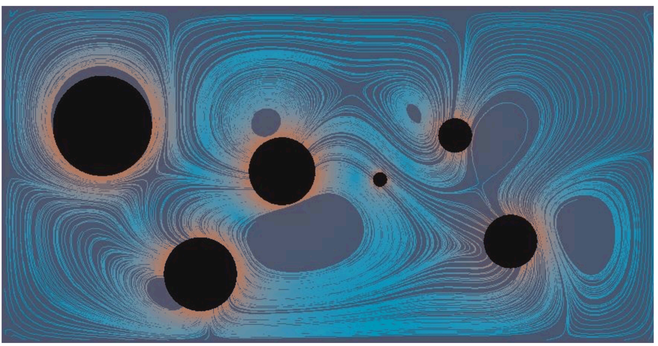
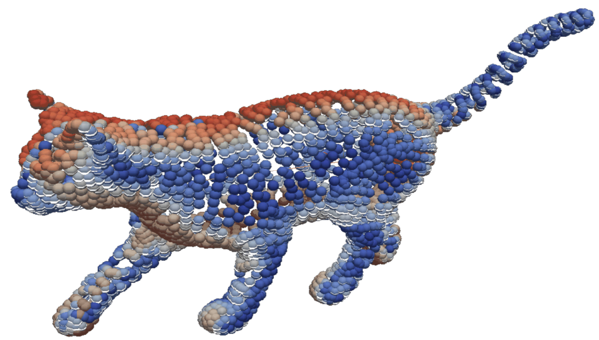
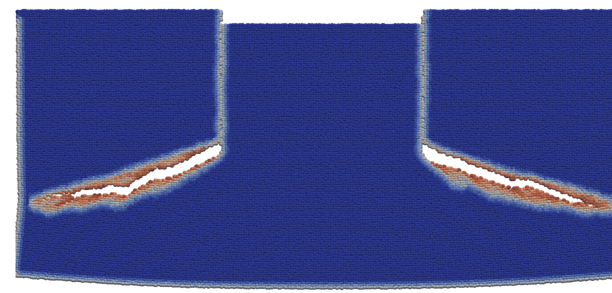
SAND2017-13553C







Consistent + Conservative Meshfree Discretization

Nat Trask

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.

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)
  - "Compatible Meshless Methods" Structural Eng. Seminar
- Kara Peterson
  - "Improving the accuracy of MPM"
- Mauro Perego
  - "Approximation properties of functional reconstruction using GMLS"
- Paul Kuberry
  - "The Compadre toolkit"
- Pete Bosler
  - In Albuquerque, interested in particle discretization for climate applications

Key tools:

- Optimization based approaches to develop meshfree discretizations with reproduction properties
- Primarily strong form discretizations, to avoid expensive quadrature

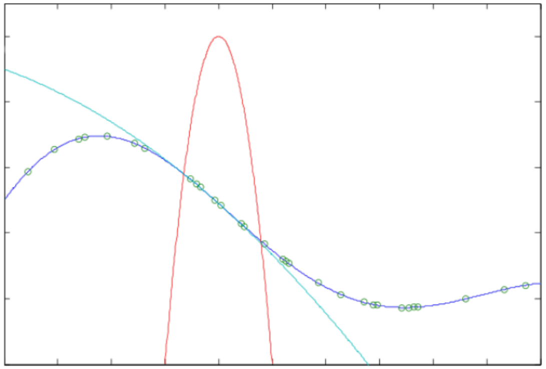
Generalized moving least squares (GMLS)

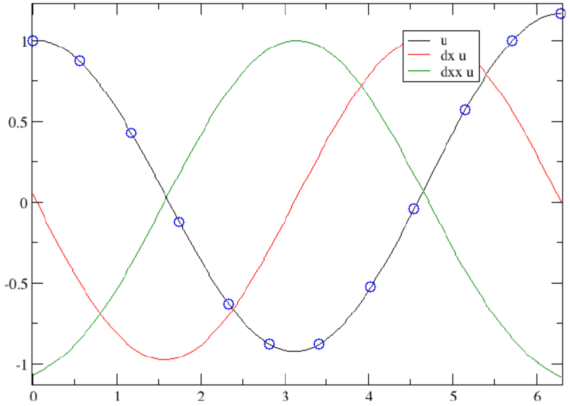
$$\tau(u) \approx \tau^h(u)$$
$$p^* = \underset{p \in \mathbf{V}}{\operatorname{argmin}} \left(\sum_j \lambda_j(p) - \lambda_j(u) \right)^2 W(\tau, \lambda_j)$$
$$\tau^h(u) := \tau(p^*)$$

