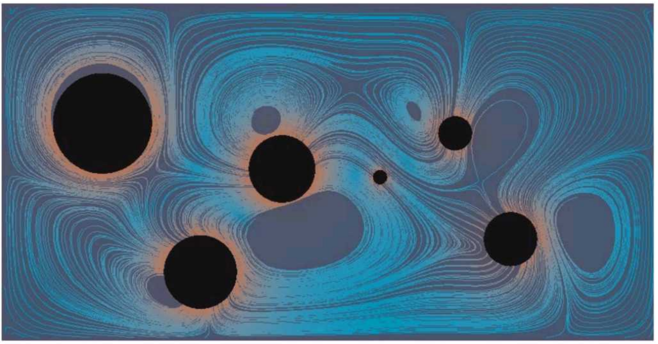
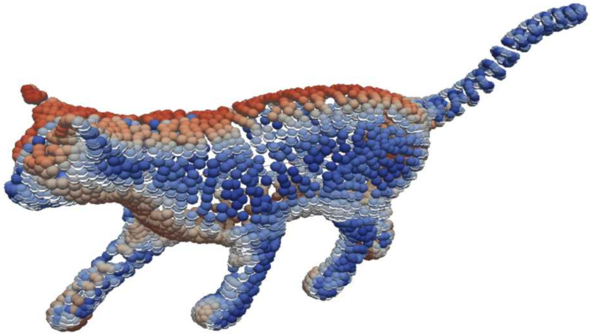
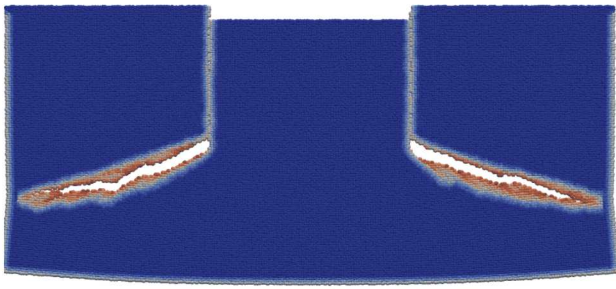
SAND2019-1062PE







Spatially compatible meshfree discretization

CCR
Center for Computing Research

Nat Trask

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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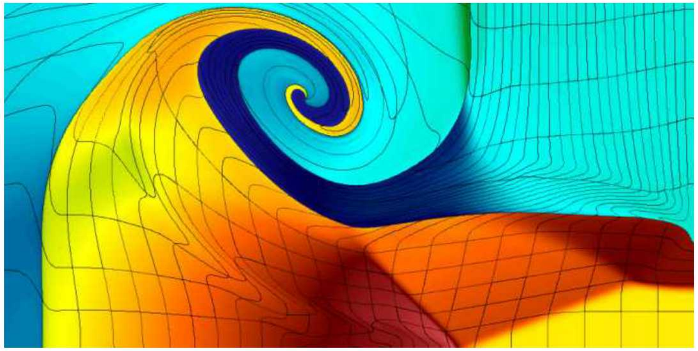
Talk overview

- An introduction to generalized moving least squares (GMLS)
  - A high-level summary of approximation theory
  - A brief survey of our ongoing work
- Conservation principles for meshfree discretization
  - How to obtain a conservative method, when we don't have a mesh to apply the Gauss divergence theorem to
- Asymptotically compatible strong-form discretizations of non-local mechanics
  - An integral theory of continuum mechanics
  - Combining in a meshfree framework allows for consistent coupling of multiphysics+fracture

Why use 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

Compadre – **Com**patible **Par**ticle **D**iscr**e**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

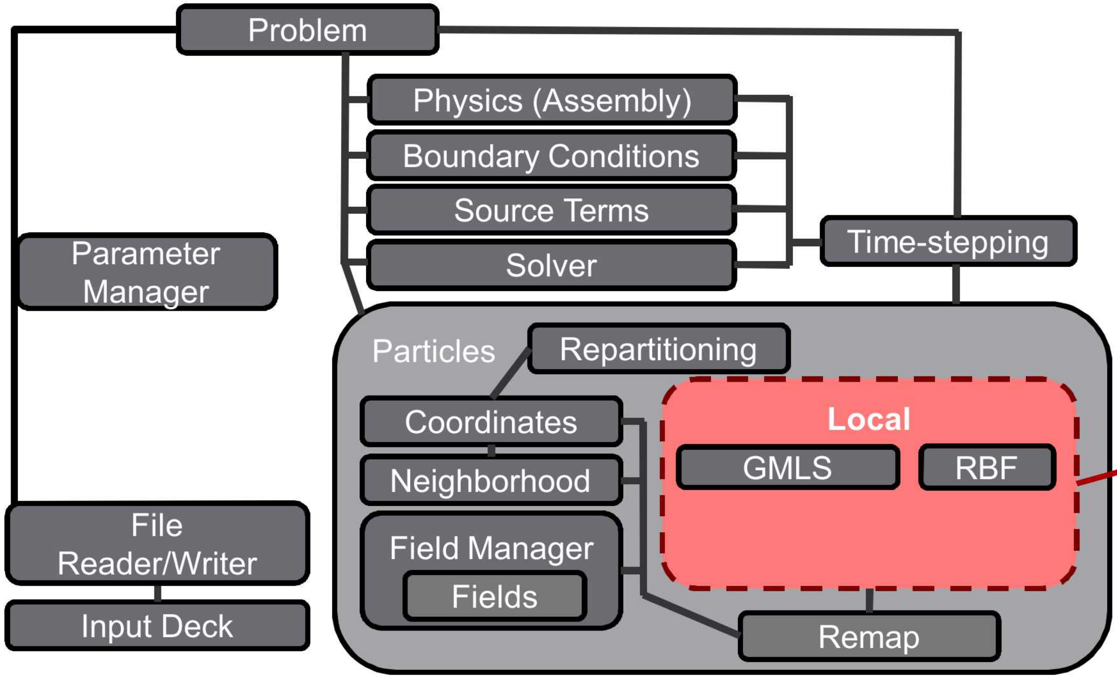
Students/collaborators:

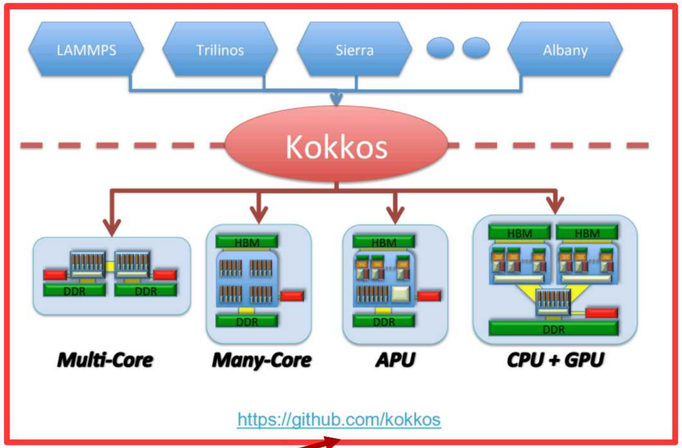
- Huaiqian You, Yue Yu – Lehigh
- Amanda Howard, Martin Maxey – Brown
- Wenxiao Pan – UW Madison
- Paul Atzberger – UC Santa Barbara
- J.S. Chen – UC San Diego

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

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:

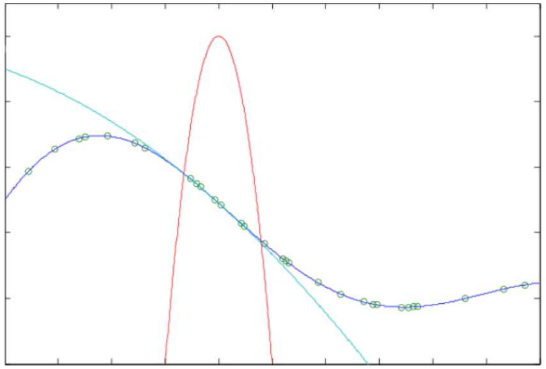
Approximate point evaluation of derivatives:

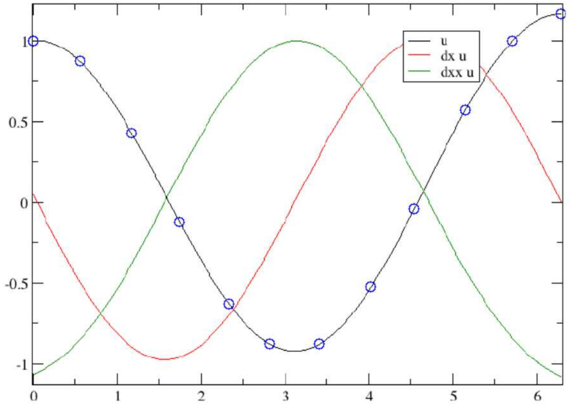
Target functional $\tau_i = D^\alpha \circ \delta_{x_i}$

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:

$$\tau^h(u) := \sum_j \alpha_j \lambda_j(u)$$

Approximation theory sketch: local reproduction

Given linear bounded functional τ, and an approximation $\tau_h = \sum_j s_{\lambda_j,\tau} \lambda_j(u)$.

We assume τ may be associated with a point x. A process for generating the coefficients $\{s_{\lambda_j,\tau}\}$ is a local reproduction over V if:

1. $\sum_j s_{\lambda_j,\tau} \lambda_j(p) = \tau(p)$ for all $p \in V$
2. $\sum_j |s_{\lambda_j,\tau}| < C_1 \, h^{-\alpha}$
3. $s_{\lambda_j,\tau}$ if $||x - x_j|| < C_2 h$

- GMLS may be shown to satisfy condition one, provided a solution exists to the optimization problem, and condition three by choice of kernel.
- Satisfaction of condition two depends upon the target and sampling functionals under consideration.

Truncation error sketch

Let $p \in V$.

$$\begin{aligned}|\tau(u) - \tau_h(u)| \leq & |\tau(u) - \tau(p)| + |\tau_h(p) - \tau_h(u)| \\ \leq & |\tau(u) - \tau(p)| + \sum_j |s_{\lambda_j,\tau}| \, |\lambda_j(p) - \lambda(u)| \\ \leq & ||\tau(u) - \tau(p)||_{L^\infty(\Omega)} + C_1 h^{-\alpha} ||\lambda_j(u) - \lambda(p)||_{L^\infty(\Omega)}\end{aligned}$$

To proceed, a specific choice must be made for operators. For example, Mirzaei estimates point evaluation of derivatives from point evaluation of functions.

$$\text{Let } u \in C^m(\Omega), \tau := D^\alpha \circ \delta_i, \lambda_j := \delta_j, V := P_m$$

Taking p as the Taylor series about x_i leads to the following estimate

$$||D^\alpha u - D_h^\alpha u||_{L^\infty(\Omega)} \leq C h^{m+1-|\alpha|} |u|_{C^{m+1}(\Omega)}$$

Mirzaei, Schacback, Dehghan. “On generalized moving least squares and diffuse derivatives” IMA Journal of Numerical Analysis (2012)

A rigorous framework for designing schemes

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

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

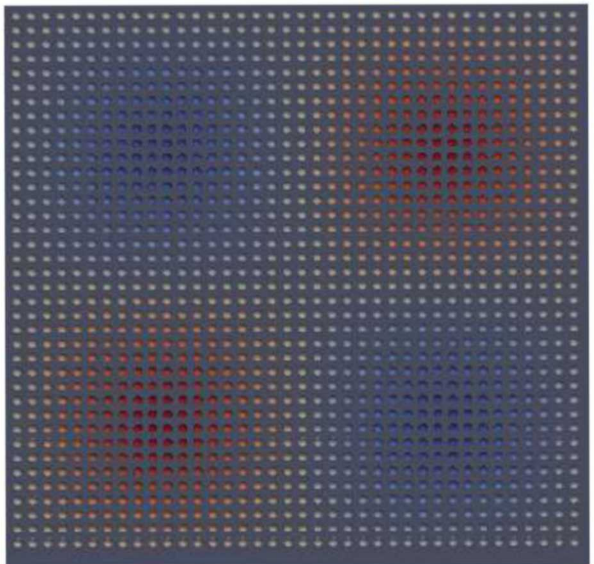
$\tau(u) = div(u)$ $\quad$ $\tau(u) = \int_{B(x)} K(x,y)u(y) - u(x)dy$ $\quad$ $\tau(u) = \int_{\partial\Omega} \sigma(u) \cdot d\mathbf{A}$

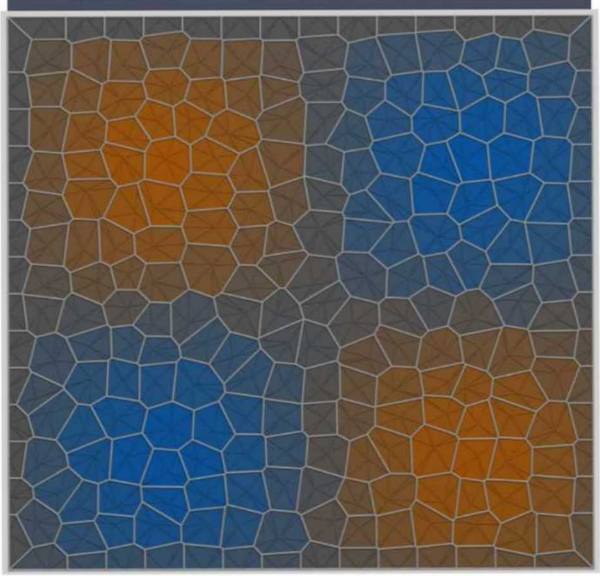
$\lambda_i^e(\mathbf{u}) := \frac{1}{|e_i|} \int_{e_i} \mathbf{u} \cdot \mathbf{t}_i$ $\quad$ $\lambda_i^f(\mathbf{u}) = \frac{1}{|f_i|} \int_{f_i} \mathbf{u} \cdot \mathbf{n}_i$ $\quad$ $\lambda_i^v(u) := \frac{1}{|V_i|} \int_{V_i} u(y)\, dy$

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

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

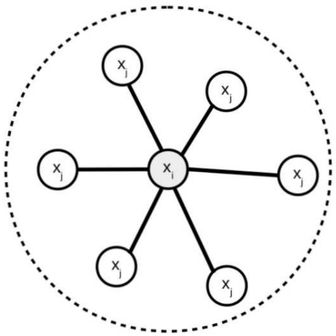
Solving PDEs with or without a mesh

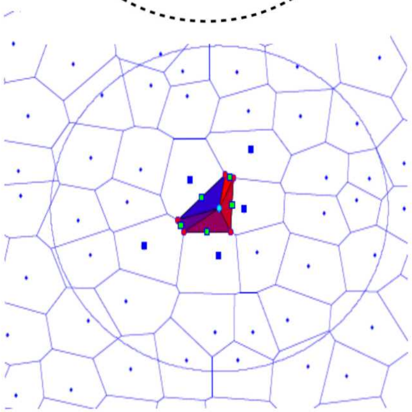


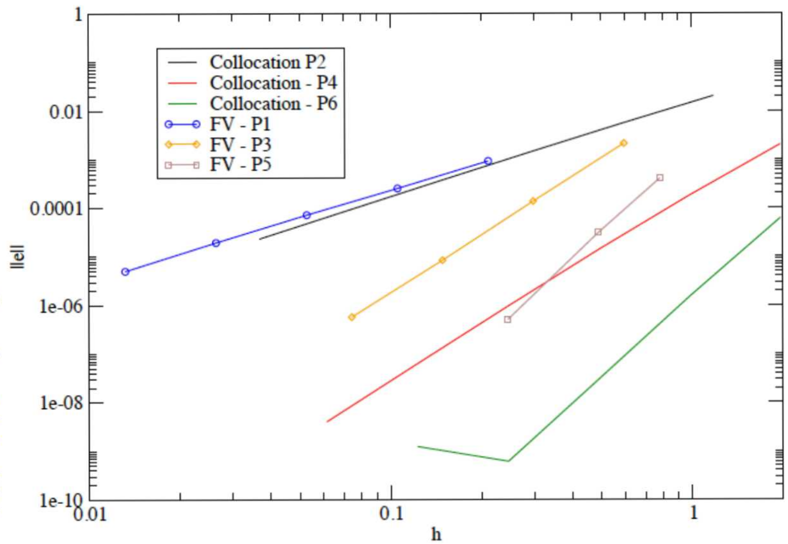


To generate mesh free schemes for $\nabla^2 \phi = f$:

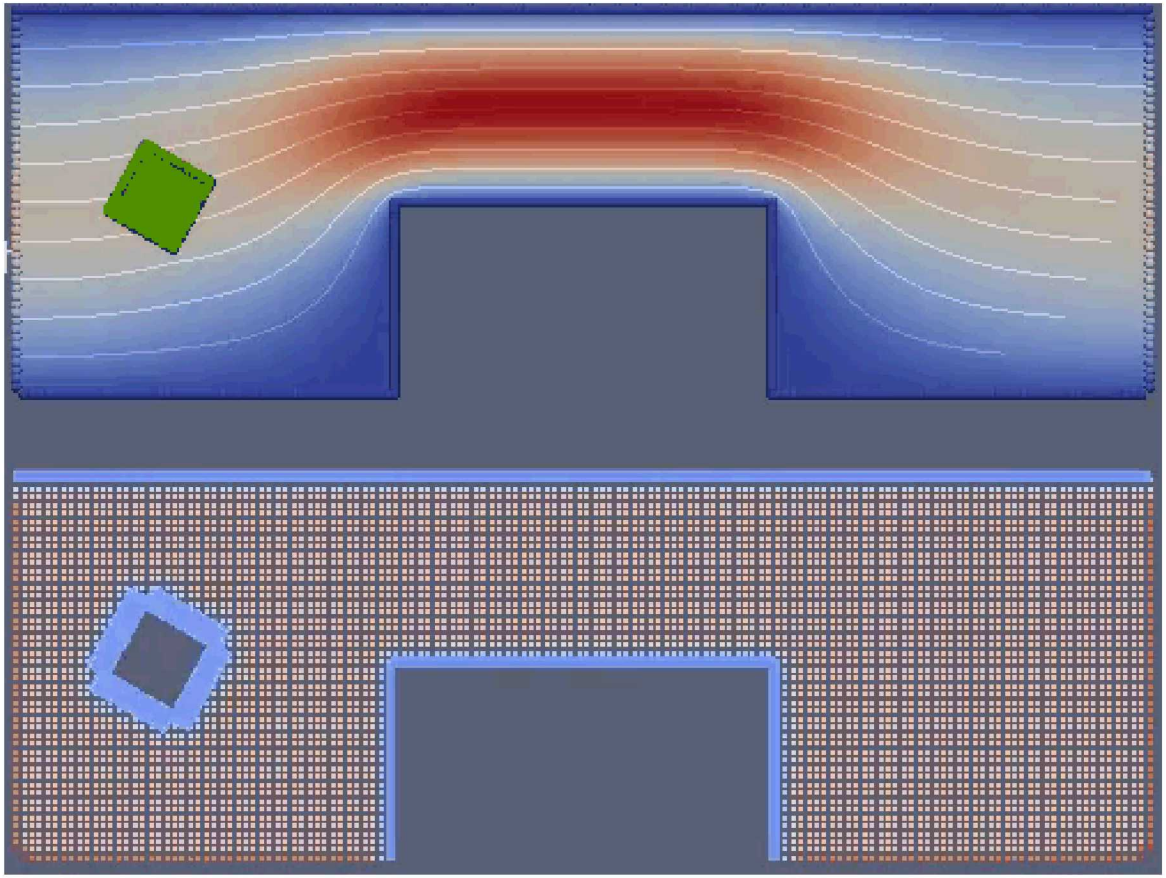
		Finite difference	Finite volume
Target functional	τ_i	$\nabla^2 \phi(\boldsymbol{x}_i)$	$\int_{face} \nabla \phi \cdot d\boldsymbol{A}$
Reconstruction space	$\mathbf{V}$	P_m	P_m
Sampling functional	λ_j	$\phi(\boldsymbol{x}_j)$	$\phi(\boldsymbol{x}_j)$
Weighting function	W	$W(\lVert \boldsymbol{x}_j -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







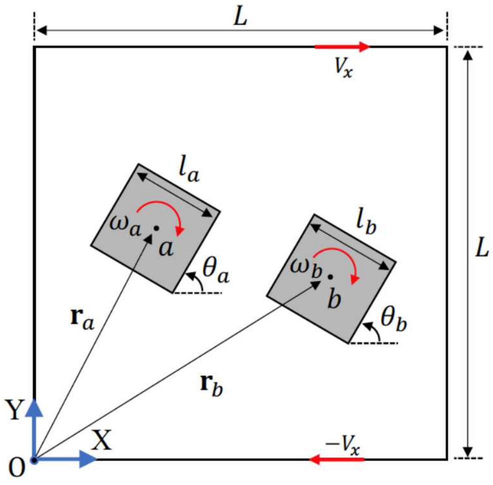
Example: Choosing approximation space

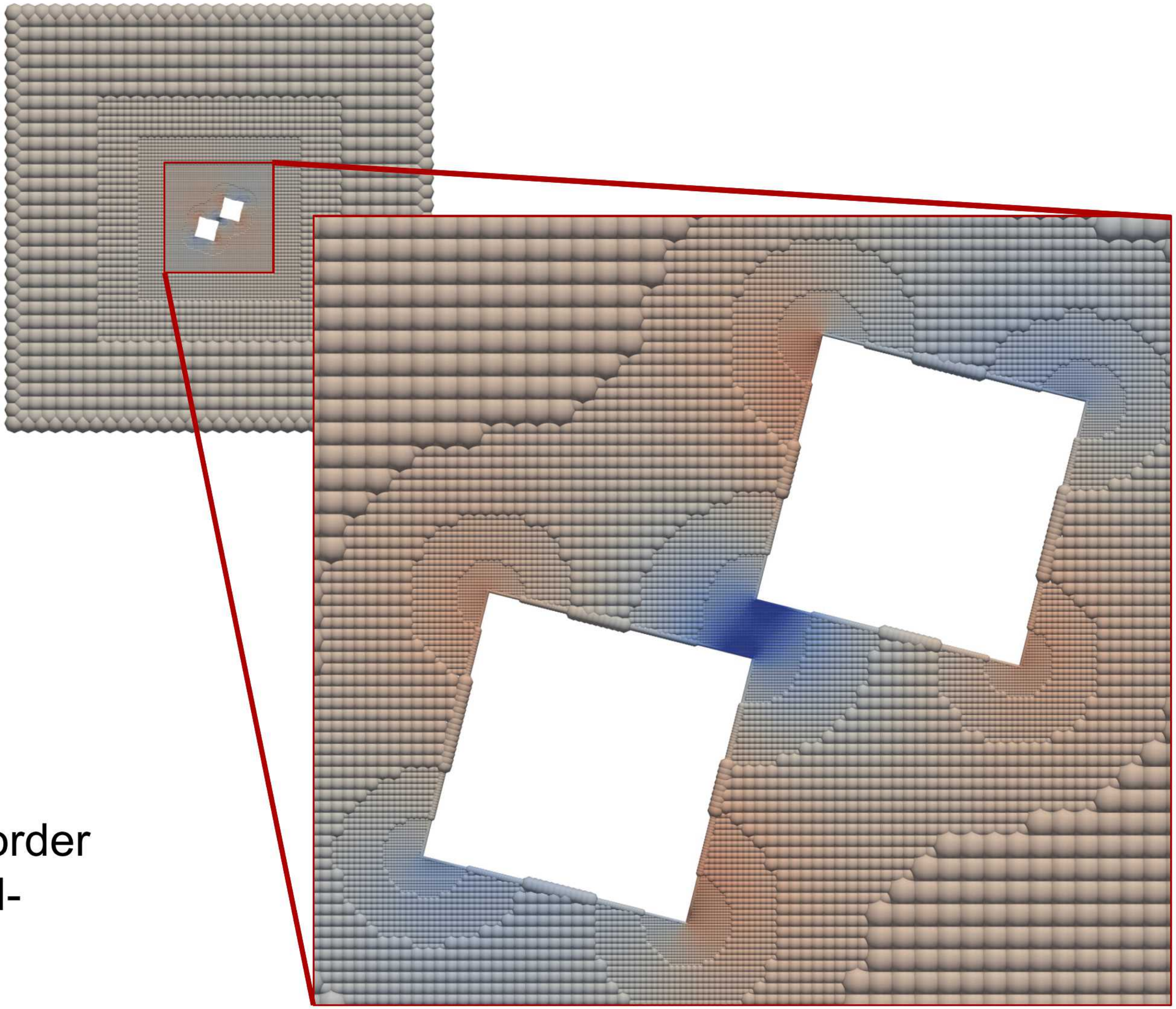


$$\begin{cases} -\nabla^2 \mathbf{u} + \nabla p = \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \\ \mathbf{u}|_{\partial\omega} = \mathbf{U} + (x - \mathbf{X}) \times \Omega \\ \int_{\partial\omega} \sigma \cdot d\mathbf{A} = 0 \end{cases}$$

Trask, N., Maxey, M.,, and Hu, X. "A compatible high-order meshless method for the Stokes equations with applications to suspension flows." *Journal of Computational Physics* 355 (2018): 310-326.

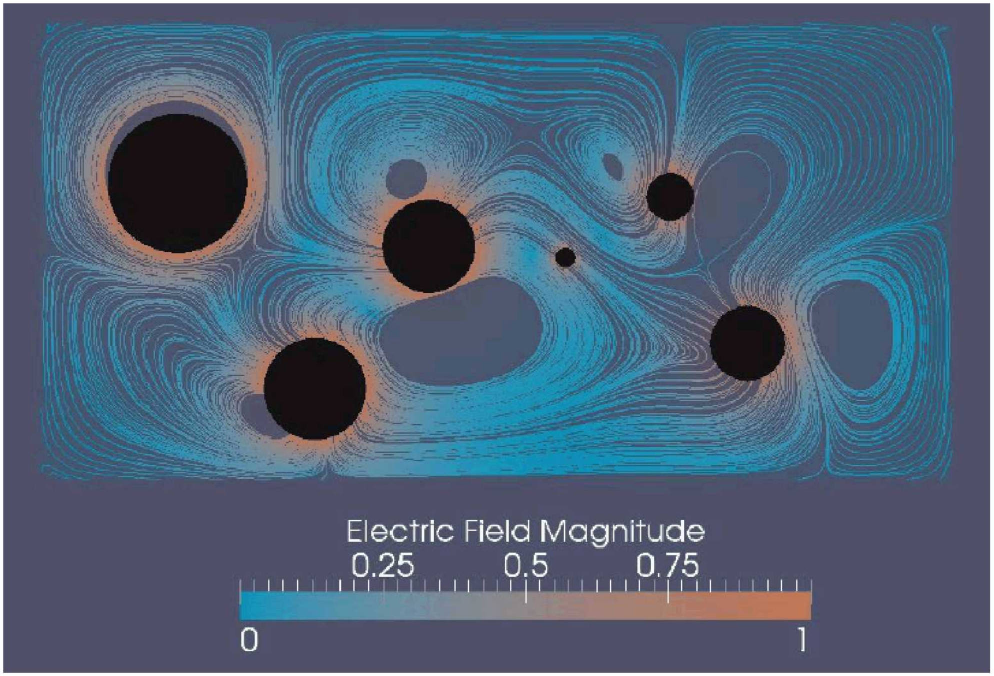
Example: Choosing kernel





Hu, Trask, Hu, Pan
“A spatially adaptive high-order meshless methods for fluid-structure interactions”
(In review, CMAME)

Example: Choosing approximation space



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

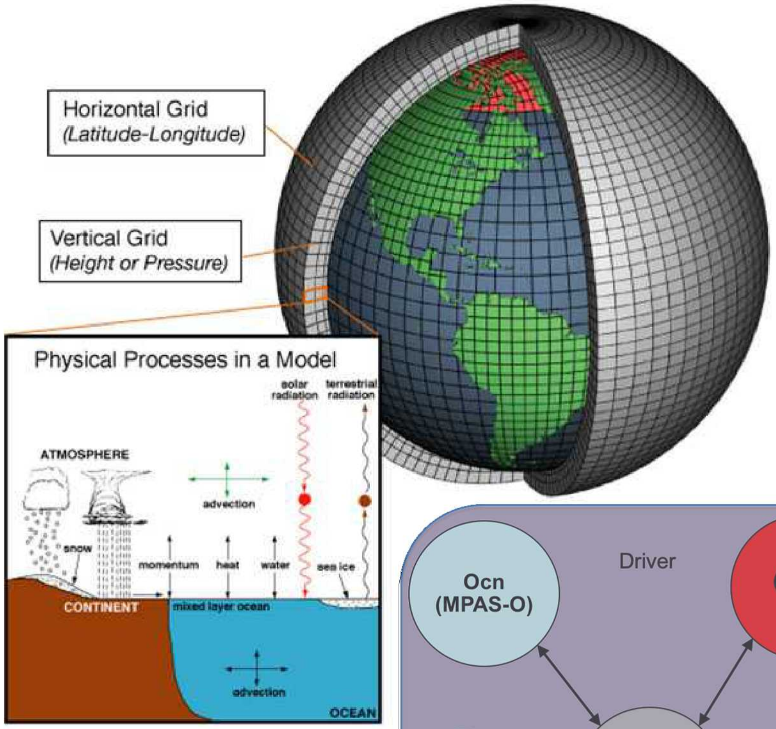
$$
-l_c^2\nabla^4\phi + \nabla^2\phi = -\frac{\rho_e(\phi)}{\epsilon}
$$

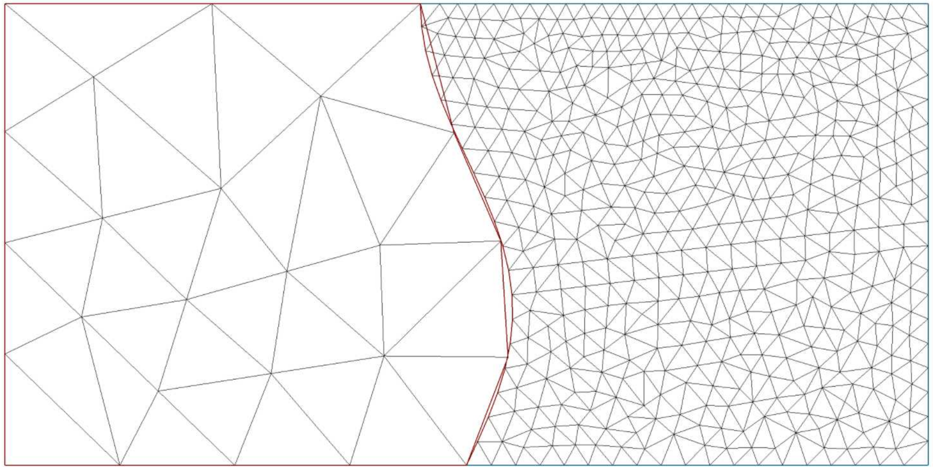
$$
\begin{cases}
0 = \int_{\partial\Omega_i} \overline{\overline{\sigma}}\cdot d\mathbf{A} \\
0 = \int_{\partial\Omega_i} \overline{\overline{\sigma}}\times(x - \mathbf{X}_i)\cdot d\mathbf{A}
\end{cases}
$$

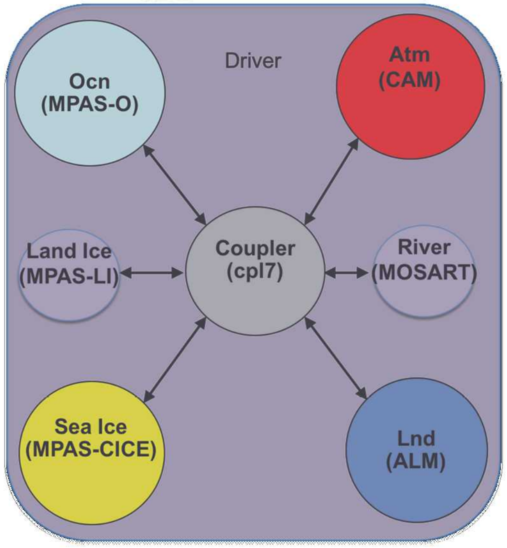
$$
\overline{\overline{\sigma}} = -\epsilon_0\left(\mathbf{E}\otimes\mathbf{E} + E^2\mathbf{I}\right) + -p\mathbf{I} + \frac{\nu}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^\intercal\right)
$$

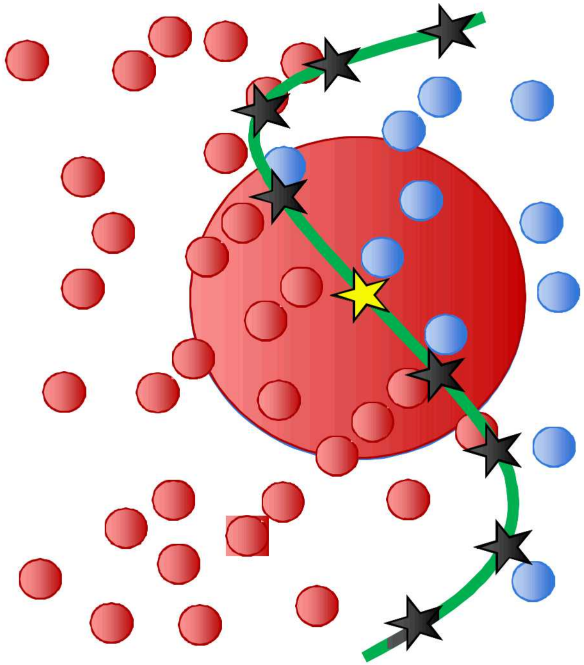
A compatible Stokes solver provides a high-order foundation for multiphysics problems in FSI

Example: Choosing sampling functional

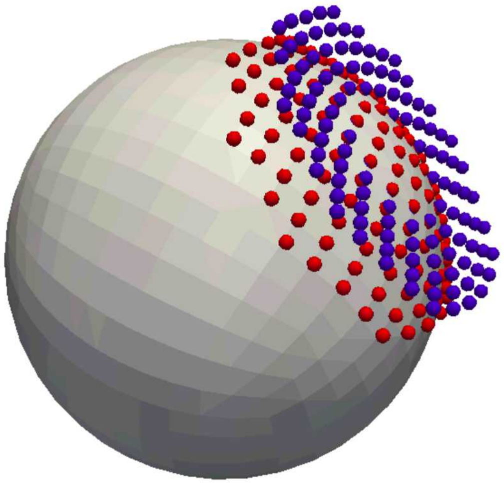


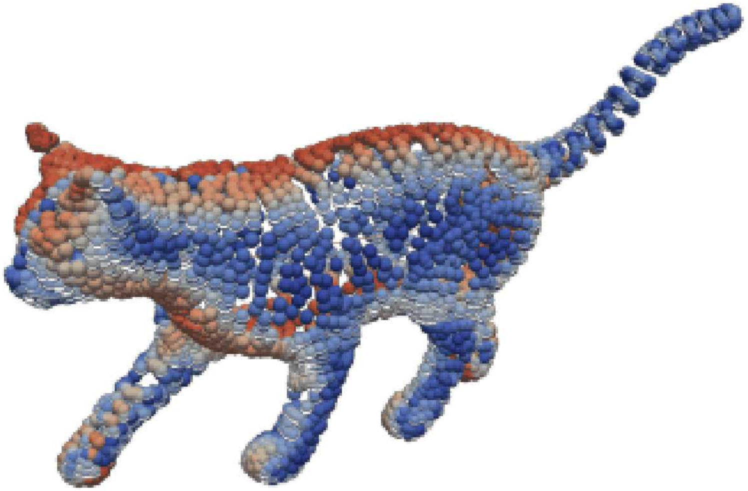


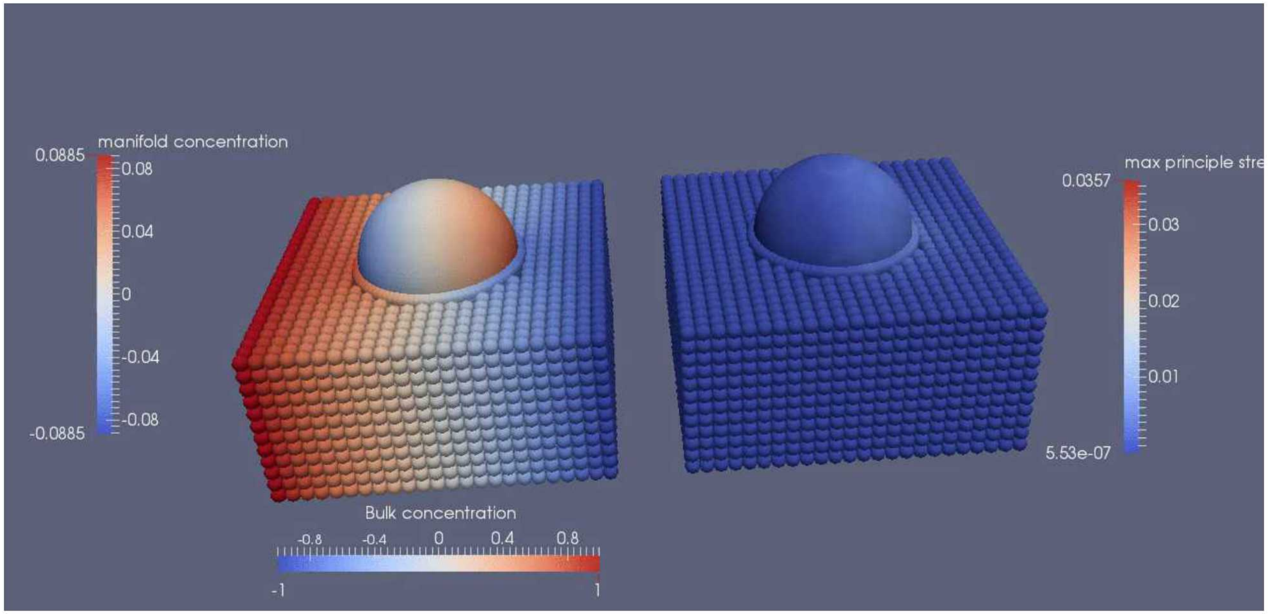




Example: Choosing target functional





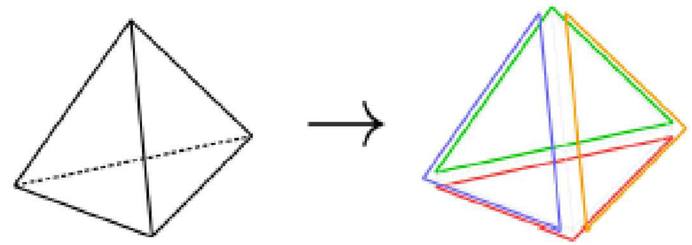


Why is conservation hard in meshfree?

