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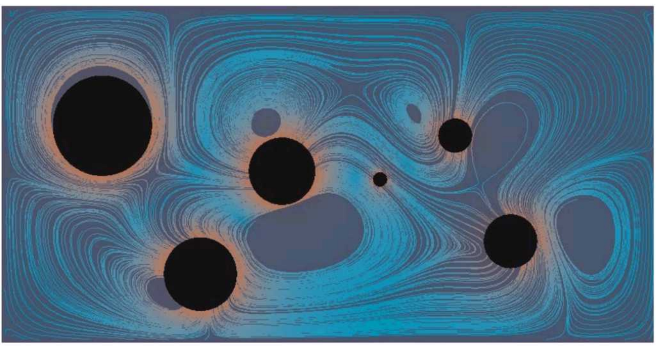
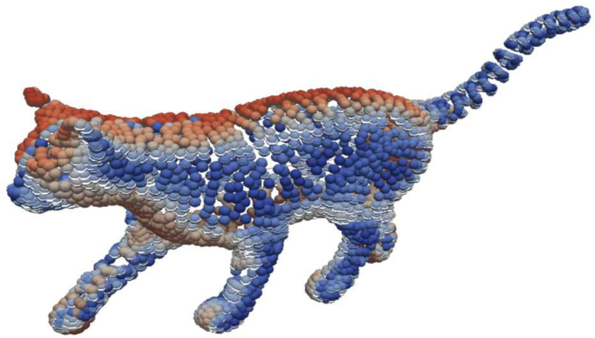
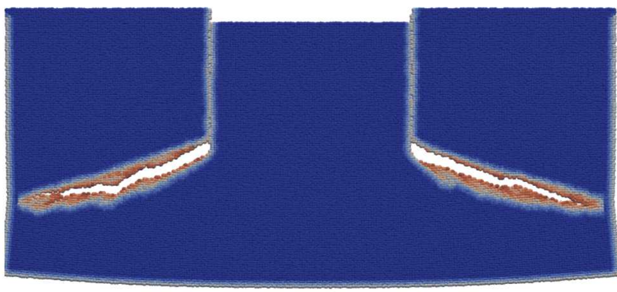






Spatially compatible meshfree discretization

Center for Computing Research

Nat Trask

Sandia National Laboratories

Talk overview

- An overview of the Compadre project
  - What is meshfree/why meshfree?
- 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
  - How to obtain accurate quadrature rules for non-local singular operators, with no reference to an underlying mesh

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
- 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

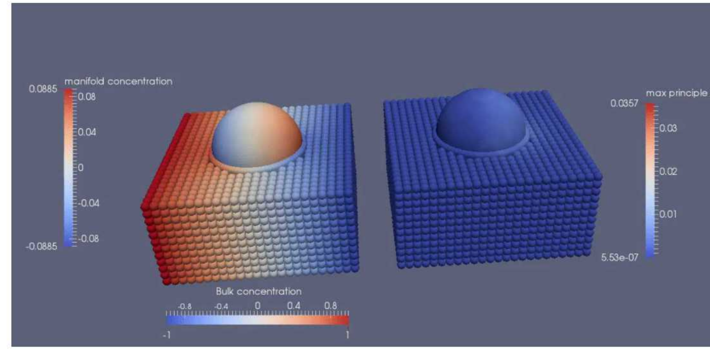
Key tools:

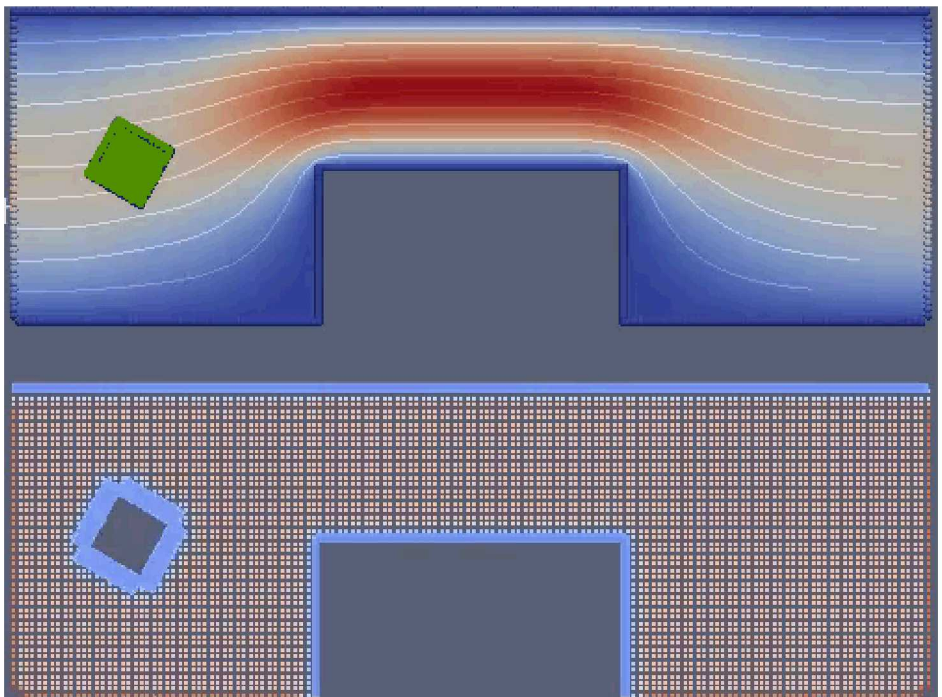
- Optimization based approaches to develop meshfree discretizations with reproduction properties
- The Compadre Trilinos library – open source library for scalable implementation of meshfree methods

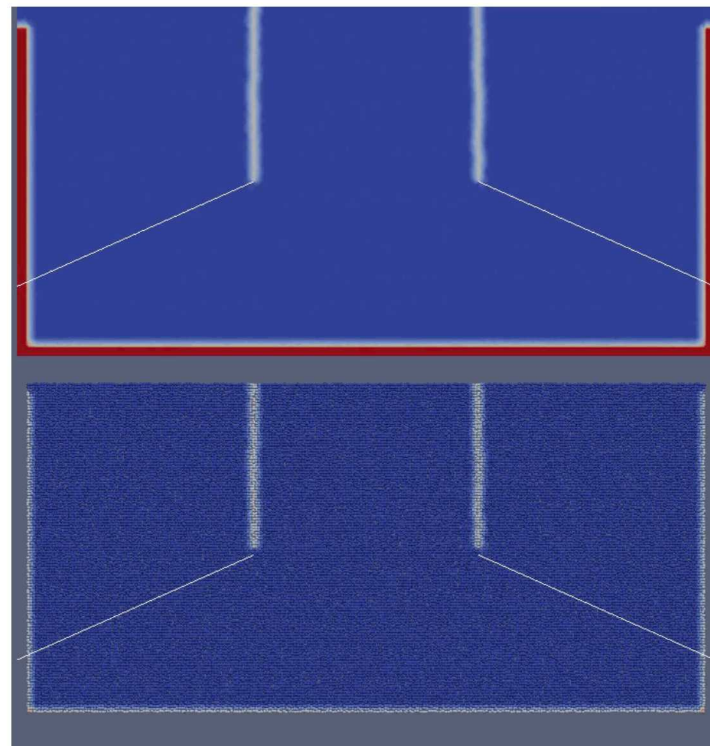
Why meshfree? Large deformation problems

- Saddle point problems
  - div-grad, div-curl, stationary Stokes
- Surface PDE
  - Bulk-manifold coupling, deposition
- Local/Non-local Lagrangian mechanics
  - Asymptotically compatible discretization

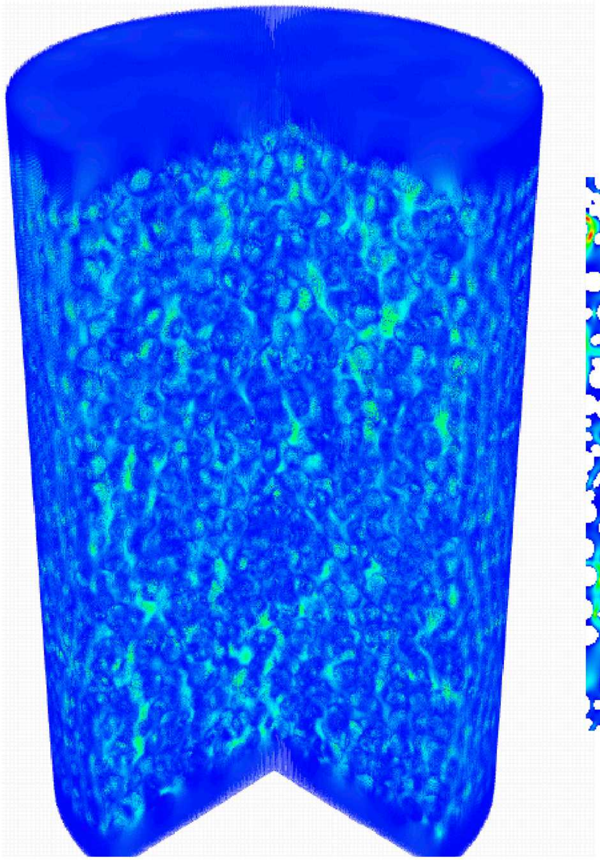
Hard to say anything without a mesh!

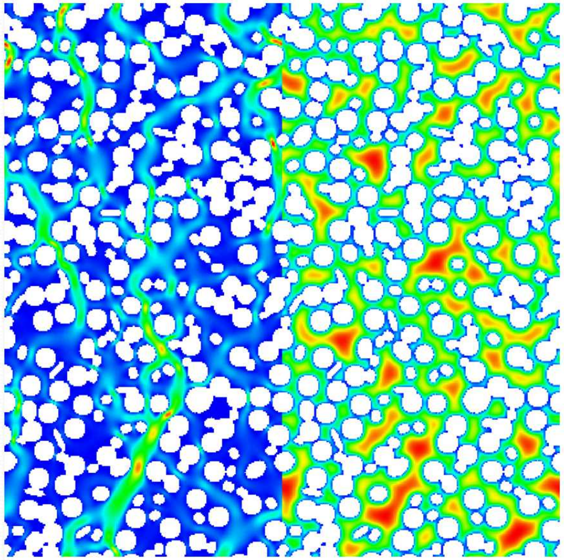






Why meshfree? Automated geometry discretization



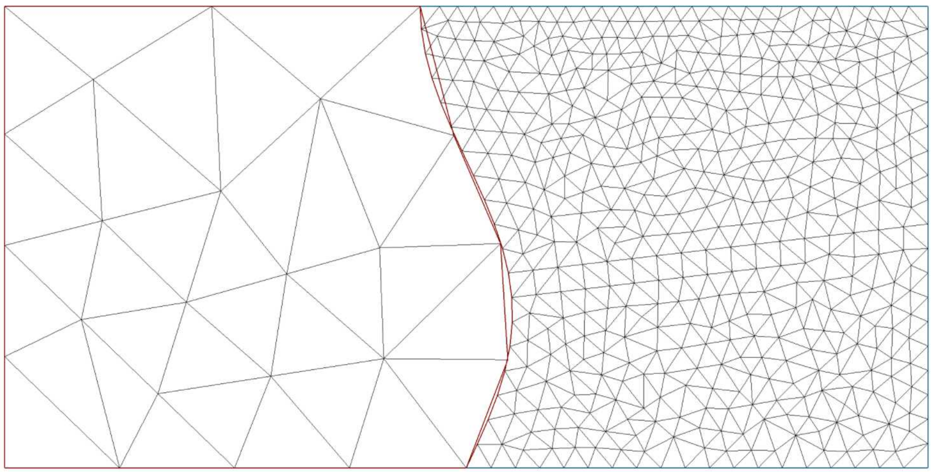


- For even experienced computational engineers, meshing is still bottleneck in workflow [1]
- Robust automated geometry discretization important as we move beyond forward simulation
- For uncertainty quantification, mesh generation scales exponentially with dimension
- For many meshfree methods, high ratio of local to global computation maps well onto modern architectures

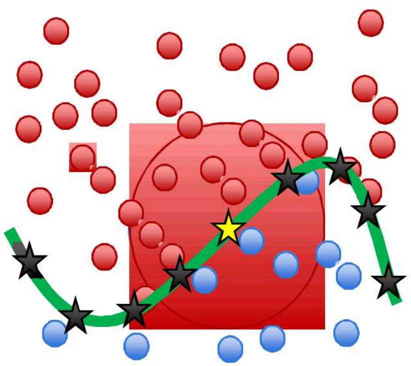
Discretization			Per Processor		
N	dx	# Particles	# Processor	# Particles	Load balance
128	6.875e-05	6,083,687	432	14,083	1.0003
192	4.583e-05	19,701,287	1,440	13,682	1.0004
256	3.437e-05	45,803,537	3,432	13,347	1.0007
384	2.291e-05	151,438,991	11,376	13,313	1.0006

