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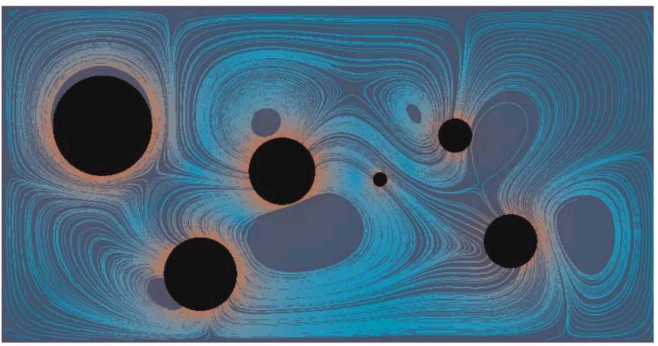

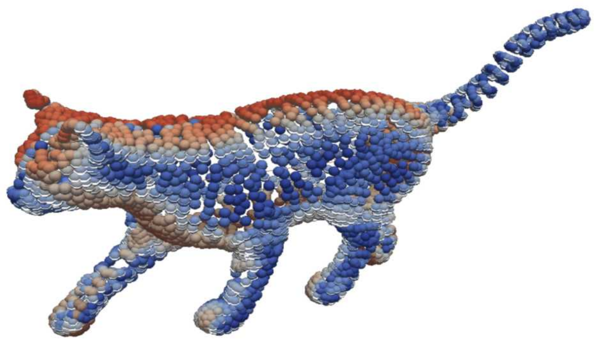

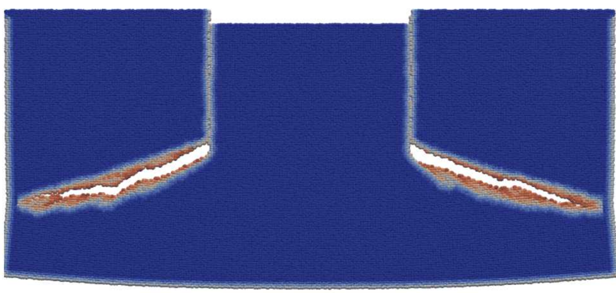

Asymptotically compatible foundations for nonlocal mechanics

Center for Computing Research

Nat Trask

Sandia National Laboratories

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Collaborators+Acknowledgements

AsCeND LDRD – Asymptotically **C**ompatible foundations for **N**onlocal **D**iscretization

- **Objective:** mathematical framework for provably convergent nonlocal schemes, with applications+software (ductile fracture, subsurface flow/fracture, failure in lithium ion batteries)
- **People:** Nat Trask, Marta D'Elia, Dave Littlewood, Stewart Silling, Mike Tupek, John Foster (UT:Austin)

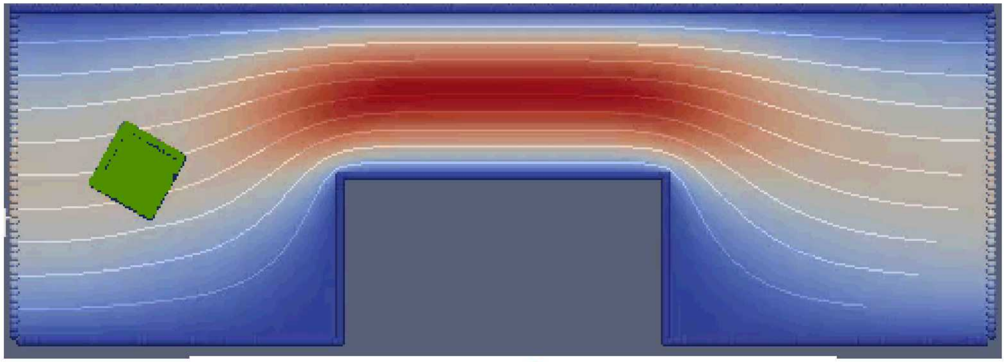
Compadre LDRD – Compatible **Pa**rticle **D**isc**re**tization

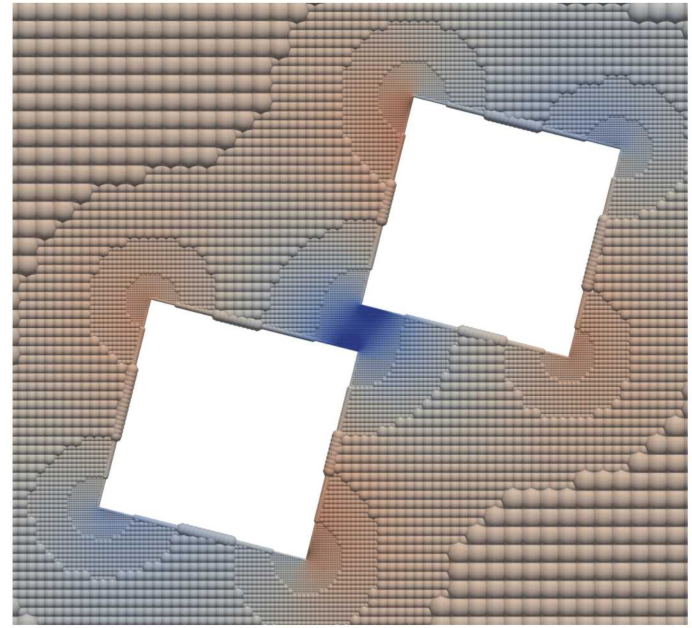
- **Objective:** approximation theory, meshless methods with mimetic properties mirroring compatible mesh-based bethods, scalable Trilinos library
- **People:** Pavel Bochev (PI), Pete Bosler, Paul Kuberry, Mauro Perego, Kara Peterson, Nat Trask

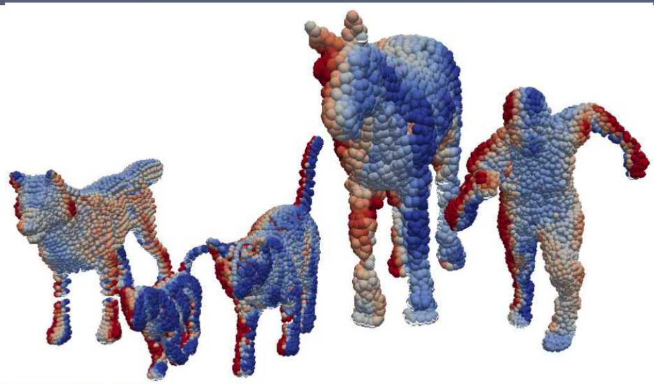
Academic collaborations

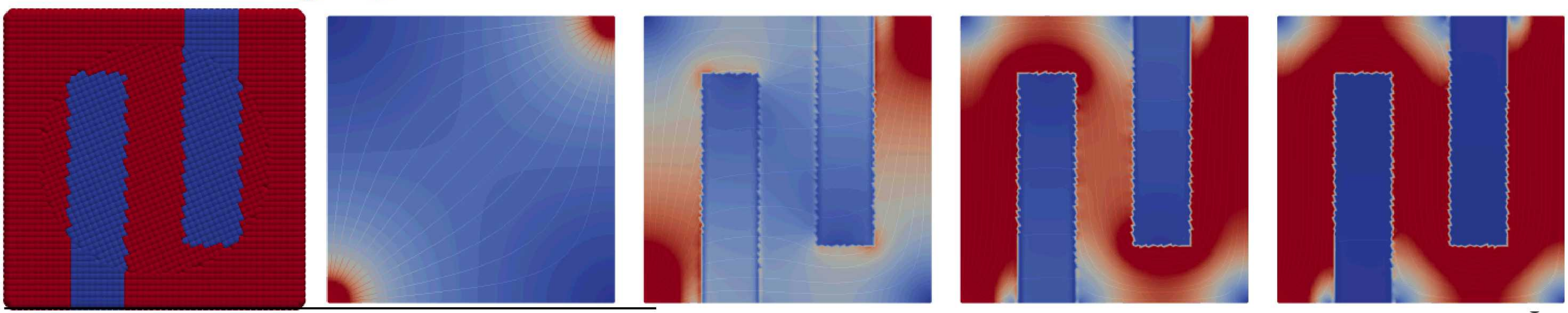
- **Lehigh:** Huaiqian You, Yue Yu
- **UT:Austin:** John Foster, Xiaochuan Tian

