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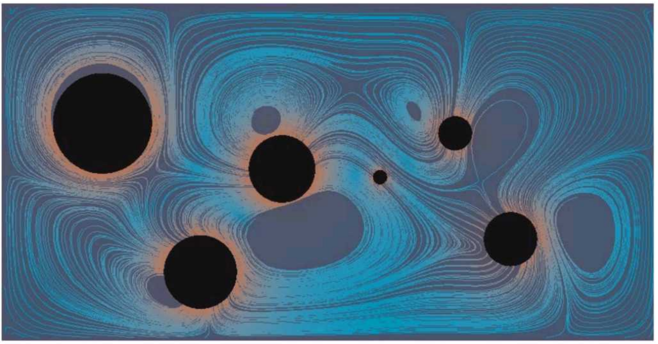

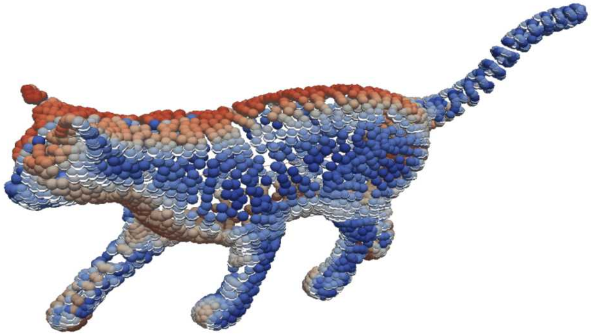

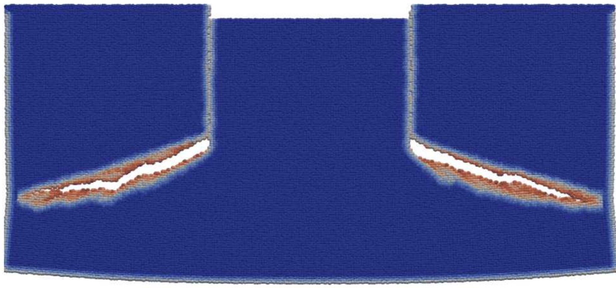

Mimetic Conservation Principles for Meshfree Approximation

Center for Computing Research

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Sandia National Laboratories

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Outline

- Scattered data approximation theory is accurate, but lacks conservation principles
- Combinatorial Hodge theory has de Rham complex, but is purely topological with no notion of convergence
- We will provide a construction of a mimetic meshfree divergence operator acting on point clouds that is consistent and provides a local conservation principle
- We will recast the construction in terms of combinatorial Hodge theory, revealing a connection to algebraic topology of graphs
- Sketch construction of consistent meshfree differential operators that inherit the exact sequence of combinatorial ones

Trask, Nathaniel, Pavel Bochev, and Mauro Perego. "A conservative, consistent, and scalable meshfree mimetic method."

arXiv preprint arXiv:1903.04621(2019).

Generalized moving least squares (GMLS)

$$\tau(u) \approx \tau^h(u)$$

$$p^* = \underset{p \in \mathbf{V}}{\text{argmin}} \left(\sum_j \lambda_j(p) - \lambda_j(u) \right)^2 W(\tau, \lambda_j)$$

$$\tau^h(u) := \tau(p^*)$$

Example:

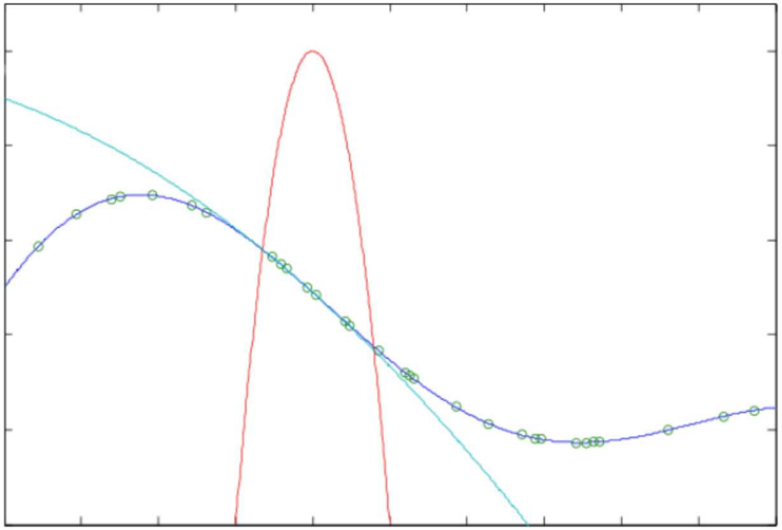
Approximate point evaluation of derivatives:

