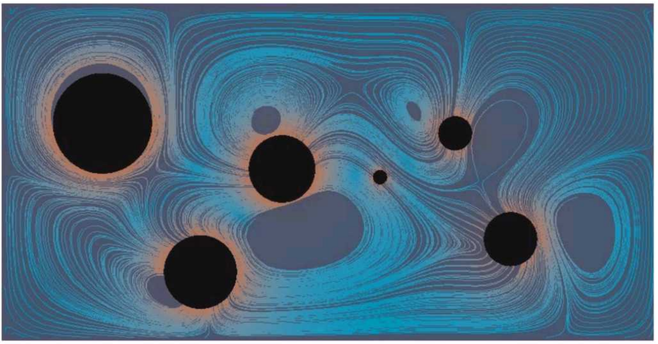
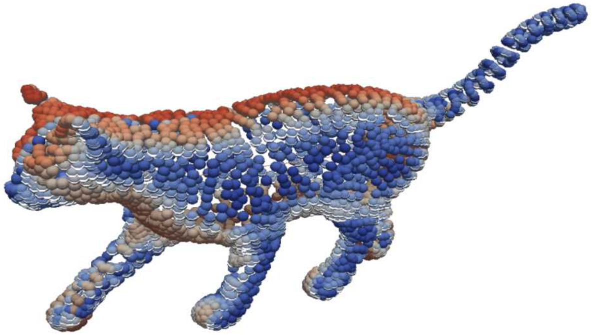
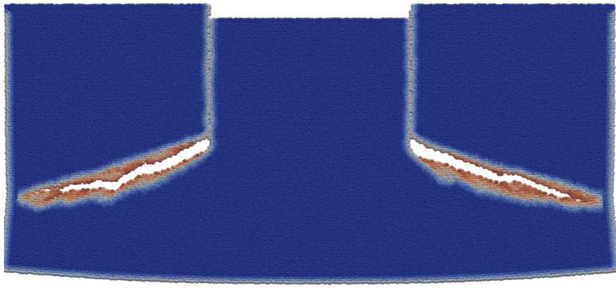
SAND2018-13525PE







Spatially compatible meshfree discretization through GMLS and graph theory

Nat Trask
Center for Computing Research
Sandia National Laboratories

Center for Computing Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Talk overview

- For the uninitiated – why would we want to use meshfree?
  - A non-technical survey of our current meshfree projects
  - General takeaway: exchange a nice mathematical setting for nice models
    - Good for stubborn engineering problems, bad for mathematical analysis
- What is "compatible discretization"?
  - Conservation principles, and why are they hard to get in meshfree?
- Our tools:
  - Generalized moving least squares – meshfree approximation
  - Combinatorial Hodge theory – meshfree topology
- Key result:
  - A conservative meshfree divergence theorem defined on a graph
- Final product:
  - A compatible meshfree finite volume method

Compadre – **Com**patible **Pa**rticle **D**isc**re**tization

Objectives:

- Meshless schemes with rigorous approximation theory and mimetic properties like compatible mesh-based methods
- Software library supporting solution of general meshless schemes with tools for coarse+fine grain parallelism and preconditioning

People:

- Pavel Bochev (PI)
- Pete Bosler
- Paul Kuberry
- Mauro Perego
- Kara Peterson
- Nat Trask

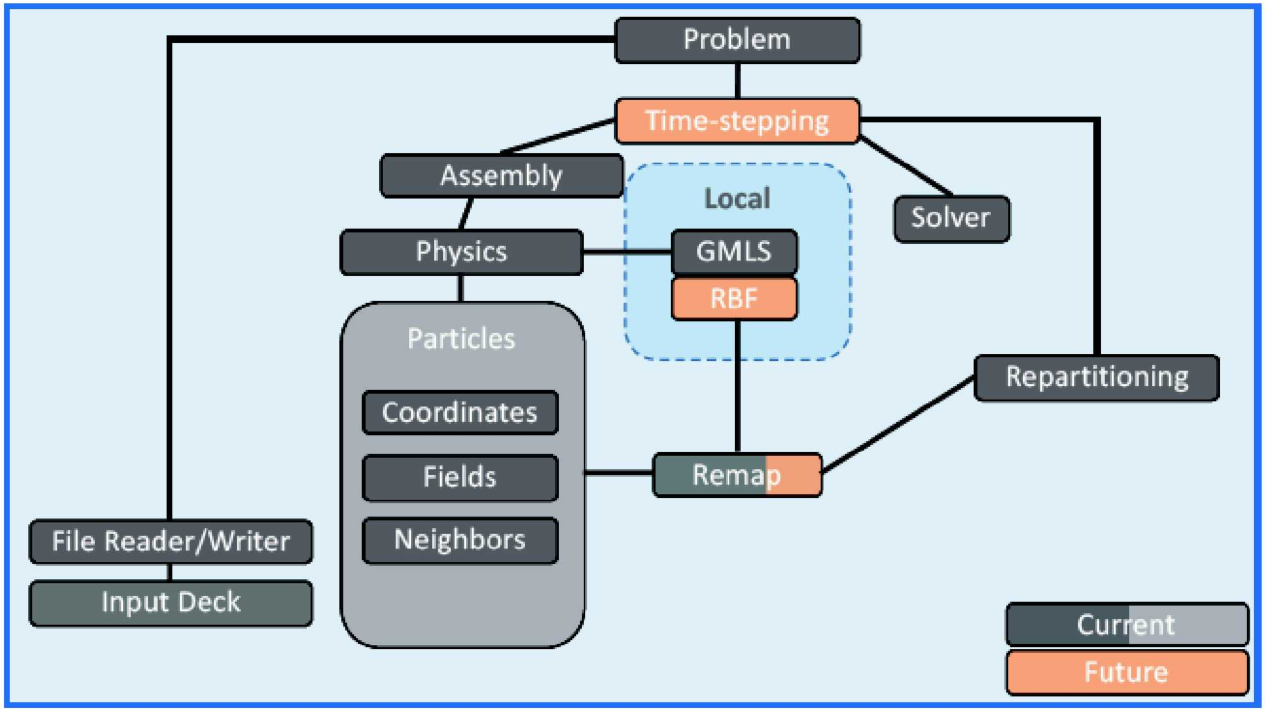
Students/collaborators:

- Huaiqian You, Yue Yu – Lehigh
- Amanda Howard, Martin Maxey – Brown
- Wenxiao Pan – UW Madison
- Paul Atzberger – UC Santa Barbara
- J.S. Chen – UC San Diego

Key tools:

- Optimization based approaches to develop meshfree discretizations with reproduction properties
- The Compadre Trilinos library – open source library for scalable implementation of meshfree methods

Compadre Trilinos package



Collection of modules for general meshfree discretizations + heterogeneous architectures

- **Local modules for efficiently solving small optimization problems on each particle**
  - Kokkos implementation gives fine grained thread/GPU parallelism
- **Global modules for assembling global matrices and applying fast solvers**
  - MPI based domain decomposition for coarse grained parallelism
  - Interfaces to MueLu for fast solvers

ASCeND –

Asymptotically **c**ompatible foundations for **n**onlocal **d**iscretization

Objectives:

- Develop mathematical underpinnings for meshfree nonlocal models

People:

- Nat Trask (PI)
- Marta D'Elia
- David Littlewood
- Stewart Silling
- Michael Tupek

PhiLMs DoE MMICCs center–

Phys**i**cs-based **L**earning **M**achines for scientific computing

Objectives:

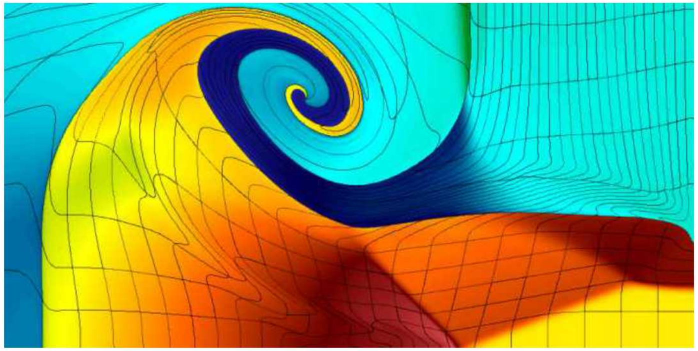
- Develop approximation theory for deep neural networks in multiscale applications

People:

- George Karniadakis (Brown University – head PI)
- Sandia Team
  - Michael Parks (Institutional PI)
  - Pavel Bochev
  - Marta D'Elia
  - Mauro Perego
  - Nat Trask

What is meshfree?

- In classical methods, a mesh gives you a lot:
  - Easy construction of basis functions
  - A partition of unity
  - Simple quadrature
  - A simplicial complex and associated exterior calculus structures
    - i.e. cells, faces, edges, nodes linked together through a boundary operator + generalized Stokes theorems
- Usually the best option, but for many applications its infeasible/annoying to efficiently build a mesh
  - Lagrangian large-deformation problems
  - Automated design-to-analysis
    - (~50% of analyst time!)[1]
  - Non-intrusive multiphysics coupling for legacy code



[1] "DART system analysis" SAND2005-4647

Meshfree – restricting ourselves to 0-forms

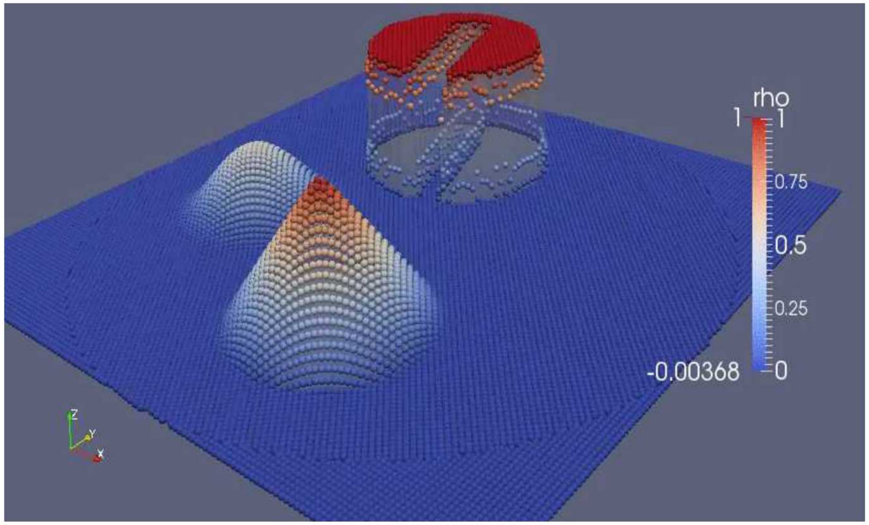
- Lots of versions of meshfree out there!
- Recall examples of differential k-forms:
  - For a polygonal mesh in 3D