Example:

To recover classical MLS approximation:

$$\text{Target functional } \tau_i = D^\alpha \circ \delta_{x_i}$$
$$\text{Reconstruction space } \mathbf{V} = P^m$$
$$\text{Sampling functional } \lambda_j = \delta_{x_j}$$
$$\text{Weighting function } W = W(\|x_i - x_j\|)$$



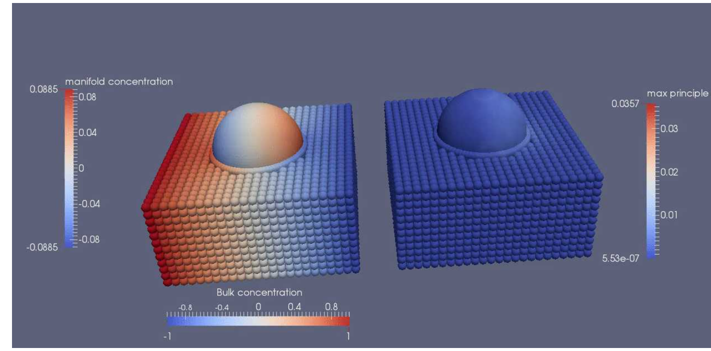


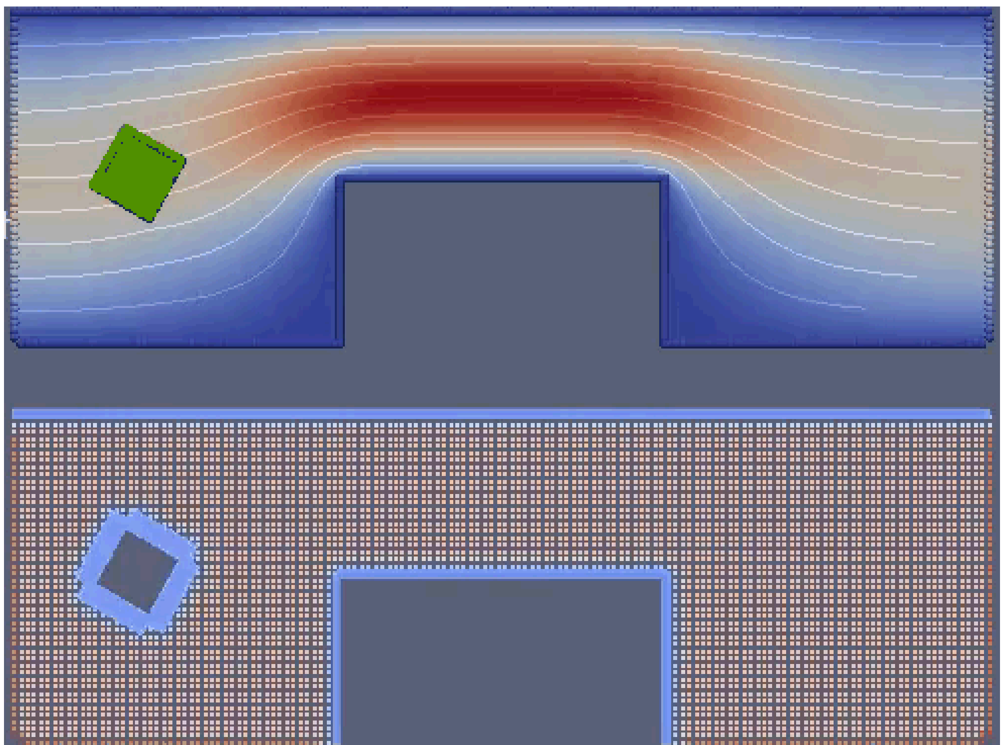
Generalization:

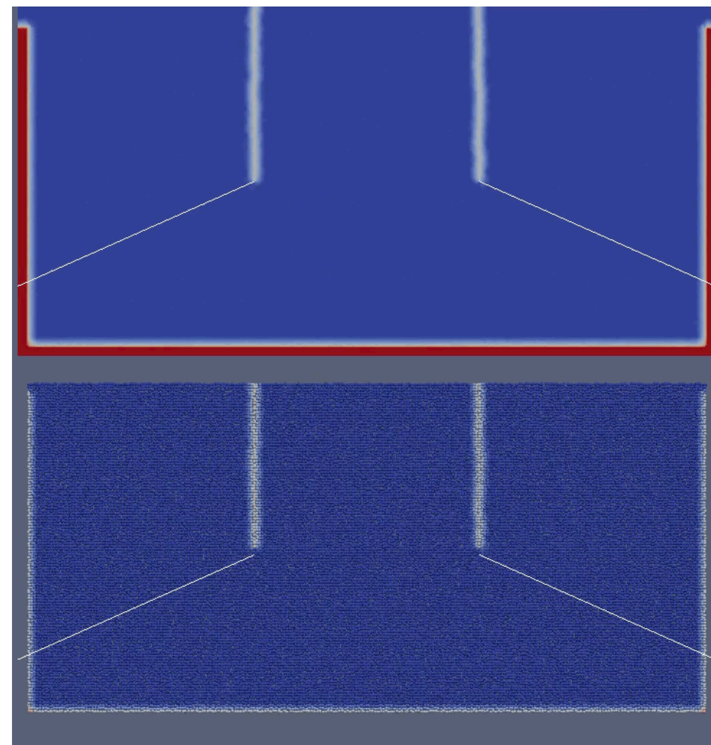
Pick e.g. integral targets, div-free V, etc