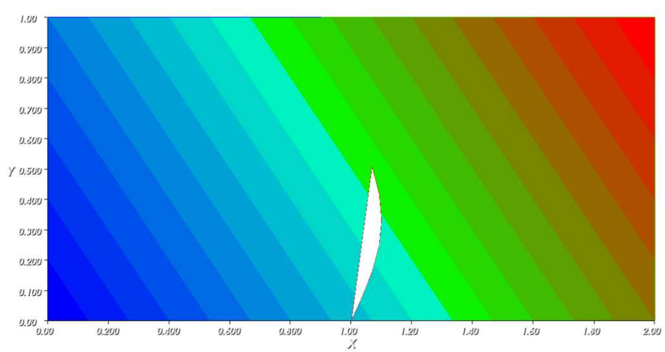
[1] "DART system analysis" M. Hardwick et al. SAND2005-4647

Why meshfree? Data transfer

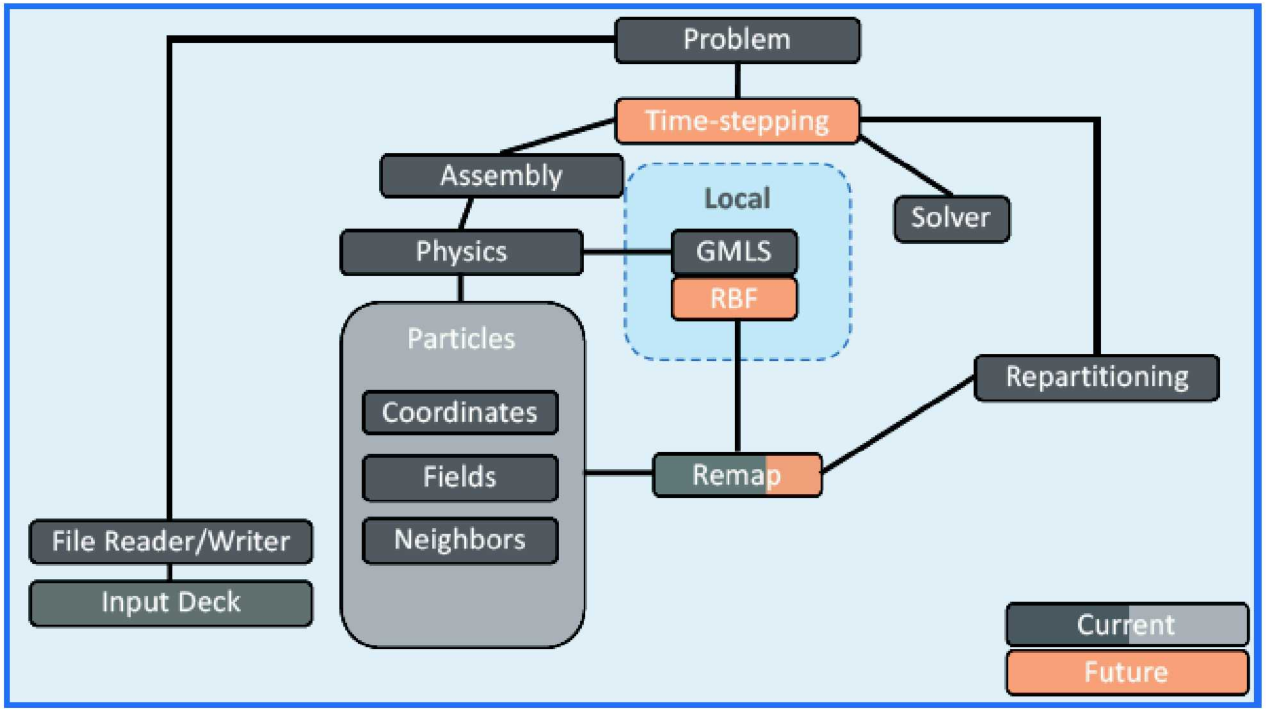


- As codes get bigger and more complex, multiphysics coupling becomes cumbersome
- Meshfree data transfer provides a non-intrusive way to transfer fluxes between codes with no assumption of underlying DOFs/boundary conformity





Compadre Trilinos package



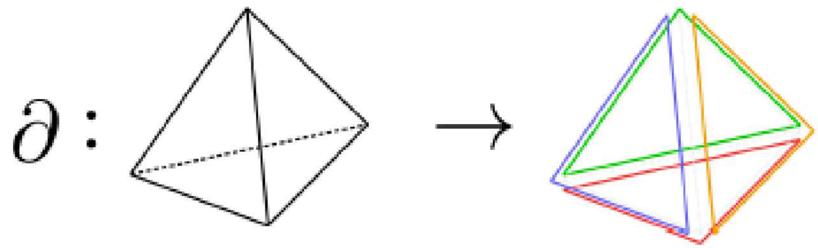
Collection of modules for general meshfree discretizations + heterogeneous architectures

- 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 efficient AMG preconditioning yielding O(N) solves

Why is conservation hard in meshfree?

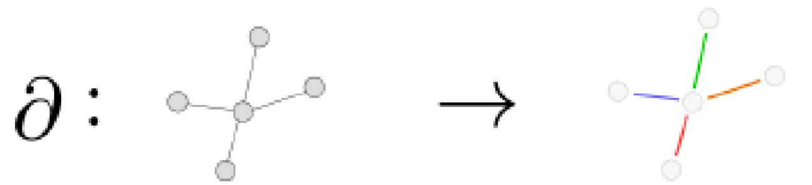
Generalized Stokes theorem

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



Gauss divergence theorem

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



Two ingredients:

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

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 $\mathbf{V} = P^m$

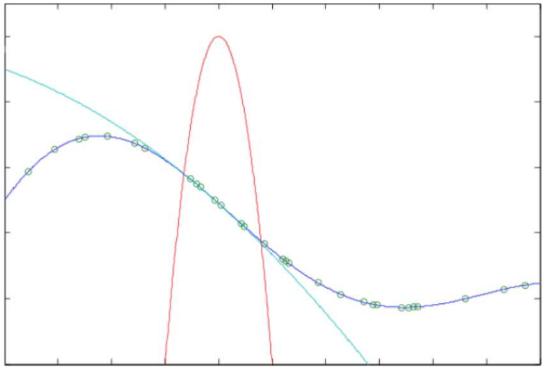
Sampling functional $\lambda_j = \delta_{x_j}$

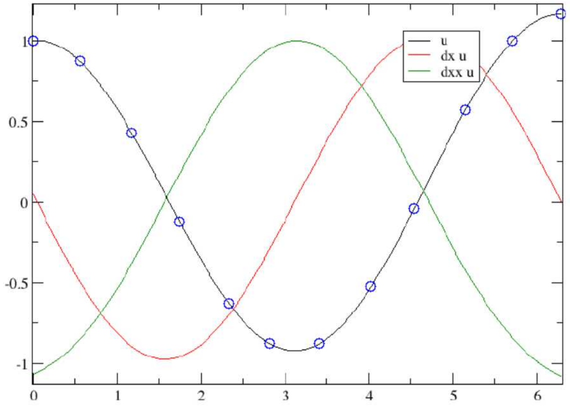
Weighting function $W = W(\|x_i - x_j\|)$

Takeaway:

A rigorous way to obtain formulas that look like:

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





Dual problem: equality constrained optimization

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

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

$$\underset{\alpha}{\text{minimize}} \quad \sum_j \frac{\alpha_j^2}{W(\tau, \lambda_j)}$$

$$\text{subject to} \quad \tau(p) = \sum_j \alpha_j \lambda_j(p), \ \forall p \in \mathbf{V}.$$

Example:

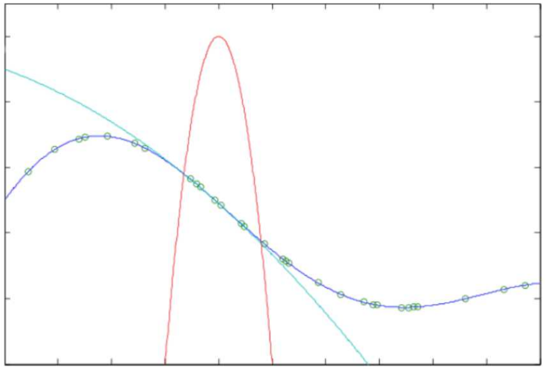
Approximate point evaluation of derivatives:

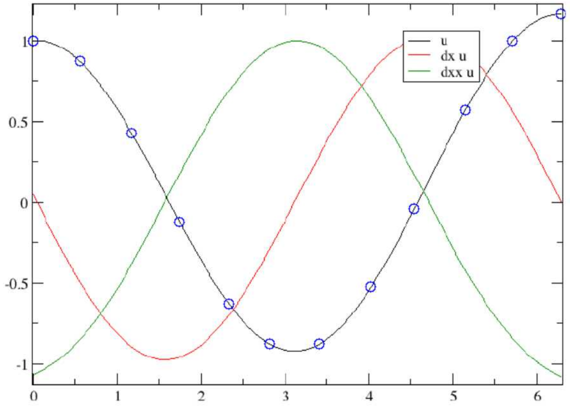
Target functional $\tau_i = D^\alpha \circ \delta_{x_i}$

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.

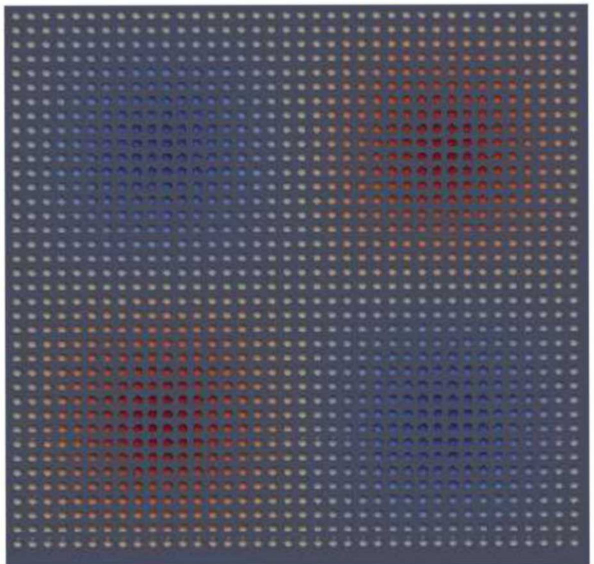
$$
\text{Let } u \in C^m(\Omega), \tau := D^\alpha \circ \delta_i, \lambda_j := \delta_j, V := P_m
$$

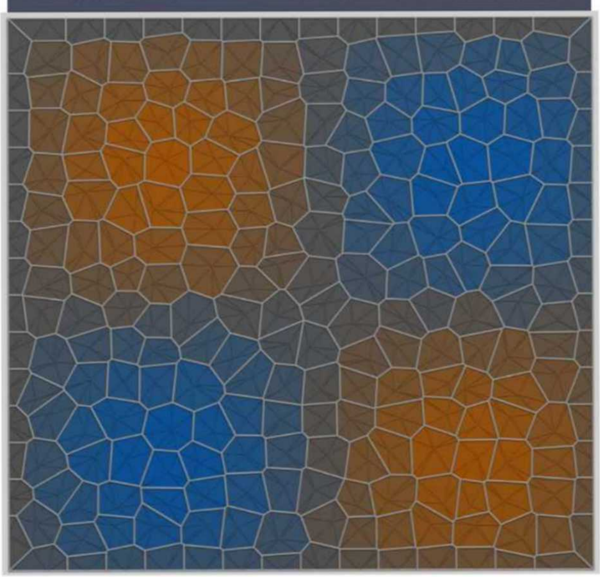
Taking p as the Taylor series about x_i leads to the following estimate