Taking advantage of previous meshfree machinery…









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:

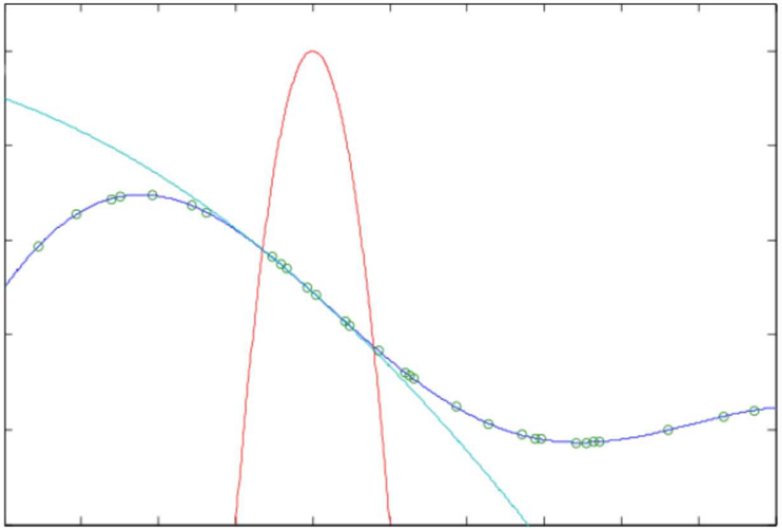
Approximate point evaluation of derivatives:

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



Abstract approximation theory:

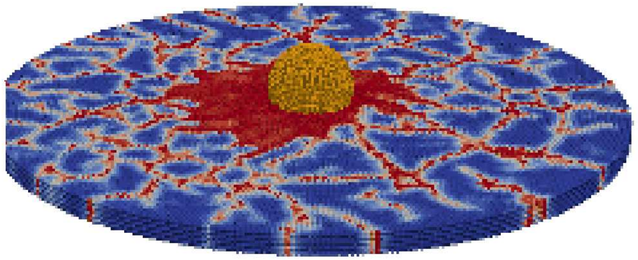
$$|\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}^h(u)| \leq |\tau_{\mathbf{x}}(u-p)| + C_W \|\tau_{\mathbf{x}}\|_{P^*} \|\Lambda_{\mathbf{x}}^{-1}\| \max_{i \in I_{\mathbf{x}}} |\lambda_i(u-p)|, \quad p \in P$$

Objective: Preserve limit to corresponding local model

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 $\boldsymbol{u} \in L^2$

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

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

No physical nonlocality – consider peridynamics as a nonlocal regularization of continuum mechanics for fracture problems

Non-local setting and notation

Consider a family of integral equations of the form:

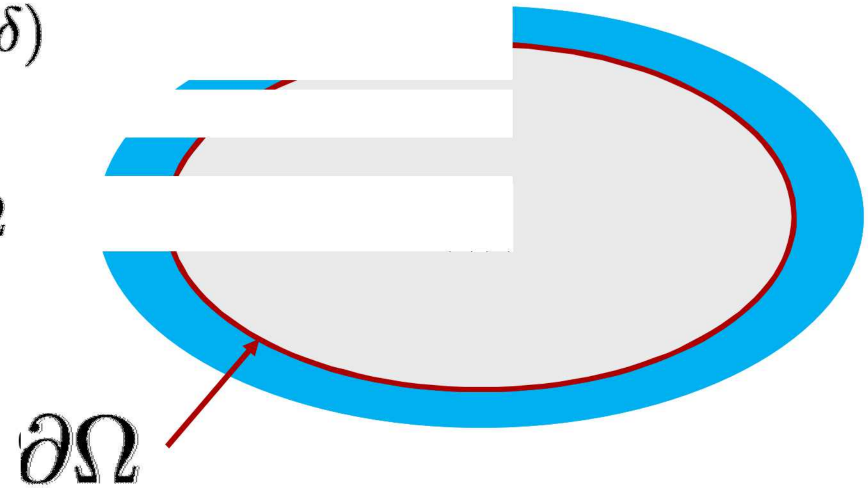
$$\mathcal{L}_\delta[u](\mathbf{x}) = \int_{B(\mathbf{x},\delta)} K(\mathbf{x},\mathbf{y})\,(u(\mathbf{y}) - u(\mathbf{x}))\; d\mathbf{y} = \mathbf{f}(\mathbf{x})$$

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

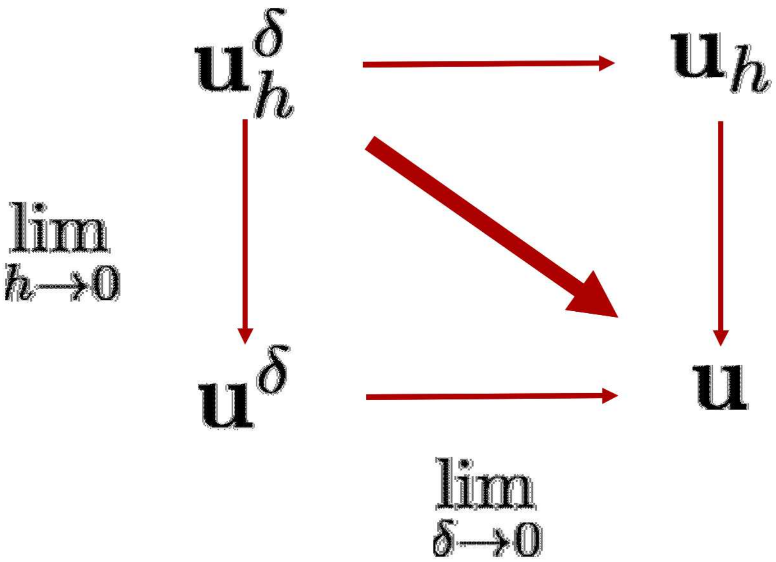
$$K(\mathbf{x},\mathbf{y}) = \frac{n(\mathbf{x},\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^\alpha}, \text{ where } n(\mathbf{x},\mathbf{y}) \le C_n$$

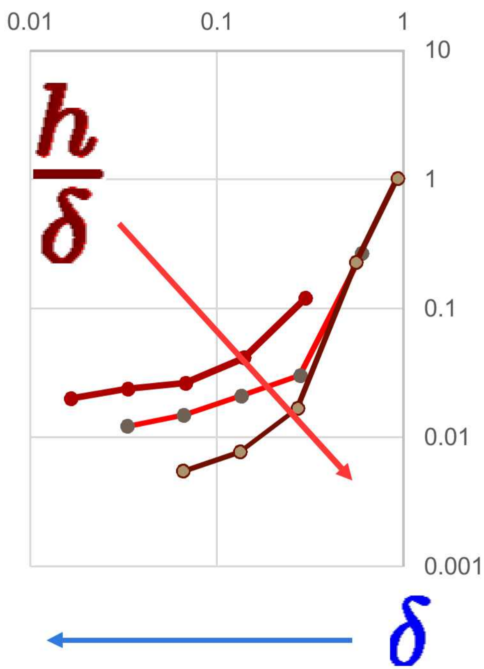
$$\Omega^\delta = \bigcup_{\mathbf{x}\in\Omega} B(\mathbf{x},\delta)$$

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



Asymptotic compatibility





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

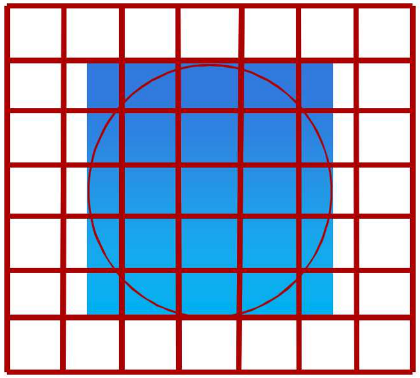
Tian, Xiaochuan, and Qiang Du. "Asymptotically compatible schemes and applications to robust discretization of nonlocal models." *SIAM Journal on Numerical Analysis* 52.4 (2014): 1641-1665.