$$\textbf{Zero-form:} \quad \delta_{\mathbf{x}_i} \circ \mathbf{u}$$

$$\textbf{One-form:} \quad \int_E \mathbf{u} \cdot d\mathbf{l}$$

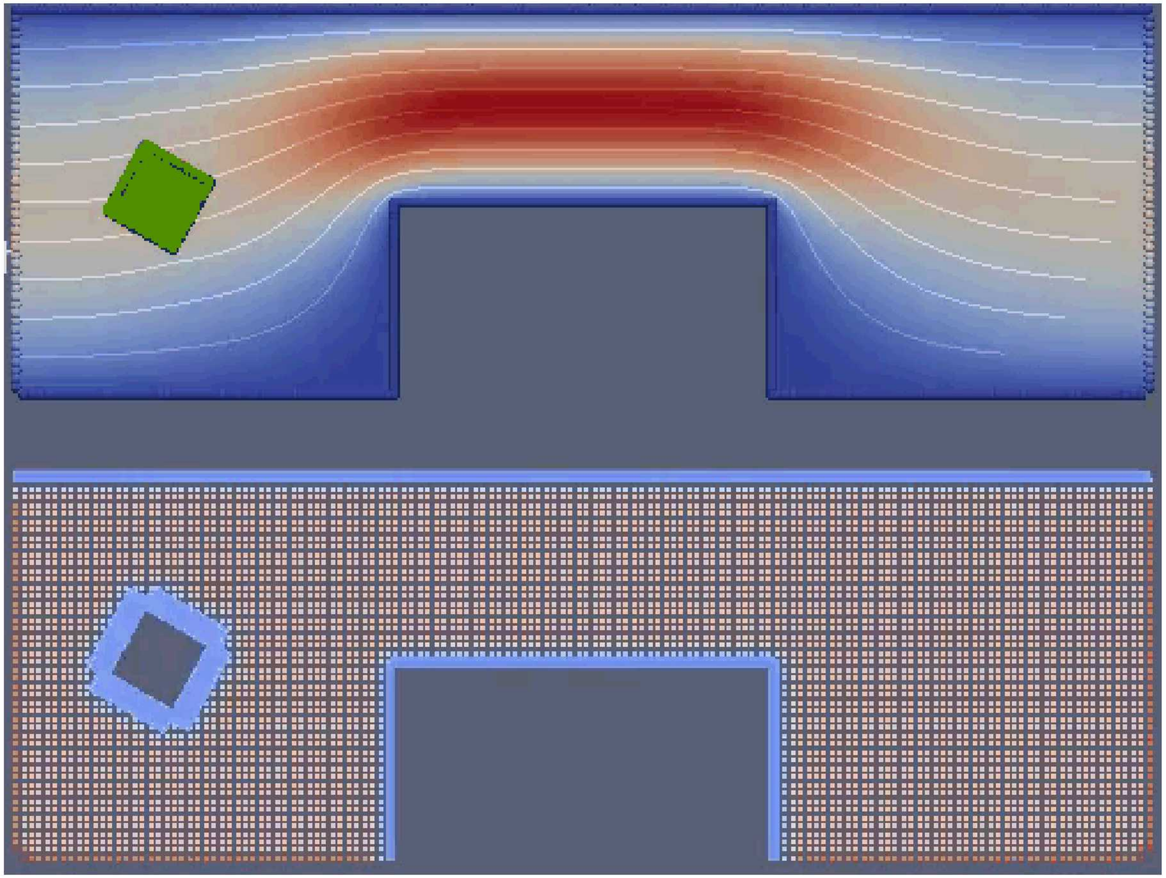
$$\textbf{Two-form:} \quad \int_F \mathbf{u} \cdot d\mathbf{A}$$

$$\textbf{Three-form:} \quad \int_C \mathbf{u} dV$$



- For our purposes, define meshfree as restricting ourselves to describing solution only in terms of zero-forms
  - Easy to push points around if you don't care about preserving a mesh
  - Exchange nice mathematical setting to get more descriptive models

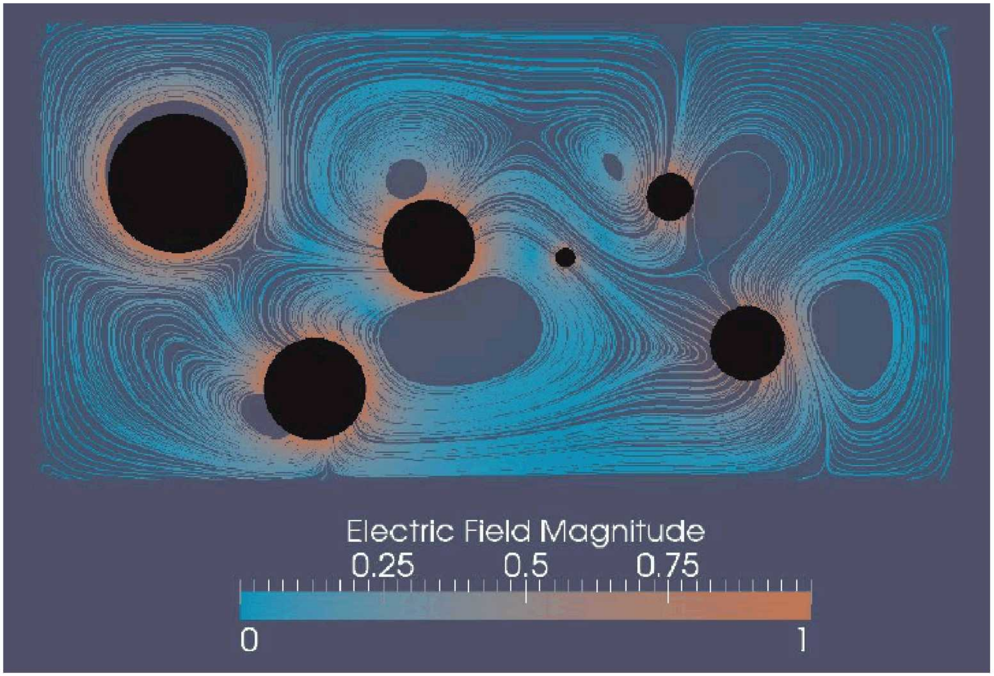
Why meshfree? Large deformation problems



$$\begin{cases} -\nabla^2 \mathbf{u} + \nabla p = \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \\ \mathbf{u}|_{\partial\omega} = \mathbf{U} + (x - \mathbf{X}) \times \Omega \\ \int_{\partial\omega} \sigma \cdot d\mathbf{A} = 0 \end{cases}$$

Meshfree: great for moving boundaries, but **how do we handle inf-sup stability?**

Why meshfree? Large deformation problems



$$\begin{cases} -\nu \nabla^2 \mathbf{u} + \nabla p = -\rho_e(\phi)\nabla\phi \\ \nabla \cdot \mathbf{u} = 0 \\ \mathbf{u} = \mathbf{w} \\ \mathbf{u} = \mathbf{V}_i + (x - \mathbf{X}_i) \times \mathbf{\Omega}_i \end{cases}$$

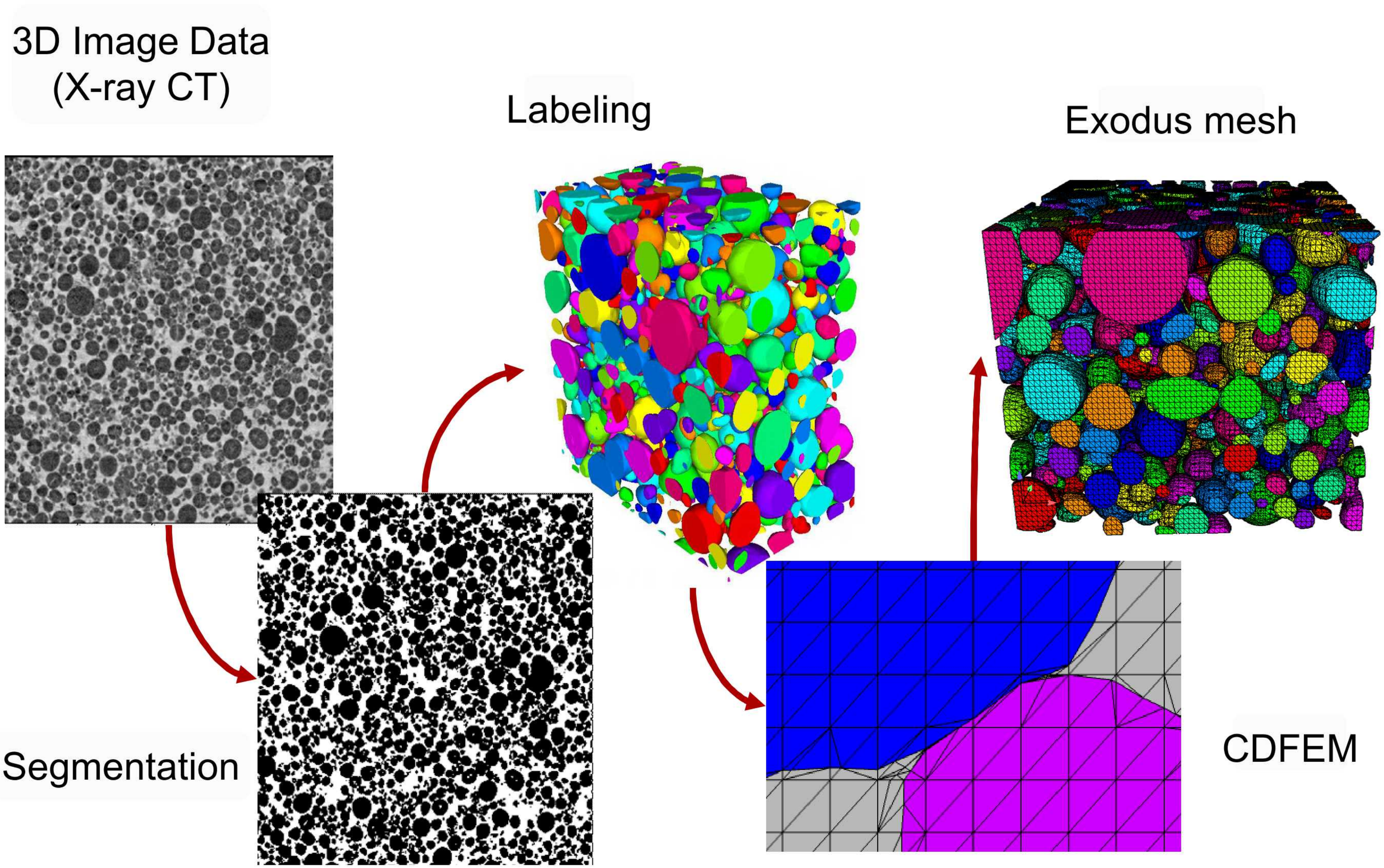
$$-l_c^2 \nabla^4 \phi + \nabla^2 \phi = -\frac{\rho_e(\phi)}{\epsilon}$$

$$\begin{cases} 0 = \int_{\partial\Omega_i} \overline{\overline{\sigma}} \cdot d\mathbf{A} \\ 0 = \int_{\partial\Omega_i} \overline{\overline{\sigma}} \times (x - \mathbf{X}_i) \cdot d\mathbf{A} \end{cases}$$

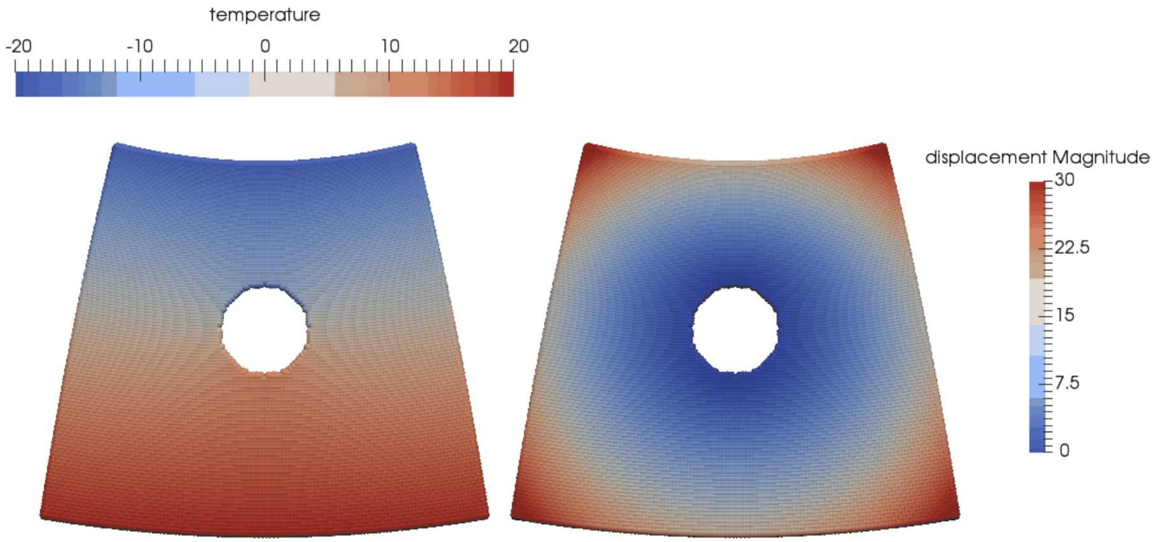
$$\overline{\overline{\sigma}} = -\epsilon_0 \left(\mathbf{E} \otimes \mathbf{E} + E^2 \mathbf{I} \right) + -p\mathbf{I} + \frac{\nu}{2} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right)$$