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

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

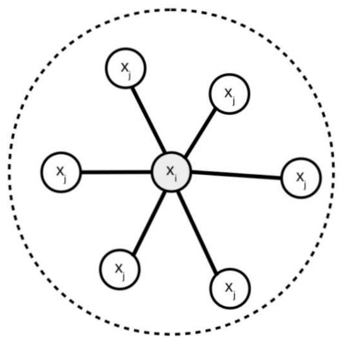
Solving PDEs with or without a mesh

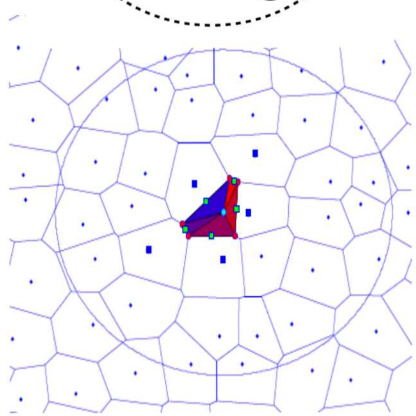


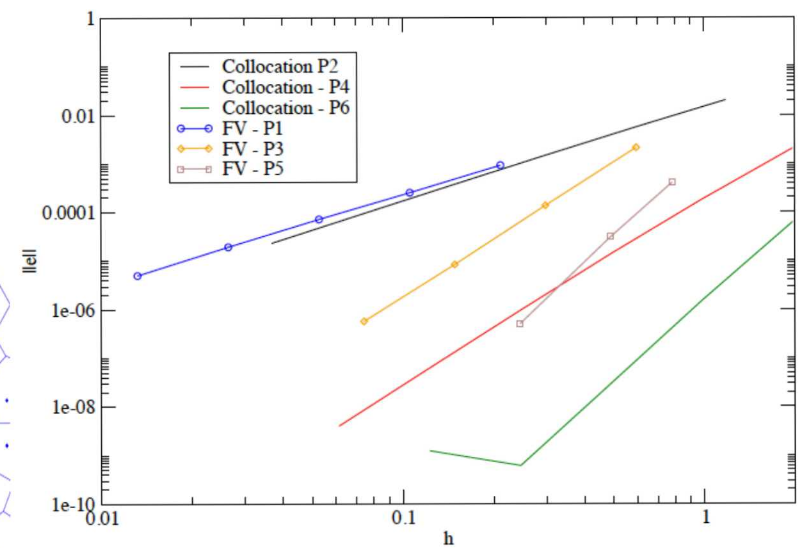


To generate mesh free schemes for $\nabla^2\phi = f$:

		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	$W(\lVert\boldsymbol{x}_j-\boldsymbol{x}_i\rVert)$	$W(\lVert\boldsymbol{x}_j-\boldsymbol{x}_i\rVert)$







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

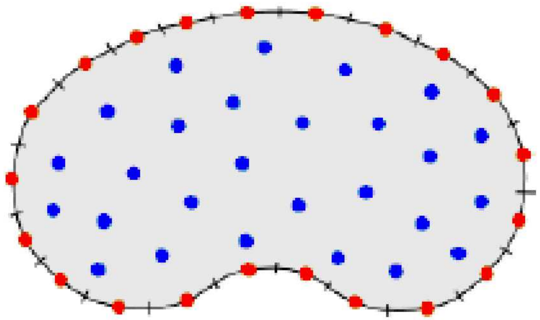
$$\mathbf{v}_c = \int_c \mathbf{P} dx$$

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.

A meshfree Gauss 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.*

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

where

- V_i and $v_{f_{ij}} = -v_{f_{ij}}$ are virtual volumes and face areas to be determined
- $c_{ij}^{\beta}(u)$ 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

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

Proof (skip)

Proof. For an arbitrary $\boldsymbol{p} \in (\Pi)^d$,

$$|V_i\,(\nabla \cdot \boldsymbol{u} - \nabla_h \cdot \boldsymbol{u})\,| \leq |V_i\,(\nabla \cdot \boldsymbol{u} - \nabla \cdot \boldsymbol{p})\,| + |V_i\,(\nabla_h \cdot \boldsymbol{p} - \nabla_h \cdot \boldsymbol{u})\,|$$

Take p^α as the Taylor expansion of the α^{th}-component of $\boldsymbol{u}$ about $\boldsymbol{x}_i$ so that

$$u^\alpha = p^\alpha + \sum_{|\gamma|=2} \frac{1}{\gamma!} D^\gamma u^\alpha(\xi)(\boldsymbol{x} - \boldsymbol{x}_i)$$

so that $|u^\alpha - p^\alpha| \leq C_\alpha \sum_{\gamma=2} (\boldsymbol{x} - \boldsymbol{x}_i)^\gamma$. Let $C_{TS} = \max_\alpha C_\alpha$. Then

$$|V_i\,(\nabla \cdot \boldsymbol{u} - \nabla_h \cdot \boldsymbol{u})\,| \leq \sum_{\gamma=2} C_{TS}\,|V_i\,(\nabla_h \cdot (\boldsymbol{x} - \boldsymbol{x}_i)^\gamma)|$$

Expanding the definition of the discrete divergence

$$|V_i\,(\nabla_h \cdot (\boldsymbol{x} - \boldsymbol{x}_i)^\gamma)| = \left| \sum_{j,\alpha,\beta} \left(\psi_j^{\alpha,\beta} - \psi_i^{\alpha,\beta}\right) c_{ij}^\beta\,((\boldsymbol{x} - \boldsymbol{x}_i)^\gamma)\,\phi^\beta(\boldsymbol{x}_{ij}) \right|$$

From the assumed scaling of the virtual areas

$$\left| \sum_{j,\alpha,\beta} \left(\psi_j^{\alpha,\beta} - \psi_i^{\alpha,\beta}\right) c_{ij}^\beta\,((\boldsymbol{x} - \boldsymbol{x}_i)^\gamma)\,\phi^\beta(\boldsymbol{x}_{ij}) \right| \leq dC_f \left| \sum_{j,\beta} c_{ij}^\beta\,((\boldsymbol{x} - \boldsymbol{x}_i)^\gamma)\,\phi^\beta(\boldsymbol{x}_{ij}) \right|.$$

From GMLS literature, there exists $C_{GMLS} > 0$ satisfying

$$\sum_j c_{ij}^\beta(f)\phi^\beta(\boldsymbol{x}_{ij}) \leq C_{gmls} h^2$$

Combining everything, we obtain

$$|V_i\,(\nabla \cdot \boldsymbol{u} - \nabla_h \cdot \boldsymbol{u})\,| \leq C_{TS} C_f h^{d-1} C_{gmls} h^2$$

$$|V_i\,(\nabla \cdot \boldsymbol{u} - \nabla_h \cdot \boldsymbol{u})\,| \leq Ch.$$

□

How to get the areas?

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

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

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?

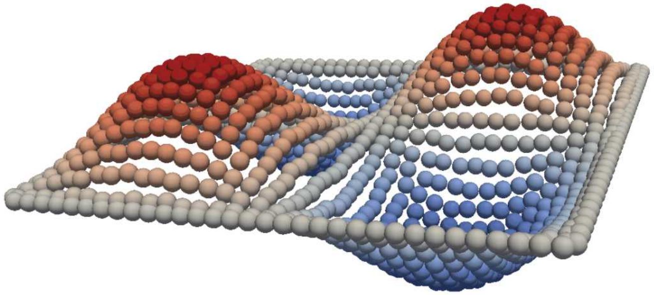
Assumed we have a process for generating volumes satisfying

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

Explored several options:

- $V_i = |\Omega|/N$
- $V_i = d_i \left(\frac{|\Omega|}{\sum d_i} \right)$, where d_i are SPH definition of volumes
- $V_i = \frac{1}{d} \left[\sum_{j,\alpha} \psi^{0\alpha} \boldsymbol{e}^{\alpha} \cdot \boldsymbol{x}_{ij} + \chi_{I \in \partial\Omega} \int_{\partial\Omega_i} \boldsymbol{x} \cdot d\boldsymbol{A} \right]$

h	Volume1	Volume2	Volume3
1/16	0.081	0.058	0.032
1/32	0.049	0.032	0.018
1/64	0.024	0.015	0.0099
1/128	0.011	0.0072	0.0046



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:**

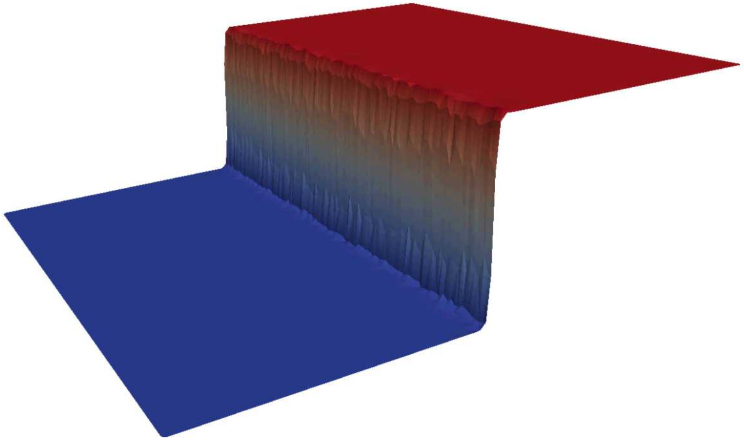
$$\boldsymbol{F} = -\mu \nabla \phi$$

- **Singularly perturbed advection diffusion:**

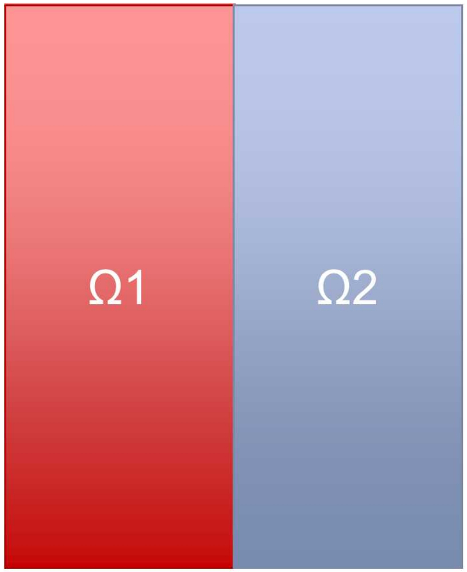
$$\boldsymbol{F} = -\mu \nabla \phi + \boldsymbol{a} \phi$$

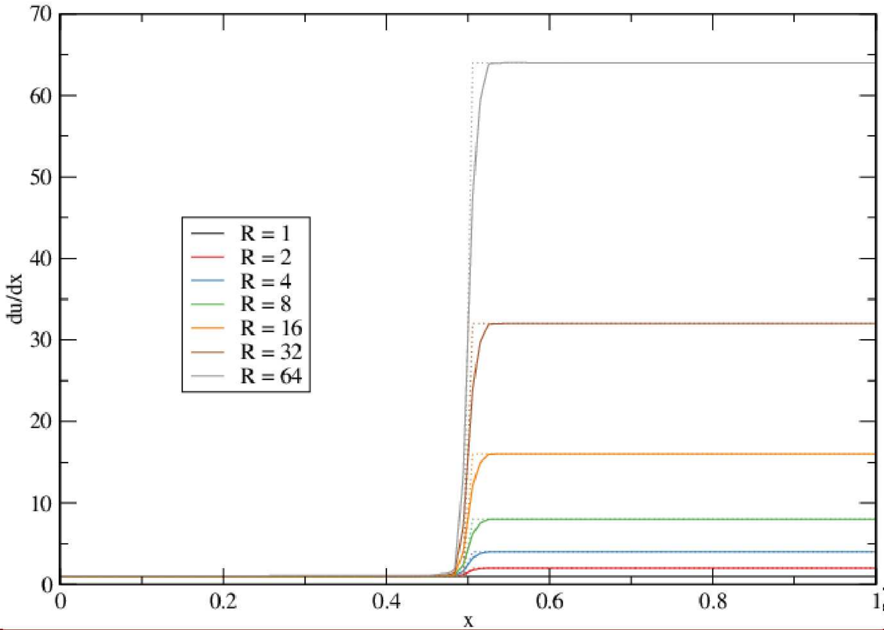
Skip lots of details: but we'll show how we handle benchmarks that challenge conventional mesh-based methods