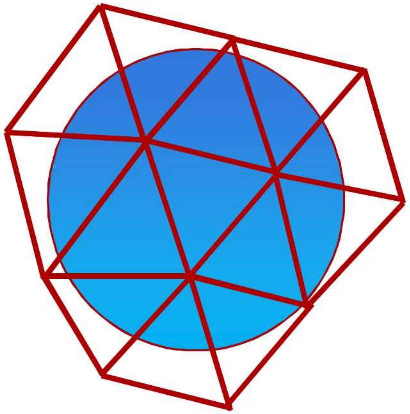
Why is this a hard quadrature problem?

Define quadrature rule:

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

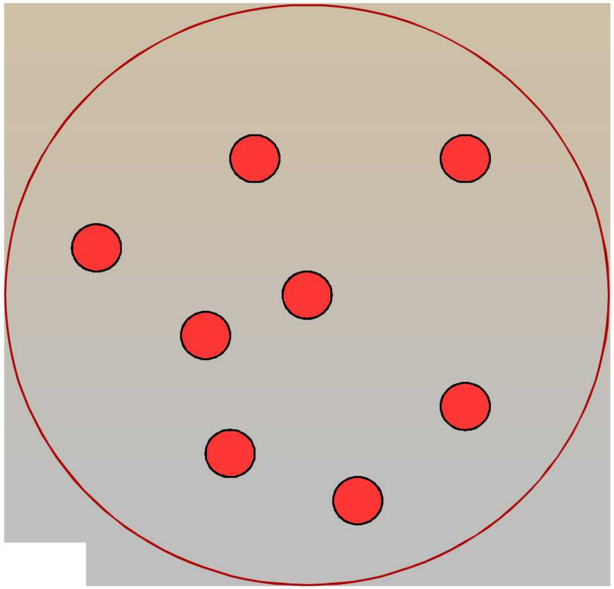
$$\mathcal{L}_\delta^h[u](\mathbf{x}_i) = \sum_{\mathbf{x}_j \in B(\mathbf{x}_q,\delta)} K(\mathbf{x}_i,\mathbf{x}_j)\,(u(\mathbf{x}_j) - u(\mathbf{x}_i))\;\omega_j$$





- Challenges in finite element setting:
  - Costly geometric intersection
  - Singularity in non-local kernel
  - Accurate treatment of null-space sensitive to symmetry in quadrature points
  - Issues compounded by double integral in weak form
- **Candidate for meshfree treatment!**

Meshfree generation of quadrature rules on balls



Idea:
- Construct rule just like Gauss quadrature
  - Can't pick points (governed by physics) but we can pick weights
- Requires knowledge of how to integrate against each member of reproducing set
- Small, easy linear systems to solve over each neighborhood

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

subject to the equality constraint

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

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

Error estimates for singular operators

- As reproducing space, select polynomials + integrand of operator

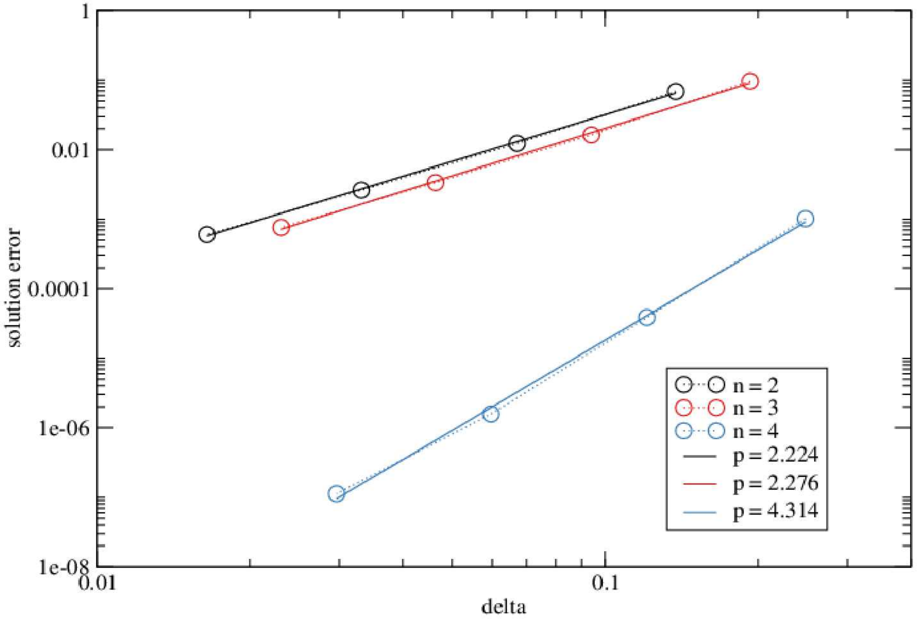
$$\mathbf{V}_h = P_m \cup S_{K,n,\mathbf{x}}, \text{ where}$$

$$S_{K,n,\mathbf{x}} := \{K(\mathbf{x},\mathbf{y})f(\mathbf{y}) \mid f \in P_n\}$$

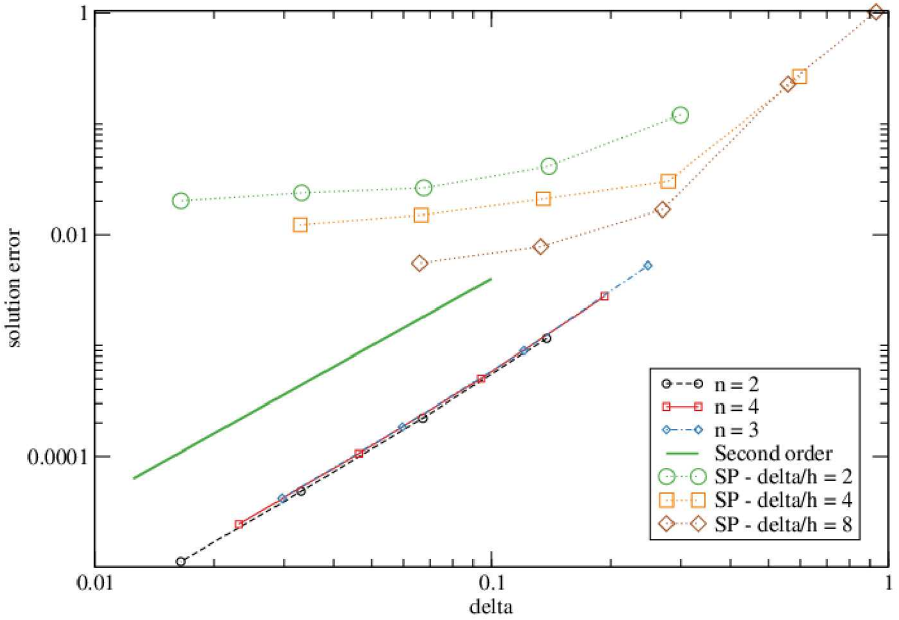
Theorem. *Consider for fixed* $\mathbf{x}$ *a kernel of the form* $K(\mathbf{x},\mathbf{y}) = \frac{n(\mathbf{x},\mathbf{y})}{|\mathbf{y}-\mathbf{x}|^\alpha}$, *where the numerator* n *satisfies* $n(\mathbf{x},\mathbf{y}) \leq C_n$ *for all* $\mathbf{y} \in B(\mathbf{x},\delta)$. *A set of quadrature 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.*