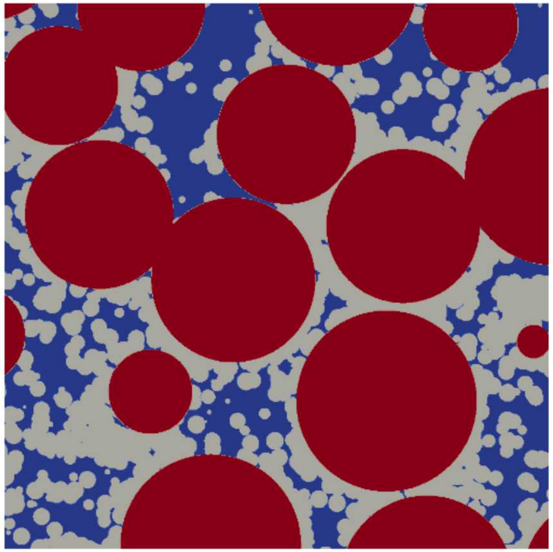
Meshfree: a nice multiphysics platform for Lagrangian models, **but how do we analyze stability of coupling?**

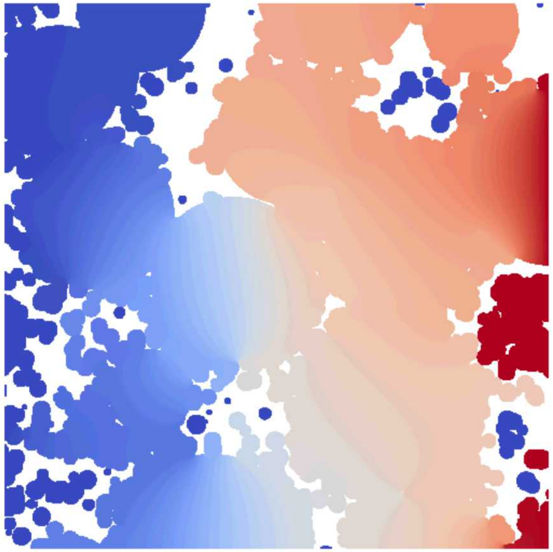
Why meshfree? Automatic geometry discretization



Why meshfree? Automatic geometry discretization

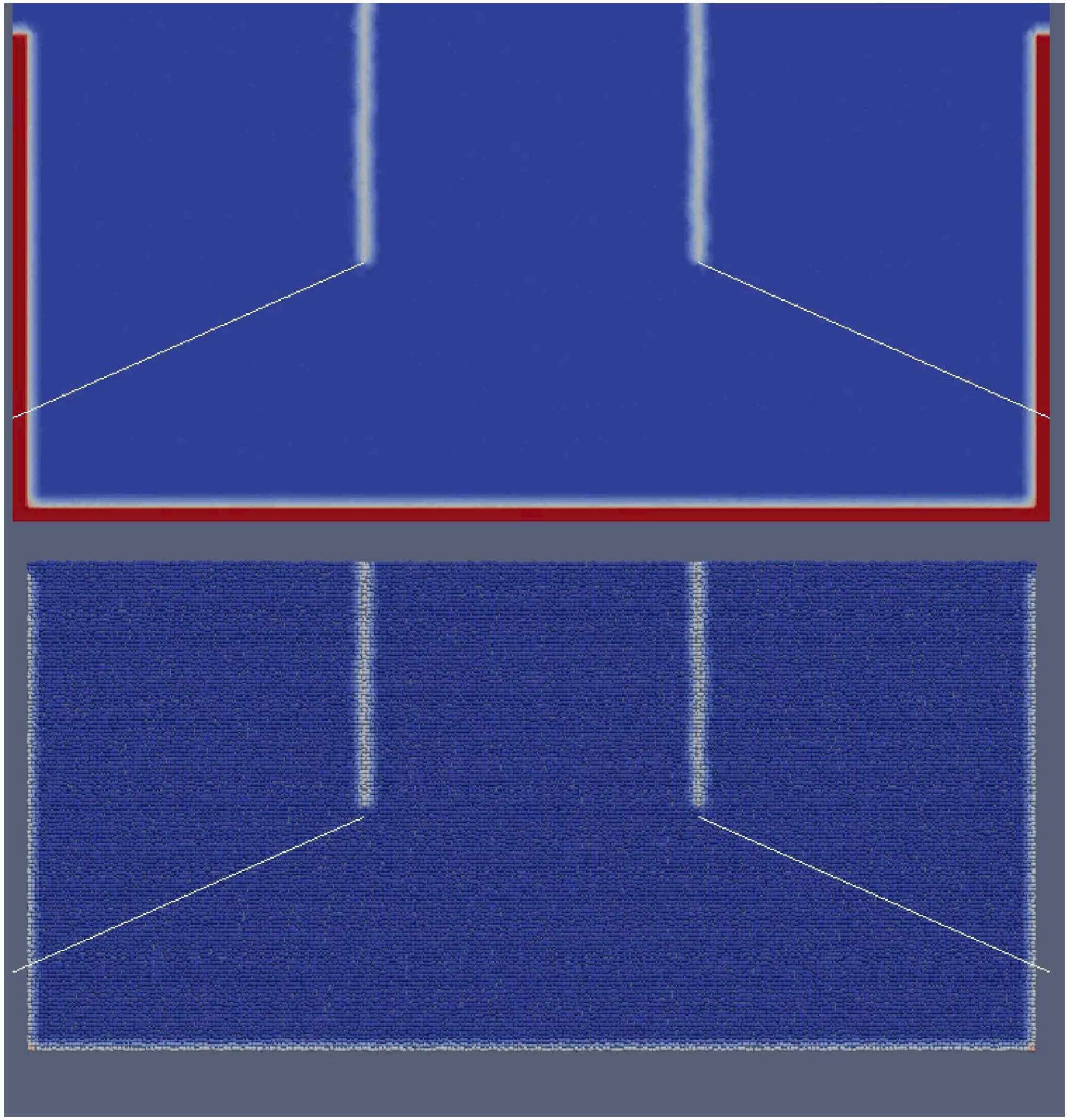






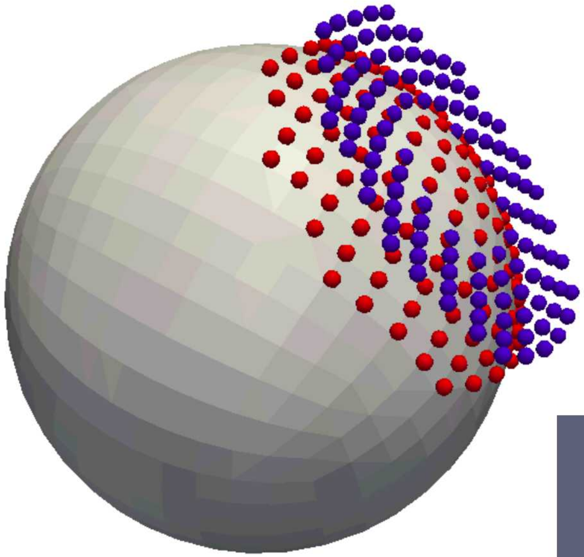
Meshfree:
Great for automatically handling internal interfaces, but **how do we make sense of conservation?**

Why meshfree? Fracture mechanics

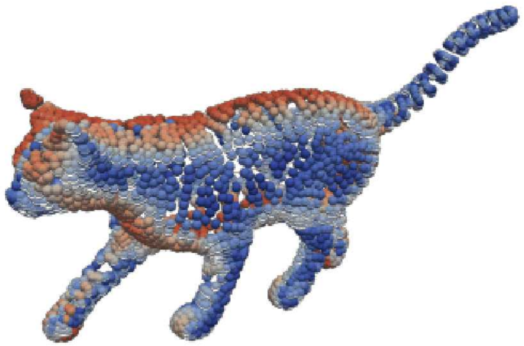


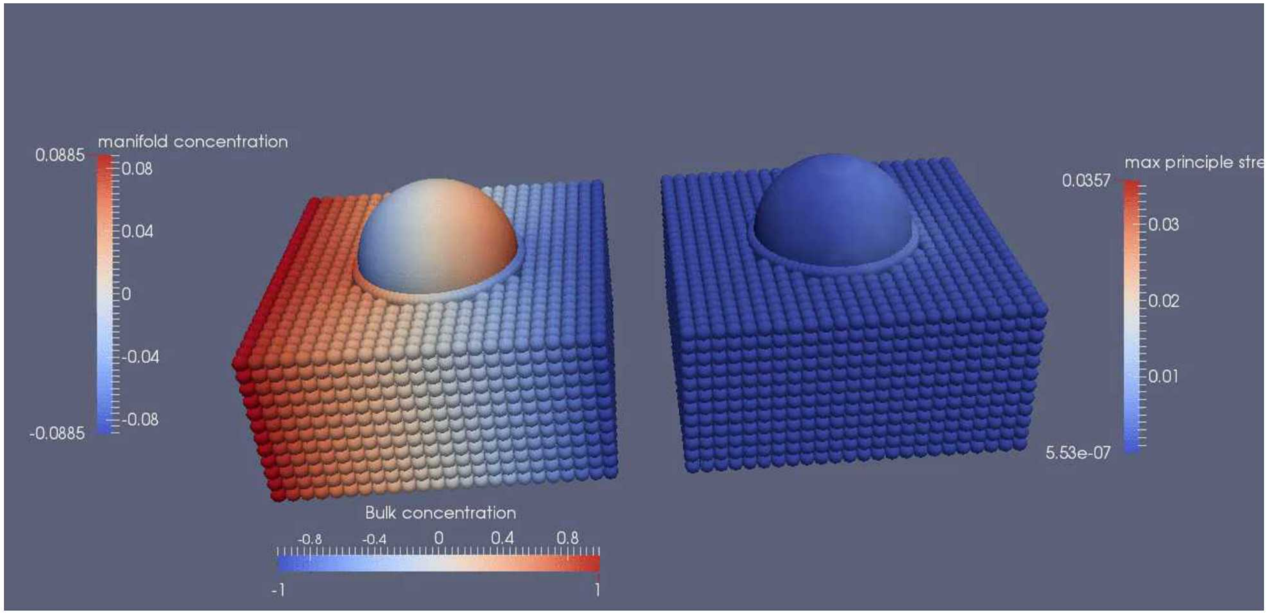
Meshfree:
Automatic treatment of topology changes, but **we may lose variational principles for nonlinear problems**