Generalized Stokes theorem

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

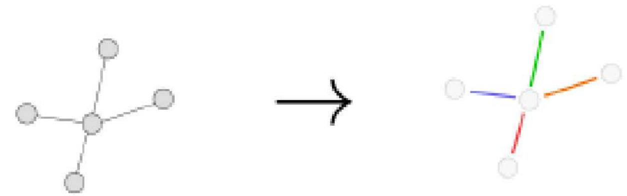
$\partial :$



Gauss divergence theorem

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

$\partial :$



Two ingredients:

- A chain complex
    - A topological structure with a well-defined boundary operator
- An exterior derivative
    - A consistent definition of a divergence

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

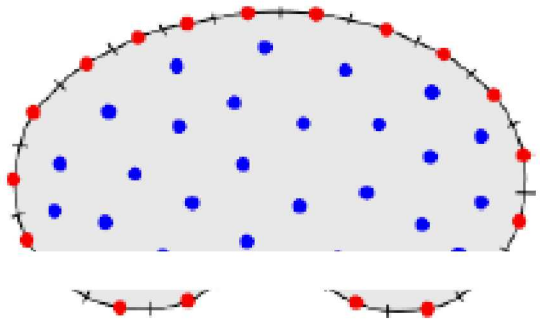
$$\mathbf{v}_c = \int_c \mathbf{P} dx$$

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.

Ansatz for a meshless Gauss divergence theorem



Recall classical FVM:

$$V_i \left(\nabla \cdot \mathbf{u}\right)_i = \sum_{f_{ij} \in \partial C_i} \mathbf{u}_{ij} \cdot \mathbf{A}_{ij}$$

Want to define ***virtual metric information****, so that* $\forall \mathbf{u} \in P^1$

$$\mu_i \left(\nabla \cdot \mathbf{u}\right)_i = \sum_{j \in B(x_i)} \mathbf{c}_{ij} \cdot \mu_{ij}$$

Assume physical metric information on domain boundary, and $\mu_{ij} = -\mu_{ji}$*, then*

$$\sum_i \mu_i \left(\nabla \cdot \mathbf{u}\right)_i = \sum_{i,j \in B(x_i)} \mathbf{c}_{ij} \cdot \mu_{ij} = \int_{\partial \Omega} \mathbf{u} \cdot d\mathbf{A}$$

An ansatz for orientable virtual faces

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

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

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

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

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

How to get the areas?

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

$$\sum_j \left(\psi_j^\alpha - \psi_i^\alpha\right) \phi^\alpha(\boldsymbol{x}_{ij}) = \mu_i \left(\nabla \cdot \phi^\alpha\right)_i - \chi_{I \in \partial\Omega} \int_{\partial\Omega_i} \phi^\alpha \cdot d\mathbf{A}$$

Assume we have a process for generating volumes satisfying

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

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.

Results: singularly perturbed advection-diffusion

Consider conservation laws

$$\partial_t \phi + \nabla \cdot \mathbf{F}(\phi) = 0$$

Where we will assume steady state and the following fluxes:

- **Darcy:**

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

- **Singularly perturbed advection diffusion:**

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

Skip lots of details: but we'll show how we handle benchmarks that challenge conventional mesh-based methods

How to get the volumes?

Assumed we have a process for generating volumes satisfying

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

Pose as a constrained quadratic program

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

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

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

With analytic solution

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

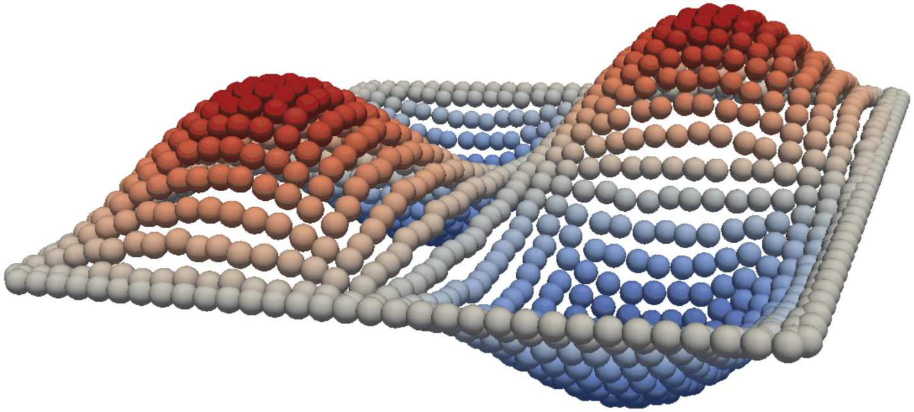
Lemma. *Assume a quasi-uniform set of points X. Then there exist* $C_1, C_2 > 0$ *satisfying*

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

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:**

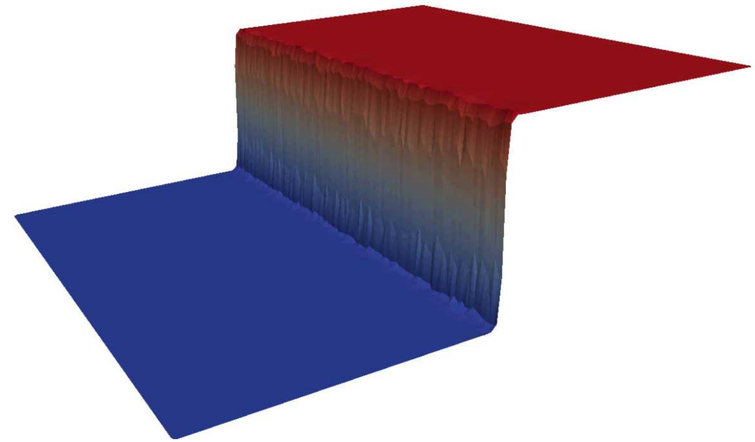
$$\boldsymbol{F} = \lambda \left(\nabla \cdot \boldsymbol{u} \right) \boldsymbol{I} + \mu \left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}} \right)$$

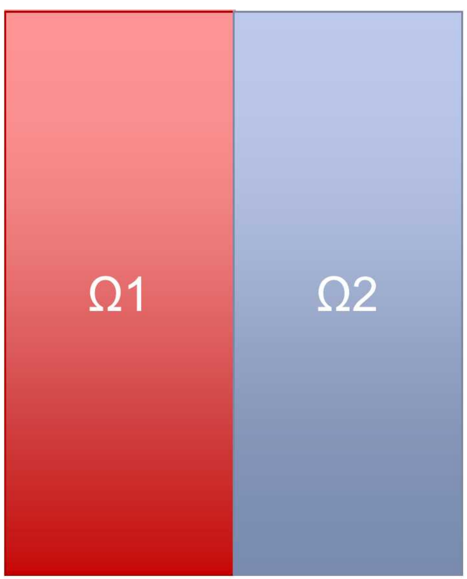
All problems will be shown for discontinuous material properties to highlight flux continuity of approach.