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

Manufactured solution to BVP in bond based



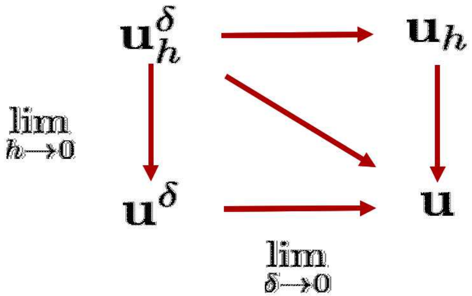
$$u_h^\delta \to u^\delta$$



$$u_h^\delta \to u$$

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

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



Damage modelling

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

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

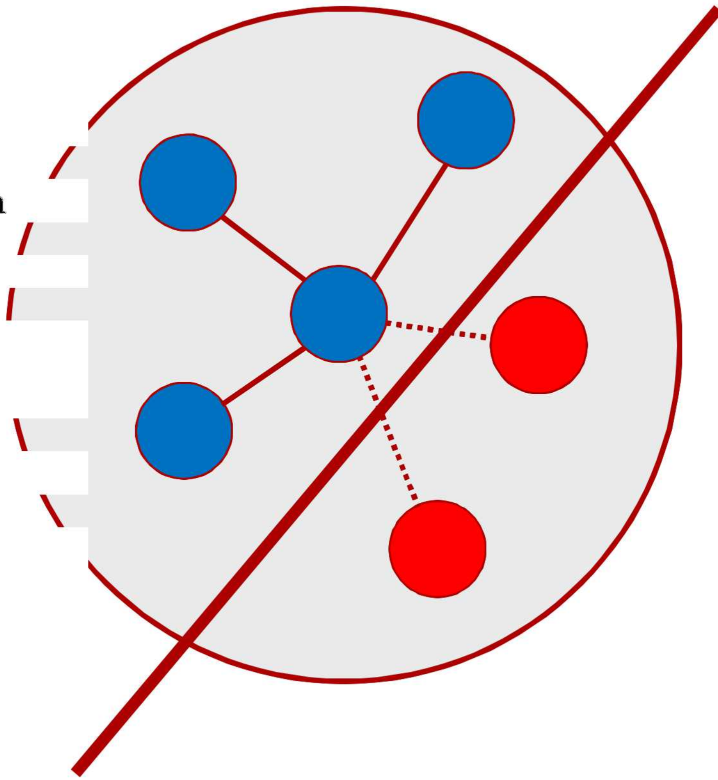
Bonds are either

- 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

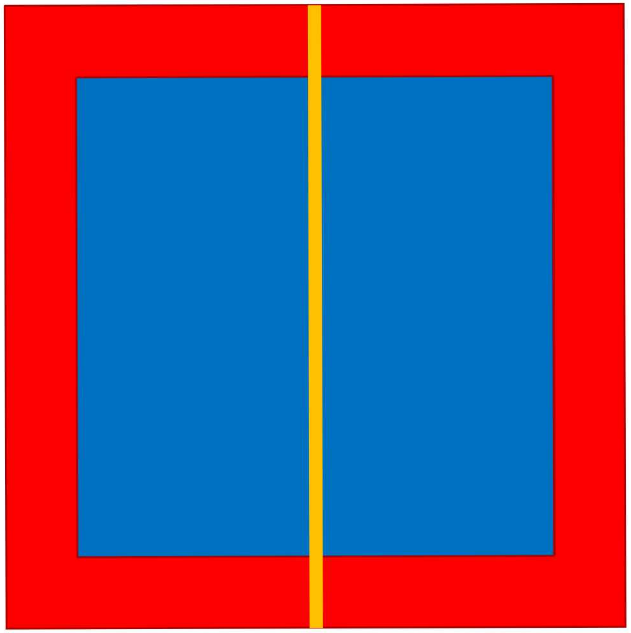
$$s_0 = \begin{cases} \sqrt{\frac{G_c}{\left(\frac{6\mu}{\pi} + \frac{16}{9\pi^2}(\kappa - 2\mu)\right)\delta}}, & \mathrm{d} = 2 \\ \sqrt{\frac{G_c}{\left(3\mu + \left(\frac{3}{4}\right)^4\left(\kappa - \frac{5\mu}{3}\right)\right)\delta}}, & \mathrm{d} = 3 . \end{cases}$$

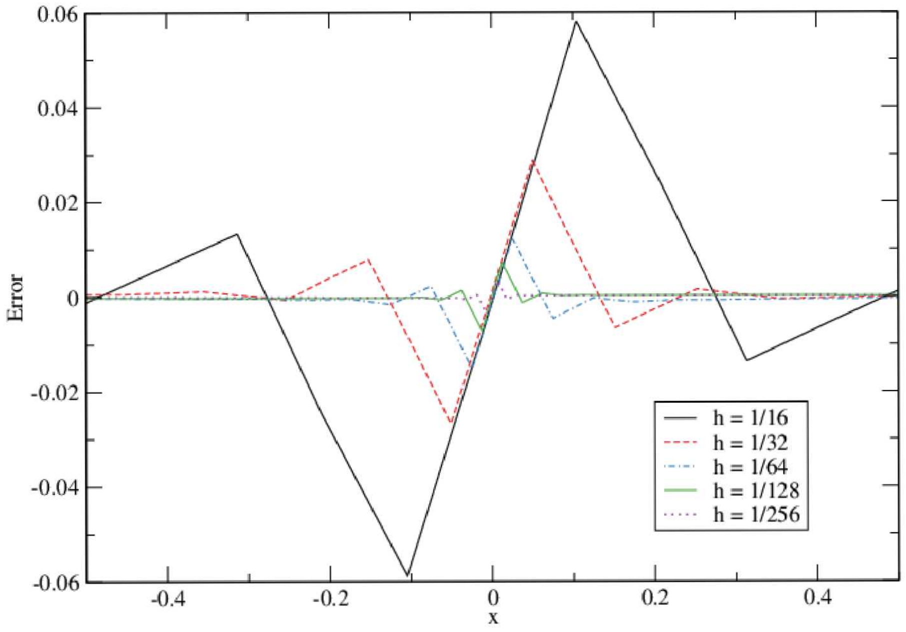


Resolution of surface effects in bond-based

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

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





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

Preserving AC in state-based linear materials

$$
-\frac{C_\alpha}{m(\delta)}\int_{B_\delta(\mathbf{x})}(\lambda(x,y)-\mu(x,y))\,K(|\mathbf{y}-\mathbf{x}|)\,(\mathbf{y}-\mathbf{x})\,(\theta(\mathbf{x})+\theta(\mathbf{y}))\,d\mathbf{y}
$$

$$
+\frac{C_\beta}{m(\delta)}\int_{B_\delta(\mathbf{x})}\mu(x,y)K(|\mathbf{y}-\mathbf{x}|)\frac{(\mathbf{y}-\mathbf{x})\otimes(\mathbf{y}-\mathbf{x})}{|\mathbf{y}-\mathbf{x}|^2}\cdot(\mathbf{u}(\mathbf{x})-\mathbf{u}(\mathbf{y}))\,d\mathbf{y}=\mathbf{f},
$$