Target functional $\tau_i = D^\alpha \circ \delta_{x_i}$

Reconstruction space $\mathbf{V} = P^m$

Sampling functional $\lambda_j = \delta_{x_j}$

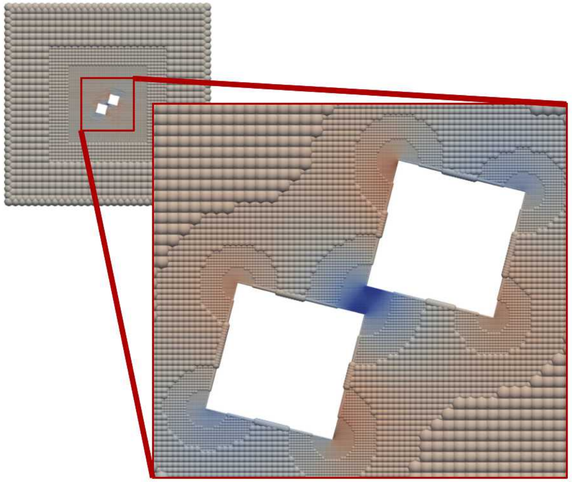
Weighting function $W = W(\|x_i - x_j\|)$

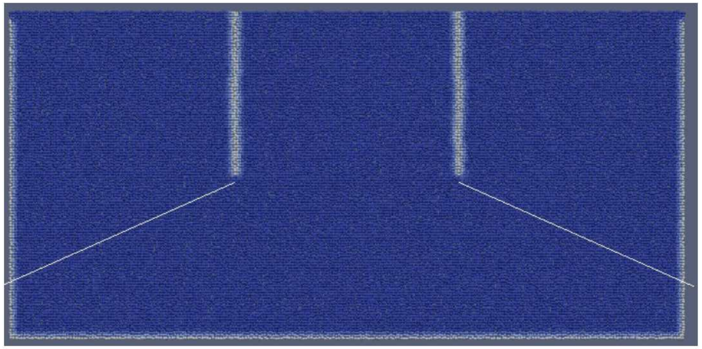


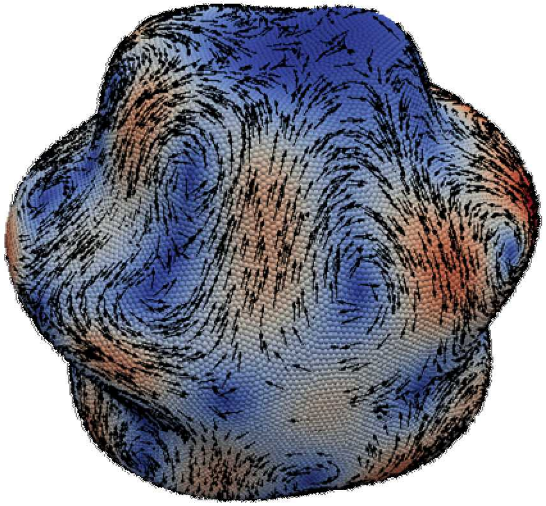
Abstract approximation theory:

$$|\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}^h(u)| \leq |\tau_{\mathbf{x}}(u-p)| + C_W \|\tau_{\mathbf{x}}\|_{P^*} \|\Lambda_{\mathbf{x}}^{-1}\| \max_{i \in I_{\mathbf{x}}} |\lambda_i(u-p)|, \quad p \in P$$