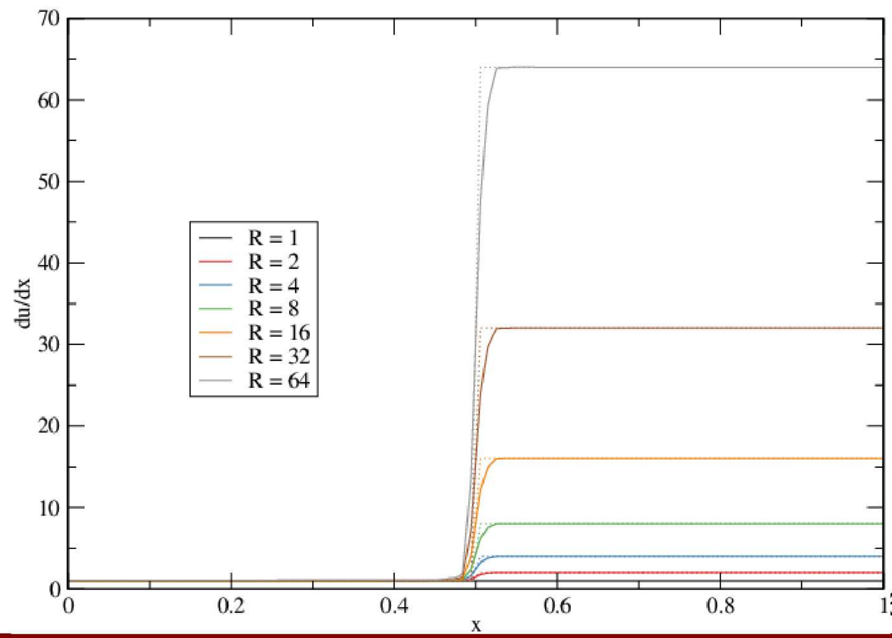
Darcy: jumps in material properties

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

$$\nabla \phi \rightarrow$$



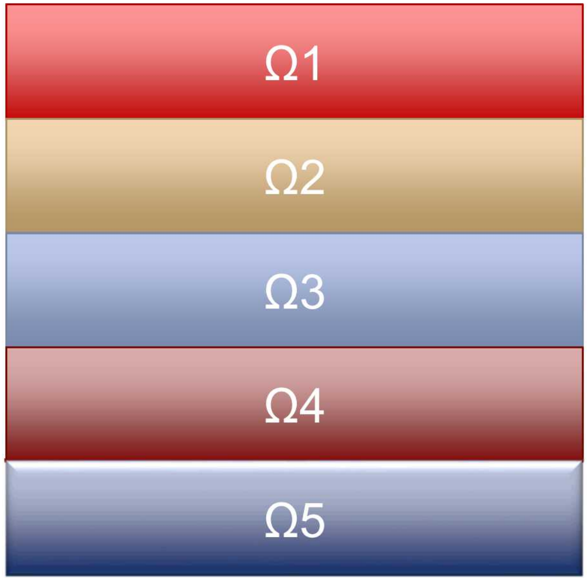


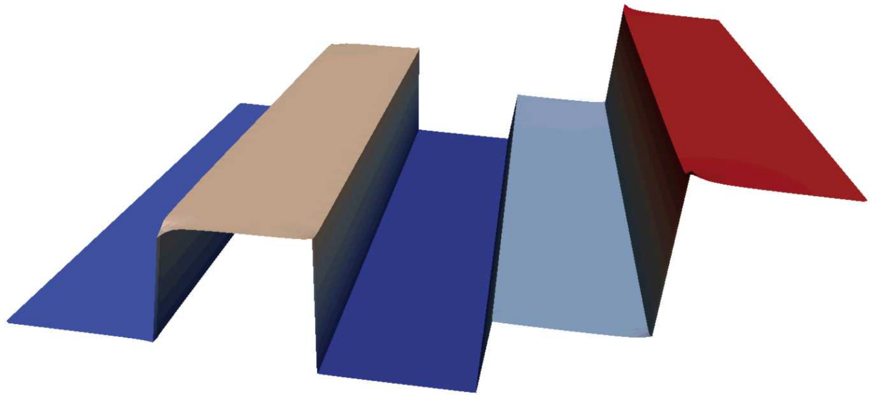


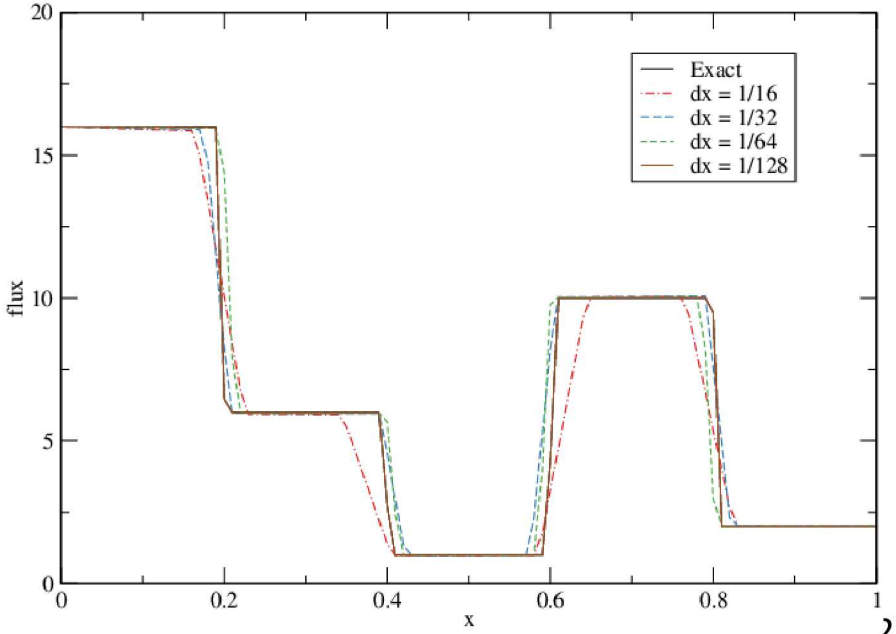
Darcy: jumps in material properties

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

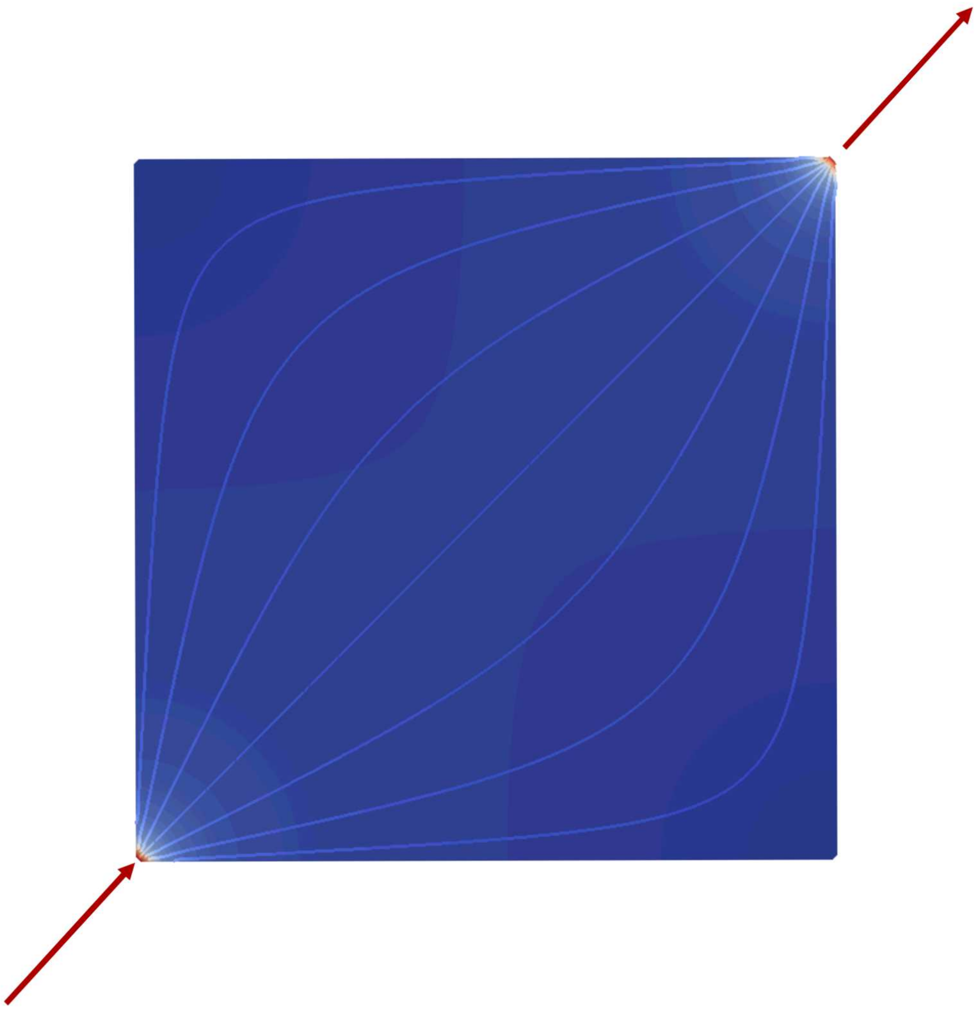
$$\nabla \phi \rightarrow$$

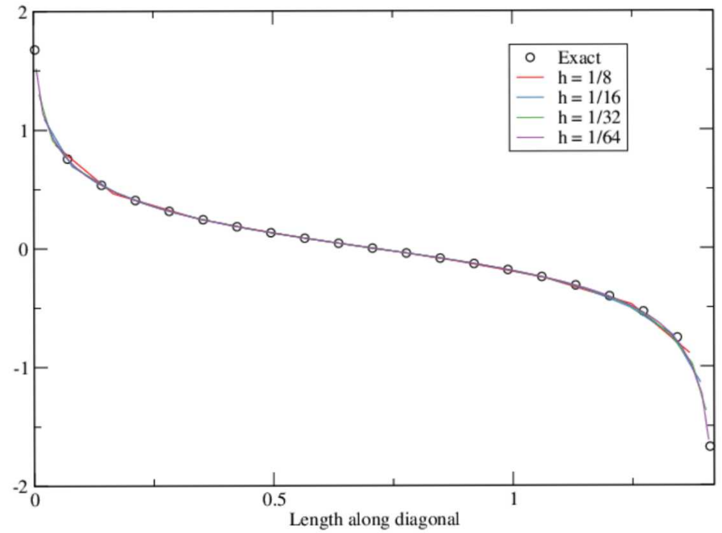


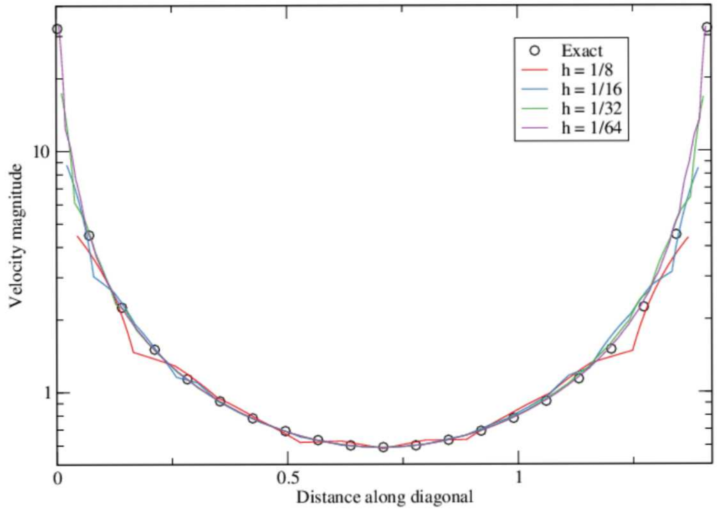




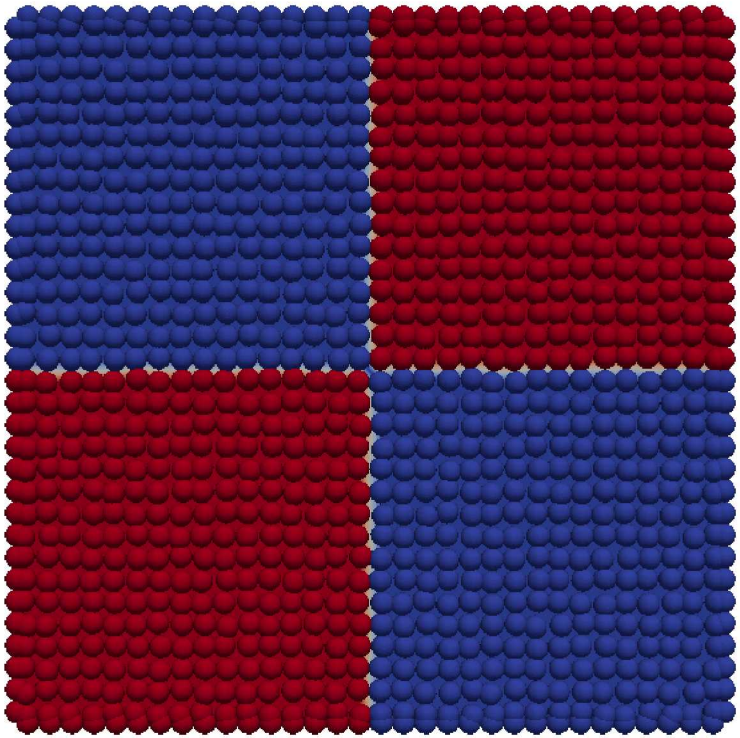
Darcy: 5-spot problem

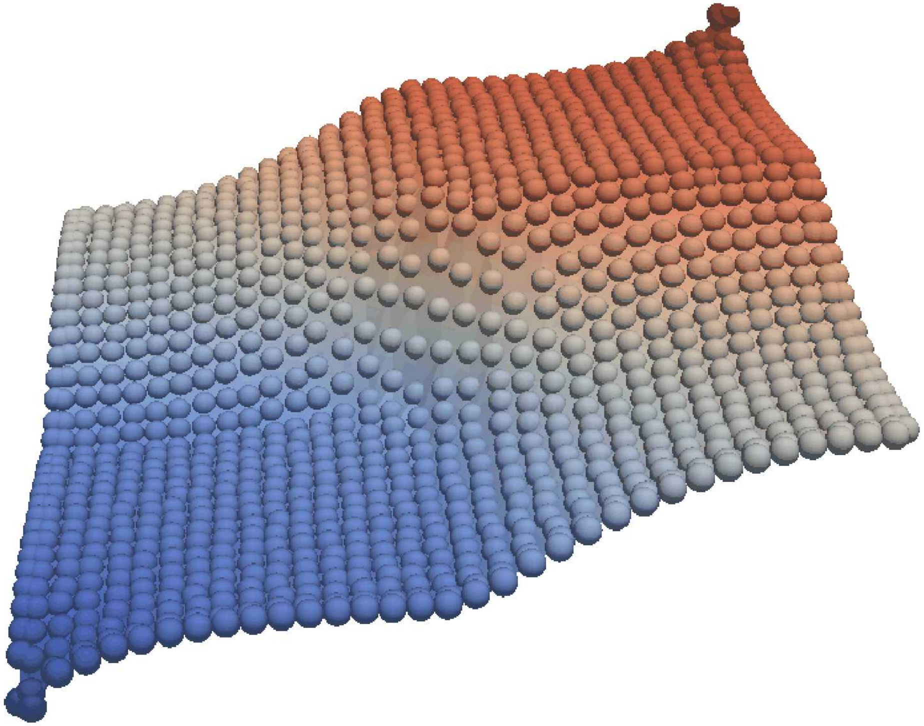




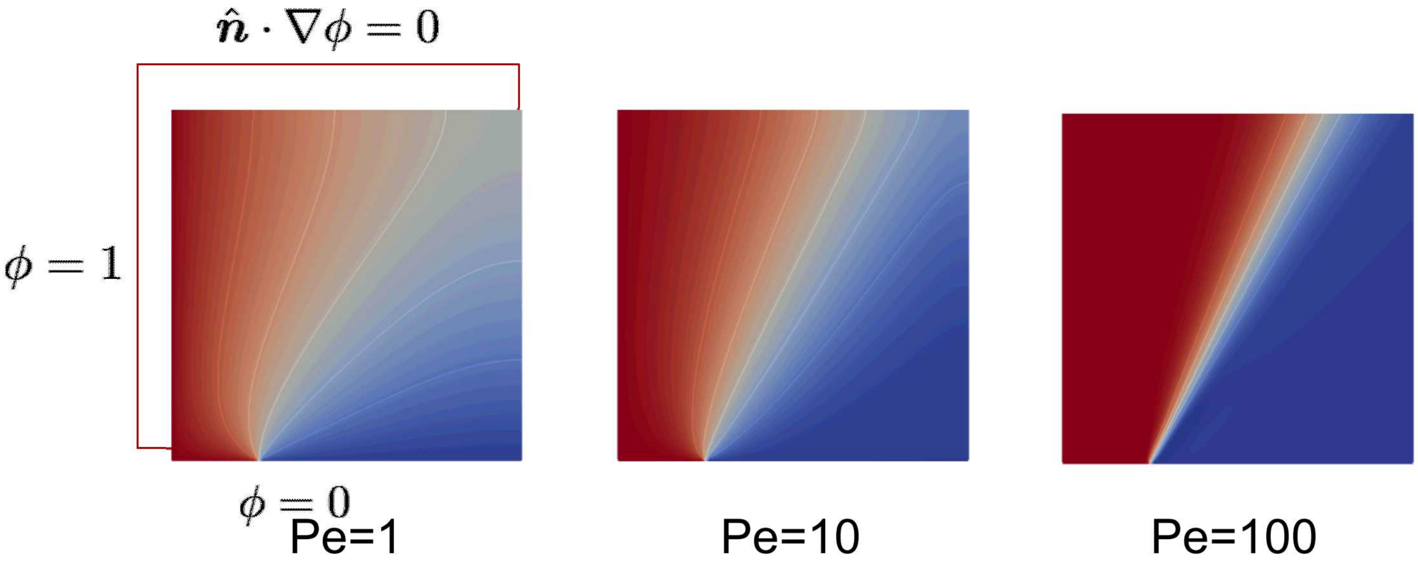


Darcy 5-spot problem





Singularly perturbed advection diffusion

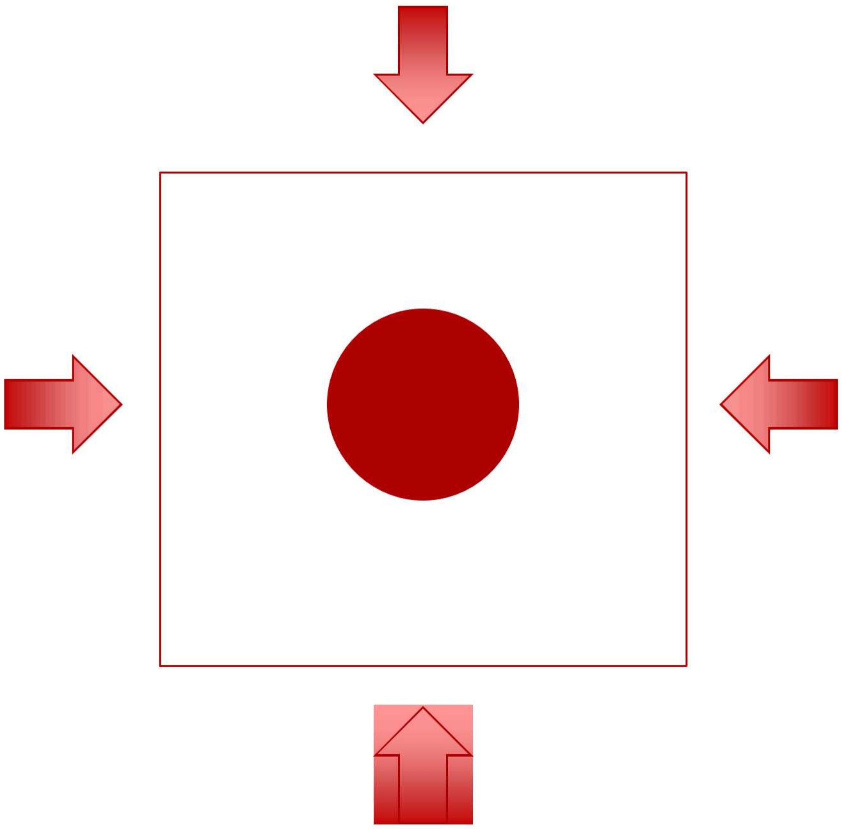


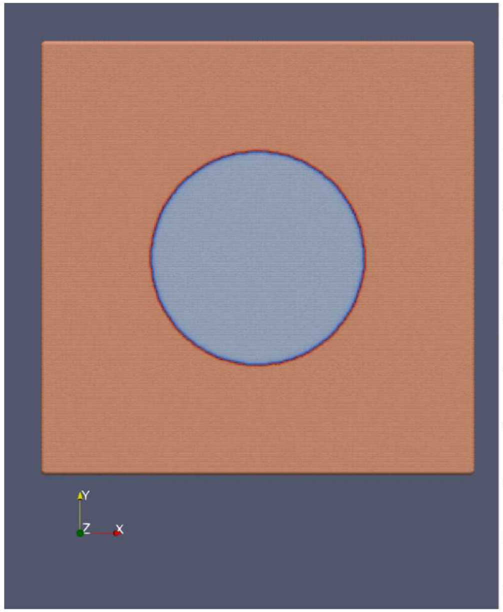
$$\frac{\partial}{\partial t}\phi + \nabla \cdot \mathbf{F} = 0$$

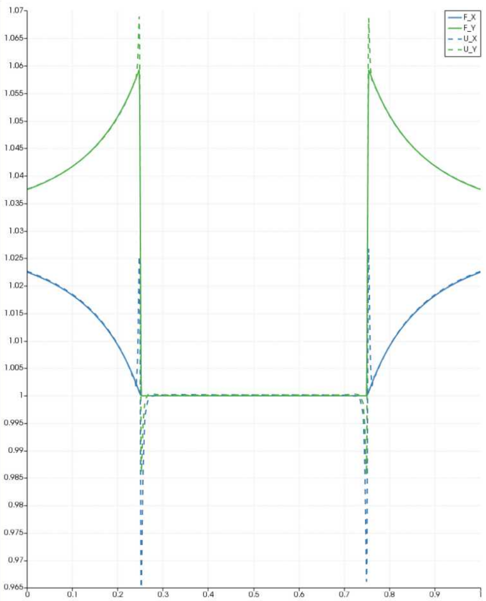
$$\mathbf{F} = \mathbf{a}\phi - \epsilon\nabla\phi$$

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

Linearly elastic composite materials



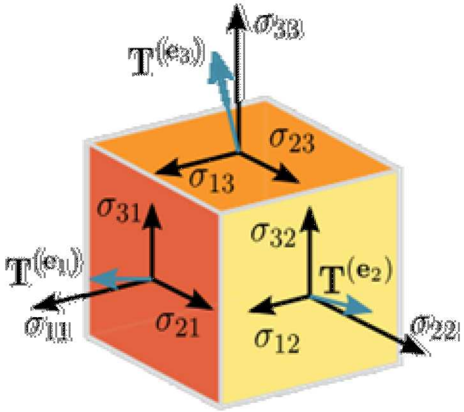


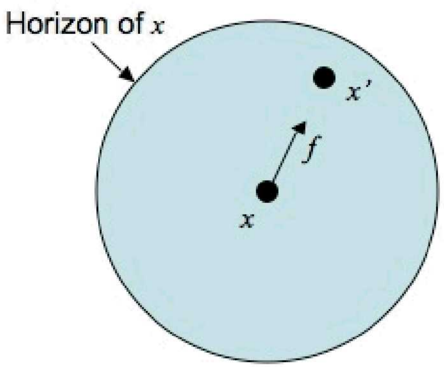


$$[\sigma \cdot \mathbf{n}] = 0$$

Talk part 2: Non-local models for the mesoscale

Peridynamics – a continuum theory based on integrals instead of derivatives





$$\rho\ddot{\mathbf{u}}(x) = \nabla \cdot \sigma(\mathbf{u})$$

$\sigma(\mathbf{u})$ - stress tensor

$$\rho\ddot{\mathbf{u}}(x) = \int \mathbf{f}(\mathbf{u}(\mathbf{y})) - \mathbf{f}(\mathbf{u}(\mathbf{x}))dy$$

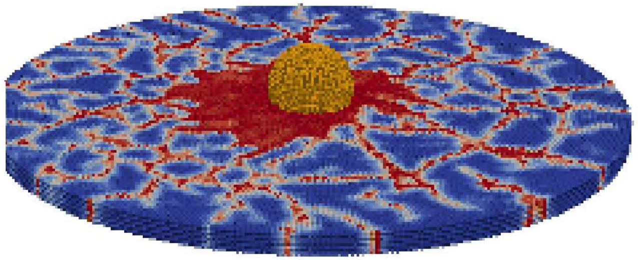
$\mathbf{f}(\mathbf{u})$ - force state

Target application: non-local fracture mechanics

Local mechanics: Natural setting $\boldsymbol{u} \in H^1$

$$\rho(\mathbf{x}) \frac{d^2}{dt^2} \mathbf{u}(\mathbf{x}) = \mathcal{L}[\mathbf{u}](\mathbf{x})$$

$$\mathcal{L}[\mathbf{u}](\mathbf{x}) = \frac{3K}{8} \left(\nabla^2 \mathbf{u} + \nabla \nabla \cdot \mathbf{u} \right)$$



Non-local mechanics: Natural setting $\boldsymbol{u} \in L^2$

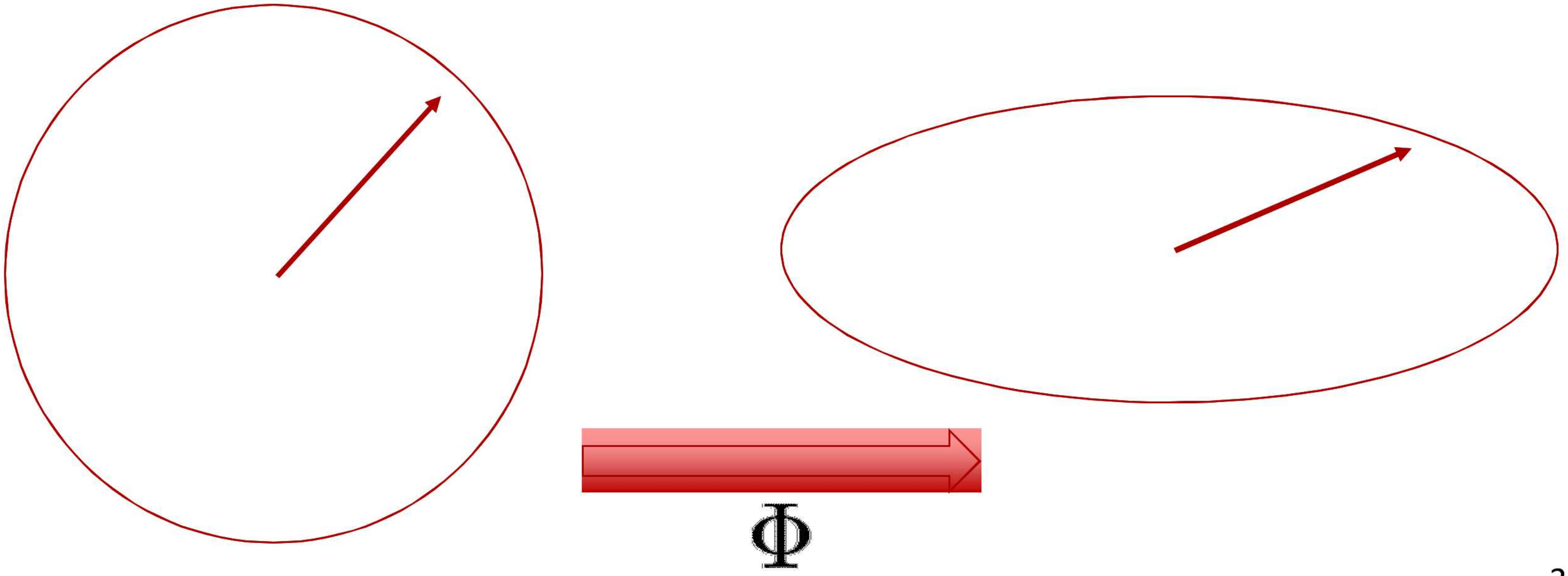
$$\rho(\mathbf{x}) \frac{d^2}{dt^2} \mathbf{u}^\delta(\mathbf{x}) = \mathcal{L}^\delta[\mathbf{u}](\mathbf{x})$$

$$\mathcal{L}^\delta[\mathbf{u}](\mathbf{x}) = \int_{B(\mathbf{x},\delta)} c \frac{\boldsymbol{\xi} \otimes \boldsymbol{\xi}}{||\boldsymbol{\xi}||^3} \left(\mathbf{u}^\delta(\mathbf{y}) - \mathbf{u}^\delta(\mathbf{x}) \right) \, d\mathbf{y}$$

In contrast to classical techniques, no need for enrichment/tracking of free surfaces/etc

Where do these models come from?