Why meshfree? Differential geometry on manifolds

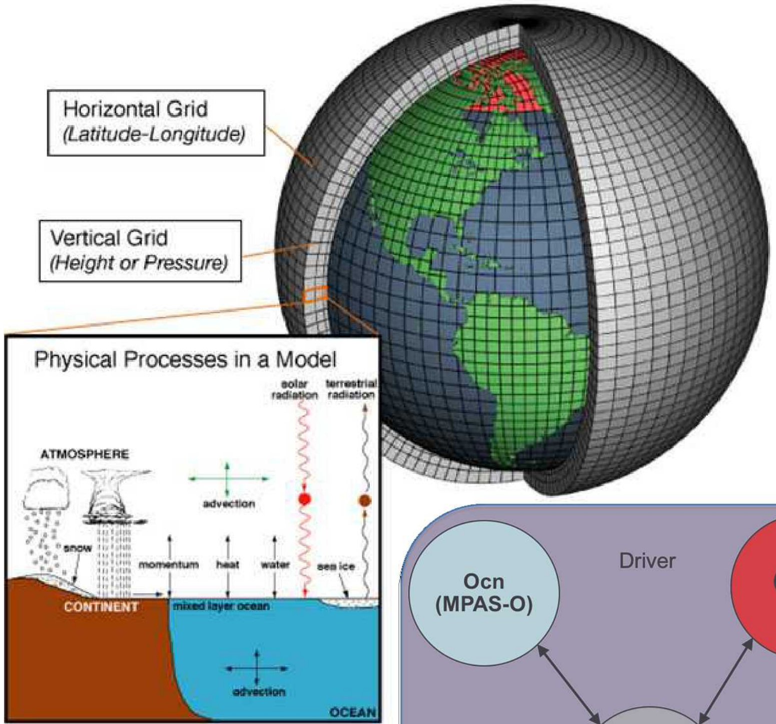


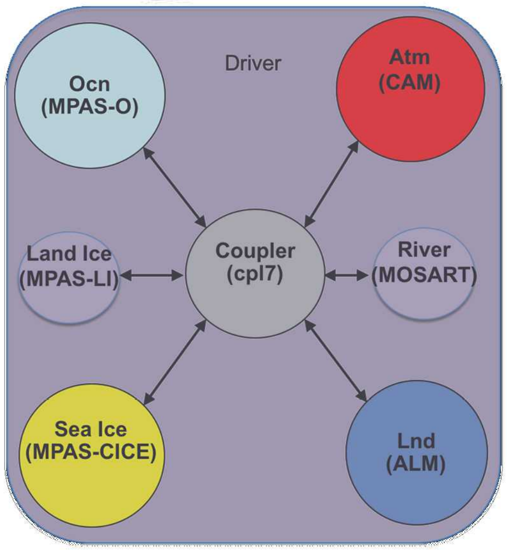
To oversimplify – mapping between local charts and tangent space can be inferred ”meshlessly” to get access to metric tensor, curvature, surface differential operators, etc.

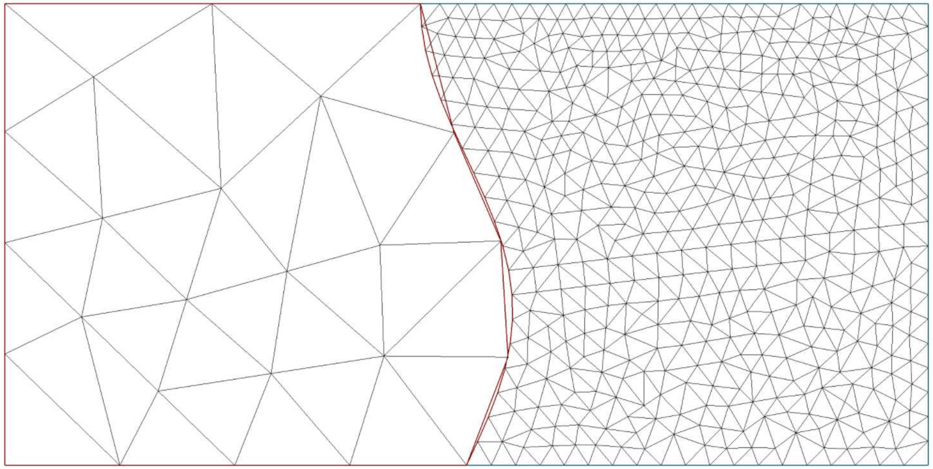


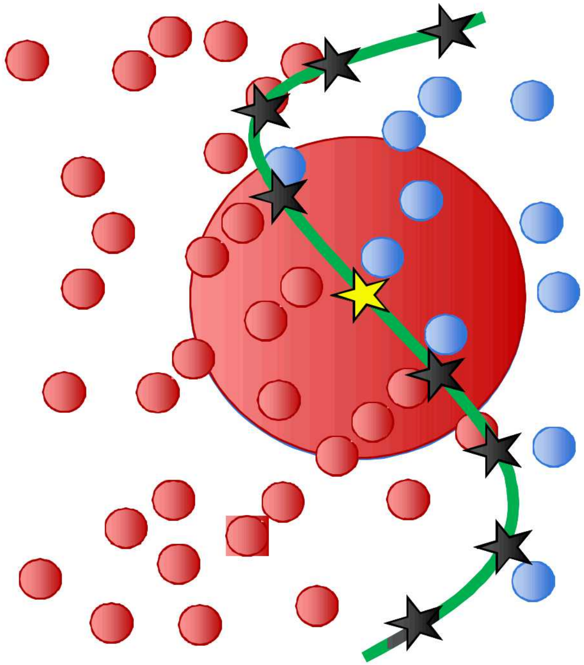


Why meshfree? Code couplers for E3SM





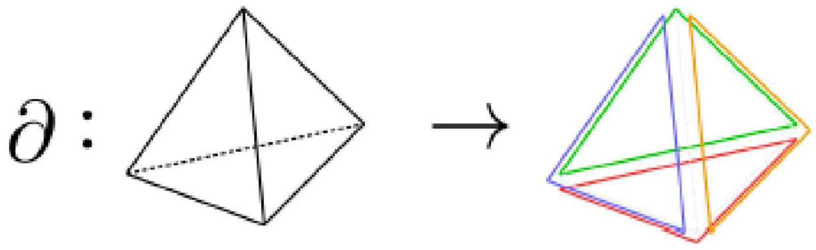




Why is conservation hard in meshfree?

Generalized Stokes theorem

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



Gauss divergence theorem

$$\int_{C} \nabla \cdot \mathbf{u} dV = \oint_{F \in C} \mathbf{u} \cdot d\mathbf{A}$$

Two ingredients to a conservative discretization:

- A chain complex – **the metric information**
    - A topological structure with a well-defined boundary operator
- An exterior derivative **– the function approximation**
    - A consistent definition of a divergence

First ingredient: function approximation

- Older meshfree approaches suffer from accuracy and stability issues
- We build all of our work on top of a framework with a rigorous approximation theory
- Give a quick overview of existing approximation theory using GMLS and our generalization to an abstract theory

---

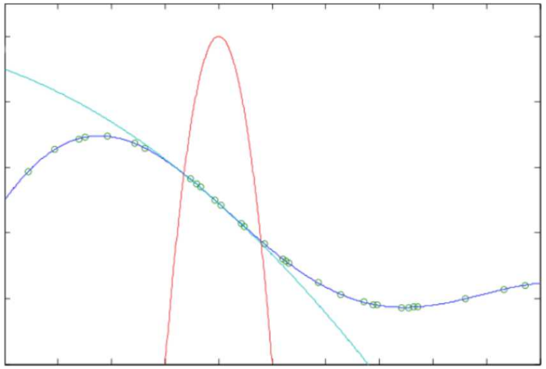
Wendland, Holger.*Scattered data approximation*. Vol. 17. Cambridge university press, 2004.
Mirzaei, Davoud, Robert Schaback, and Mehdi Dehghan. "On generalized moving least squares and diffuse derivatives."*IMA Journal of Numerical Analysis* 32.3 (2012): 983-1000.
Trask, Nathaniel, Mauro Perego, and Pavel Bochev. "A high-order staggered meshless method for elliptic problems."*SIAM Journal on Scientific Computing* 39.2 (2017): A479-A502.

Generalized moving least squares (GMLS)

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

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

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



Example:

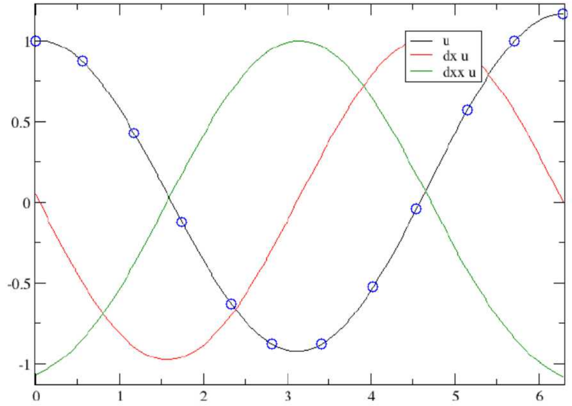
Approximate point evaluation of derivatives:

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

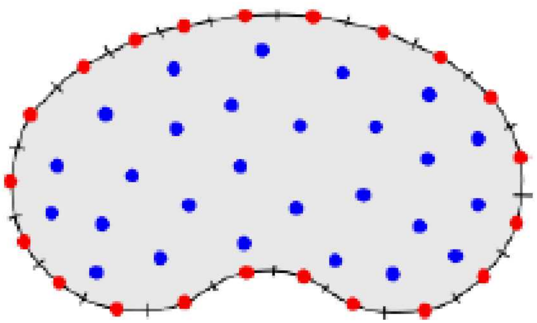


Takeaway:

A rigorous way to obtain formulas that look like:

$$\tau_i(u)_h = \sum_j \alpha_{ij} \lambda_j(u)$$

Preliminaries: Quasi-uniform point clouds



Definition 0.1. Fill+separation distances Given point cloud $X = \{x_1, \ldots, x_N\} \subset \Omega$, define distances

$$h_X = \sup_{x \in \Omega} \min_{j \in X} ||x - x_j||^2$$

$$q_X = \frac{1}{2} \min_{j \neq I} ||x_i - x_j||^2$$

Definition 0.2. Quasi-uniformity A point cloud X is *quasi-uniform with respect to* c_{qu} if

$$q_X \leq h_X \leq c_{qu} q_X$$

Proposition 0.1. *Suppose bounded* Ω *and quasi-uniform* X *w.r.t.* $c_{qu} > 0$. *Then there exist* $c_1, c_2 > 0$ *such that*

$$c_1 N^{-\frac{1}{d}} \leq h_X \leq c_2 N^{-\frac{1}{d}}$$

Classical MLS: quasi-interpolants [Wendland04]

Definition 0.1. Local polynomial reproduction: A process defining $\forall x_i \in X$ an approximation $u(x) = \sum_j \phi_j u(x_j)$ Is a local polynomial reproduction if there exist $C_1, C2 > 0$.

1. $\sum_j \phi_j P_j = P(x)$ for all $P \in V_h$
2. $\sum_j |\phi_j| \leq C_1$ for all $x \in \Omega$
3. $\phi_j(x) = 0$ if $||x - x_j||_2 > C_2 h_X$ and $x \in \Omega$

Theorem 0.1. *For bounded Ω, define $\Omega^* = \underset{x\in\Omega}{\cup} B(x, C_2 h_X)$. If s_f is a local polynomial reproduction of order m and $f \in C^{m+1}(\Omega^*)$ then*

$$|f(x) - s_f(x)| \leq C h_X^{m+1} |f|_{C^{m+1}(\Omega^*)}$$

Theorem 0.2. *Consider the GMLS process with $\tau = \delta_x$, $\lambda_j(u) = u(x_j)$, and $V = \Pi_m$. If Ω is compact and satisfies a cone condition, and X is quasi-uniform, then there exists a constant $C > 0$ such that supp$(W) = C\, h_X$ where the GMLS problem is solvable and forms a local polynomial reproduction.*

Classical MLS: derivative approximation [Mirzaei12]

Definition 0.1. Local polynomial reproduction: A process defining $\forall x_i \in X$ an approximation $D^\alpha u(x) = \sum_j \phi_j u(x_j)$ Is a local polynomial reproduction if there exist $C_1, C2 > 0$.