A rigorous meshfree approximation framework

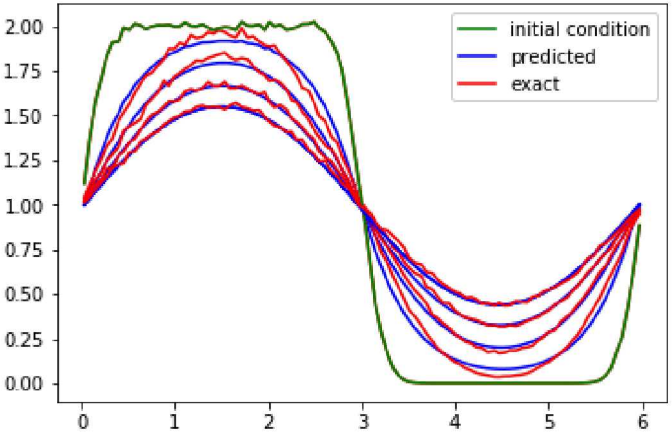






Foundation to build provably consistent schemes:

- Naturally stable discretization of Stokes+Darcy
- Nonlocal discretizations of fracture mechanics
- Native data transfer for mixed FEM-type DOFS
- Functional regression to support data-driven model discovery

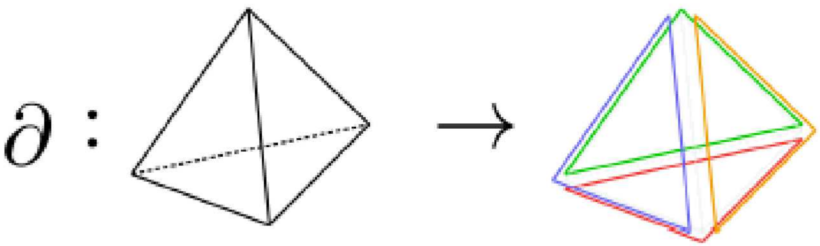


Why is conservation hard in meshfree?

Generalized Stokes theorem:

$$\int_{\Omega} d\omega = \int_{\partial\Omega} \omega$$

Gauss divergence theorem:



$$\int_{C} \nabla \cdot \mathbf{u}\, dx = \int_{F \in \partial C} \mathbf{u} \cdot d\mathbf{A}$$

Ingredients to cook up a conservative discretization:

- A chain complex – **a good boundary operator**
- A consistent coboundary operator **– good function approximation**
- A measure on each mesh entity

Quadrature with GMLS

Assume a basis, $\forall p \in \mathbf{V}$, $p = \mathbf{c}^\intercal \mathbf{P}$ and rewrite GMLS problem as

$$c^* = \underset{c \in \mathbb{R}^{dim(\mathbf{V})}}{\arg\min} \frac{1}{2} \sum_{j=1}^{N} \left(\lambda_j(u) - c^* \lambda_j(\mathbf{P})\right)^2 \omega(\tau; \lambda_j).$$

$$\tau(u) \approx c^* \tau(P^*)$$

Ex: Selecting $\tau = \int_c u \, \mathrm{dx}$, and defining the vector

$$\mathbf{v}_c = \int_c \mathbf{P} dx$$

we can see that a quadrature functionals may be represented as a pairing of the GMLS reconstruction coefficient vector with some vector in its dual space

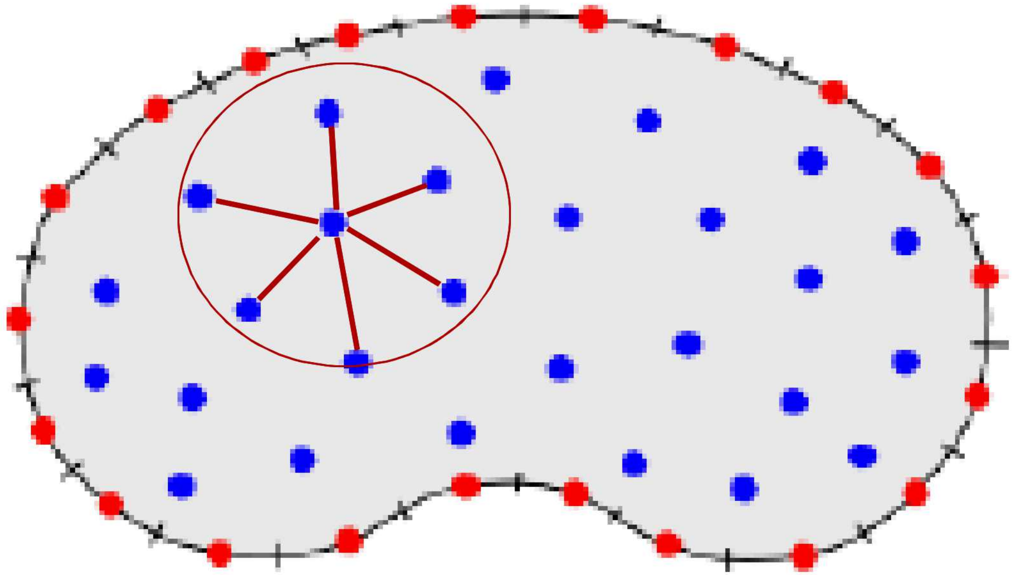
$$I_c[u] = \mathbf{v}_c^\intercal \mathbf{c}^*$$