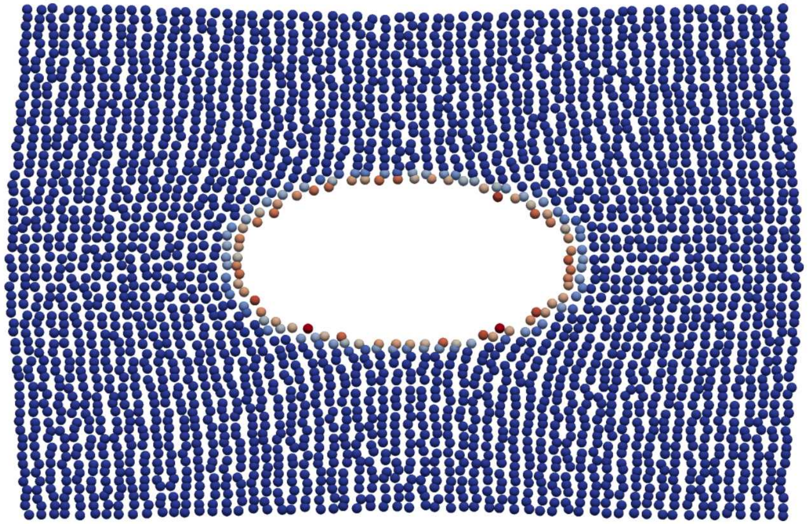
$$
\theta^{corr}(\mathbf{x})=\frac{d}{m(\delta)}\int_{B_\delta(\mathbf{x})\cap\Omega}K(|\mathbf{y}-\mathbf{x}|)\,(\mathbf{y}-\mathbf{x})\cdot\mathbf{M}(\mathbf{x})\cdot(\mathbf{u}(\mathbf{y})-\mathbf{u}(\mathbf{x}))\,d\mathbf{y},
$$

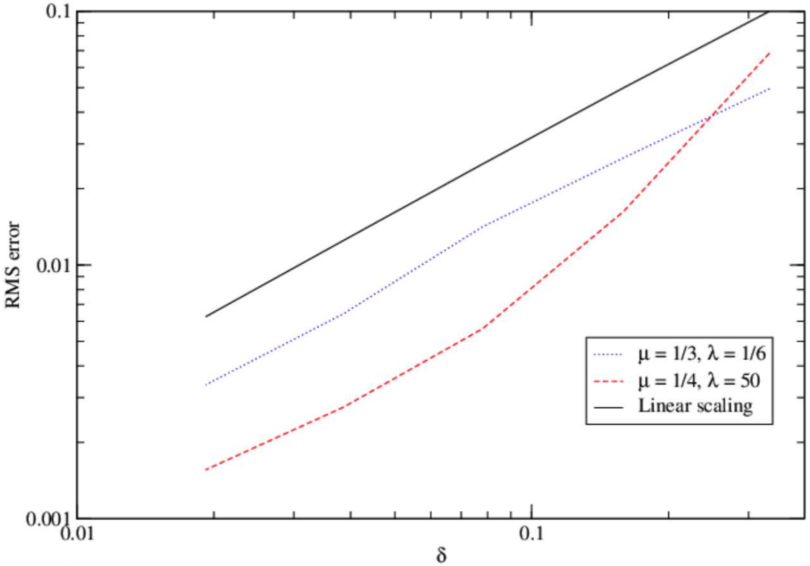
with

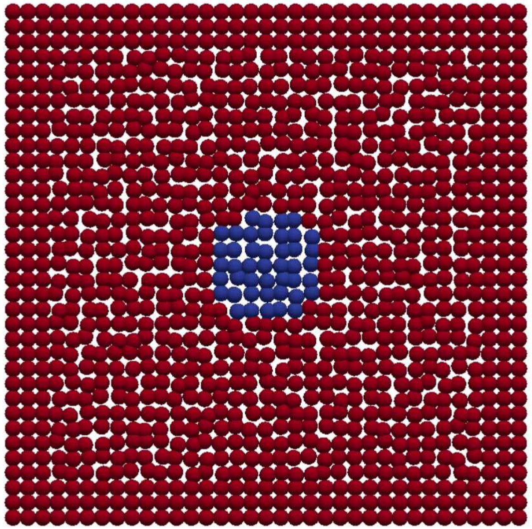
$$
\mathbf{M}(\mathbf{x})=\left[\frac{d}{m(\delta)}\int_{B_\delta(\mathbf{x})\cap\Omega}K(|\mathbf{y}-\mathbf{x}|)\,(\mathbf{y}-\mathbf{x})\otimes(\mathbf{y}-\mathbf{x})\,d\mathbf{y}\right]^{-1}.
$$

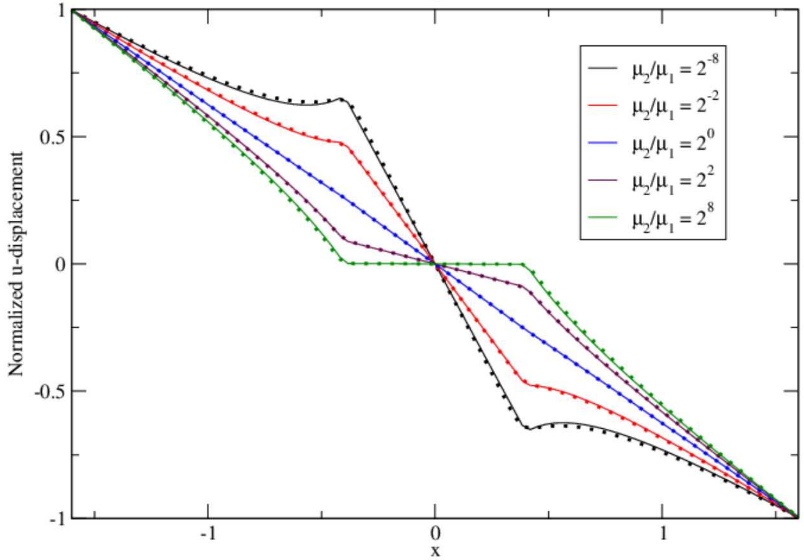
- Remove boundary effects by renormalizing dilatation
  - No modification to material model
- Apply optimization based quadrature without modification

