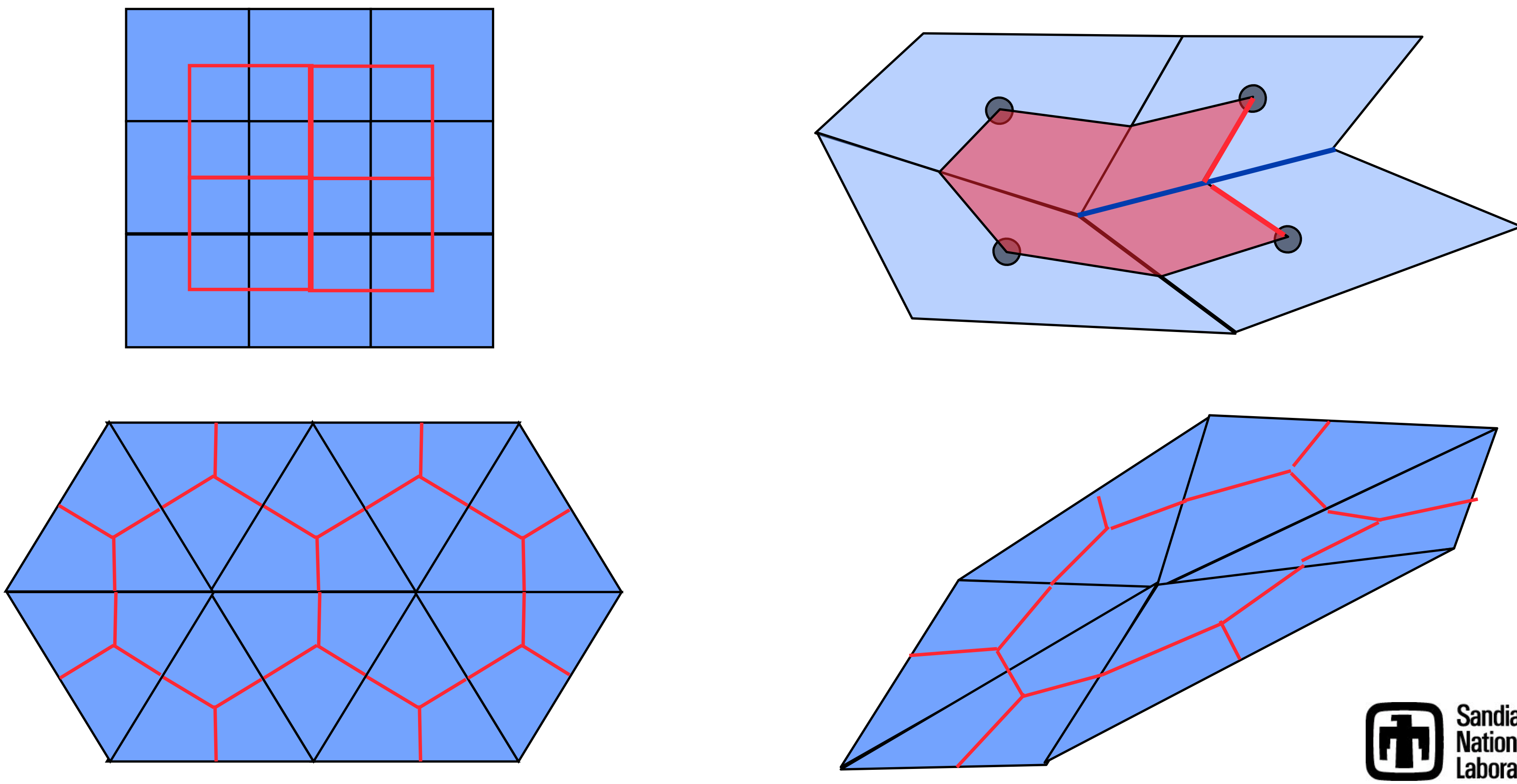
Staggered grid discretizations
Covolume (Delaunay-Voronoi)
Box Integration Method