1. $\sum_j \phi_j P_j = D^\alpha P(x)$ for all $P \in V_h$
2. $\sum_j |\phi_j| \leq C_1 h_X^{-|\alpha|}$ for all $x \in \Omega$
3. $\phi_j(x) = 0$ if $||x - x_j||_2 > C_2 h_X$ and $x \in \Omega$

Theorem 0.1. *For bounded* Ω*, define* $\Omega^* = \bigcup_{x \in \Omega} B(x, C_2 h_X)$*. If* s_f *is a local polynomial reproduction of order* m *and* $f \in C^{m+1}(\Omega^*)$ *then*

$$|f(x) - s_f(x)| \leq C h_X^{m+1-|\alpha|} |f|_{C^{m+1}(\Omega^*)}$$

Theorem 0.2. *Consider the GMLS process with* $\tau(u) = D^\alpha u(x)$*,* $\lambda_j(u) = u(x_j)$*, and* $V = \Pi_m$*. If* Ω *is compact and satisfies a cone condition, and* X *is quasi-uniform, then there exists a constant* $C > 0$ *such that* $supp(W) = C\, h_X$ *where the GMLS problem is solvable and forms a local polynomial reproduction.*

A general abstract framework

Basic technique:

$$
\begin{aligned}
|\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}^h(u)| &\leq |\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}(p)| + |\tau_{\mathbf{x}}(p) - \tau_{\mathbf{x}}^h(u)|, \quad (\forall p \in P) \\
&\leq |\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}(p)| + |\tau_{\mathbf{x}}^h(p - u)|, \quad \longleftarrow \text{ reconstruction property} \\
&\leq |\tau_{\mathbf{x}}(u - p)| + \left| \sum_{i=1}^{N_p} \lambda_i(u - p)\, a_{\tau_{\mathbf{x}}}^i \right| \quad \longleftarrow \text{ GMLS definition} \\
&\leq |\tau_{\mathbf{x}}(u - p)| + \max_{i \in I_{\mathbf{x}}} |\lambda_i(u - p)| \sum_{i \in I_{\mathbf{x}}} |a_{\tau_{\mathbf{x}}}^i|.
\end{aligned}
$$

$$\sum_{i \in I_{\mathbf{x}}} |a_{\tau_{\mathbf{x}}}^i| \leq C_W \|\tau_{\mathbf{x}}\|_{P^*} \|\Lambda_{\mathbf{x}}^{-1}\|$$

Holds for any target functional and approximation space:

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

A general abstract framework

- All examples from beginning of talk fall into this framework
  - Ex: Data transfer applications

$$\lambda_i^e(\mathbf{u}) := \frac{1}{|e_i|}\int_{e_i} \mathbf{u} \cdot \mathbf{t}_i \qquad \lambda_i^f(\mathbf{u}) = \frac{1}{|f_i|}\int_{f_i} \mathbf{u} \cdot \mathbf{n}_i \qquad \lambda_i^v(u) := \frac{1}{|V_i|}\int_{V_i} u(\boldsymbol{y})\, d\boldsymbol{y}$$

  - Ex: Solving different PDES

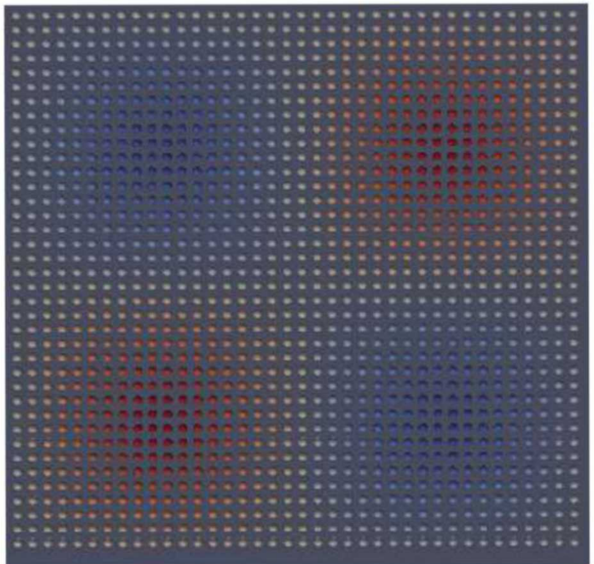
$$\tau(u) = div(u) \qquad \tau(u) = \int_{B(x)} K(x,y)u(y) - u(x)dy \qquad \tau(u) = \int_{\partial\Omega} \sigma(u) \cdot d\mathbf{A}$$

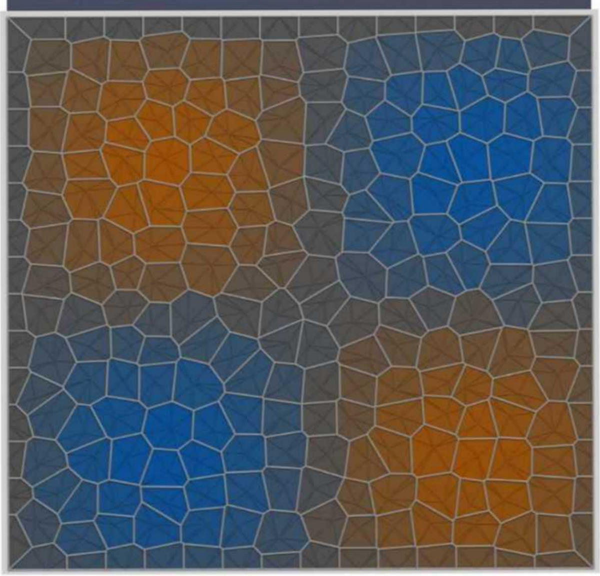
  - Ex: Handling divergence/curl constraints in saddle point problems

$$V_h = \left\{\mathbf{v} \in (\Pi_m)^d | \quad \nabla \cdot \mathbf{v} = 0\right\}$$

$$V_h = \left\{\mathbf{v} \in (\Pi_m)^d | \quad \nabla \times \mathbf{v} = 0\right\}$$

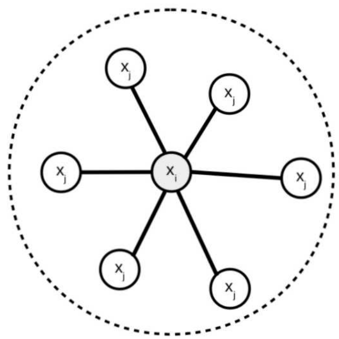
Solving PDEs with or without a mesh

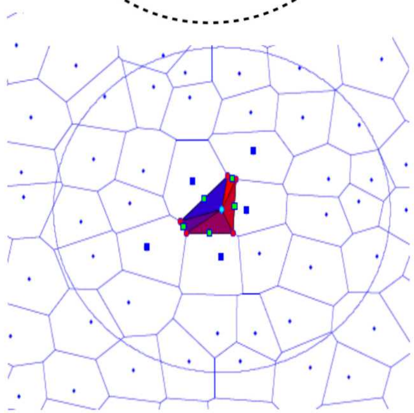


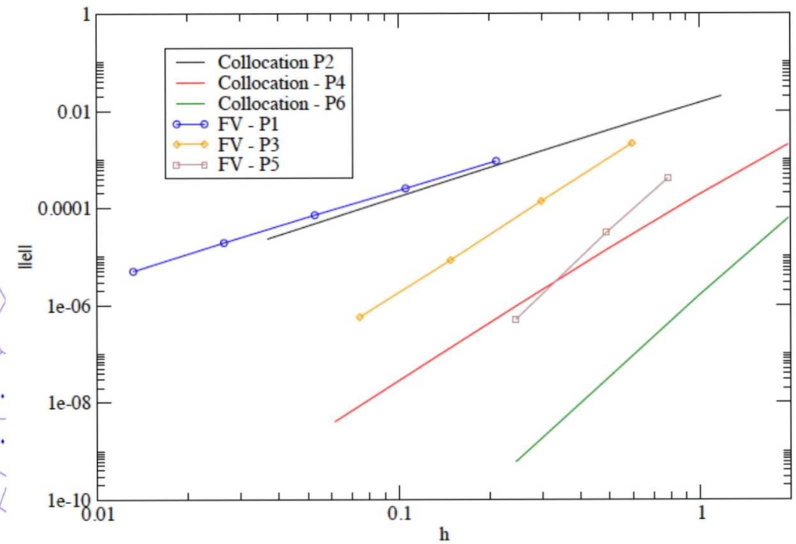


To generate mesh free schemes for $\nabla^2 \phi = f$:

		Finite difference	Finite volume
Target functional	τ_i	$\nabla^2 \phi(\boldsymbol{x}_i)$	$\int_{face} \nabla \phi \cdot d\boldsymbol{A}$
Reconstruction space	$\mathbf{V}$	P_m	P_m
Sampling functional	λ_j	$\phi(\boldsymbol{x}_j)$	$\phi(\boldsymbol{x}_j)$
Weighting function	W	$W(\lVert x_j - x_i \rVert)$	$W(\lVert x_j - x_i \rVert)$







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

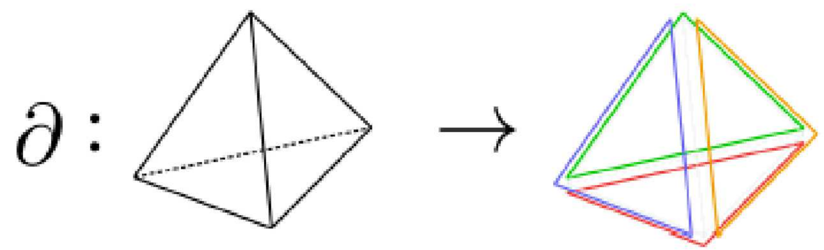
$$I_c[u] = \mathbf{v}_c^\intercal \mathbf{c}^*$$

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

Second ingredient for conservation: topology

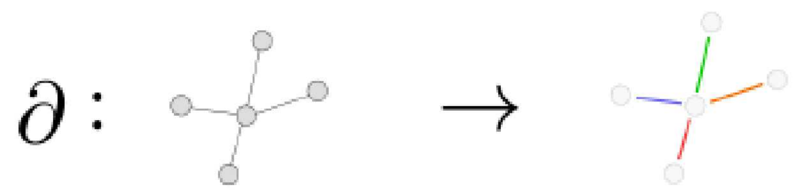
Generalized Stokes theorem

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



Gauss divergence theorem

$$\int_{C} \nabla \cdot \mathbf{u} dV = \oint_{F\in C} \mathbf{u} \cdot d\mathbf{A}$$



Definition 0.1. ϵ-ball graph: Given a point set X, consider the graph $G(N, E)$ embedded in Ω, where $N = X$ and $E = \{(i, j) \,|\, ||x_i - x_j||_2 \leq \epsilon\}$

Definition 0.2. Boundary operator: For all $n_i \in N$, define the operator

$$\partial : N \rightarrow E$$

where

$$\partial n_i = \{e(j, k) \in E \,|\, i = j \text{ or } i = k\}$$

Combinatorial Hodge theory: meshfree topology

Definition 0.1. k-clique: A k-tuple denoting a subset of k nodes $C \subset N$ such that every two distinct vertices are adjacent.

Definition 0.2. Boundary operator: A mapping ∂ from a k-clique to a $(k-1)$-clique.

Definition 0.3. Abstract simplicial complex: A collection $\mathcal{K}$ of k-cliques with associated boundary operators, satisfying $k \in \mathcal{K} \implies \partial k \in \mathcal{K}$, and $k_1, k_2 \in \mathcal{K} \implies k_1 \cap k_2 \in \partial k_1 \cap \partial k_2$.

Definition 0.4. Exterior derivative/coboundary operator: A linear map δ_k taking a k-clique to a $(k+1)$-clique, satisfying $\delta_k \delta_{k+1} = 0$.