Convergence in near incompressible limit to free-surface, inclusion problems









Diffusion for heterogeneous materials

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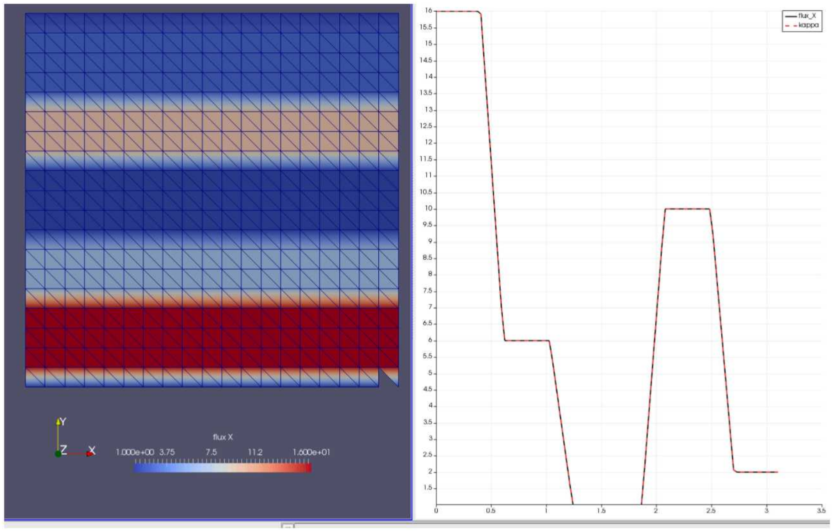
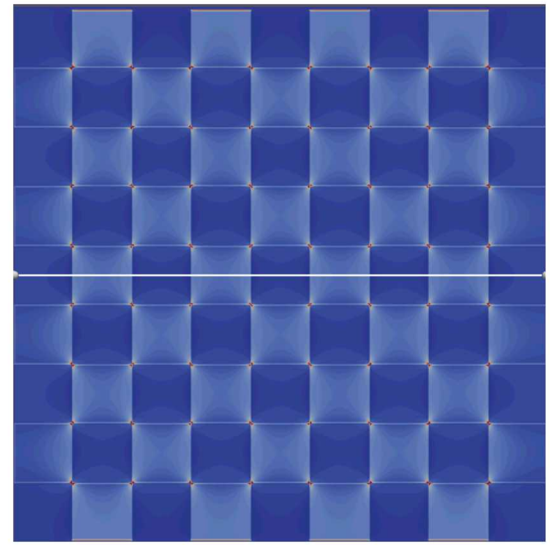
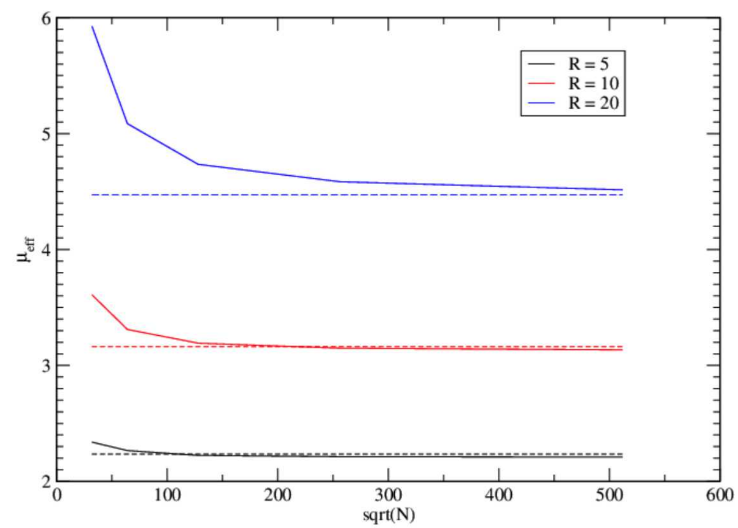


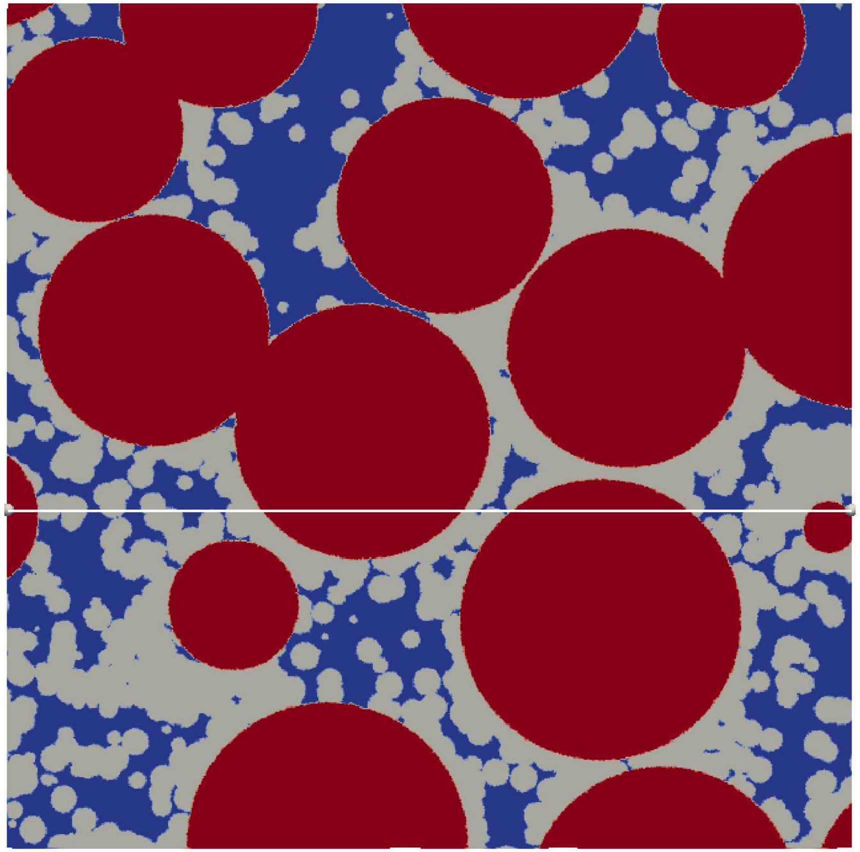


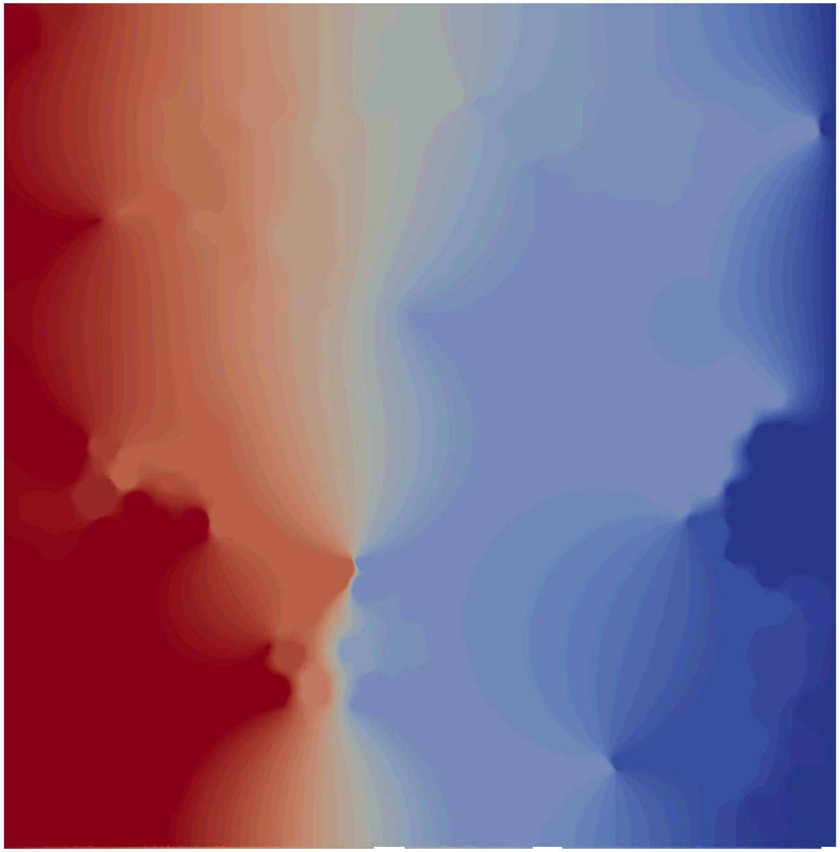
$$\nabla \cdot \kappa \nabla \phi \approx$$

$$\int_{B_\delta(\mathbf{x})} \kappa(\boldsymbol{x},\boldsymbol{y}) K(\boldsymbol{x},\boldsymbol{y}) \left(\phi(\boldsymbol{y}) - \phi(\boldsymbol{x})\right) d\boldsymbol{y}$$