Darcy: jumps in material properties



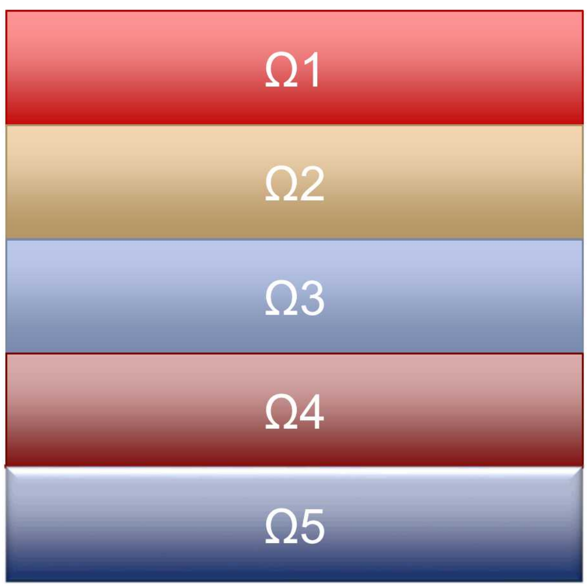
$$\nabla \phi \rightarrow$$

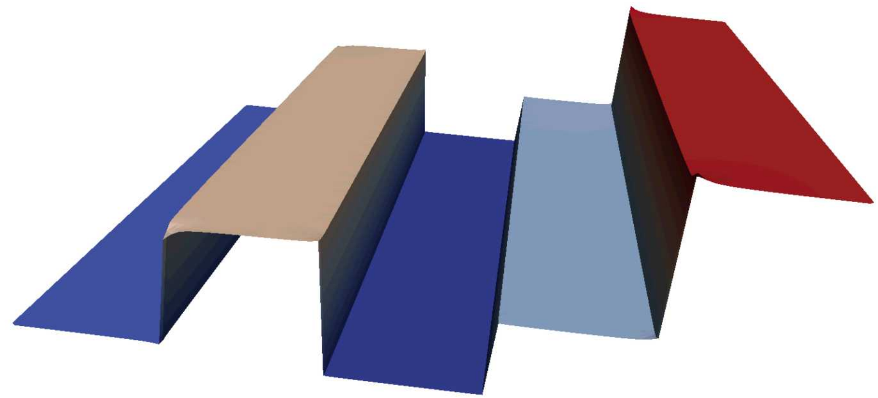


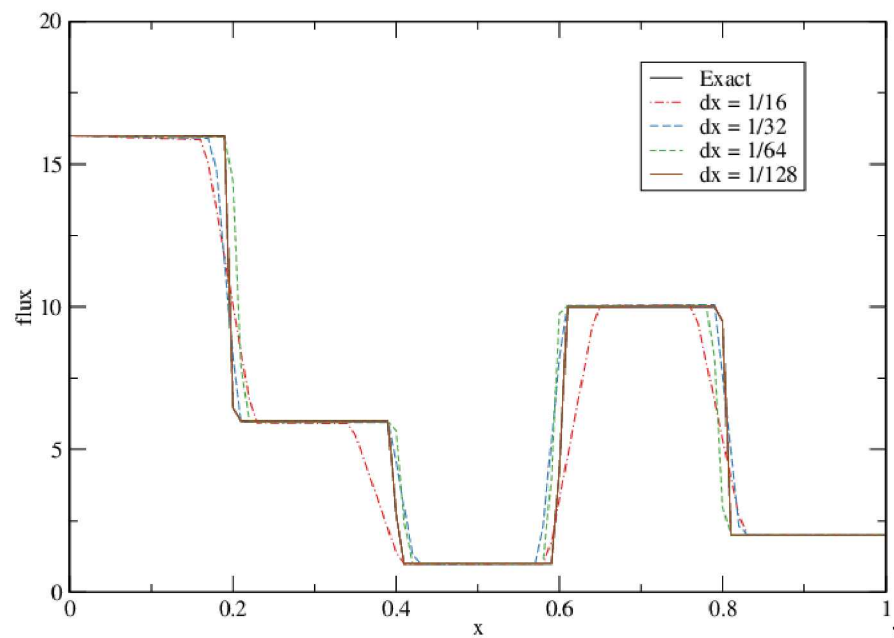


Darcy: jumps in material properties

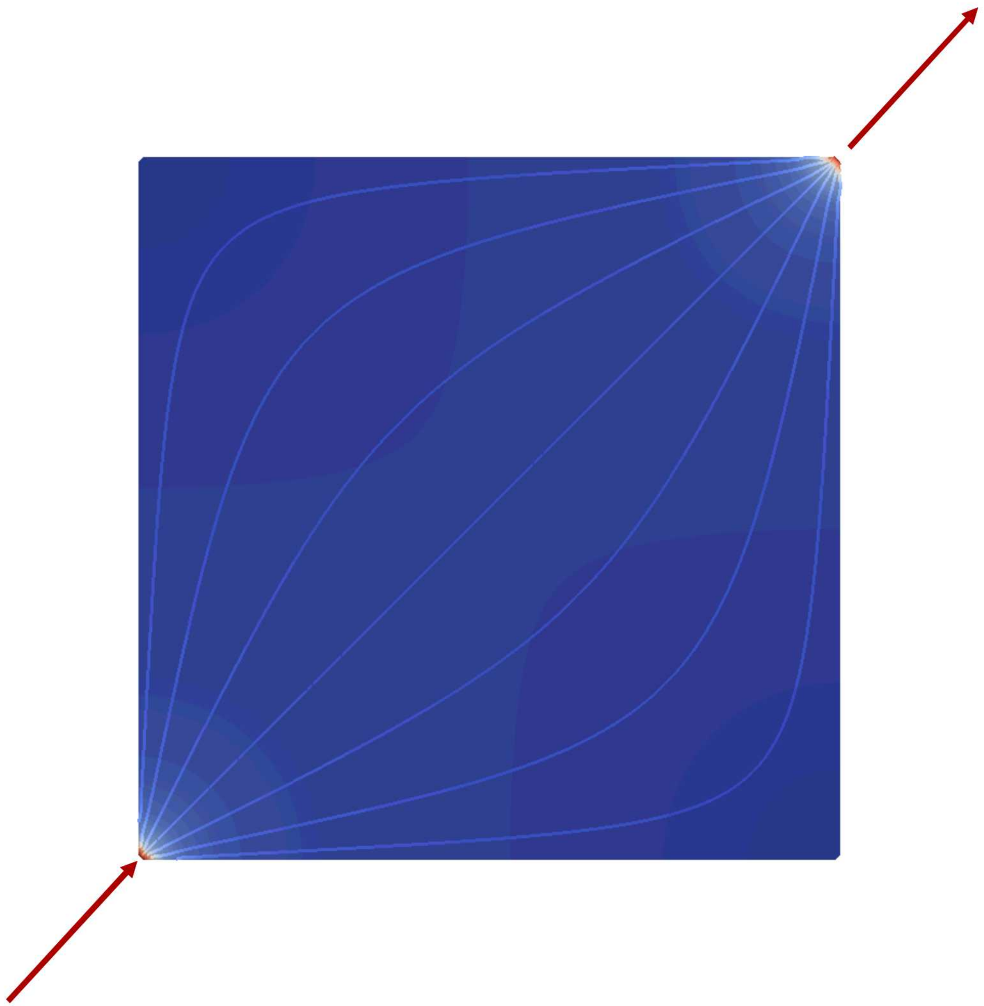
$$\nabla \phi \rightarrow$$

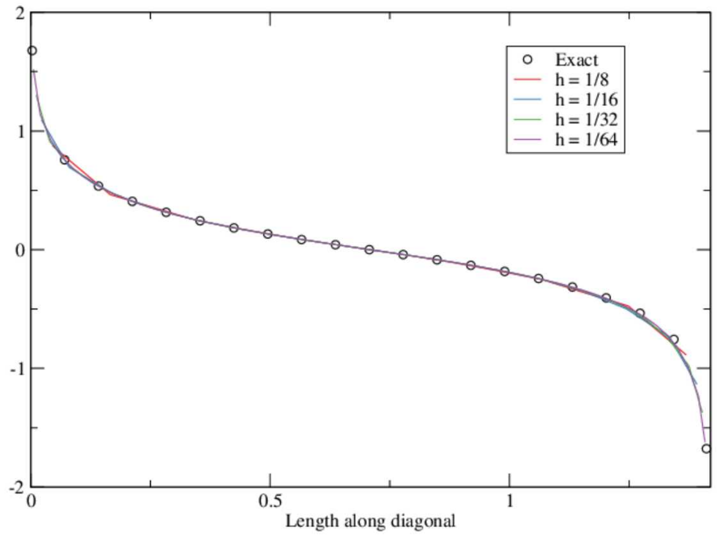


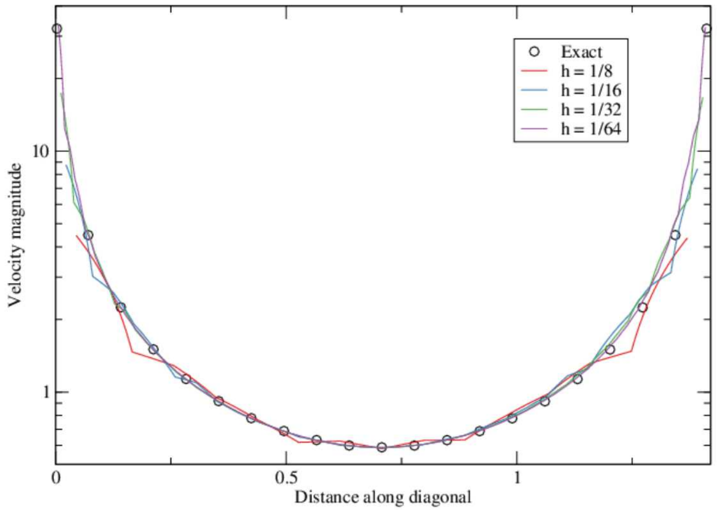




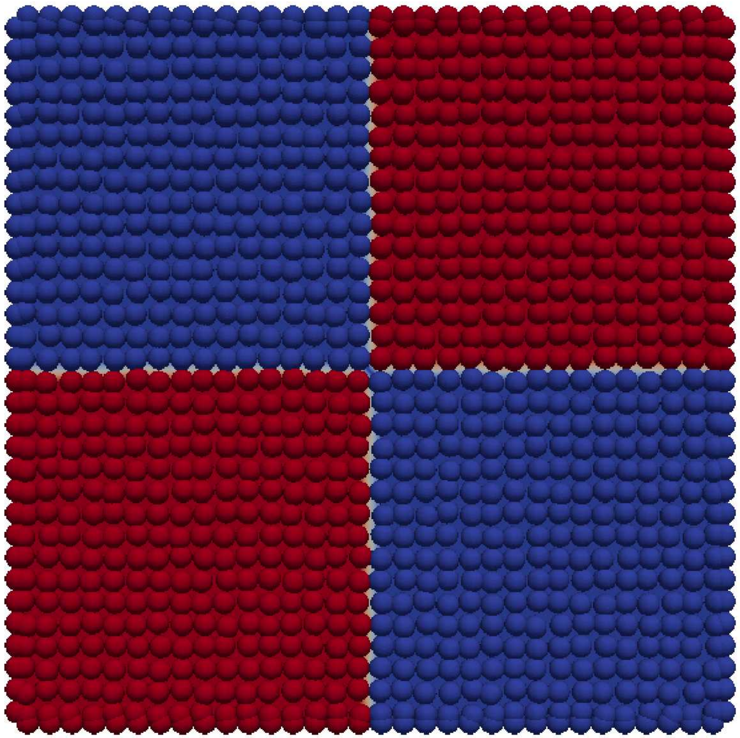
Darcy: 5-spot problem

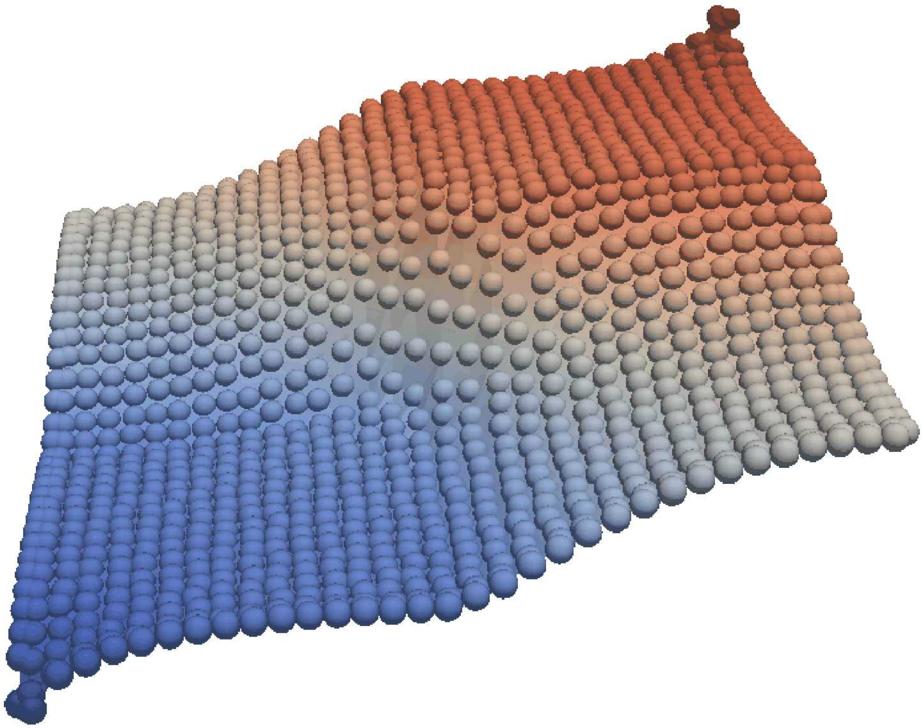




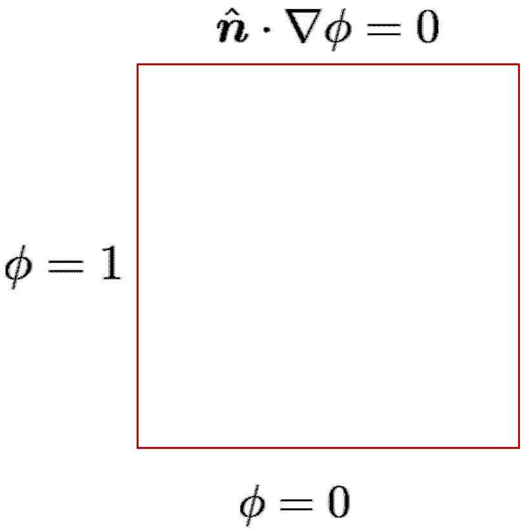


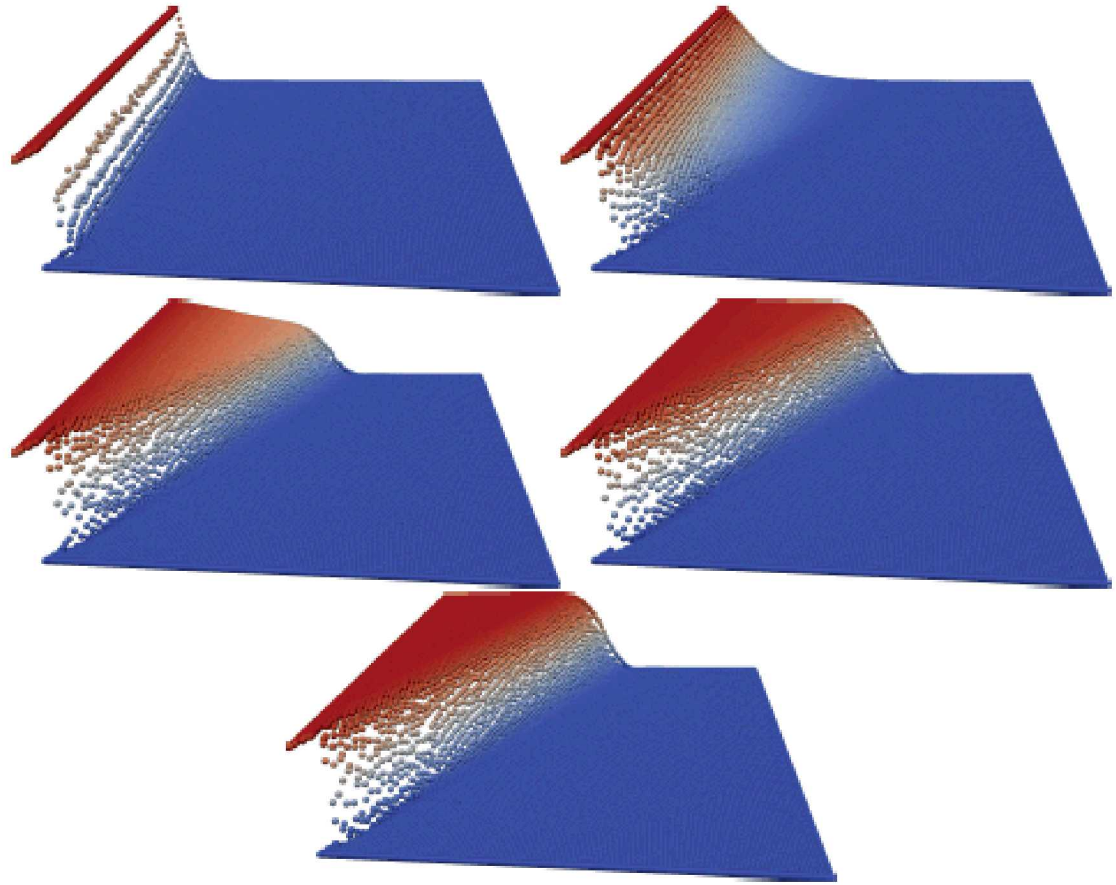
Darcy 5-spot problem





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

Talk part 2: Non-local models for mesoscale

By non-local mechanics, we mean a model which evolves according to an integral operator of the form

$$\rho \ddot{\boldsymbol{u}} = \int_{\mathbb{R}^d} K(x, y) u(y) dy$$

These types of models mainly come in two flavors:

- Physics are nonlocal: e.g. Coulombic surface tension models, density functional theory
- A local theory is more conveniently expressed via integral operators than derivatives, for regularity reasons

Target application: non-local fracture mechanics

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

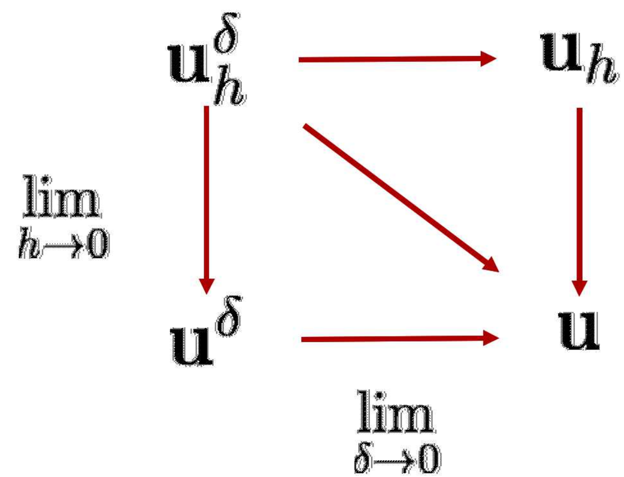
$$\rho(\mathbf{x}) \frac{d^2}{dt^2} \mathbf{u}(\mathbf{x}) = \mathcal{L}[\mathbf{u}](\mathbf{x})$$

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