- **Ansatz:** Assume a functional form for pairwise interactions
  - **Ex:** Bond-based peridynamics
  - Assume elastic response analogous to Hooke's law
    - Force state is proportional to displacement from reference configuration
    - By calculating strain energy, may relate stiffness to classical local properties



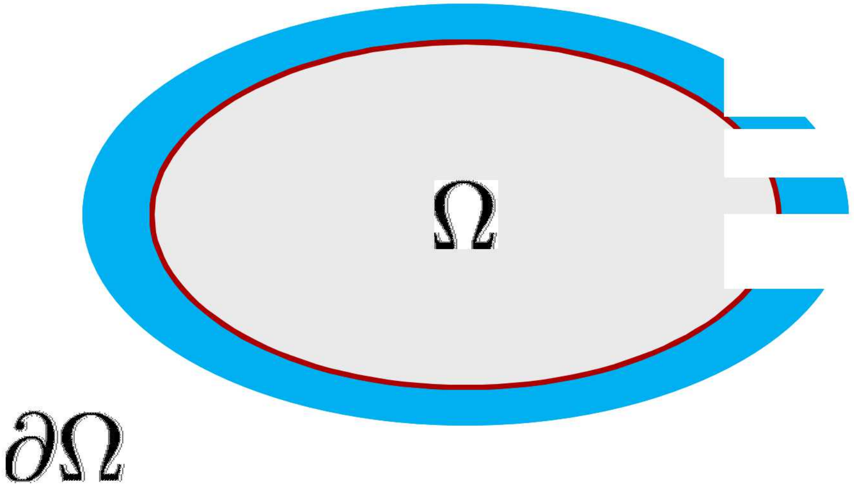
Non-local setting and notation

Consider a family of integral equations of the form:

$$\mathcal{L}_\delta[u](\mathbf{x}) = \int_{\mathbb{R}^d} K(\mathbf{x},\mathbf{y})u(\mathbf{y})\,d\mathbf{y} = \mathbf{f}(\mathbf{x})$$

$$supp(K(x,\cdot)) = B_\delta(\mathbf{x})$$

$$K(\mathbf{x},\mathbf{y}) = \frac{n(\mathbf{x},\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^\alpha},\ \text{where } n(\mathbf{x},\mathbf{y}) \le C_n$$



$$\Omega^\delta = \bigcup_{\mathbf{x}\in\Omega} B(\mathbf{x},\delta)$$

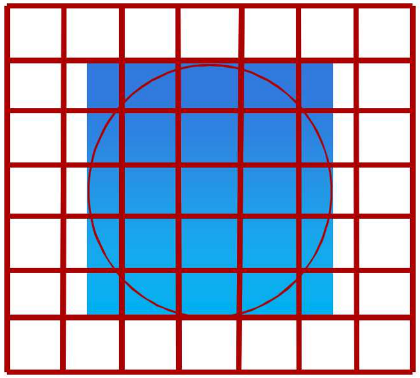
$$\partial^\delta\Omega = \Omega^\delta \setminus \Omega$$

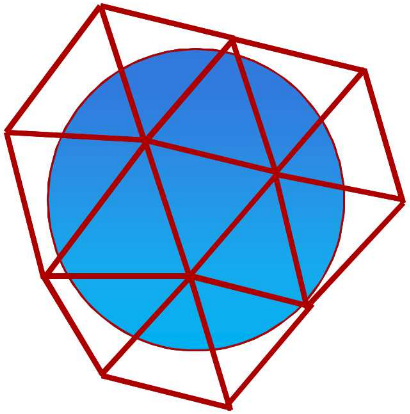
Motivation: non-local quadrature on mesh

Define quadrature rule:

$$\mathcal{L}_\delta[u](\mathbf{x}) = \int_{B(\mathbf{x},\delta)} K(\mathbf{x},\mathbf{y})u(\mathbf{y})\,d\mathbf{y}$$

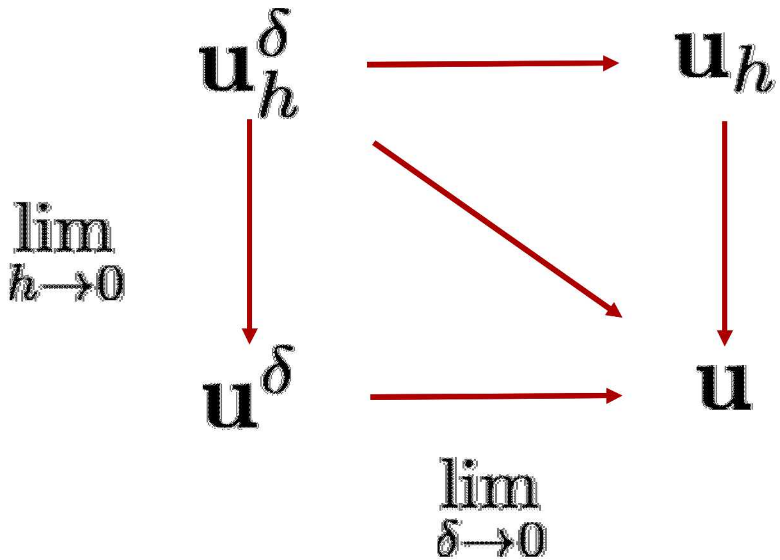
$$\mathcal{L}_\delta^h[u](\mathbf{x}_i) = \sum_{\mathbf{x}_j \in \mathbf{X}_q \subset B(\mathbf{x}_q,\delta)} K(\mathbf{x}_i,\mathbf{x}_j)u(\mathbf{x}_j)\,\omega_j$$

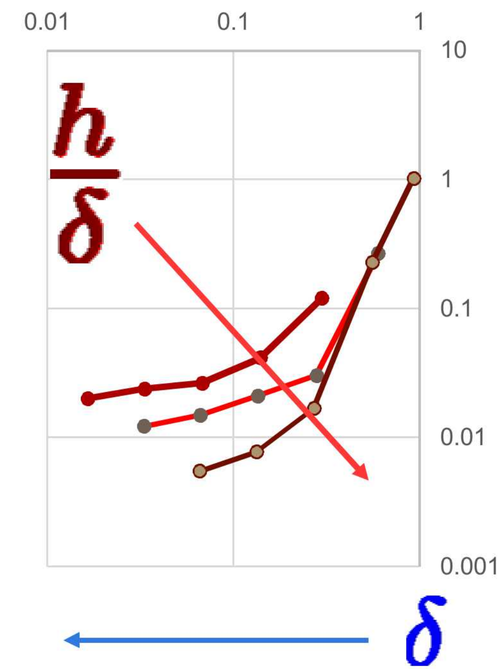




- Challenges in finite element setting:
  - Costly geometric intersection
  - Singularity in non-local kernel – **particularly hard on unstructured meshes**

Asymptotically compatible discretization





Seek a discretization that recovers local solution as nonlocal + local length scales both tend to zero at same rate

Tian, Xiaochuan, and Qiang Du. "Asymptotically compatible schemes and applications to robust discretization of nonlocal models." *SIAM Journal on Numerical Analysis* 52.4 (2014): 1641-1665.

Meshfree generation of quadrature rules on balls

$$I[f] \approx I_h[f] = \sum_j f_j \, \omega_j$$

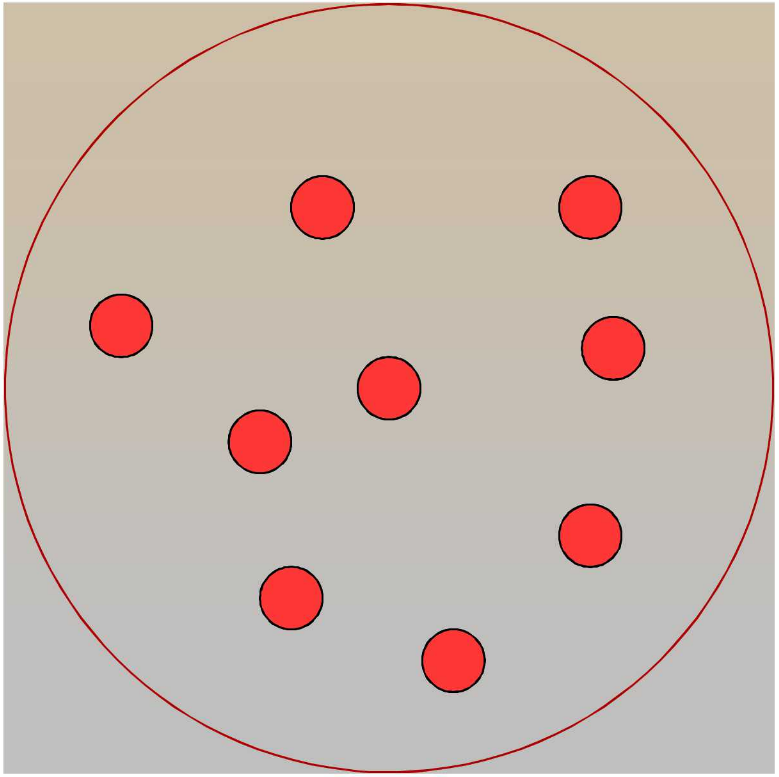
$$\underset{\omega}{\text{minimize}} \sum_j \omega_j^2$$

subject to

$$I[f] = \sum_j f_j \omega_j, \; \forall p \in \mathbf{V}$$

where

$$I[f] = \int_{B(x,\delta)} f \, dx$$



Idea:

- Construct rule just like Gauss quadrature
- Requires knowledge of how to integrate against each member of reproducing set

Singular integrals

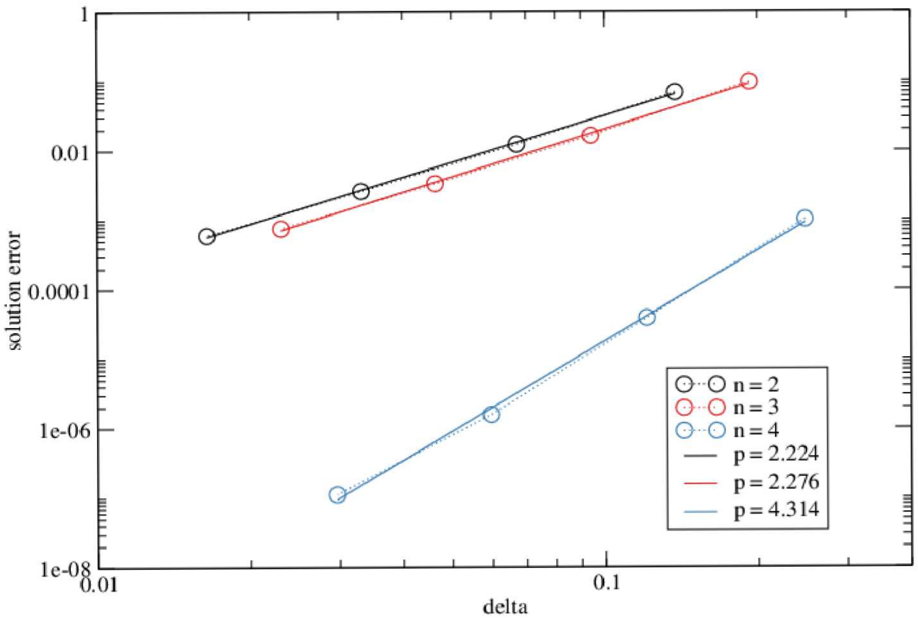
- As reproducing space, select polynomials + integrand of operator

$$\mathbf{V}_h = P_m \cup S_{K,n,\mathbf{x}}, \text{ where}$$
$$S_{K,n,\mathbf{x}} := \{K(\mathbf{x},\mathbf{y})f(\mathbf{y}) \,|\, f \in P_n\}$$

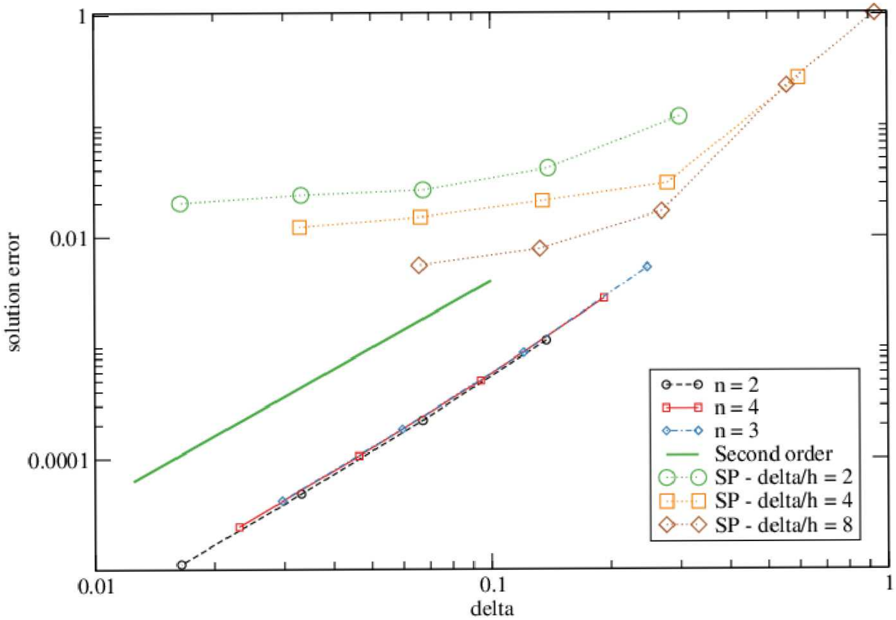
Theorem. *Consider for fixed* $\mathbf{x}$ *a kernel of the form* $K(\mathbf{x},\mathbf{y}) = \frac{n(\mathbf{x},\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^\alpha}$, *where the numerator* n *satisfies* $n(\mathbf{x},\mathbf{y}) \le C_n$ *for all* $\mathbf{y} \in B(\mathbf{x},\delta)$. *A set of quadrature weights obtained from the GMLS process with the choice of* $\mathbf{V}_h = P_m \cup S_{K,n,\mathbf{x}}$ *for* $u \in C^m$ *and* $m > n$ *satisfies the following pointwise error estimate, with* $C > 0$ *independent of the particle arrangement.*

$$\left| \int_{B(\boldsymbol{x},\delta)} K(\boldsymbol{x},\boldsymbol{y})u(\boldsymbol{y})d\boldsymbol{y} - \sum_{j \in \mathbf{X}_q} K(\boldsymbol{x},\boldsymbol{x}_j)u_j\omega_j \right| \le C\delta^{n-\alpha+d+1}$$

Manufactured solution to BVP



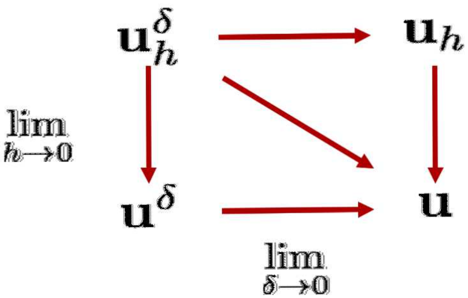
$$u_h^\delta \to u^\delta$$



$$u_h^\delta \to u$$

$$-c \sum_{j \in B(\mathbf{x}_i,\delta)} K_{ij}(\mathbf{u}_j - \mathbf{u}_i)\omega_{j,i} = \mathcal{L}^\delta[\mathbf{u}](\mathbf{x}_i)$$