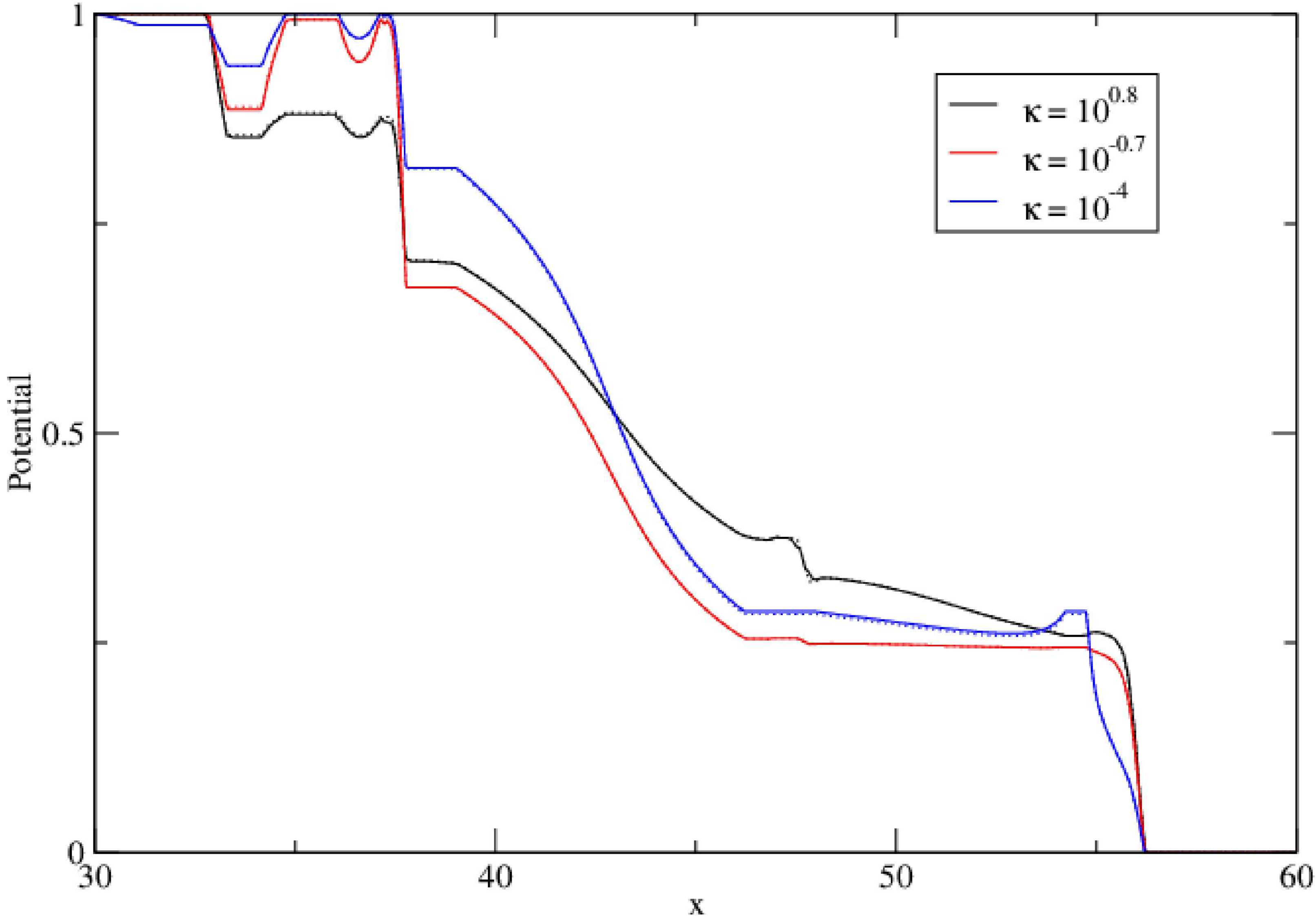


Comparison to microstructural data





Comparison to finite element solution



A microstructure framework for transport induced fracture

Diffusion process

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

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

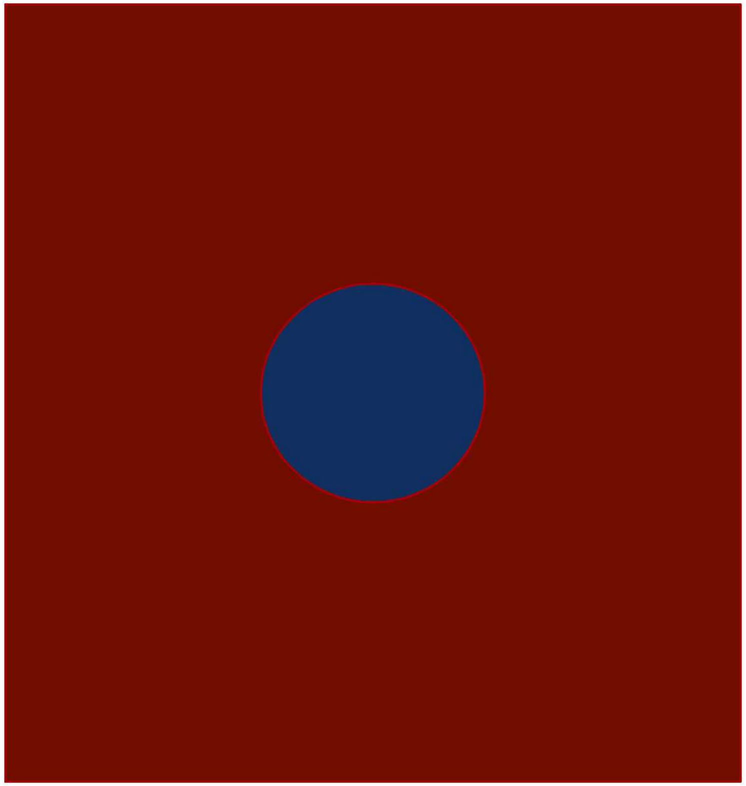
$$[\hat{\mathbf{n}} \cdot \kappa \nabla \phi] = h$$