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

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

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



For reduced regularity in modelling fracture, we care about so-called *asymptotic compatibility* where discrete nonlocal model converges to the continuous local model

Non-local setting and notation

Consider a family of integral equations of the form:

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

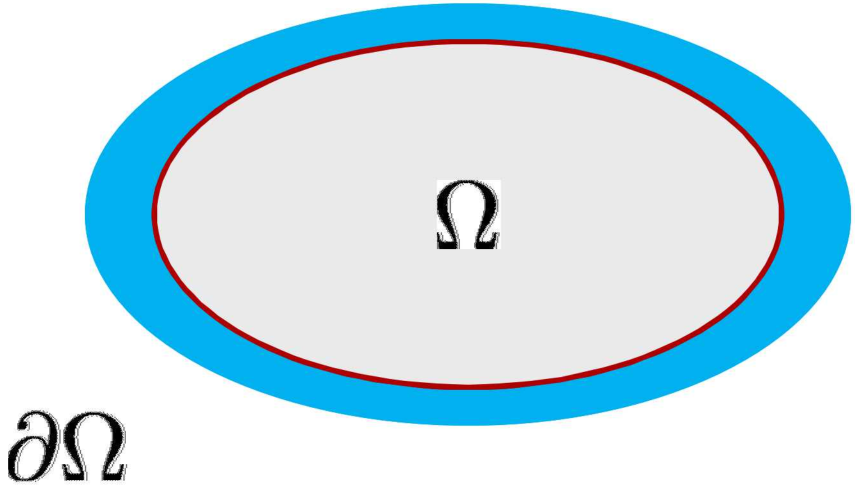
$$supp(K(x,\cdot)) = \delta$$

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

Discretized over the domain:

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

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

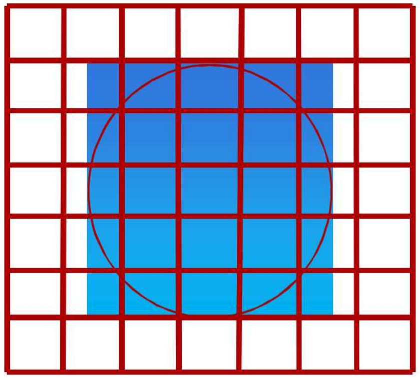


Motivation: non-local quadrature on mesh

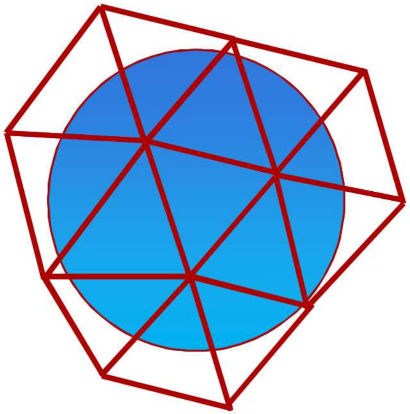
Define quadrature rule:

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

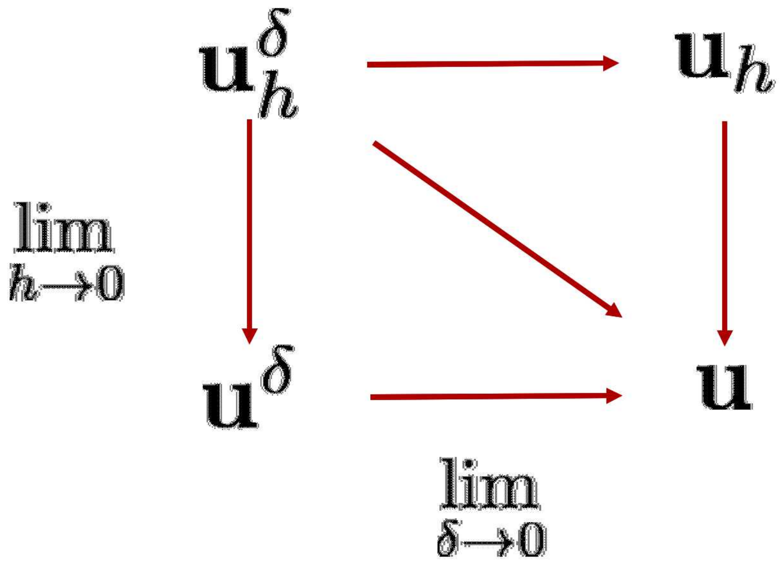
$$\mathcal{L}_\delta^h[u](\mathbf{x}_i) = \sum_{\mathbf{x}_j \in \mathbf{X}_q \subset B(\mathbf{x}_q,\delta)} K(\mathbf{x}_i,\mathbf{x}_j)u(\mathbf{x}_j)\,\omega_j$$

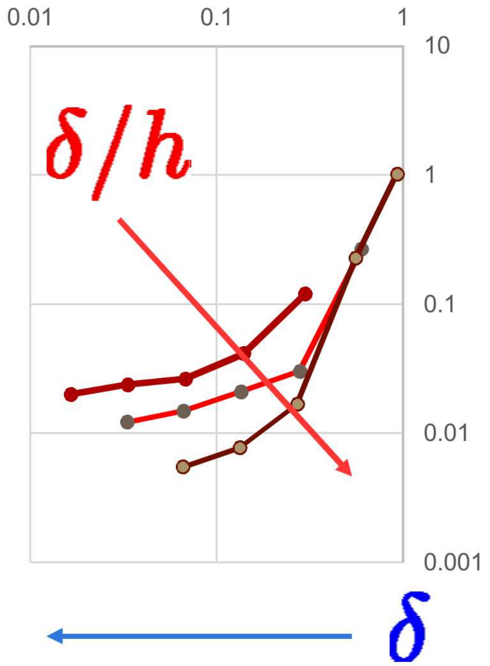


- Challenges in finite element setting:
  - Costly geometric intersection
  - Singularity in non-local kernel – **particularly hard on unstructured meshes**
    - **Ex:** P0 discontinuous approximation, u = 1