We seek to similarly define *meshfree quadrature functionals* with summation by parts properties.

Desired functional form to get summation-by-parts

Construct ε-ball graph:

- **Virtual cells (nodes)**
- **Virtual faces (edges)**
- **Physical boundary faces (red)**



$$I_{c_i}[\nabla \cdot \mathbf{F}] = \sum_{j \in N_i^{\epsilon}} I_{f_{ij}}[\mathbf{F}]$$

$$I_{f_{ij}}[\mathbf{F}] = -I_{f_{ji}}[\mathbf{F}]$$

$$\sum_i I_{c_i}[\nabla \cdot \mathbf{F}] = \sum_{\substack{i \\ j \in \partial\Omega^c}} I_{f_{ij}}[\mathbf{F}] + \sum_{i \in \partial\Omega} \int_{\partial\Omega_i} \mathbf{F} \cdot d\mathbf{A}$$

$$= \int_{\partial\Omega} \mathbf{F} \cdot d\mathbf{A}$$

Virtual divergence theorem construction

Let $\mathbf{F} \in P_1(\Omega)^d$. We assume the following ansatz for our *virtual divergence theorem.*

$$\mu_i \left(div\, \mathbf{F}\right)_i = \sum_{j,\beta} \mu_{ij}^{\intercal} \mathbf{c}_{ij}(\mathbf{F})$$

where

- μ_i and $\mu_{ij} = -\mu_{ij}$ are measures **to be determined** corresponding to virtual volumes and face areas
- $\mathbf{c}_{ij}(\mathbf{F})$ is a vector of coefficients associated with the GMLS reconstruction of $\mathbf{F}$ over $P_1(\Omega)^d$ at virtual face f_{ij}
- Due to the polynomial reproduction property of GMLS, this VDT is exact for first-order polynomials

How to get the areas?

Assume virtual areas μ_{ij}^{α} may be expressed in terms of a *virtual area potential* multiplied by point evaluation of basis function at virtual face

$$\mu_{ij}^{\alpha} = \left(\psi_j^{\alpha} - \psi_i^{\alpha}\right) \phi^{\alpha}(\boldsymbol{x}_{ij})$$

Then we obtain the following **weighted graph Laplacian** problem for each basis function

$$\sum_j \left(\psi_j^{\alpha} - \psi_i^{\alpha}\right) \phi^{\alpha}(\boldsymbol{x}_{ij}) = \mu_i div\, \phi_i^{\alpha}$$

Following Fredholm alternative, this has solution if

- $\sum_i \mu_i = \mu(\Omega)$
- $\mu_i > 0$

O(N) solution using black-box AMG

How to get the volumes?

Assumed we have a process for generating volumes satisfying

- $\sum \mu_i = \mu(\Omega)$
- $\mu_i > 0$

Solve the following equality constrained QP

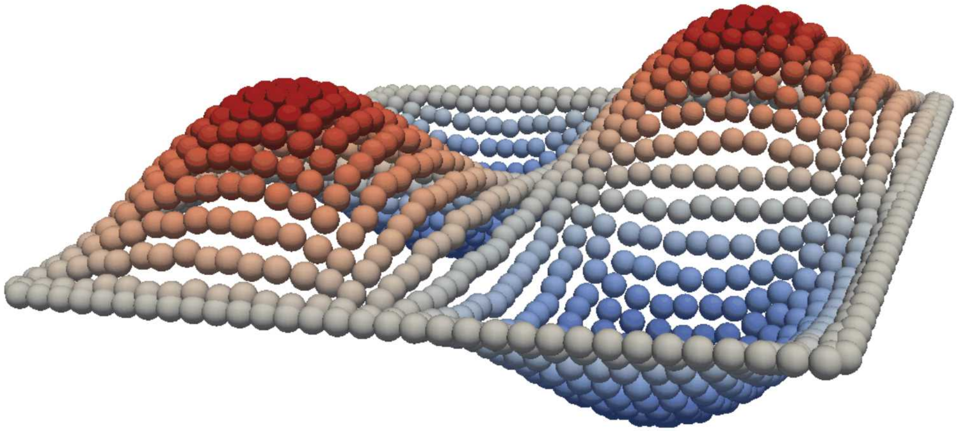
$$\mu^* = \underset{\mu}{argmin} \sum_i \mu_i^2 \omega_i$$