Mechanics process

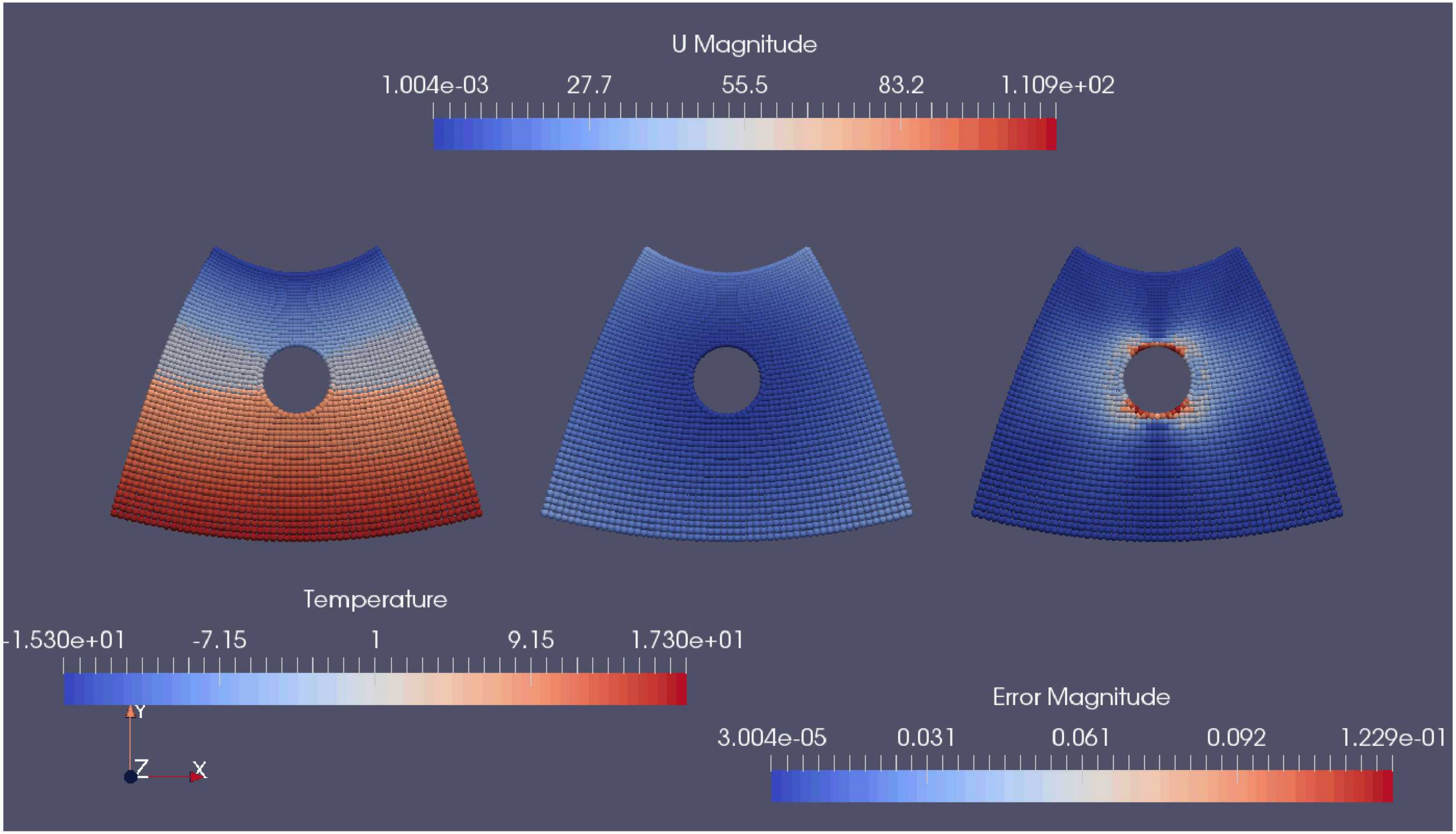
$$\nabla \cdot \sigma = f$$

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

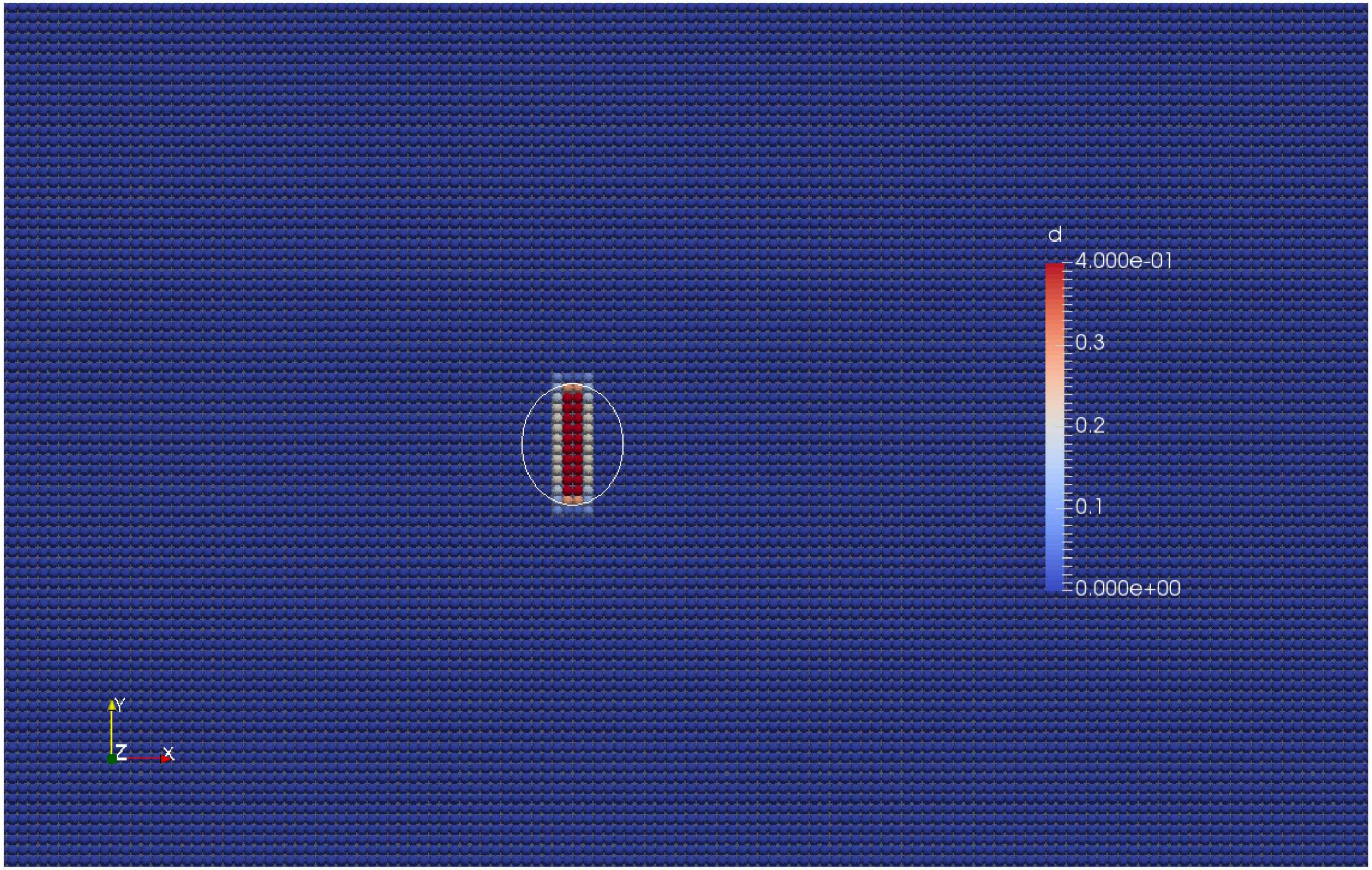
$$\hat{\mathbf{n}} \cdot \sigma \; = \mathbf{t}$$



Consistent coupling to mechanics



Consistent pressure loading of cracks



See talks by Yue Yu, Huaiqian You for details regarding mathematics
- well-posedness, error estimates, and discretization with our scheme

Conclusions

- Continuum peridynamic theory is robust, but lacks aproper discretization to support modeling efforts
  - For practitioners, this is often misinterpreted as a physical effect
- We have introduced a new optimization based quadrature rooted in GMLS approximation theory
- Swapping out quadrature weights in standard peridynamics codes with new scheme restores convergence in sense of asymptotic compatibility
- Therefore, with a slight perturbation, we can restore accuracy to a number of methods
- Fixes: surface effects, consistency, near incompressible limits
- Future work: still strong form, so analysis is limited to truncation error and special cases of particle distribution
  - Extensions to variational forms