Not always feasible

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



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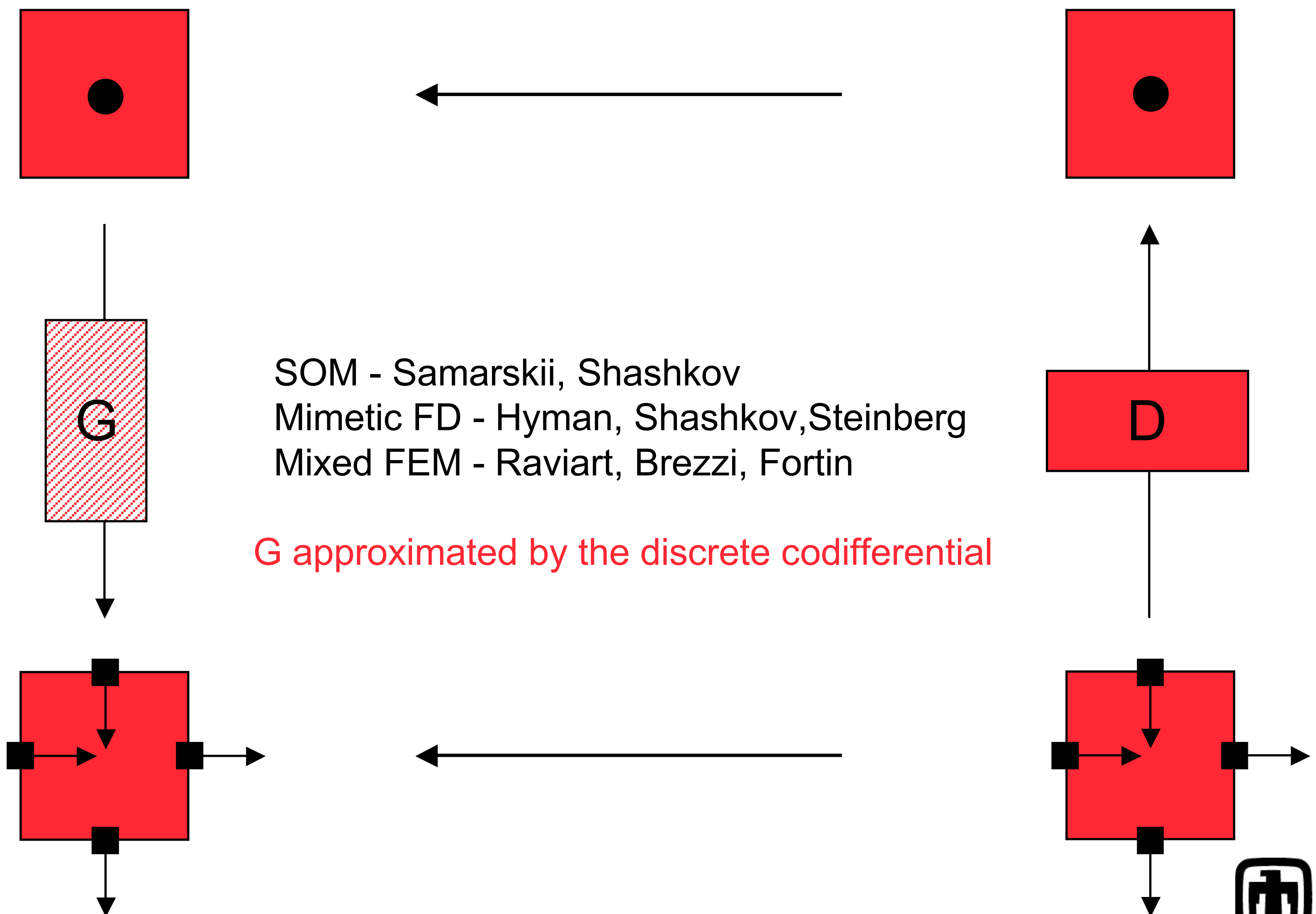
Solution #2: cheat cleverly



SOM - Samarskii, Shashkov
Mimetic FD - Hyman, Shashkov,Steinberg
Mixed FEM - Raviart, Brezzi, Fortin

G approximated by the discrete codifferential

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:

$$\nabla \cdot \mathbf{v} = 0 \qquad \mathbf{u} + \nabla p = 0 \qquad \mathbf{v} - \rho\mathbf{u} = 0 \quad \Longrightarrow \quad \mathbf{v} = \rho\mathbf{u} \quad \Longrightarrow \quad \nabla \cdot \rho\mathbf{u} = 0 \qquad \mathbf{u} + \nabla p = 0$$

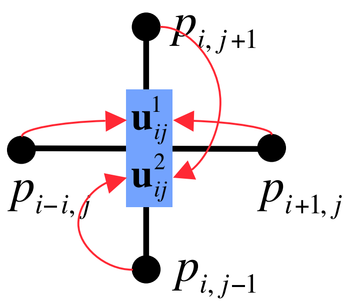
Unfortunately, in the discrete world line and surface fields cannot coexist at the same grid location