$$\text{such that } \sum_i \mu_i = \mu(\Omega)$$

For any weight $\omega_i > 0$, this provides the definition

$$\mu_i = \frac{\omega_i}{\sum_k \omega_k} \mu(\Omega)$$

First order truncation error for discrete divergence



H	unweighted	weighted
1/16	0.081	0.058
1/32	0.049	0.032
1/64	0.024	0.015
1/128	0.011	0.0072

$$\mathbf{F} = -\langle \cos x \sin y, \sin x \cos y \rangle$$

Can use to build up discretizations of conservation laws

Consider conservation laws for conserved variable q

$$\partial_t q + \nabla \cdot \mathbf{F} = 0$$

Where we will assume steady state and the following fluxes:

- **Darcy:**

$$\boldsymbol{F} = -\mu \nabla \phi$$

- **Singularly perturbed advection diffusion:**

$$\boldsymbol{F} = -\mu \nabla \phi + \boldsymbol{a} \phi$$

- **Linear elasticity:**

$$\boldsymbol{F} = \lambda \left(\nabla \cdot \boldsymbol{u} \right) \boldsymbol{I} + \mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}} \right)$$

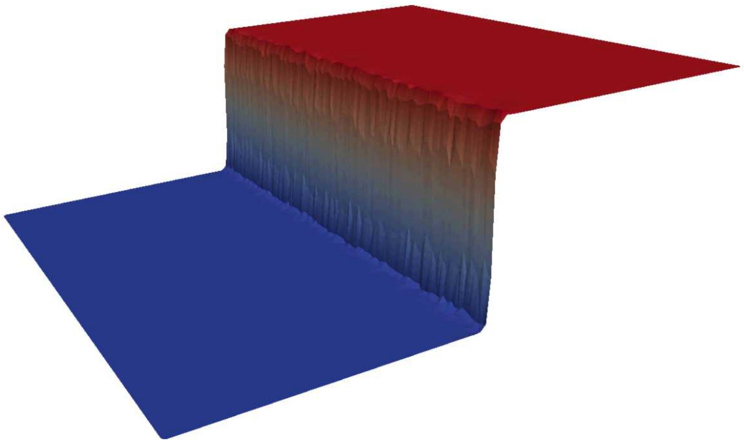
All problems will be shown for discontinuous material properties to highlight flux continuity of approach.