- $\delta_0 = grad[s](i,j) := s_j - s_i$
- $\delta_1 = curl[X](i,j,k) := X_{ij} + X_{jk} + X_{ki}$

Definition 0.5. Adjoint operator: A linear map δ_k^* from k-cliques to $(k-1)$-cliques.

- $-div := \delta_0^*$

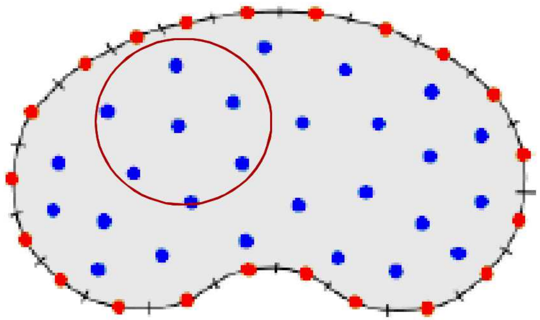
Jiang, Xiaoye, et al. "Statistical ranking and combinatorial Hodge theory." Mathematical Programming 127.1 (2011): 203-244.

Gameplan

- From our easily constructed graph, we have access to operators in combinatorial Hodge theory
  - Nice operators – exact sequence, summation-by-parts properties, etc
- Unfortunately – pure topological objects
  - We want a conservative approximation to the divergence
  - Combinatorial divergence does not converge to actual divergence
- Solution: Use GMLS to define integration functionals that use combinatorial divergence to define *virtual face areas* and *virtual cell volume* at nodes and edges to define an operator analogous to the mimetic divergence

$$DIV_h(\mathbf{u}) = \frac{1}{V} \sum_{F \in \partial C} \mathbf{A}_f \cdot \mathbf{u}_f$$

A virtual meshfree divergence theorem



We assume a collection of particles partitioned over the interior and boundary of the domain and characterized by a spacing lengthscale h ($\mathbf{X}_h = \mathbf{X}_i \cup \mathbf{X}_b$), and for each particle on the boundary x_b we associate a portion of the boundary ($\partial\Omega = \cup\Omega_b$).

Select a velocity space $\mathbf{V}_h = (\pi_1)^d$ and define $\mathbf{M}_h = div(\mathbf{V}_h)$.

Seek to define a discrete divergence theorem ansatz in terms of *virtual cells, virtual faces* and *physical boundary faces.*

$$I_c[\nabla \cdot \mathbf{F}] = \sum_{f \in \partial c} I_f[\mathbf{F}] + \chi_{c \in \mathbf{X}_b} \int_{\partial\Omega_c} \mathbf{F} \cdot d\mathbf{A}$$

which, under the assumption that $I_{f_{ij}} = -I_{f_{ji}}$ provides the following global conservation statement

$$\sum_c I_c[\nabla \cdot \mathbf{F}] = \sum_{c, f \in \partial c} I_f[\mathbf{F}] + \sum_{c \in \mathbf{X}_b} \int_{\partial\Omega_c} \mathbf{F} \cdot d\mathbf{A}$$

$$= \sum_{c \in \mathbf{X}_b} \int_{\partial\Omega_c} \mathbf{F} \cdot d\mathbf{A} = \int_{\partial\Omega} \mathbf{F} \cdot d\mathbf{A}$$

Truncation error of ansatz

Let $u \in C^1(\Omega)$. We assume the following ansatz for our *virtual divergence theorem.*

$$V_i \left(\partial_{x_\alpha} u\right)_i = \sum_{j,\beta} \boldsymbol{v}^{\alpha,\beta}_{f_{ij}} c^{\beta}_{ij}(u) + \chi_{i \in \partial\Omega} \int_{\partial\Omega_i} u \, dA^{\alpha}$$

where

- V_i and $v_{f_{ij}} = -v_{f_{ij}}$ are virtual volumes and face areas to be determined
- $c^{\beta}_{ij}(u)$ are GMLS coefficients associated with the β^{th} basis function of the GMLS reconstruction of u at the virtual face f_{ij}
- $\alpha \in 1, ..., d$ denotes the component of the gradient and virtual face normal

Objective:

Define V_i and $v_{f_{ij}}$ such that our VDT holds for any $u \in P_1$

Summation-by-parts ansatz

Assume virtual areas $v_{f_{ij}}$ may be expressed in terms of *virtual area potentials* multiplied by point evaluation of basis function at virtual face

$$\boldsymbol{v}_{f_{ij}}^{\alpha,\beta} = \left(\psi_j^{\alpha,\beta} - \psi_i^{\alpha,\beta}\right)\phi^\beta(\boldsymbol{x}_{ij})$$

Theorem. *Let $\boldsymbol{u} \in C_1(\Omega)$, and consider a set of virtual metric information $\left(\{V_i\}, \left\{\boldsymbol{v}_{f_{ij}}^{\alpha,\beta}\right\}\right)$ that define a P_1-reproducing SBP operator. Assume that the virtual face moments satisfy the scalings, $|\psi_j^{\alpha,\beta} - \psi_i^{\alpha,\beta}| \leq C_f h^{d-1}$ and $|V_i| \leq C_c h^d$ for all α, β, i, j. If $P_1 \subset \Pi$, then there exists $C > 0$ such that the following estimate holds at each virtual cell*

$$|\nabla \cdot \boldsymbol{u} - \nabla_h \cdot \boldsymbol{u}|_i \leq Ch$$

where $\nabla_h \cdot \boldsymbol{u} = \sum_\alpha (\partial_{x_\alpha} u^\alpha)_i$.

How to get the areas?

For each $\phi^\beta \in V$, plug into ansatz and get

$$\sum_j \left(\psi_j^{\alpha,\beta} - \psi_i^{\alpha,\beta}\right) \phi^\beta(\boldsymbol{x}_{ij}) = V_i \left(\partial_{x_\alpha} \phi^\beta\right)_i - \chi_{I \in \partial\Omega} \int_{\partial\Omega_i} \phi^\beta \, dA^\alpha$$

Assume we have a process for generating volumes satisfying

- $\sum V_i = |\Omega|$
- $V_i > 0$

then this provides a weighted-graph Laplacian problem for each area moment, with RHS satisfying Fredholm alternative necessary for singularity.

Solve $d+1$ graph Laplacian problems, each with d RHSs, using AMG for $O(N)$ work.

How to get the volumes?

Assumed we have a process for generating volumes satisfying

- $\sum V_i = |\Omega|$
- $V_i > 0$

Solve

$$V_i = \text{argmin} \sum_i V_i^2 w_i$$

Such that

$$\sum_i V_i = |\Omega|$$

where

$$w_i = \sum_j \phi(|x_i - x_j|)$$

$$V_i = \frac{1}{w_i} \left(\frac{|\Omega|}{\sum_j \frac{1}{w_j}} \right)$$

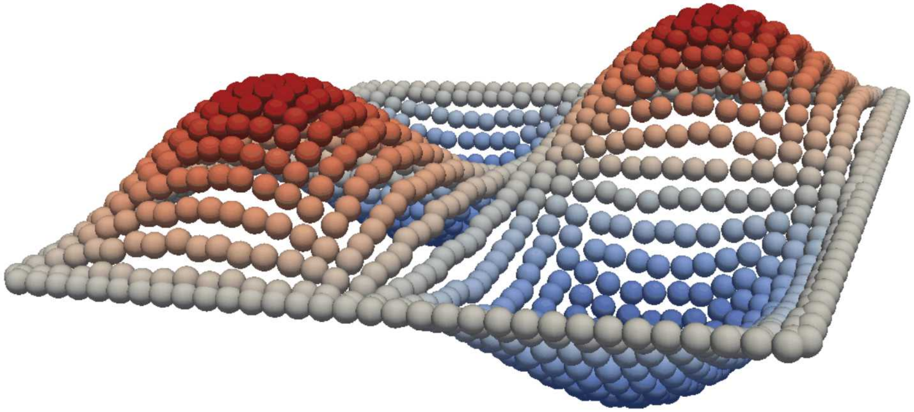
Lemma 0.1. *Assume a quasi-uniform points X. Then there exist $C_1, C_2 > 0$ such that*

$$C_1 h^d \leq V_i \leq C_2 h^d$$

Convergence of divergence operator

$$V_i = \frac{1}{w_i}\left(\frac{|\Omega|}{\sum_j \frac{1}{w_j}}\right)$$

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



Results: singularly perturbed advection-diffusion

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:**

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

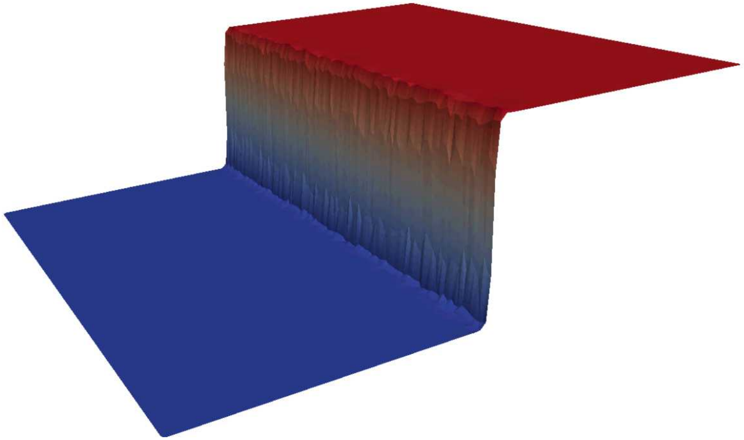
All problems will be shown for discontinuous material properties to highlight flux continuity of approach.