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

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

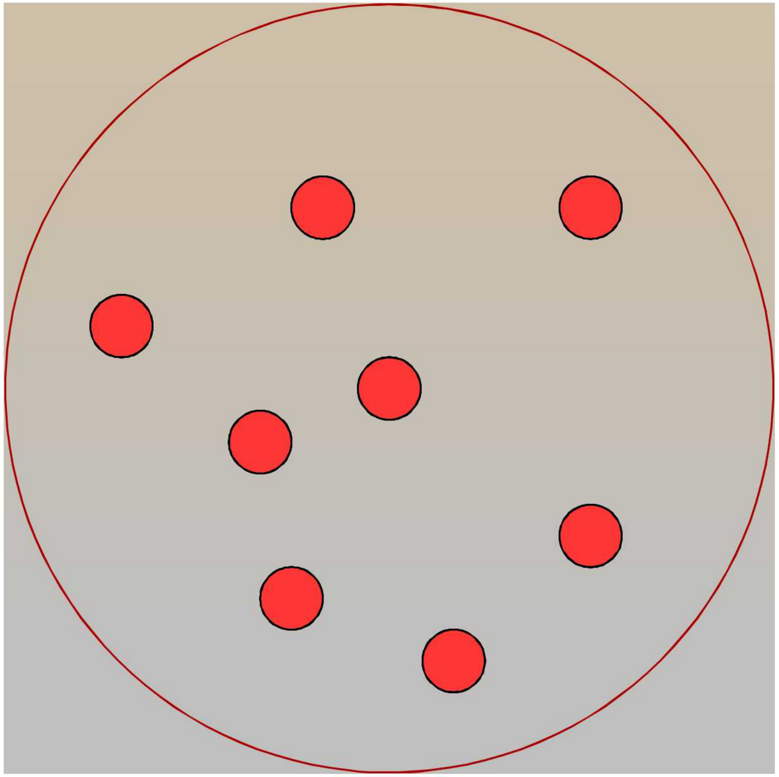
$$\underset{\omega}{\text{minimize}} \sum_j \omega_j^2$$

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

Solution of KKT system

$$\begin{bmatrix} \mathbf{I} & \mathbf{B}^\intercal \\ \mathbf{B} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\omega} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{g} \end{bmatrix}$$

- $\mathbf{I} \in \mathbb{R}^{N_q \times N_q}$ - identity matrix
- $\boldsymbol{\omega} \in \mathbb{R}^{N_q}$ - quadrature weights
- $\boldsymbol{\lambda} \in \mathbb{R}^{dim(\mathbf{V}_h)}$ - Lagrange multipliers to enforce reproduction
- $\mathbf{B} \in \mathbb{R}^{N_q \times dim(\mathbf{V}_h)}$ - reproducing set evaluated at each quadrature point
- $\mathbf{g} \in \mathbb{R}^{dim(\mathbf{V}_h)}$ integral of each function in the reproducing set over the ball

- $O(dim(V)^3)$ work using Schur complement solver
- Requires efficient means to solve g
  - Best case scenario, analytic solution available for **V** over domain
    - **Ex:** integrate some polynomials on balls
  - Worst case: need to integrate numerically on a ball

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* $n(\mathbf{x},\mathbf{y}) \leq C_n$ *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.*

$$\left| \int_{B(\mathbf{x},\delta)} K(\mathbf{x},\mathbf{y})u(\mathbf{y})\,d\mathbf{y} - \sum_{j\in X_q} K(\mathbf{x},\mathbf{x}_j)u_j\omega_j \right| \leq C\delta^{k+1-\alpha+d}$$

Truncation error for smooth displacements

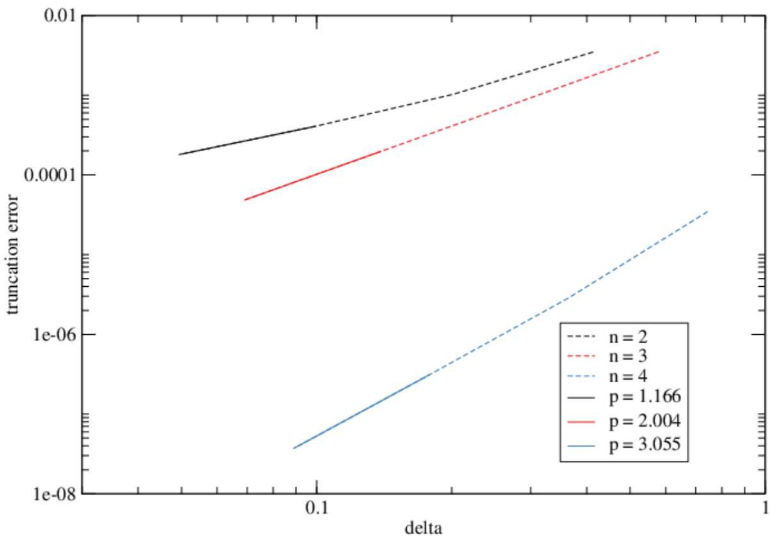
$$\mathcal{L}[\mathbf{u}](\mathbf{x}) = \frac{3K}{8}\left(\nabla^2\mathbf{u} + \nabla\nabla\cdot\mathbf{u}\right)$$

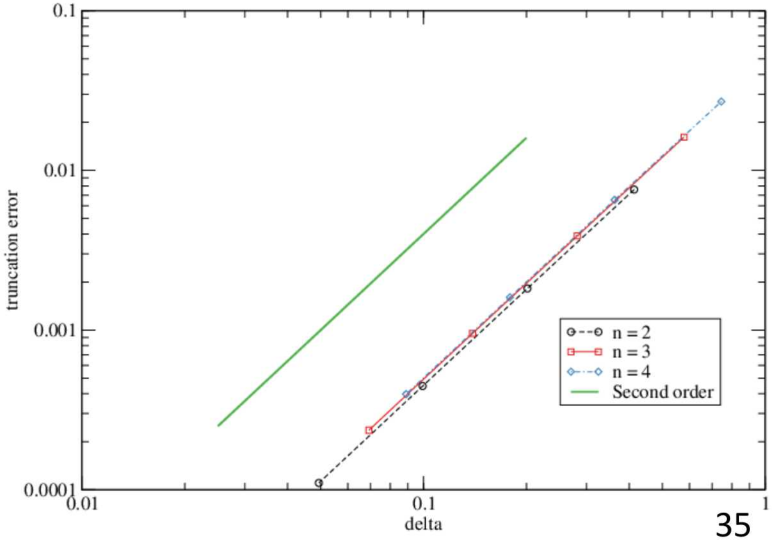
$$\mathcal{L}^\delta[\mathbf{u}^\delta](\mathbf{x}) = \int_{B(\mathbf{x},\delta)} c\frac{\boldsymbol{\xi}\otimes\boldsymbol{\xi}}{||\boldsymbol{\xi}||^3}\left(\mathbf{u}^\delta(\mathbf{y}) - \mathbf{u}^\delta(\mathbf{x})\right)\,d\mathbf{y}$$

$$c = \begin{cases} \frac{72K}{5\pi\delta^3} & d = 2 \\ \frac{18K}{\pi\delta^4} & d = 3 \end{cases}$$

$$\left|\mathcal{L}^\delta[u] - \mathcal{L}_h^\delta[u]\right| \le C\delta^{m-\alpha}$$

$$\left|\mathcal{L}[u] - \mathcal{L}_h^\delta[u]\right| \le C\delta^2$$





To recap:

- What have we achieved:
  - Replaced a difficult geometric quadrature problem with a local, easy optimization problem that maps well onto modern architectures
- Applicable to general integral equations
  - Even in the case where there is a mesh!
- Restrict ourselves now to bond-based peridynamics
  - Manufactured solutions to demonstrate asymptotic compatibility
  - Combine with damage model to get asymptotically compatible damage
  - Extend this to define an extension operator providing a means of enforcing BCs locally
  - Some mechanics examples

Manufactured solution to BVP

Let $\omega_{j,i}$ be the weight for particle i in stencil j

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

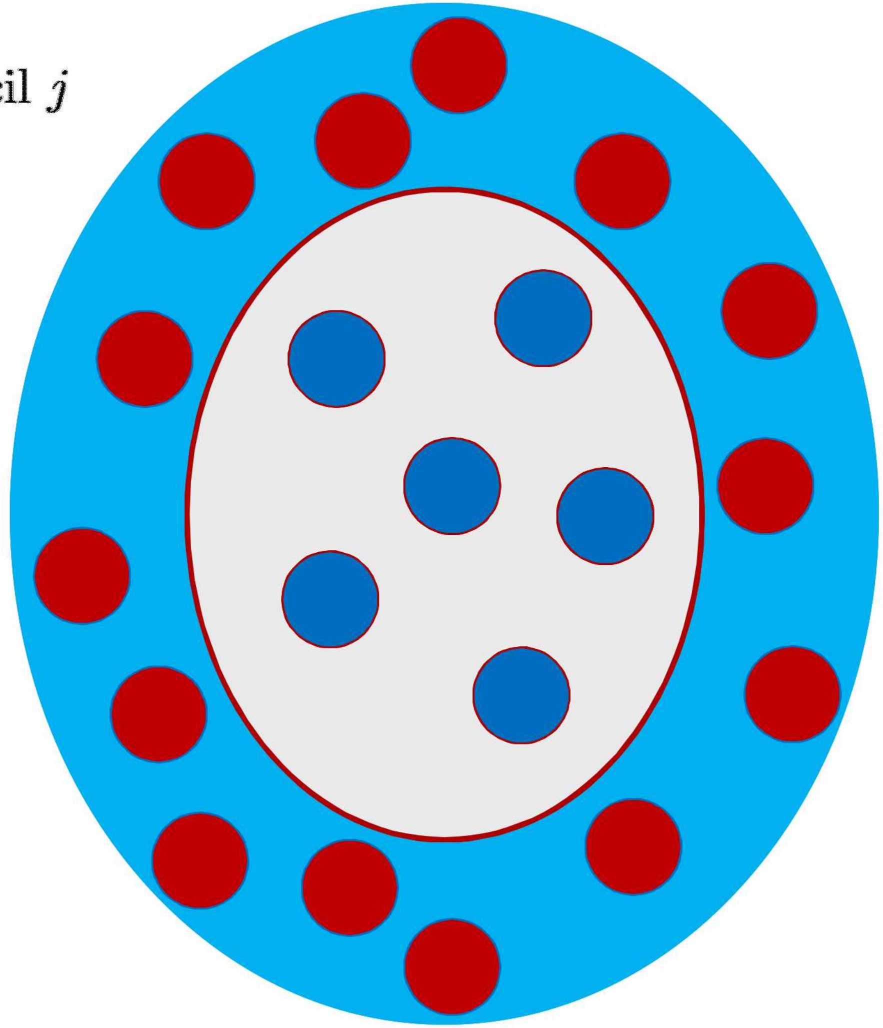
$$\mathbf{u} = \langle \sin x \sin y, \cos x \cos y \rangle$$

Characterize point cloud distribution

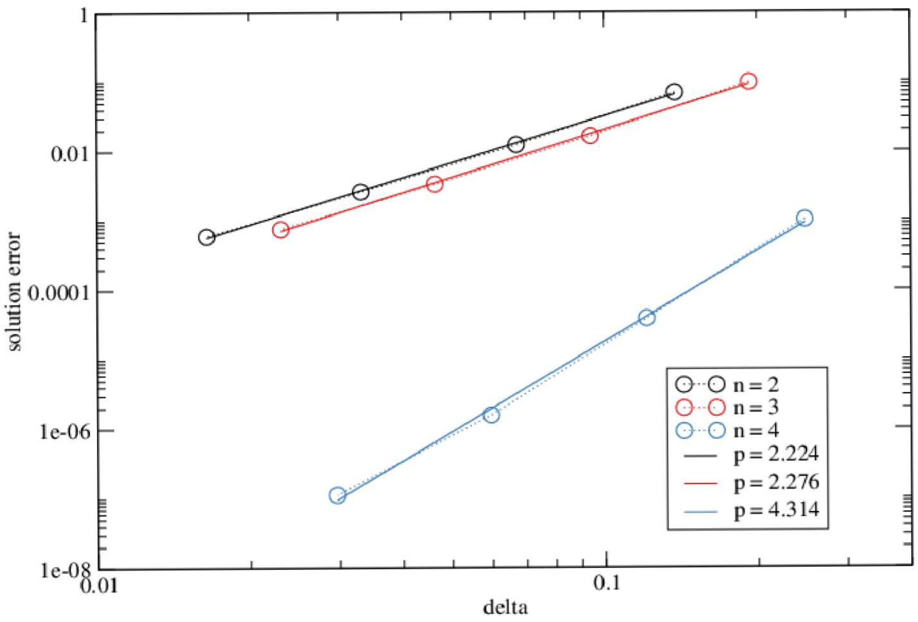
$$h = \sup_{\mathbf{x} \in \Omega^\delta} \min_{1 \le j \le N_p} ||\mathbf{x} - \mathbf{x}_j||_2$$