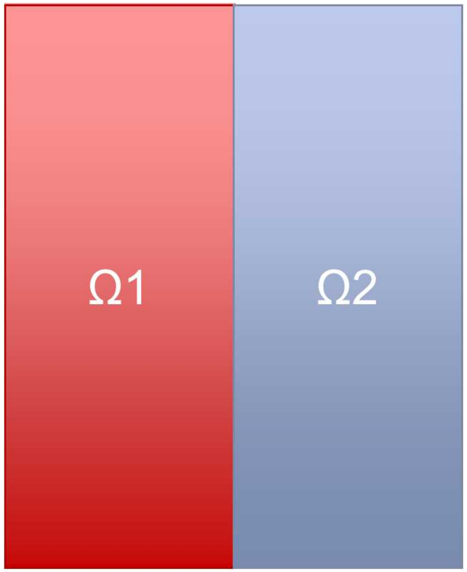
Darcy: jumps in material properties

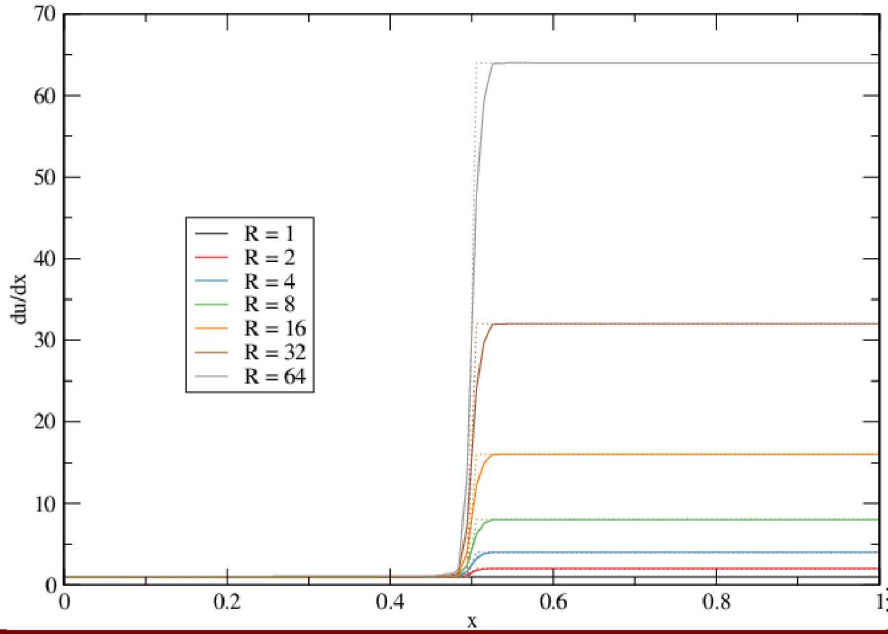
Flux continuity across interface:

$$[\kappa \nabla \phi \cdot \mathbf{n}] = 0$$

$$\nabla \phi \rightarrow$$







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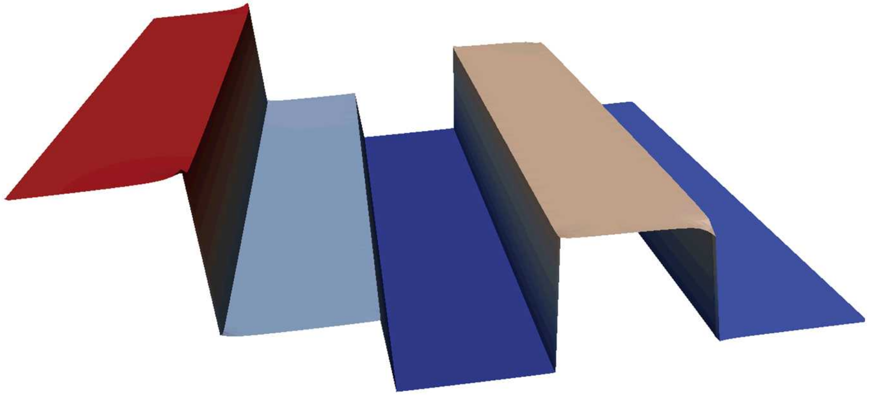
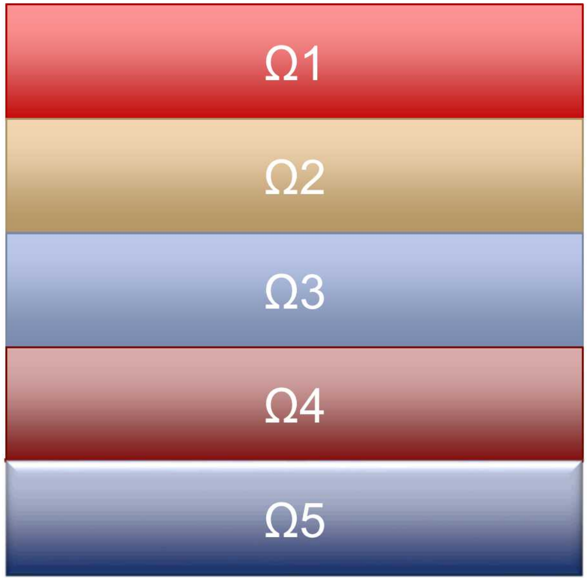
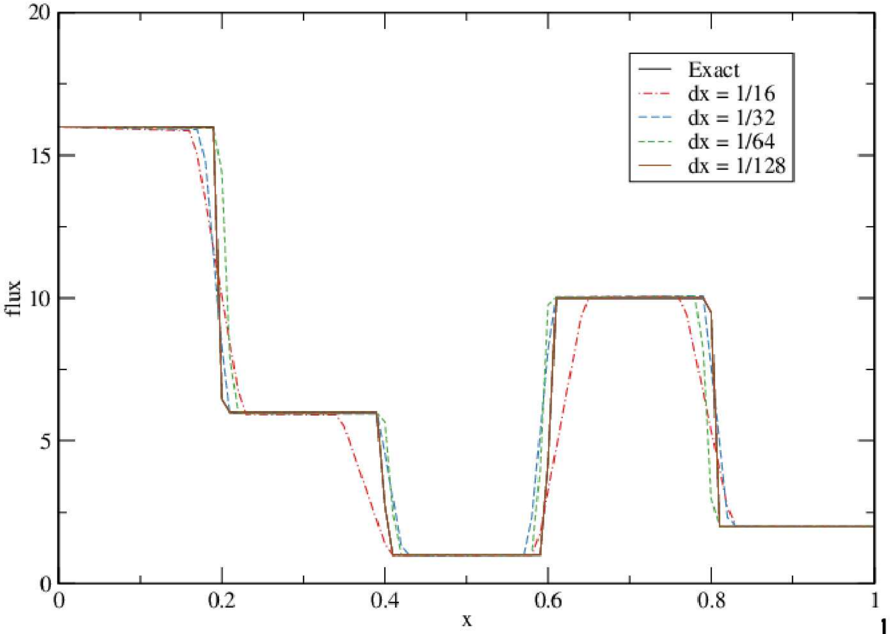
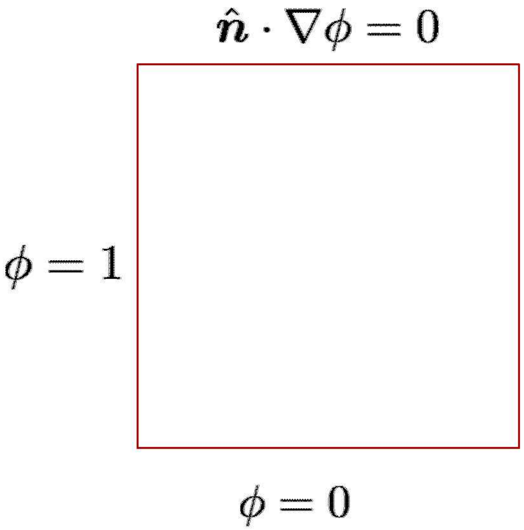