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



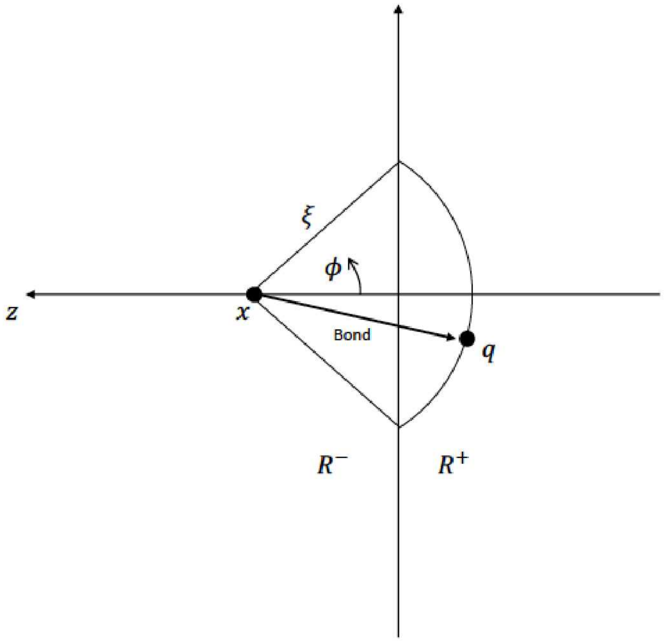
Surface effects + implicit transmission conditions

To calculate effective flux and model boundary conditions, postulate:

$$F[u](\mathbf{x}) = C \int_{\Omega^c \cap B(\mathbf{x},\delta)} K(\mathbf{x},\mathbf{y}) f(\mathbf{y}) d\mathbf{y}$$

For an infinitesimal area element near half-plane boundary, the nonlocal flux is given by

$$\mathbf{Q}/dA = \int_0^\delta \int_0^r \int_{cos^{-1}(-z/r)}^{cos^{-1}(z/r)} K(\mathbf{x},\mathbf{y}) f(\mathbf{y}) r \, d\theta \, dz \, dr$$



Damage modelling

Sandia National Laboratories

Given a pair (i,j) in $B(x_i,\delta)$, associate the state of either broken or unbroken

$$\tilde{\omega}_{j,i} = \begin{cases} \omega_{j,i}, & \text{if bond is unbroken} \\ 0, & \text{if bond is broken .} \end{cases}$$

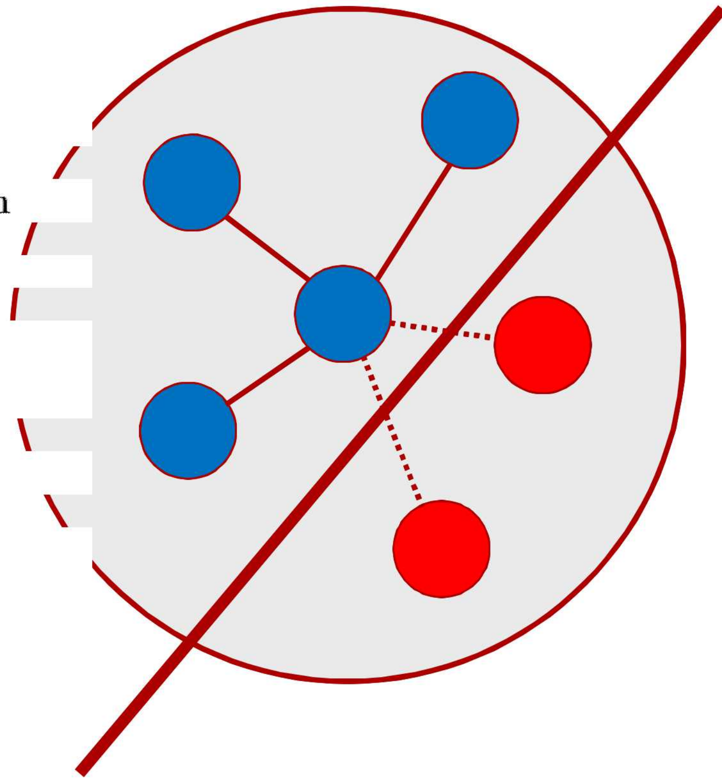
Bonds are either

- Broken as a pre-processing step to introduce a crack to the problem
- Broken over the course of the simulation if the bond strain

$$s = \frac{|\mathbf{u}_j - \mathbf{u}_i| - |\mathbf{x}_j - \mathbf{x}_i|}{|\mathbf{x}_j - \mathbf{x}_i|},$$

Exceeds a damage criteria, e.g. $s > s_0$ where

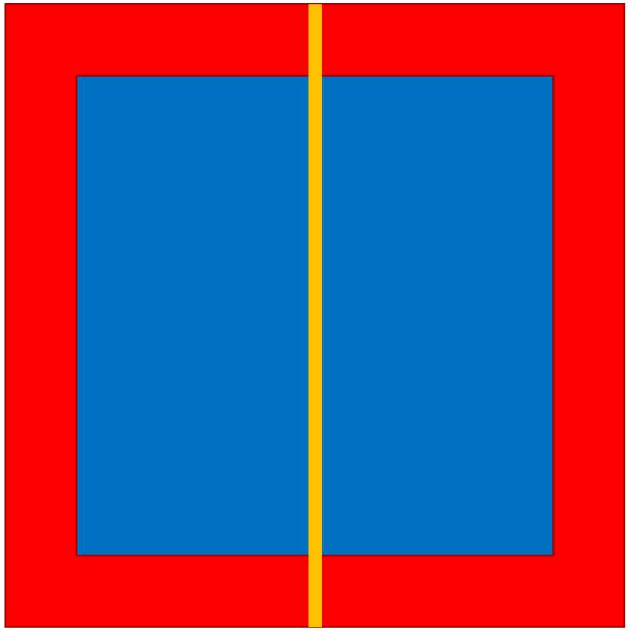
$$s_0 = \begin{cases} \sqrt{\frac{G_c}{\left(\frac{6\mu}{\pi} + \frac{16}{9\pi^2}(\kappa - 2\mu)\right)\delta}}, & \text{d} = 2 \\ \sqrt{\frac{G_c}{\left(3\mu + \left(\frac{3}{4}\right)^4\left(\kappa - \frac{5\mu}{3}\right)\right)\delta}}, & \text{d} = 3 \text{ .} \end{cases}$$

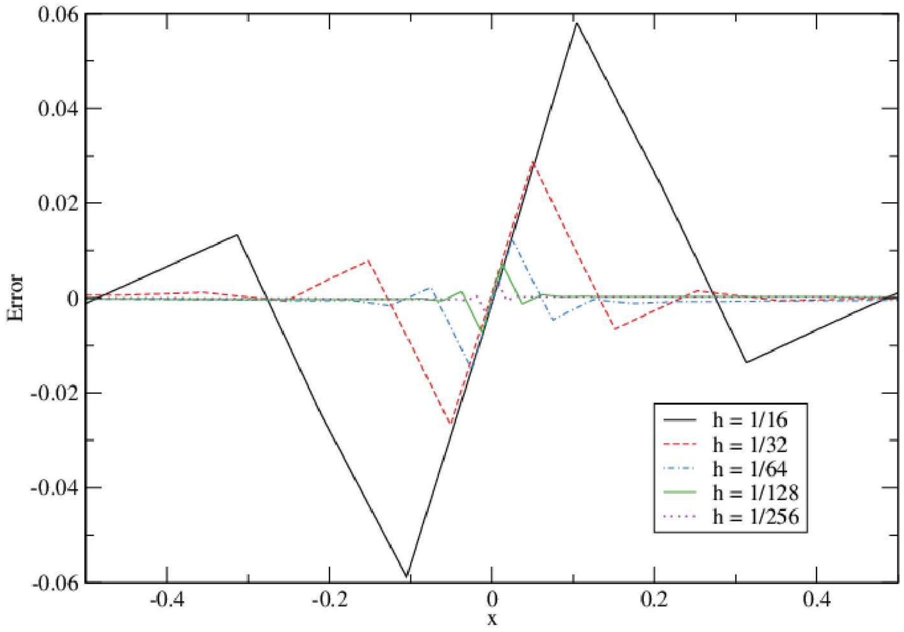


Asymptotic convergence to local condition

$$\mathbf{u}_{tf} = \langle x + y, -x - 3y) \rangle$$

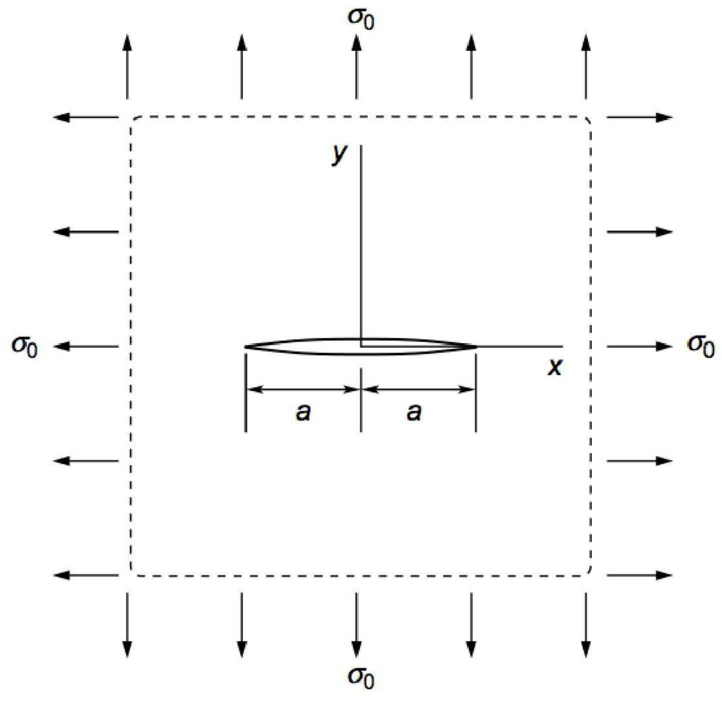
$$\sigma(u) \cdot \hat{n} = 0$$

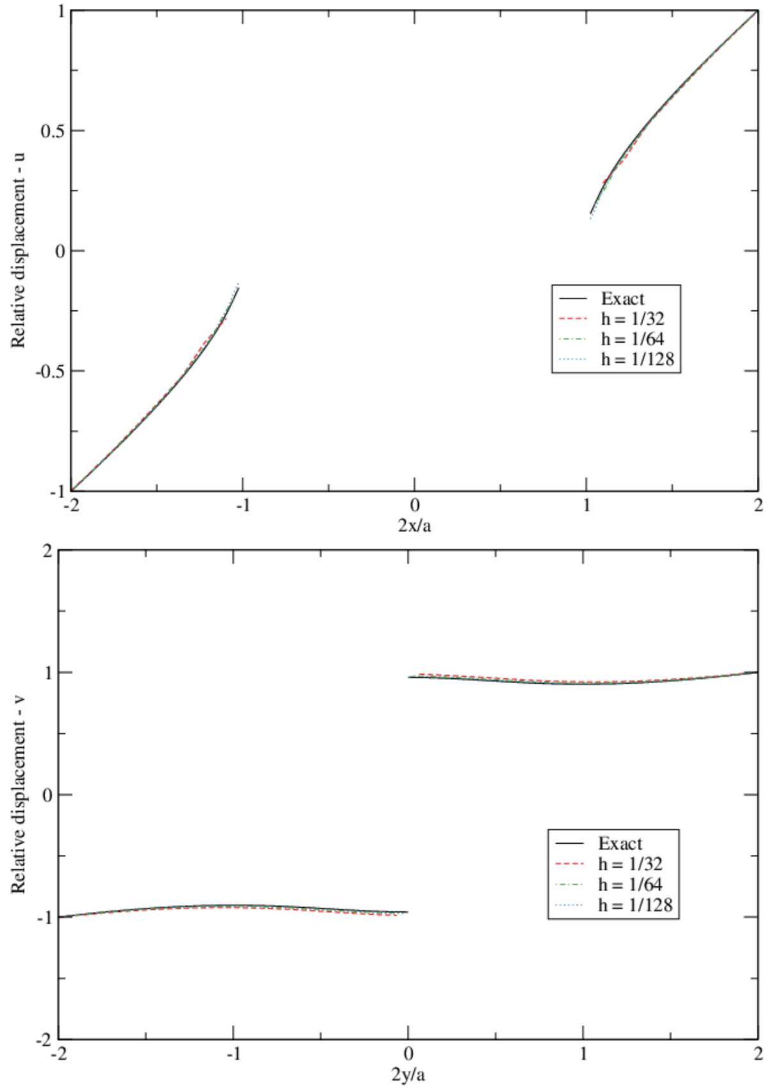




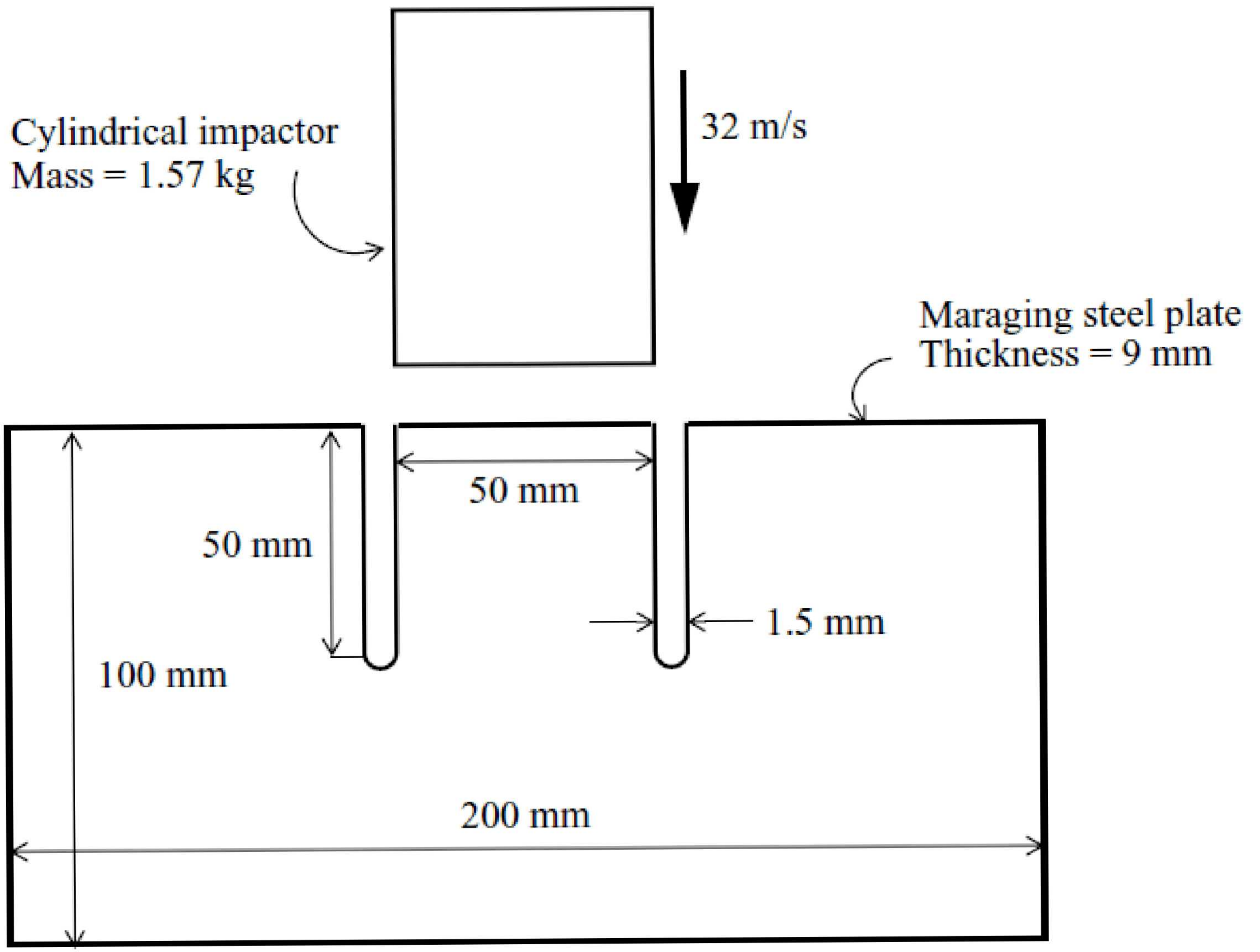
Damage model recovers analytic traction-free local solution as $O(\delta)$.