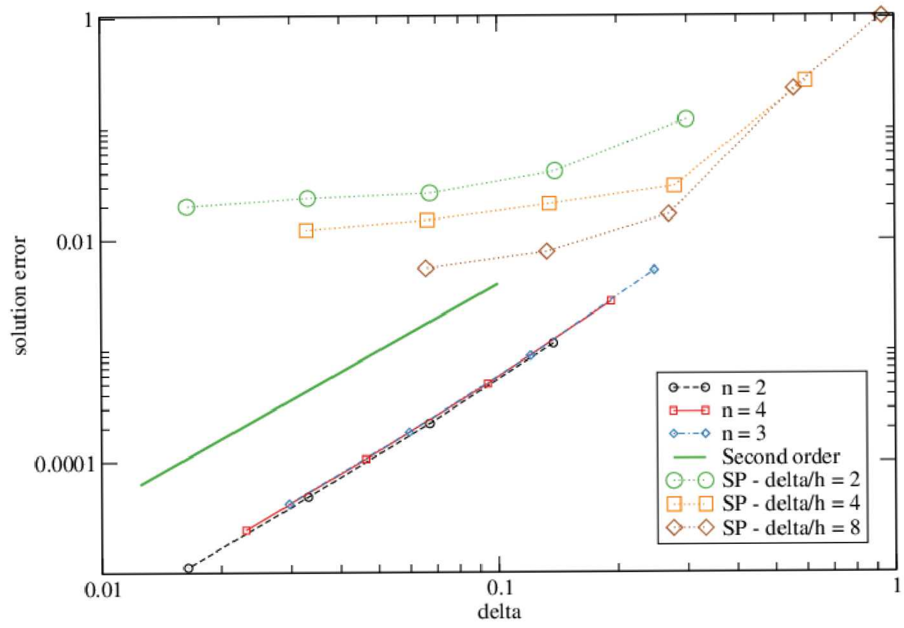
$$q_{\mathbf{X}_h} = \frac{1}{2} \min_{i \neq j} ||\mathbf{x}_i - \mathbf{x}_j||_2$$

$$q_{\mathbf{X}_h} \le h \le c_{qu} q_{\mathbf{X}_h}$$



Manufactured solution to BVP





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

$$u_h^\delta \to u$$

Damage modelling

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

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

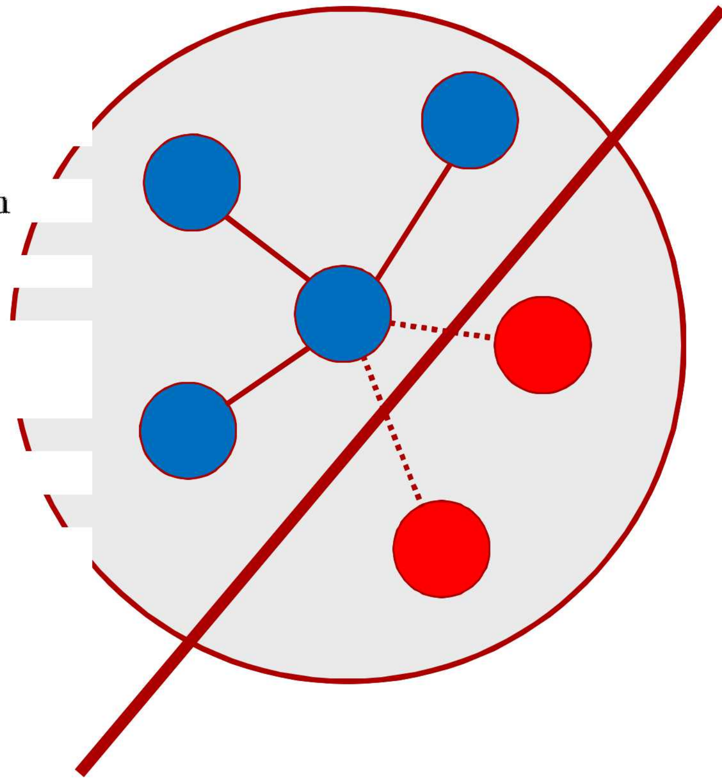
Bonds are either

- 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

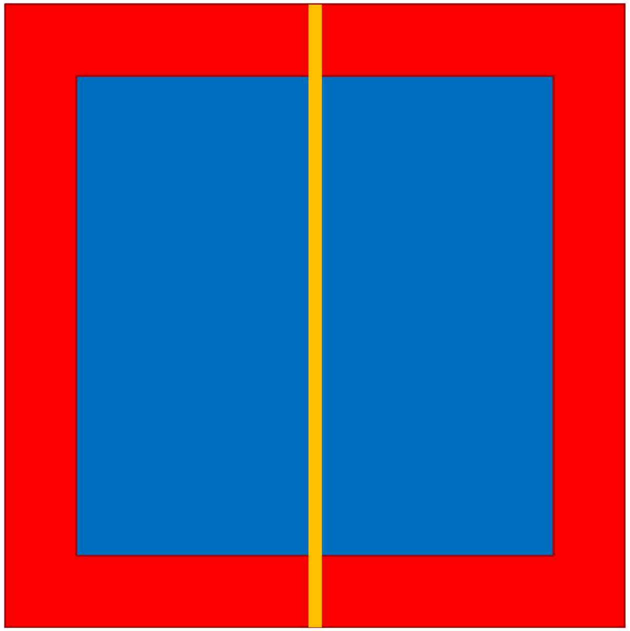
$$s_0 = \begin{cases} \sqrt{\frac{G_c}{\left(\frac{6\mu}{\pi} + \frac{16}{9\pi^2}(\kappa - 2\mu)\right)\delta}}, & \text{d} = 2 \\ \sqrt{\frac{G_c}{\left(3\mu + \left(\frac{3}{4}\right)^4\left(\kappa - \frac{5\mu}{3}\right)\right)\delta}}, & \text{d} = 3 \text{ .} \end{cases}$$