⇒ 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**

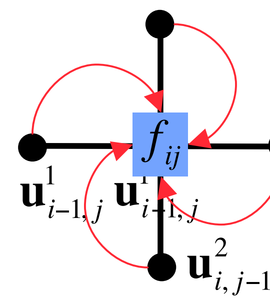
⇓

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

⇓

Non-conservative method

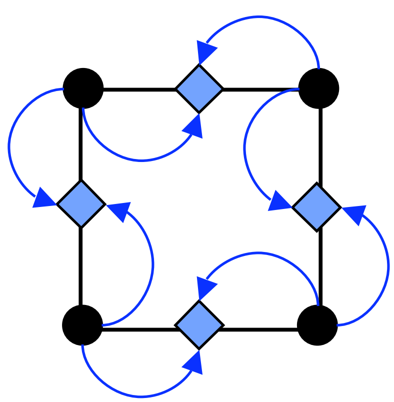
Discrete divergence



node → node

---

node → edge



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

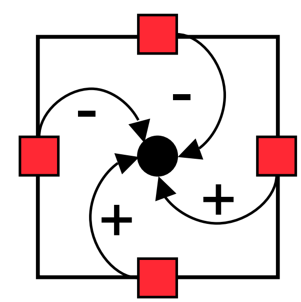
⇓

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

⇓

Conservative method

face → center



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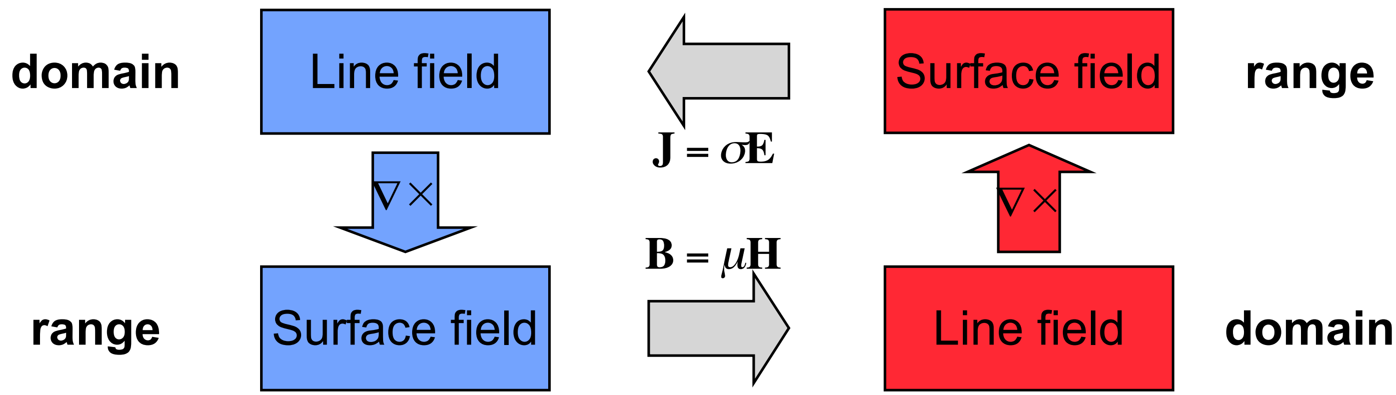
Is this stuff useful in other cases?

Many other important models have identical duality structure



$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\nabla \times \mathbf{H} = \mathbf{J}$$

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

Yee FDTD scheme (1966), FIT (Weiland), Co-volume (Nicolaides), FEM (Bossavit, Nedelec)

Conclusions

- ❑ Discretization is a model reduction
- ❑ Careless discretization causes unphysical behavior
- ❑ Compatible discretizations mimic continuum structures
- ❑ Our discussion can be formalized using Differential Geometry and Algebraic Topology
- ❑ Differential geometry provides the tools to encode this structure
- ❑ Algebraic topology provides the tools to copy the structure to discrete models
- ❑ Further details:

- ➢ Springer IMA Lecture Notes 142, **Spatial Compatible Discretizations.** Edited by D. Arnold, P. Bochev, R. Lehoucq, R. Nicolaides, M. Shashkov
- ➢ **http://www.ima.umn.edu/talks/workshops/5-11-15.2004**
- ➢ **http://www.sandia.gov/~pbboche/index.html**