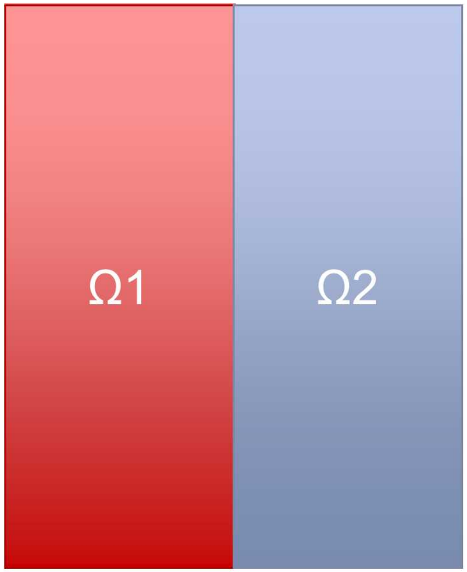
Darcy: jumps in material properties

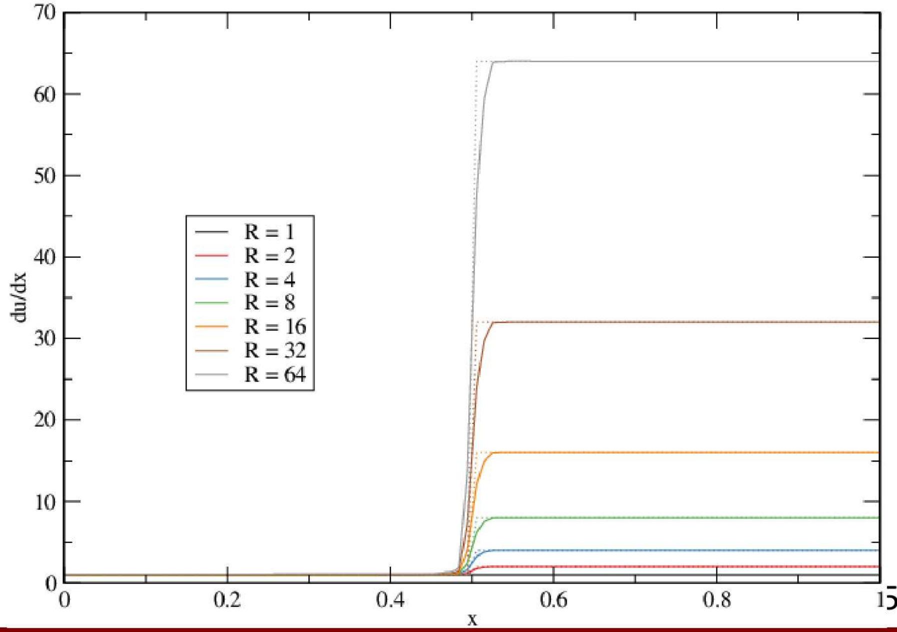
Flux continuity across interface

$$[\mu \nabla \phi \cdot \hat{n}] = 0$$

$$\nabla \phi \rightarrow$$





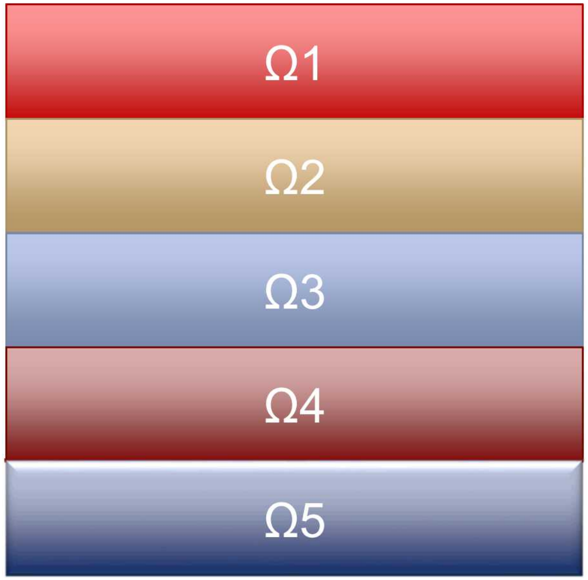


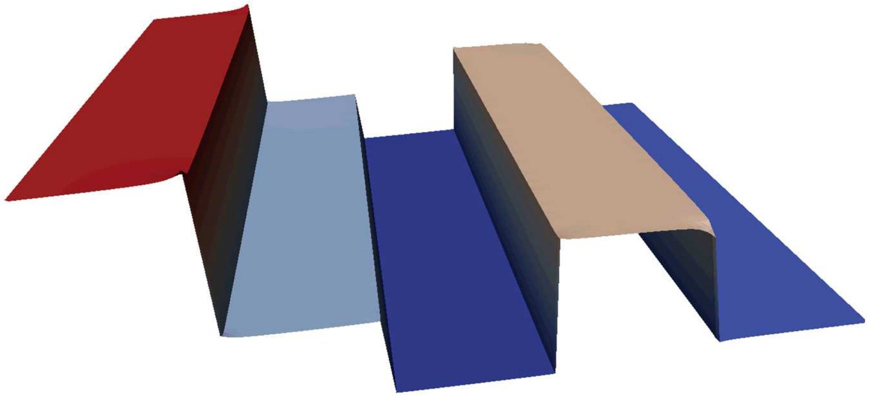
Darcy: jumps in material properties

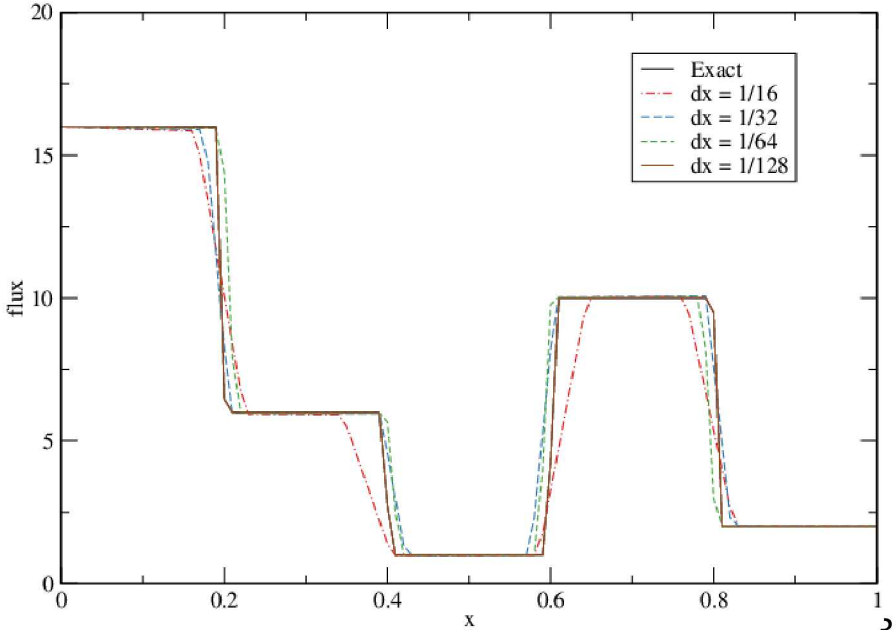
Zero flux normal to interface
admits discontinuous fluxes