Type-I crack loading

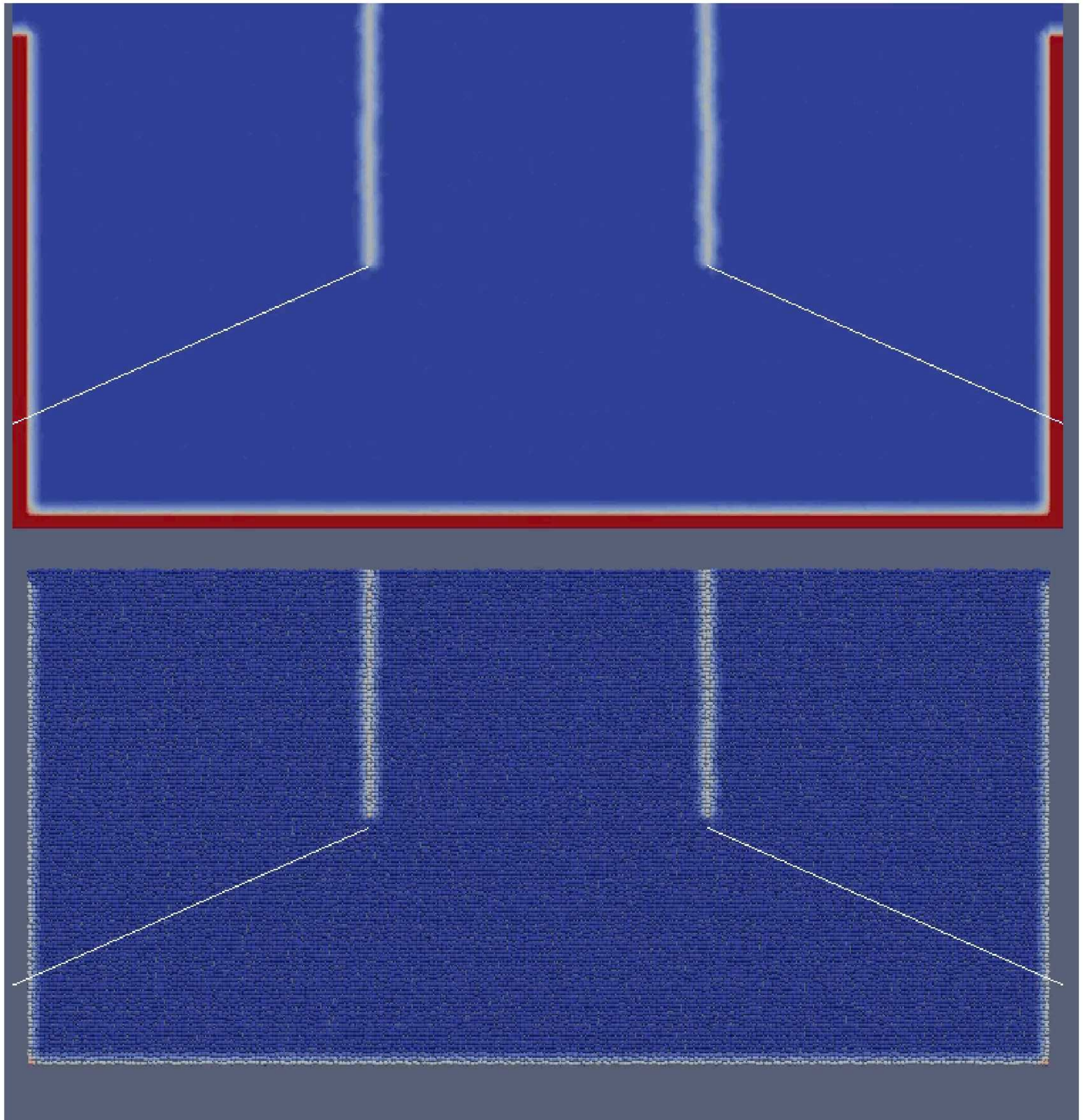




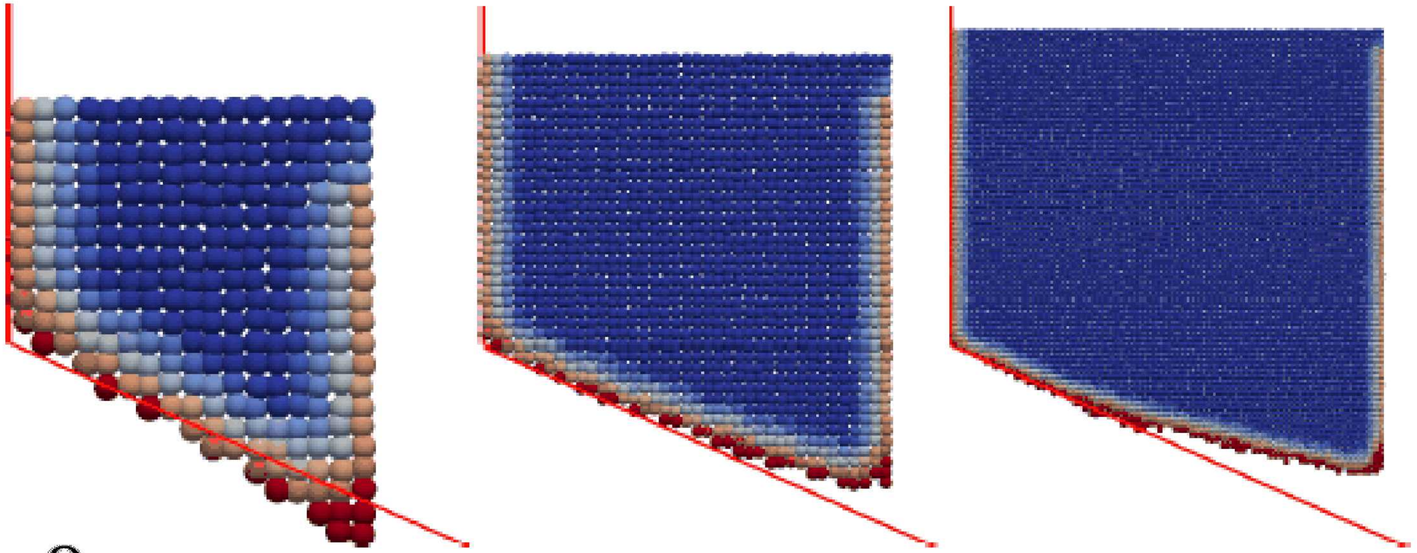
Kalthoff-Winkler experiment



Kalthoff-Winkler experiment

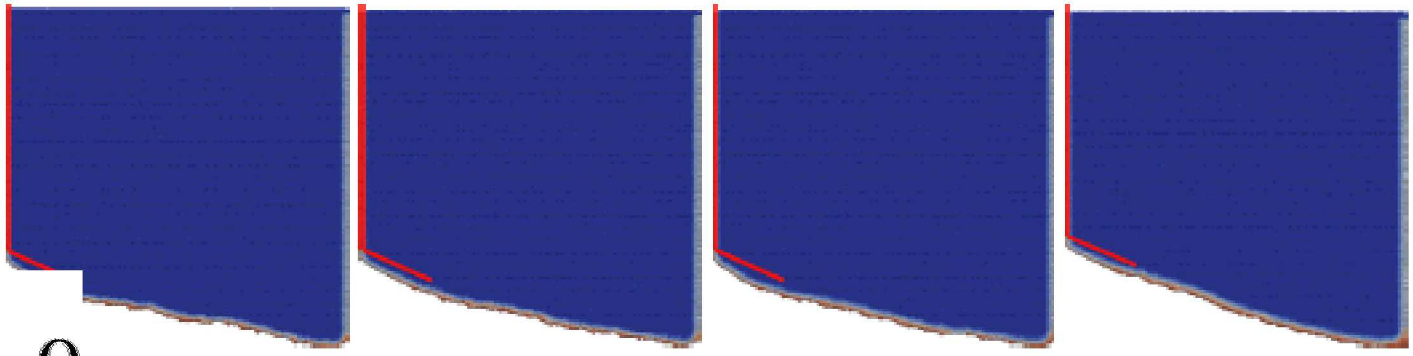


Kalthoff-Winkler experiment



$$\frac{\delta}{h} = 3$$

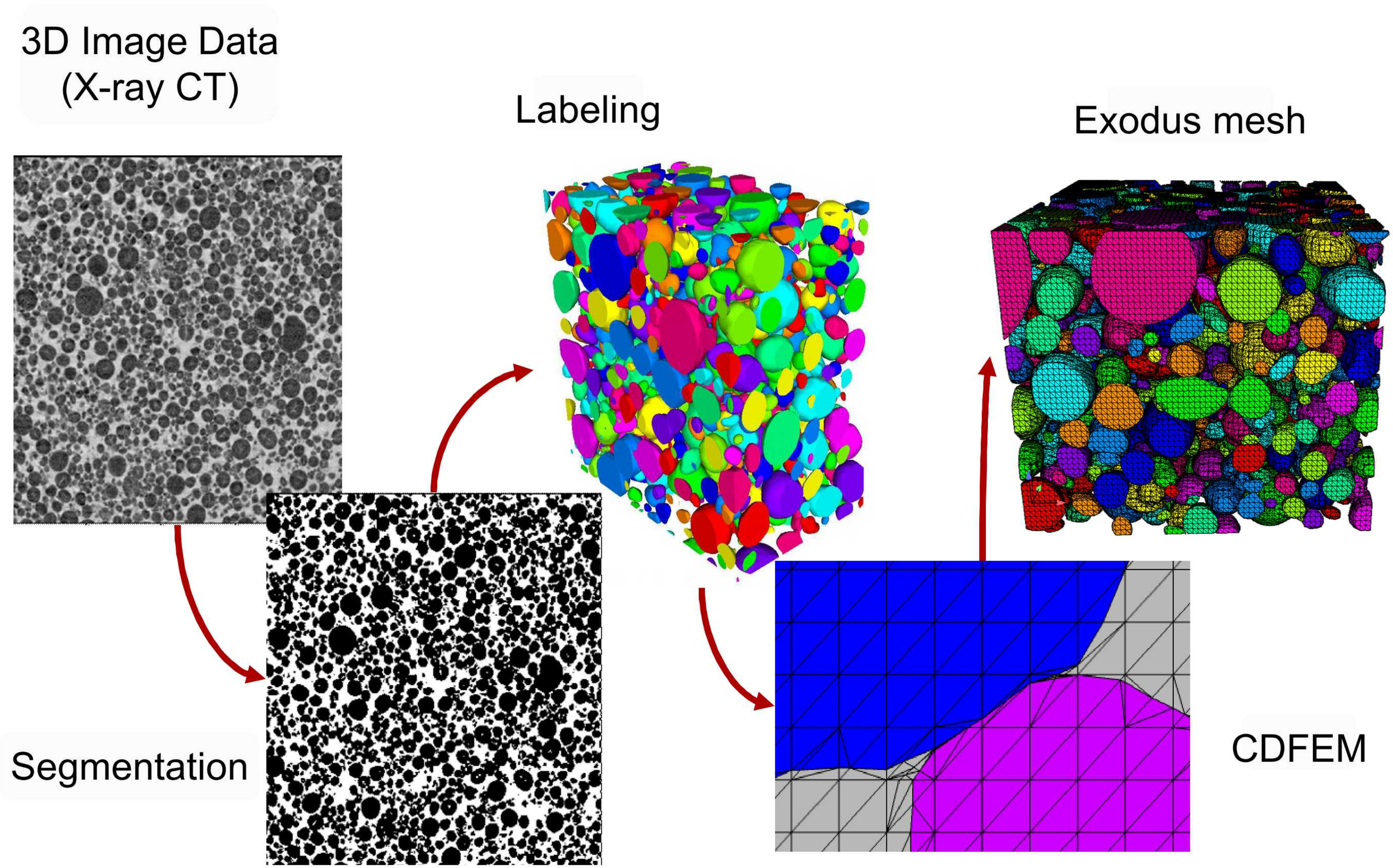
$$\delta \to 0$$



$$h = \frac{1}{256}$$

$$\frac{h}{\delta} \to 0$$

Application driver: Lithiation-induced failure



A microstructure framework for transport induced fracture

Diffusion process

$$\nabla \cdot \mathbf{F} = g$$

$$\mathbf{F} = -\kappa \nabla \phi$$

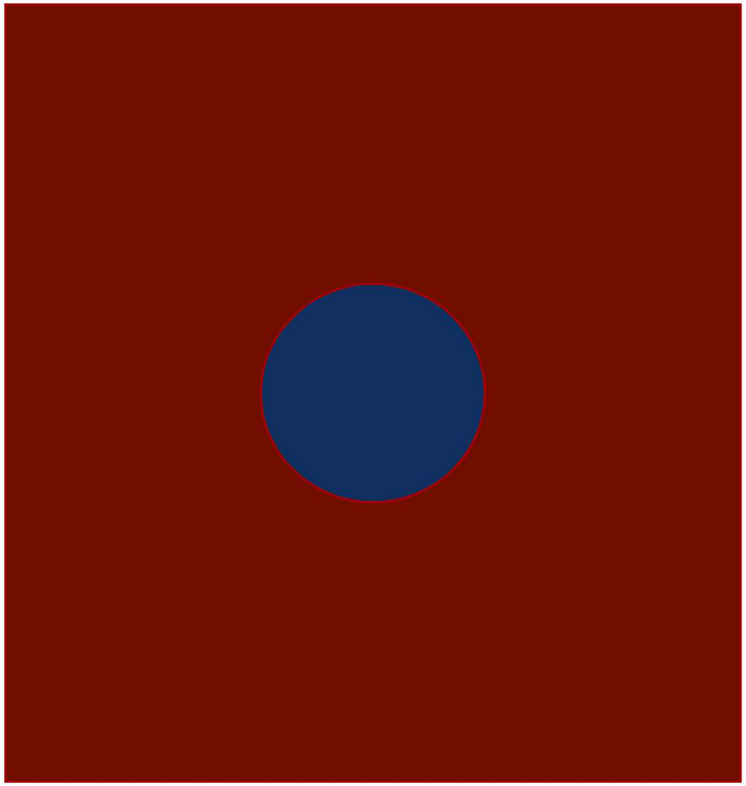
$$[\hat{\mathbf{n}} \cdot \kappa \nabla \phi] = h$$

Mechanics process

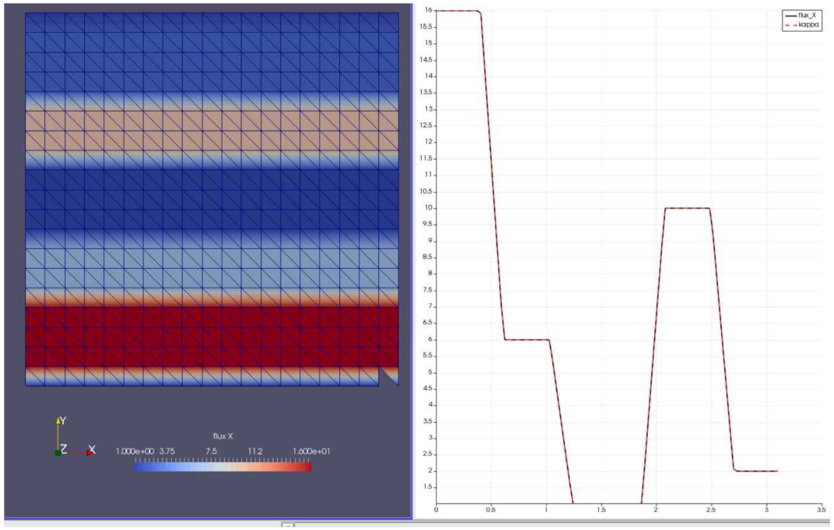
$$\nabla \cdot \sigma = f$$

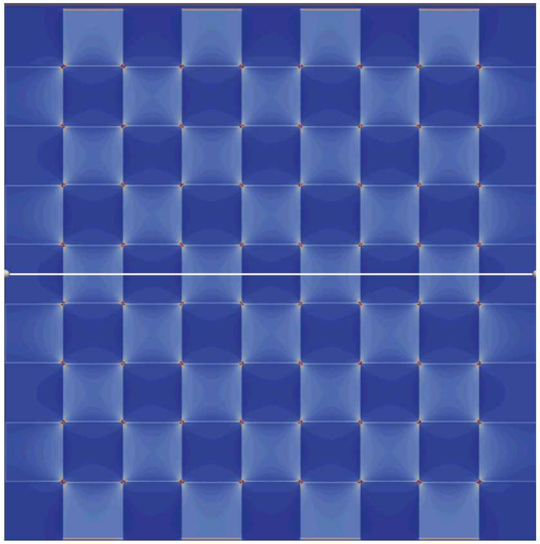
$$\sigma = \sigma_{mech}(\mathbf{u}) + \epsilon \phi \mathbb{I}$$

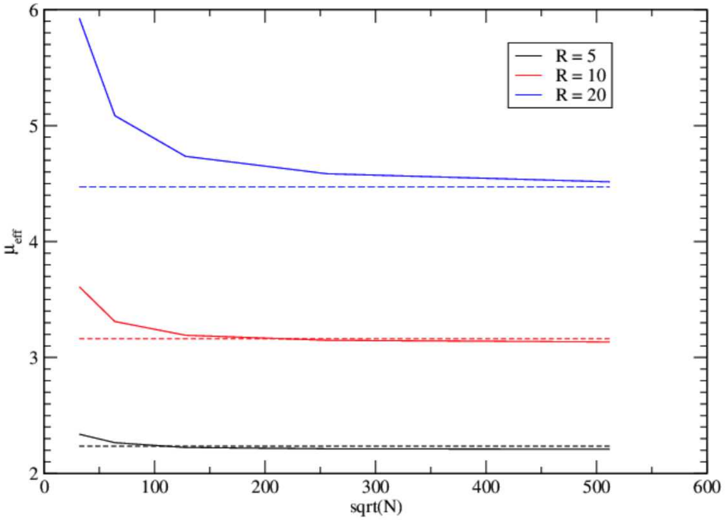
$$\hat{\mathbf{n}} \cdot \sigma \ = \mathbf{t}$$