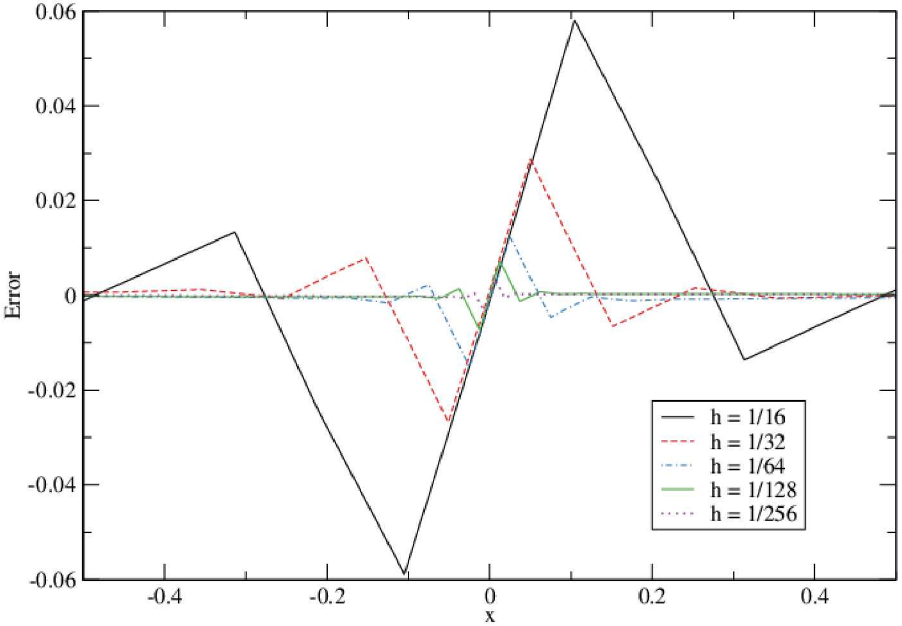


Asymptotic convergence to local condition

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

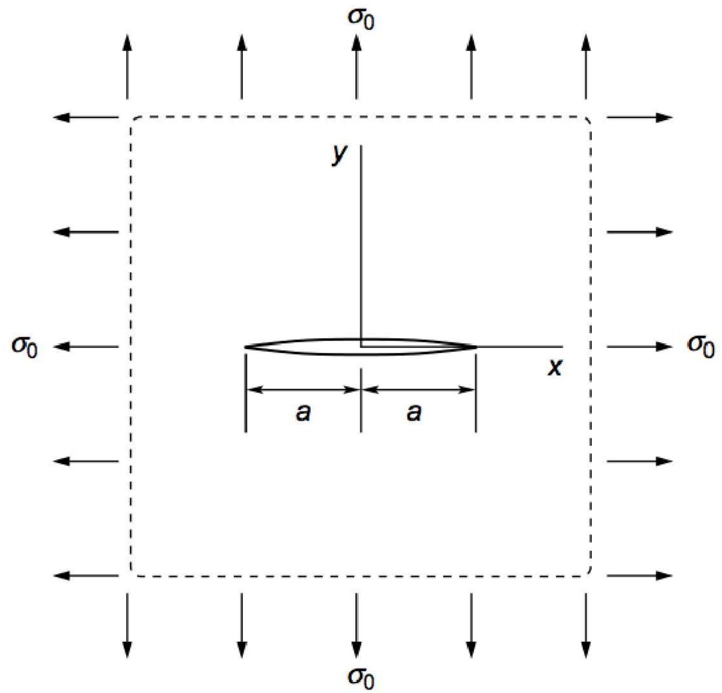
$$\sigma(u) \cdot \hat{n} = 0$$

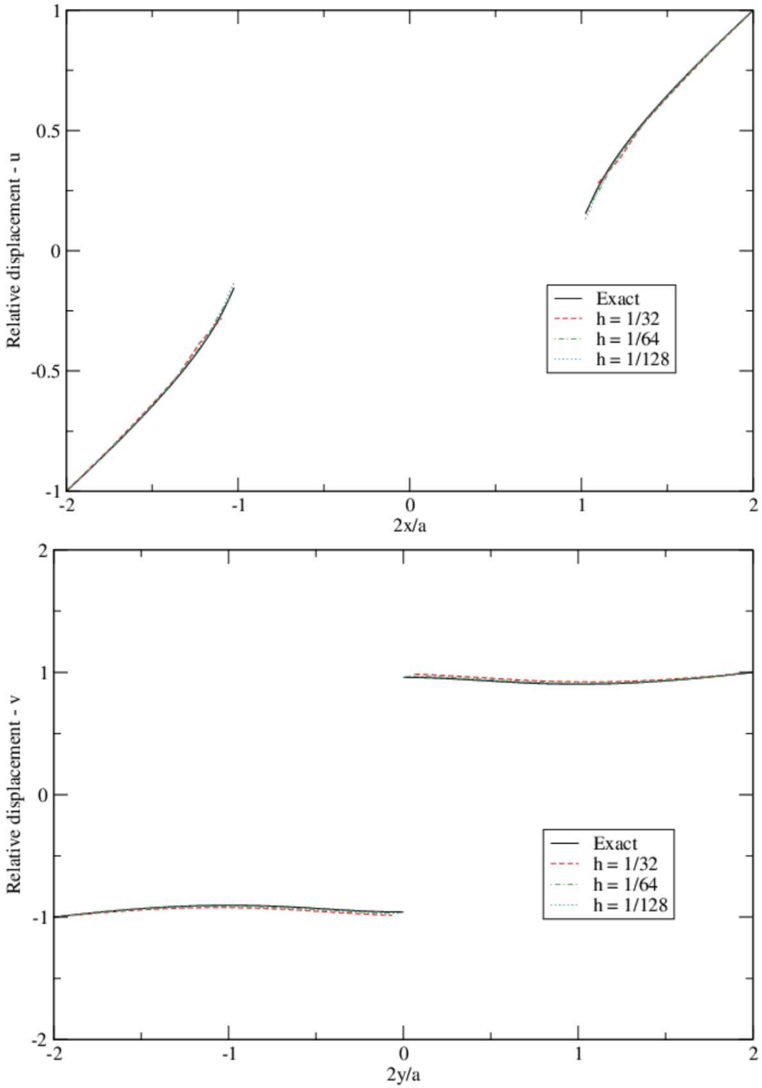




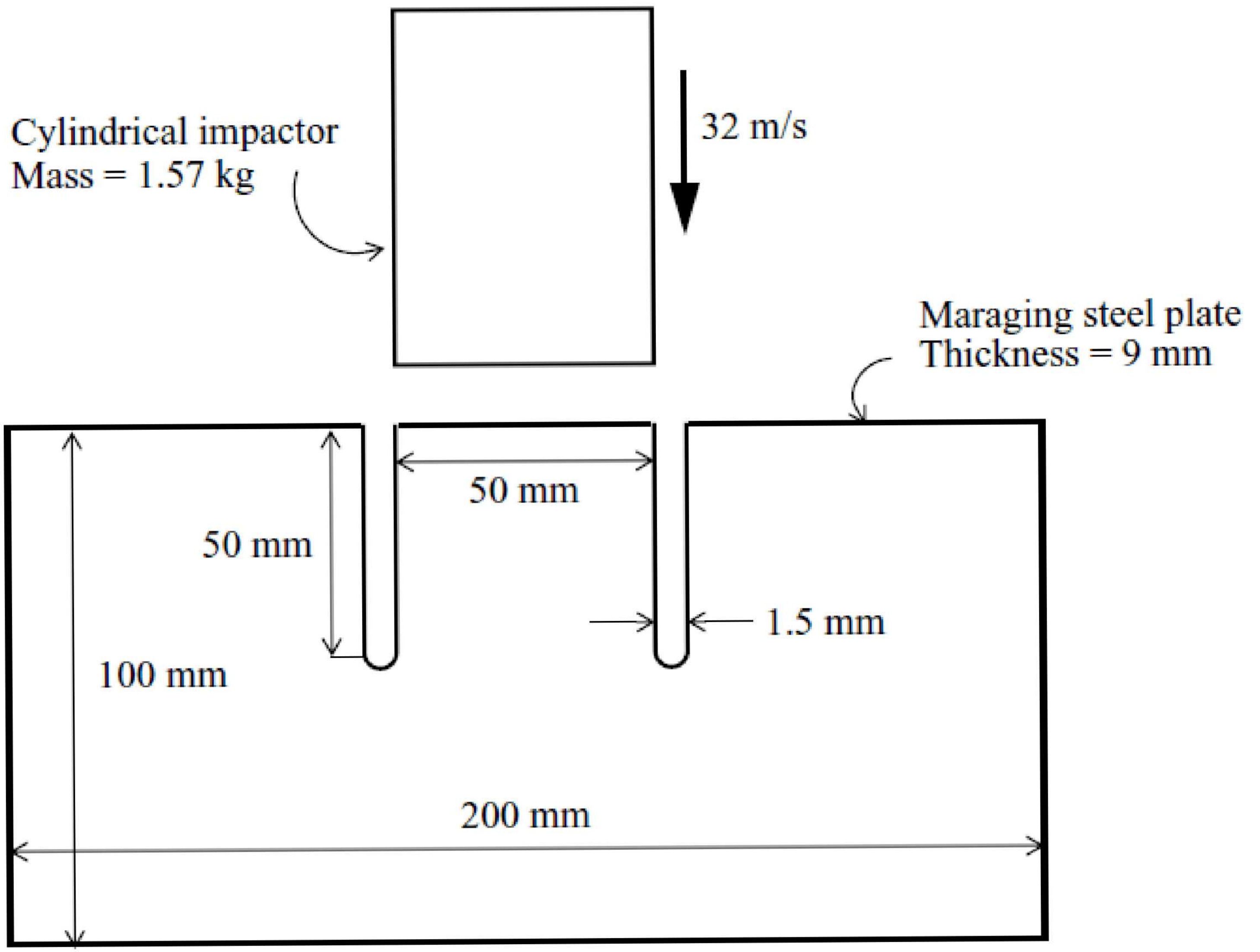
Damage model recovers analytic traction-free local solution as $O(\delta)$.

Type-I crack loading



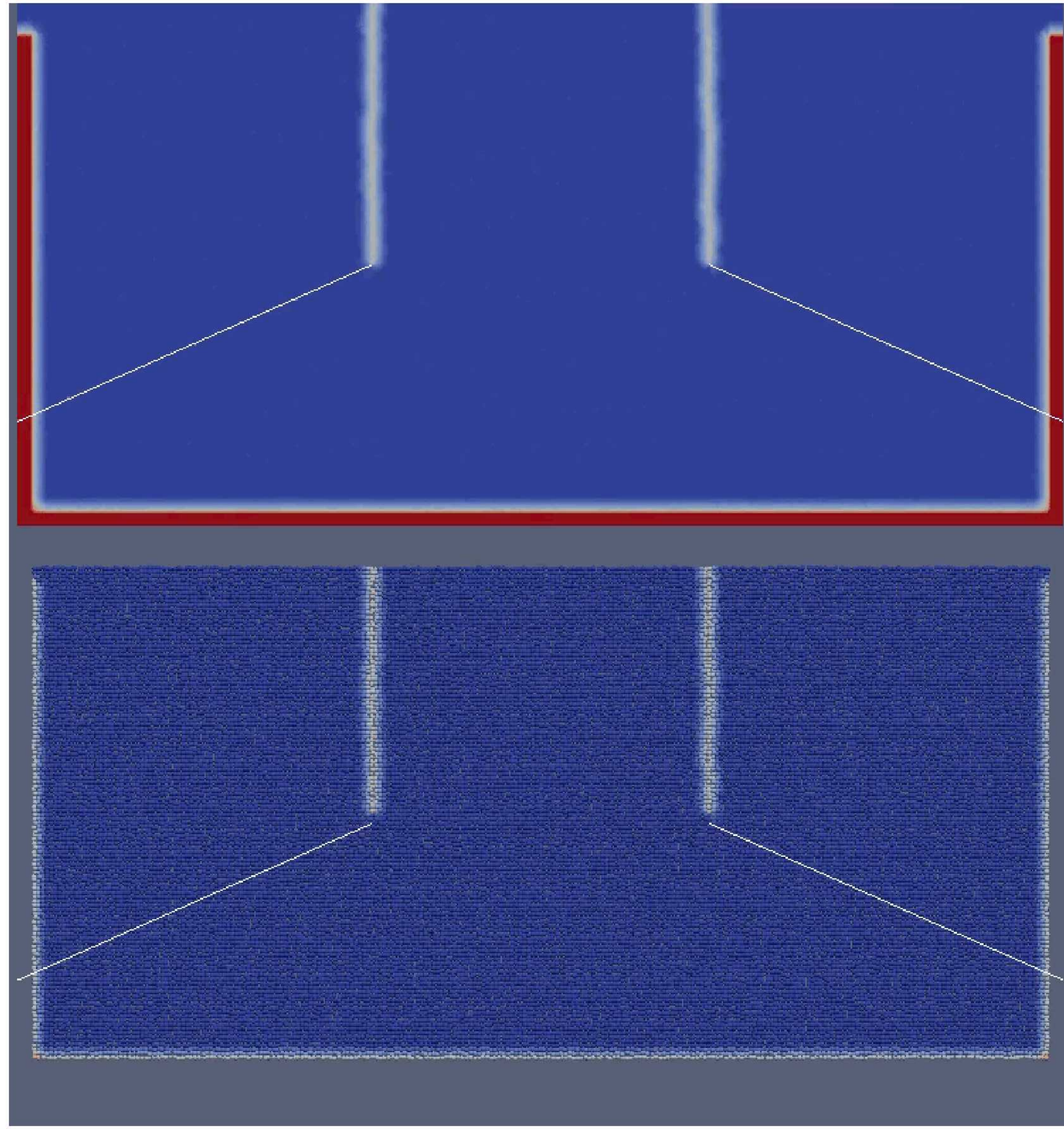


Kalthoff-Winkler experiment



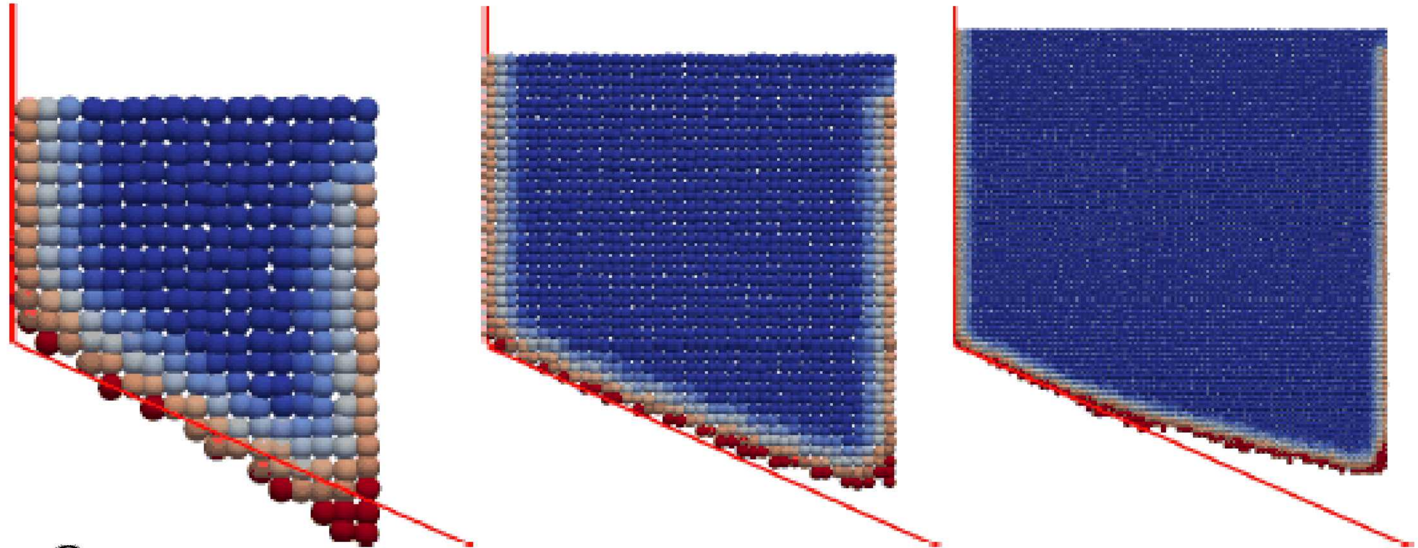
Kalthoff-Winkler experiment

Key property:
Introduction of optimization based quadrature fits into standard peridynamics workflow



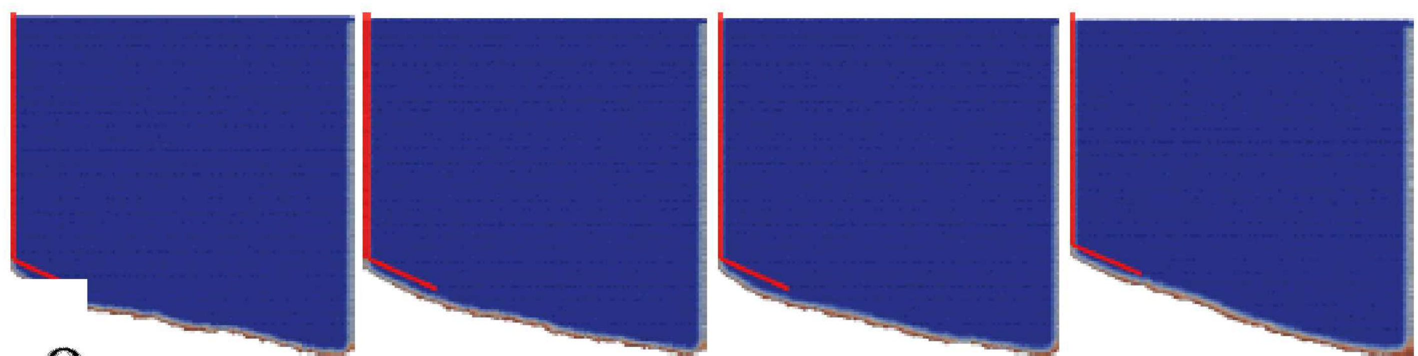
Kalthoff-Winkler experiment

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



$$\delta \to 0$$

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



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

Conclusions

- Meshfree methods provide needed flexibility for many problems, but historically struggle with notions of conservation and consistency
- We remedy this with optimization based approaches
- We provide a constructive approach to develop consistent meshfree summation-by-parts operators, utilizing GMLS to obtain accuracy and fast graph Laplacian solvers to obtain virtual definitions of metric information (a meshfree RT)
- For non-local methods, asymptotic compatibility may be achieved in a similar framework, putting peridynamic fracture models on a sound mathematical foundation
- Many other applications: surface PDE, Stokes flow, local elasticity, plasma physics