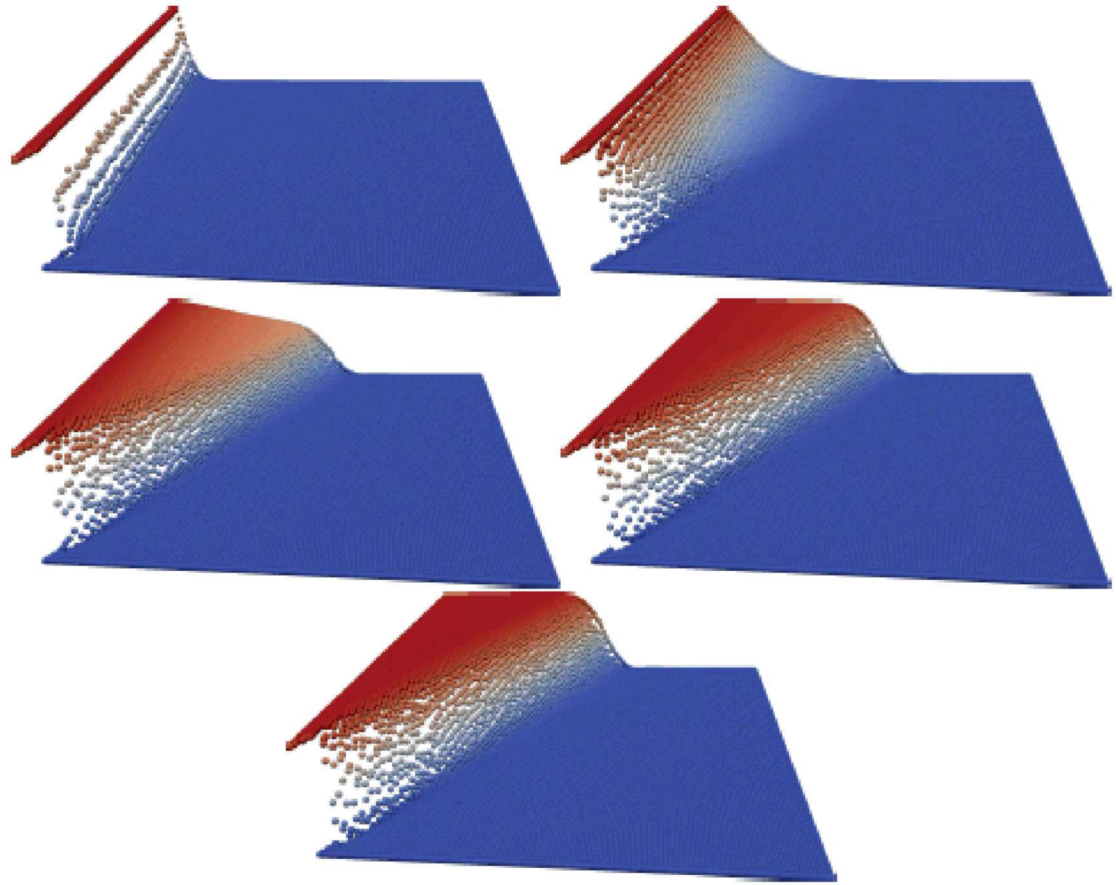
Singularly perturbed advection diffusion