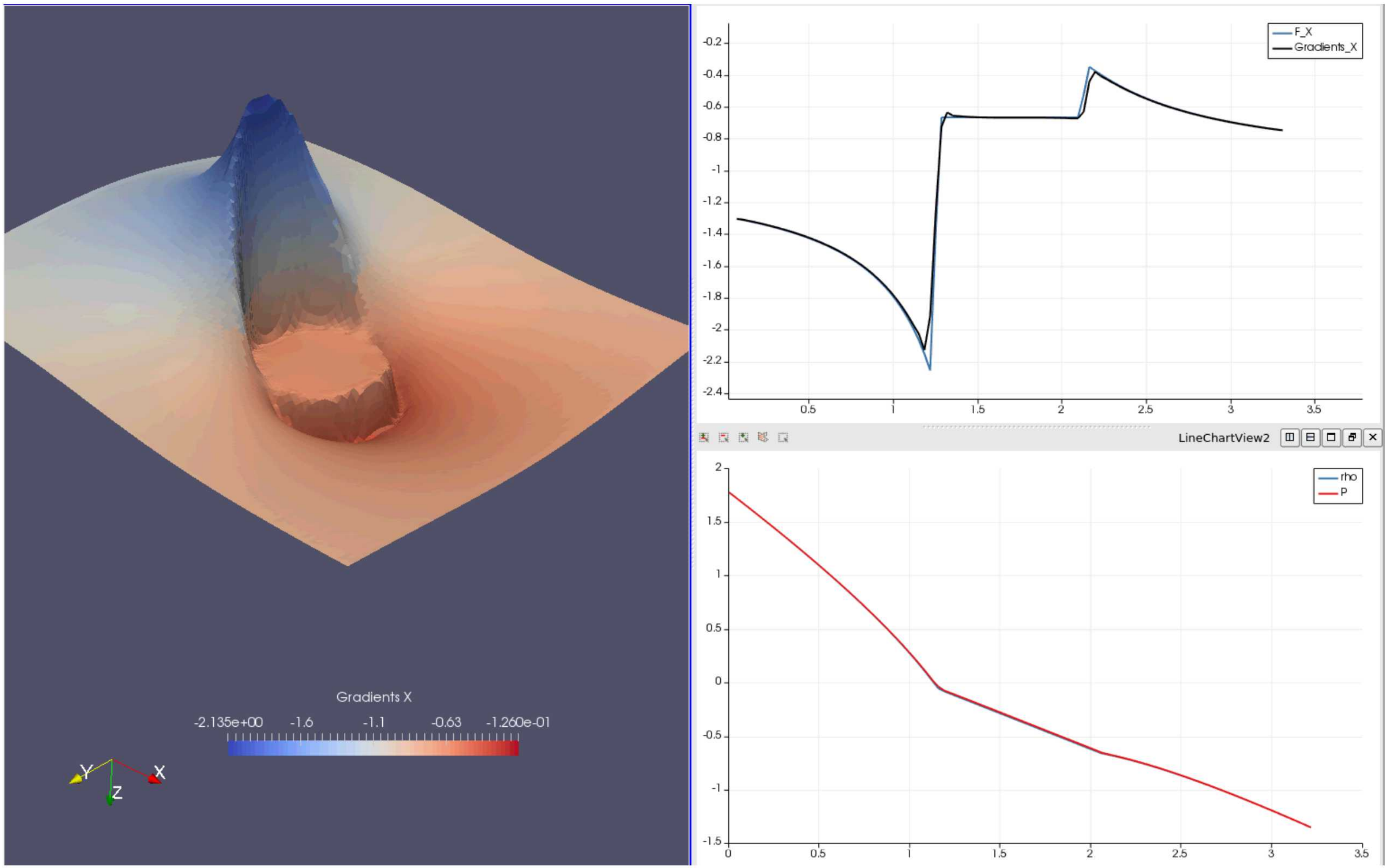
Diffusion for heterogeneous materials



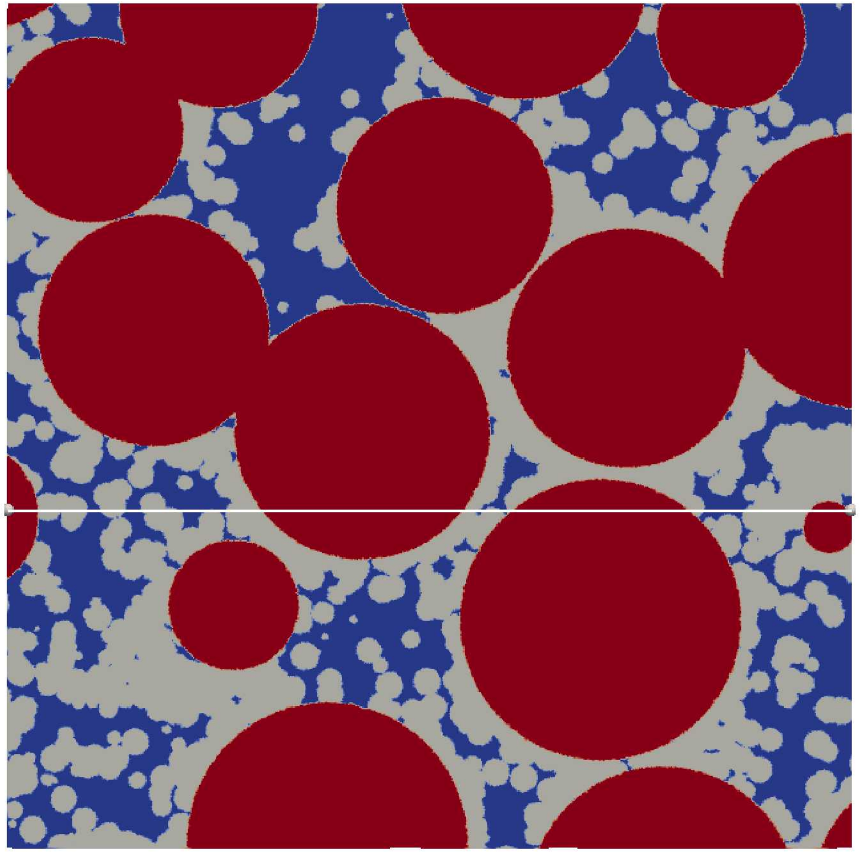


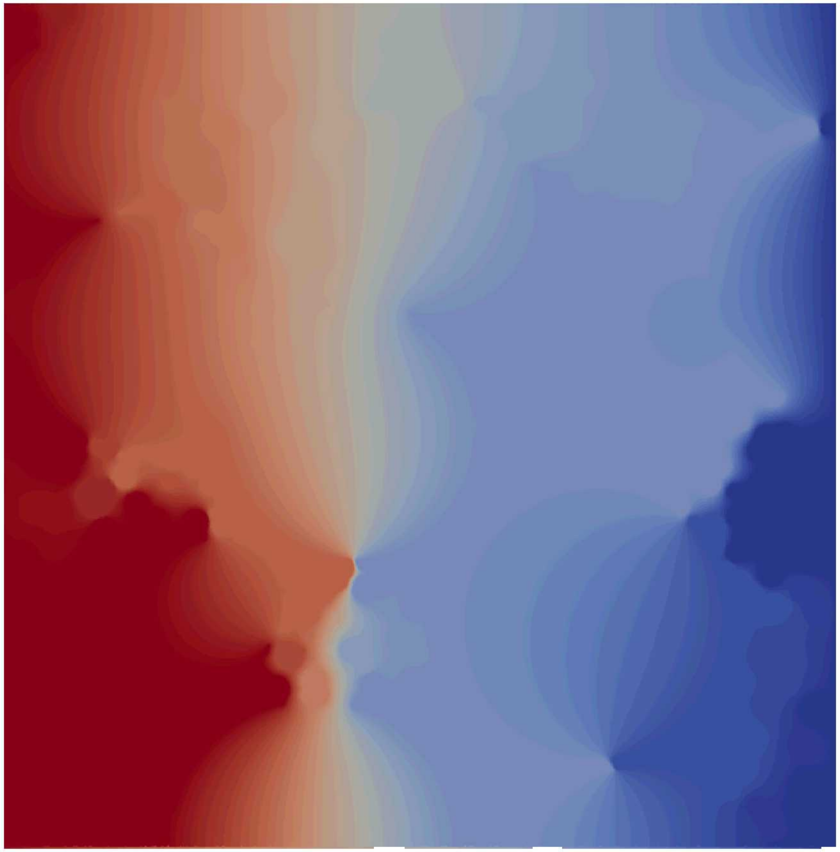


Inhomogeneous flux condition

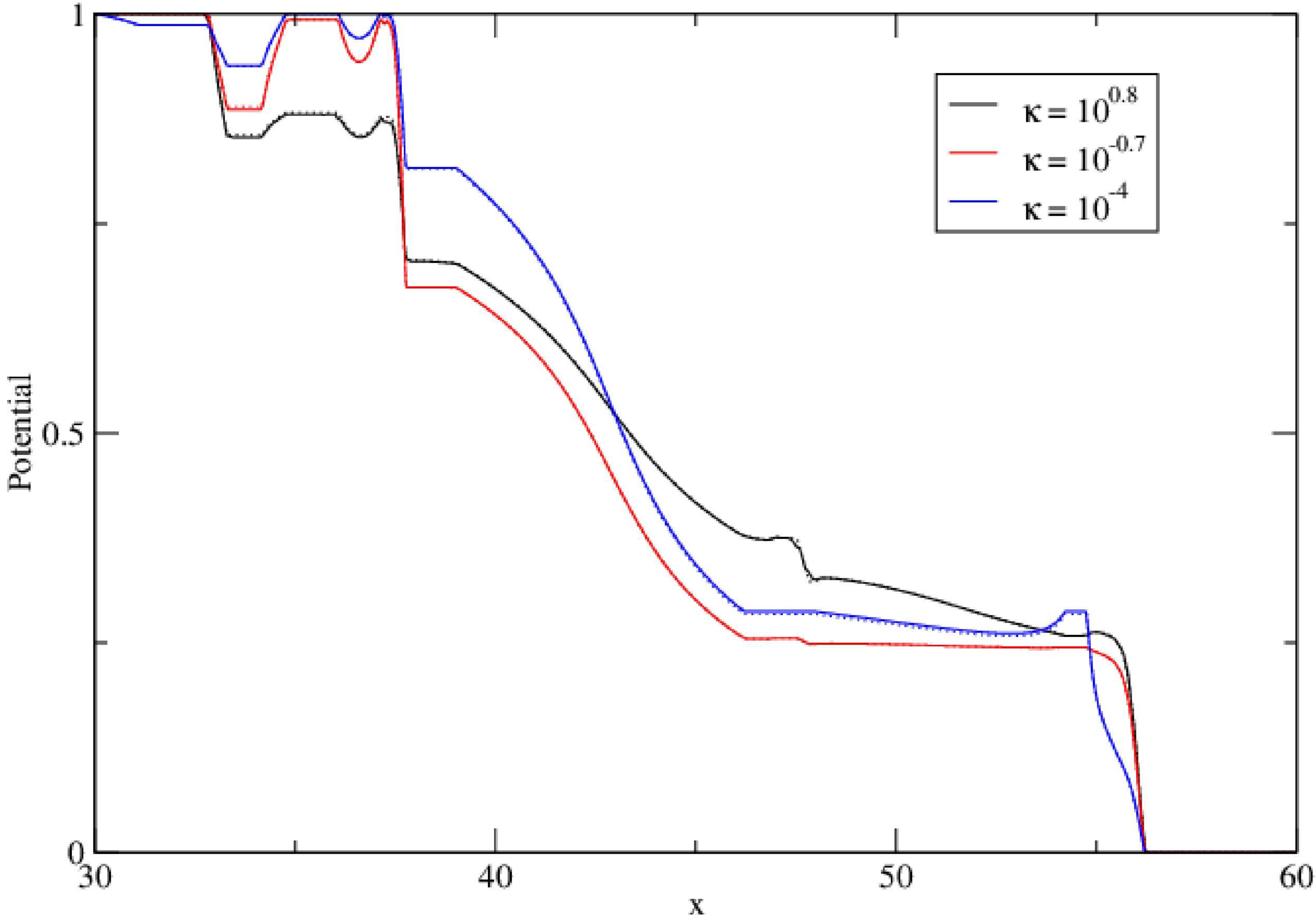


Comparison to microstructural data

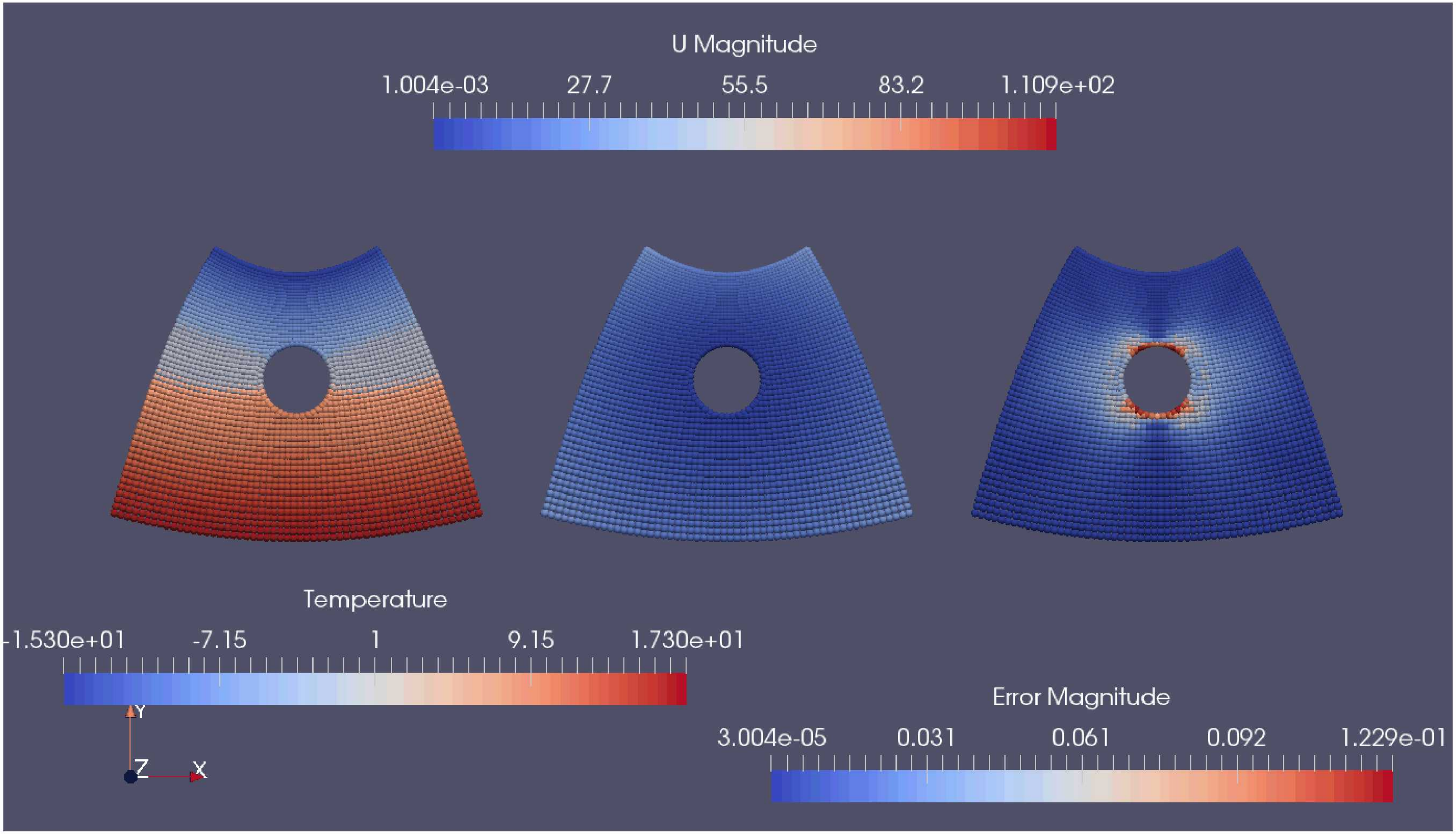




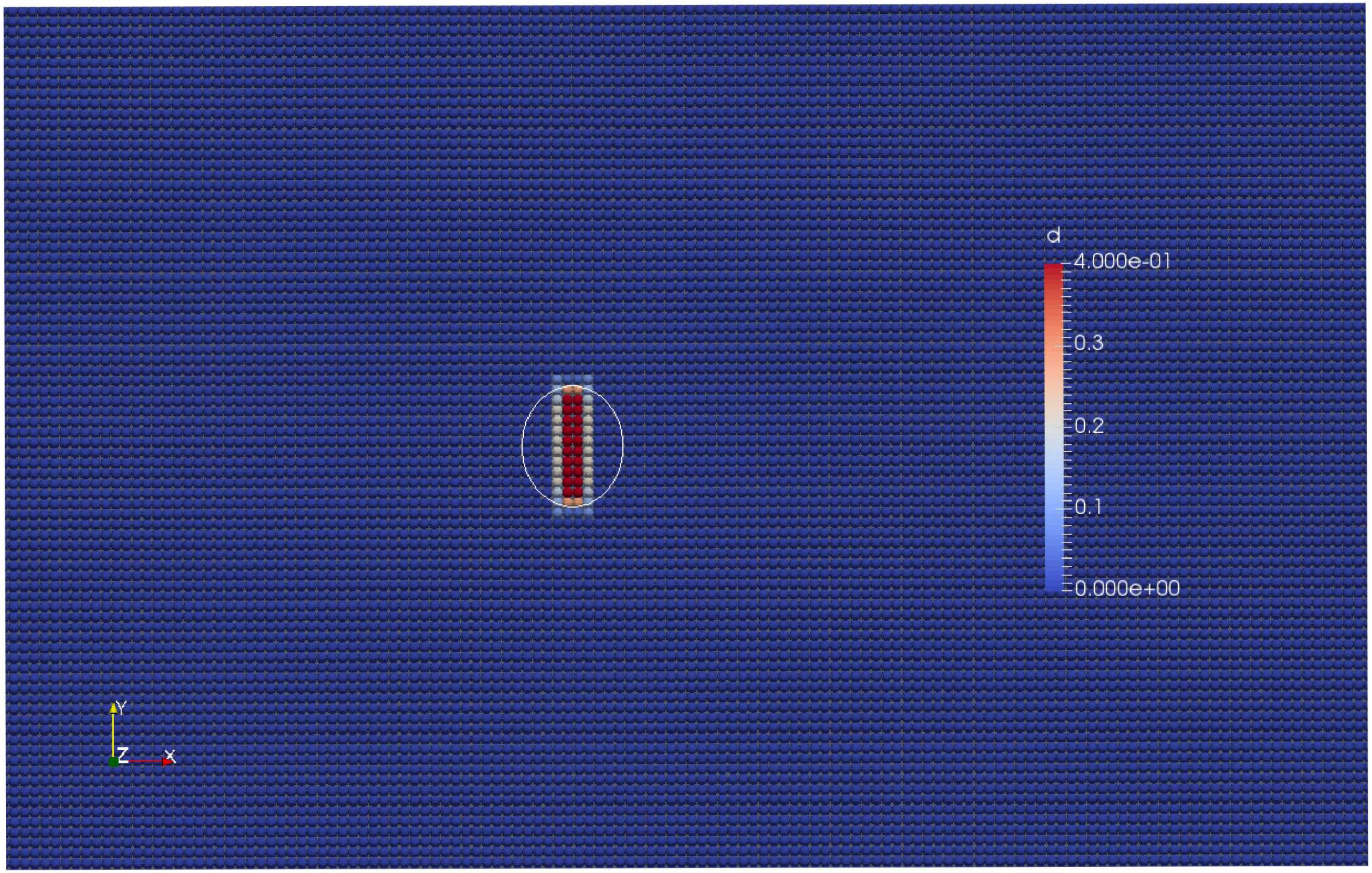
Comparison to finite element solution



Consistent coupling to mechanics



Pressure loading of cracks



Conclusions

- GMLS provides a versatile platform for rigorous meshfree recovery of functionals
- By constructing meshfree analogues to the Gauss divergence theorem, we provide a topological structure which may be paired with GMLS to obtain a purely meshfree finite volume method
  - Swap the geometric problem of mesh generation for a scalable algebraic one
- Same ideas may be used to restore consistency to nonlocal models of mechanics
- End result: a flexible and rigorous multiphysics framework well suited for large deformation problems