$$[\mu \nabla \phi \cdot \hat{n}] = 0$$

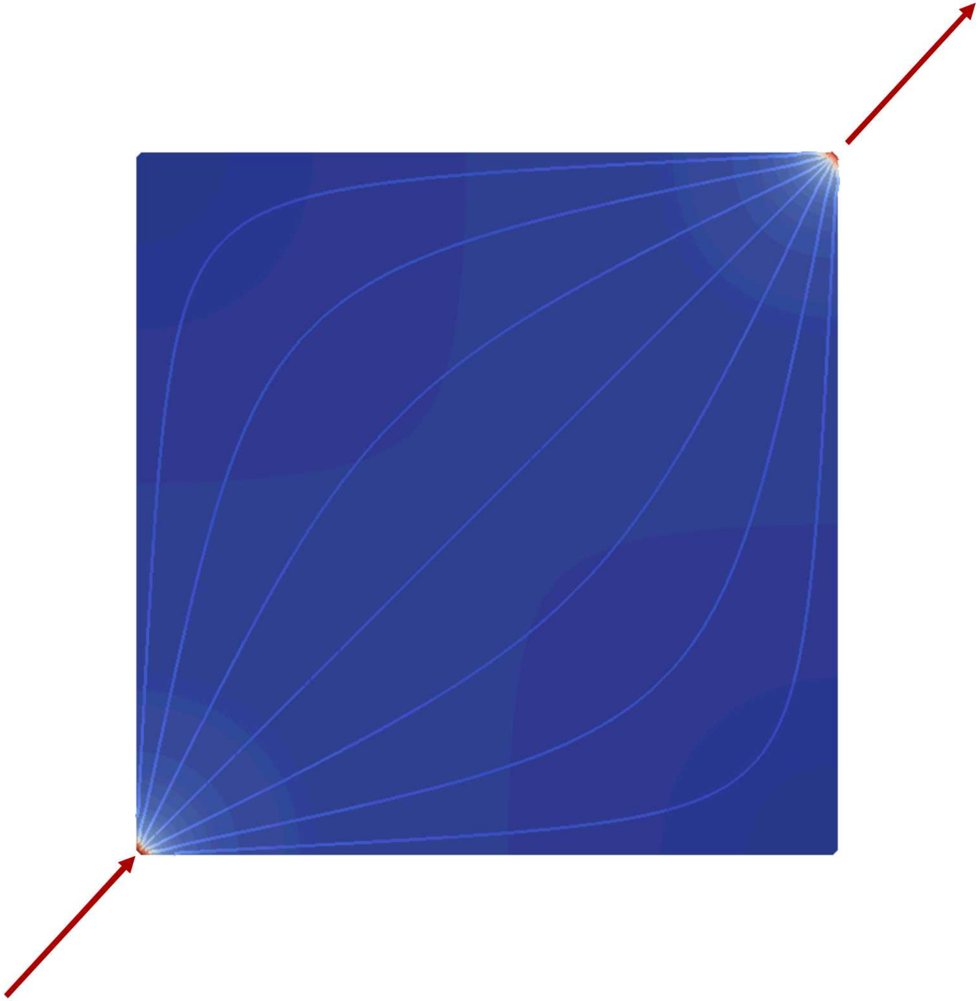
$$\nabla \phi \rightarrow$$

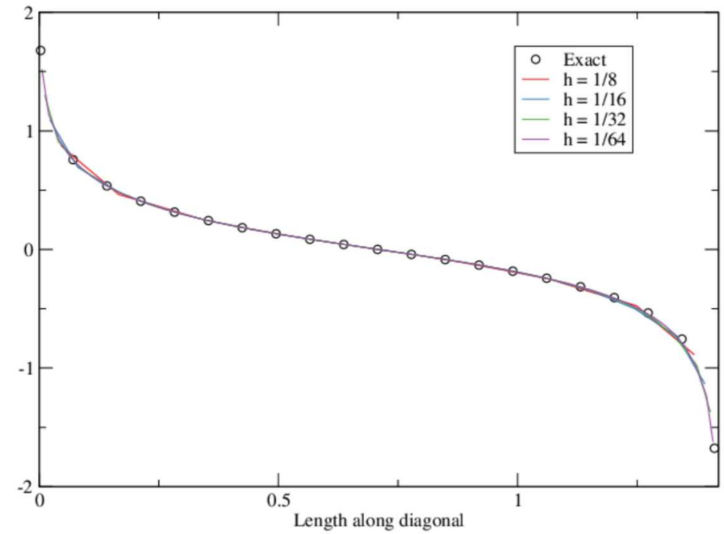


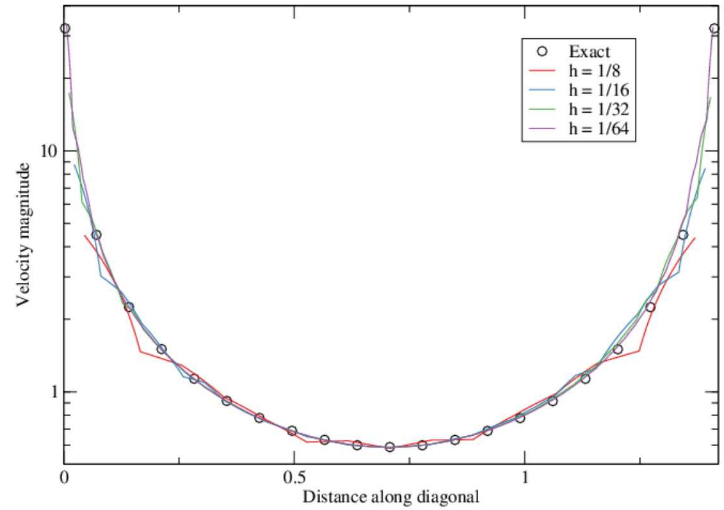




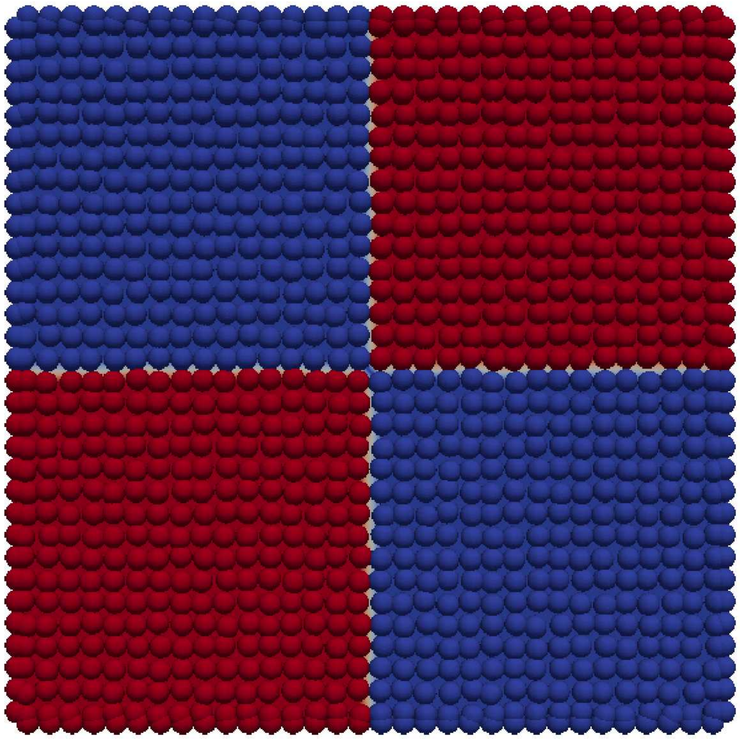
Darcy: 5-spot problem

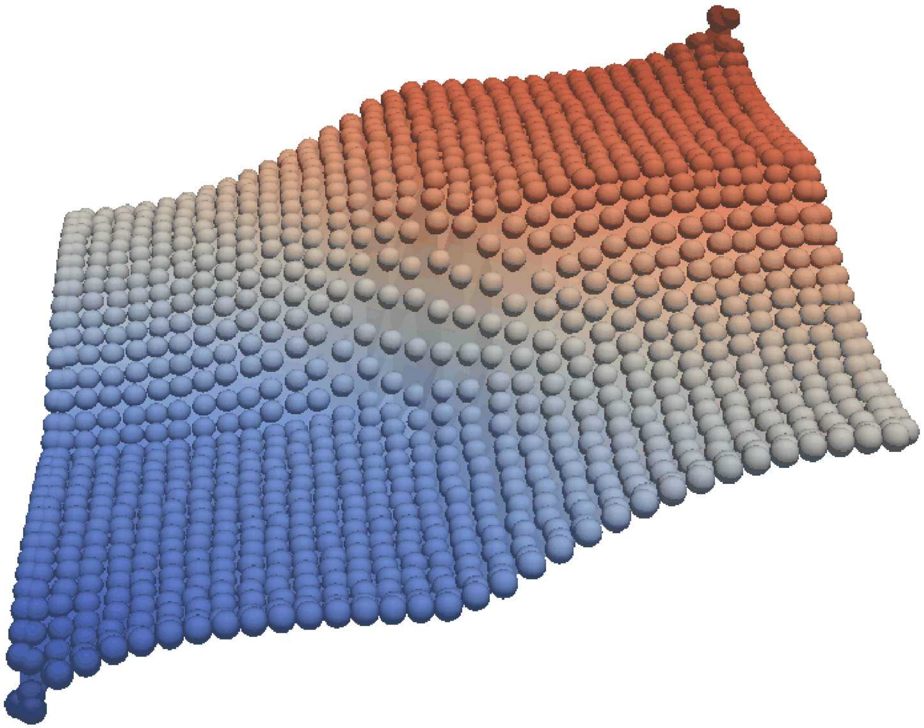




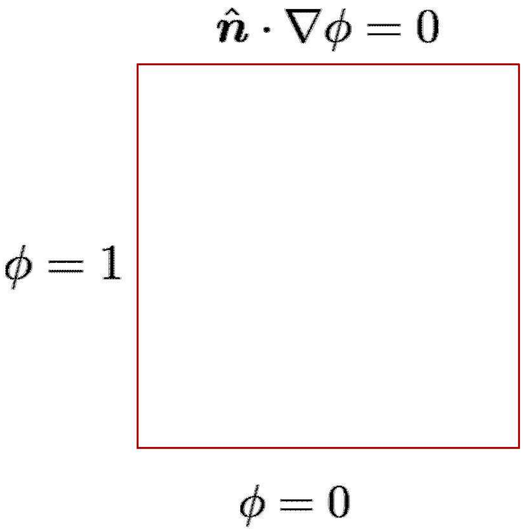


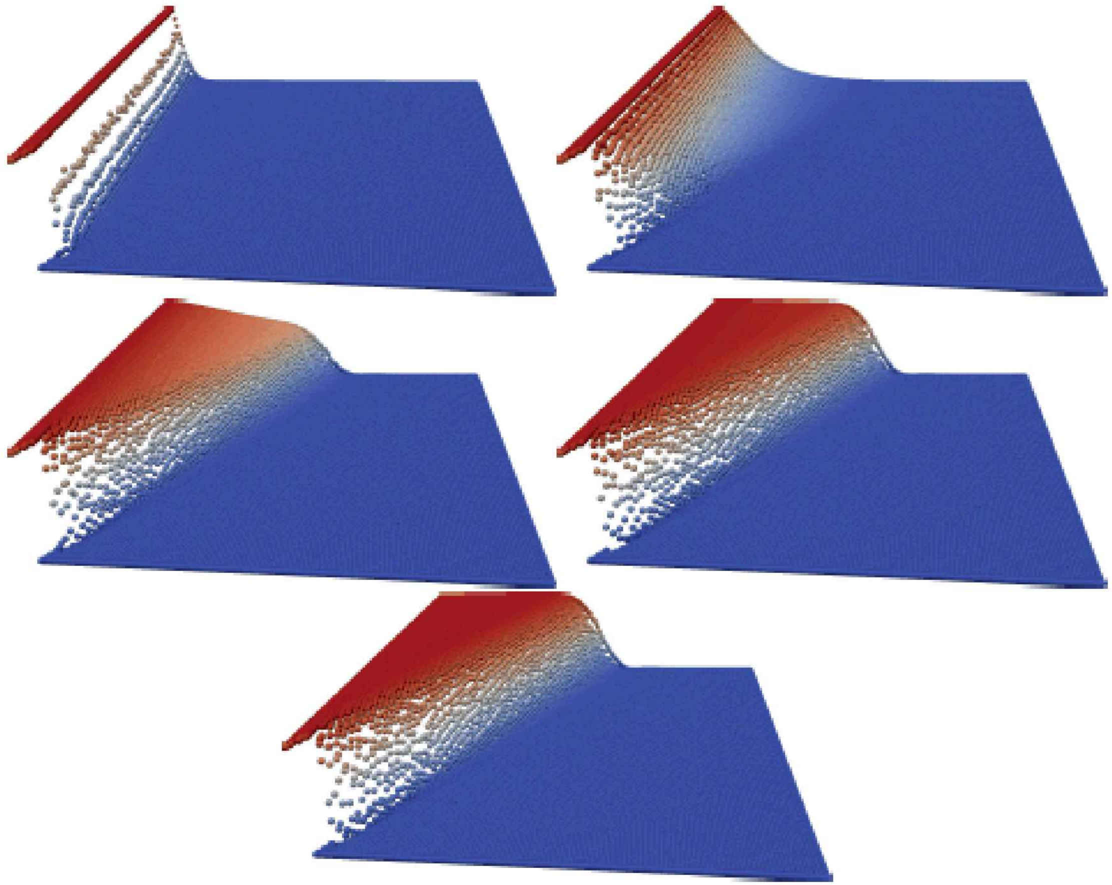
Darcy 5-spot problem





Singularly perturbed advection diffusion



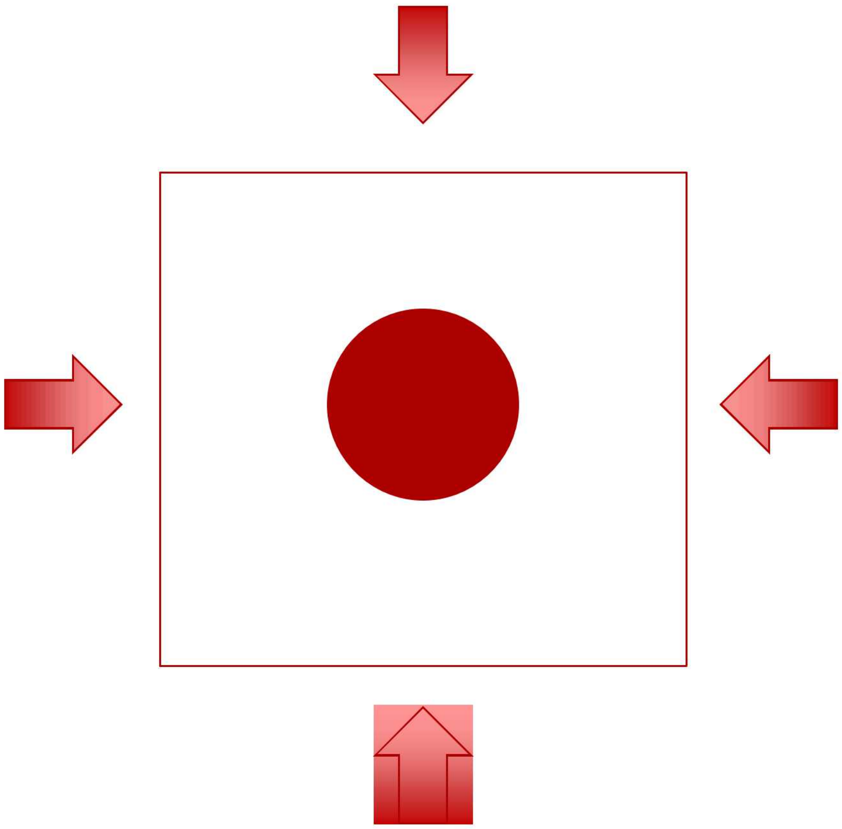


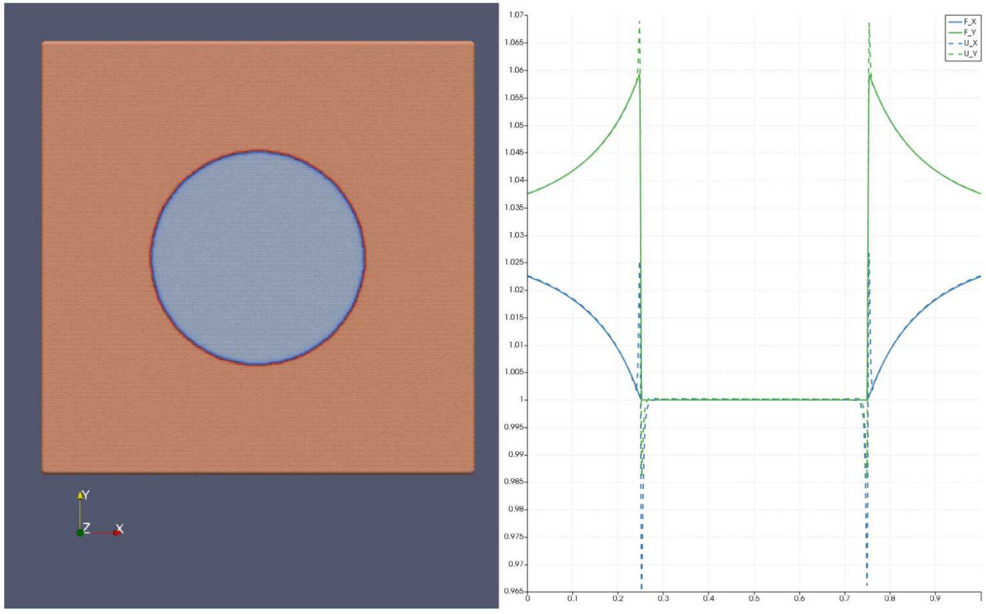
$$\frac{\partial}{\partial t}\phi + \nabla \cdot \mathbf{F} = 0$$

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

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

Linearly elastic composite materials





Hydrostatic loading of a stiff inclusion
- Normal stress continuity across interface

Conclusions

- We have illustrated how GMLS may be used to pair **metric information** together with **function approximation**, obtaining the two key ingredients to generating conservative meshfree discretizations
- We presented an ansatz for a **meshfree divergence theorem**, and illustrated how it may be solved efficiently via graph Laplacian problems
- We presented a number of applications where we are able to obtain consistent + conservative solutions for problems that present challenges for other discretizations that lack **H(div) conformity**
- For the first time, a rigorous meshfree method with discrete **conservation**, **convergence**, and **scalability**, replacing **geometric problem** of mesh generation with **scalable algebraic one**