$$\frac{\partial}{\partial t}\phi + \nabla \cdot \mathbf{F} = 0$$

$$\mathbf{F} = \mathbf{a}\phi - \epsilon\nabla\phi$$

Single timestep
$Co \in \{1, 10, 100, 1000, \infty\}$
demonstrating L-stability



Unification with Combinatorial Hodge theory

Combinatorial chain complex

$$C_0 \xleftarrow{\partial_0} C_1 \xleftarrow{\partial_1} C_2$$

Combinatorial co-chain complex

$$C^0 \xrightarrow{\delta_0} C^1 \xrightarrow{\delta_1} C^2.$$

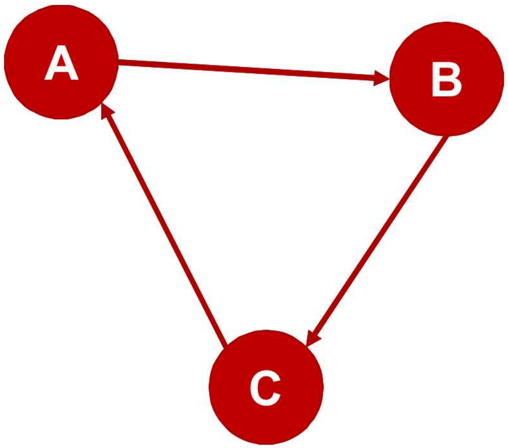
Example: combinatorial gradient

$$\delta_0 : C^1 \rightarrow C^0$$

$$\delta_0 \phi_{ij} = \phi_j - \phi_i$$

Note that:

- δ_0 does *not* converge to ∇
- $\delta_k \circ \delta_{k-1} = 0$



An example 3-clique (A, B, C) belonging to C_2

Jiang, Xiaoye, et al. "Statistical ranking and combinatorial Hodge theory." Mathematical Programming 127.1 (2011): 203-244.

Current work: a meshfree de Rham sequence

Previous scheme can be rewritten in combinatorial Hodge notation:

$$\mu_c div_h(u)_c = \delta_0^* \left[(\delta_0 \psi_f)^\intercal D_f c_f(u) \right]$$

We may similarly define a mimetic curl operator by moving to the right on the combinatorial de Rham complex

$$I_f[\nabla \times u] = \delta_1^* \left[(\delta_1 \psi_e)^\intercal D_e c_e(u) \right]$$

Choosing $I_f[\nabla \times u] = (\delta_0 \psi_f)^\intercal D_f c_f(\nabla \times u)$ we obtain

$$\mu_c div_h \circ curl_h(u)_c = \delta_0^* \delta_1^* \left[(\delta_1 \psi_e)^\intercal D_e c_e(u) \right] = 0$$

A direct extension to define virtual curl satisfying div*curl = 0