The generalized part of GMLS

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

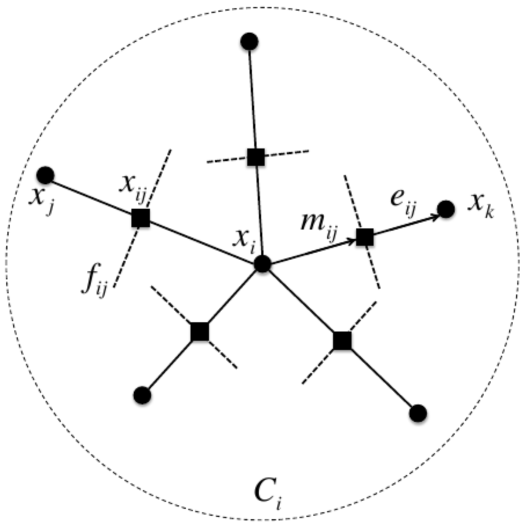


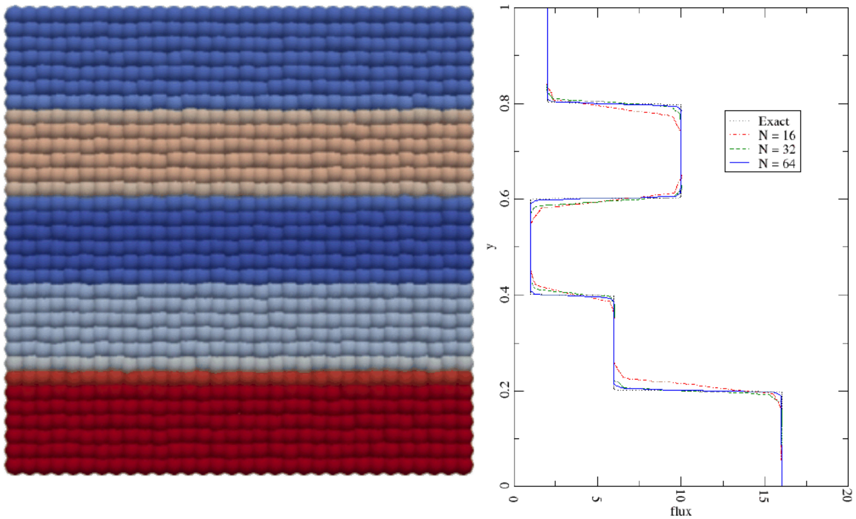




Locally compatible meshfree discretization

Sandia National Laboratories





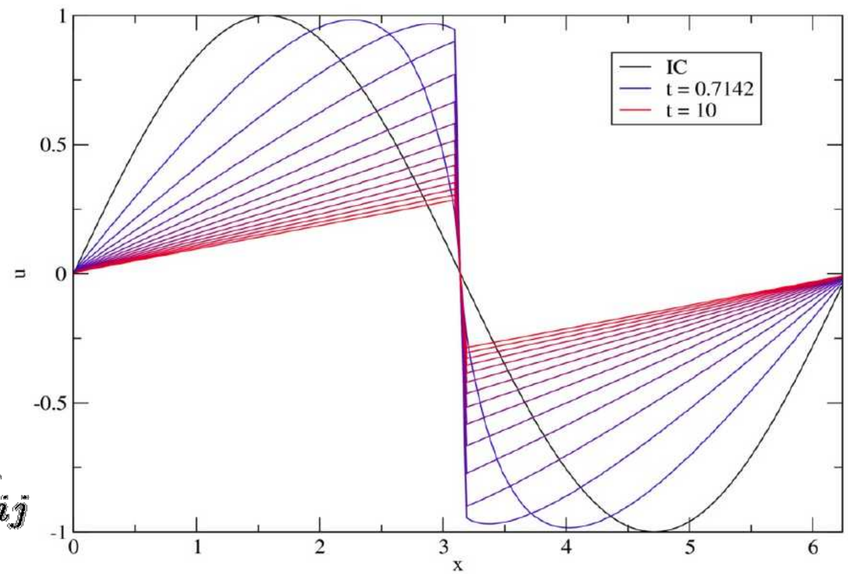
$$GRAD : V \rightarrow E$$

$$DIV : E \rightarrow V$$

$$GRAD\phi_{ij} := \int_{e_{ij}} \nabla\phi \cdot d\mathbf{s} = \phi_j - \phi_i$$

$$DIV\,\mathbf{u}_i := \nabla \cdot \mathbf{p}_i$$

$$\mathbf{p}^* = \underset{p \in \mathbf{V}}{\operatorname{argmin}} \sum_j \left(\int_{e_{ij}} (\mathbf{u} - \mathbf{p}) \cdot d\mathbf{s} \right)^2 W_{ij}$$



Objective: A globally compatible discretization

- Mesh-based physics compatible schemes are rooted in exterior calculus
- The key ingredient to these schemes is the generalized Stokes theorem (or the Gauss divergence theorem for div-grad problems)
- If we want to obtain a scheme with a discrete divergence principle, need to make sense of

$$I_c[\phi] = \int_c \phi \, dV$$

$$I_f[\mathbf{F}] = \int_f \mathbf{F} \cdot d\mathbf{A}$$

$$\underbrace{I_c[\nabla \cdot \mathbf{F}]}_{\text{3 form}} = \sum_{f \in \partial c} \underbrace{I_f[\mathbf{F}]}_{\text{2-forms}}$$

Tricky part: Particles only naturally have 0-form DOFs

how do we introduce a notion of particle volume?

Target functionals revisited: GMLS quadrature

$$\mathbf{b}^* = \underset{\mathbf{b}\in\mathbb{R}^{dim(\mathbf{V})}}{\operatorname{argmin}} \left(\sum_j \mathbf{b}^\intercal \lambda_j(\mathbf{P}) - \lambda_j(u)\right)^2 W(\|x - x_j\|)$$

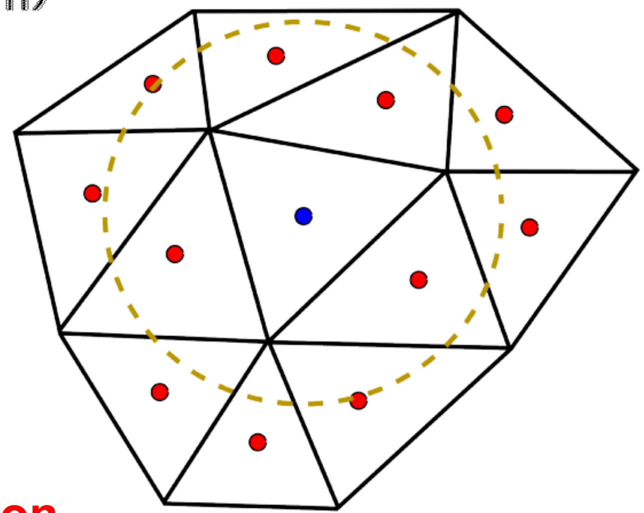
$$\mathbf{V} = span(p_1, \ldots, p_{dim(\mathbf{V})})$$

$$\mathbf{P}(x) = \{p_1(x), \ldots, p_{dim(\mathbf{V})}(x)\}$$

$$\tau_h(u) = \tau(\mathbf{P})^\intercal \mathbf{b}^* := \mathbf{v}_\tau^\intercal \mathbf{b}^*$$

metric information

function approximation



$$I_c^h[\phi] := \mathbf{v}_c^\intercal \mathbf{b}_\phi^* \qquad I_f^h[\mathbf{F}] := \mathbf{v}_f^\intercal \mathbf{b}_\mathbf{F}^*$$

$$v_c^\alpha = \int_c p_\alpha \, dx \qquad v_f^\alpha = \int_f \mathbf{p}_\alpha \cdot d\mathbf{A}$$

v encodes metric information

- can we come up with a similar vector encoding **virtual particle volume?**

Virtual particle volumes & particle quadrature

- Precompute cell moments

$$V_c^\alpha = \int_c \phi^\alpha dV$$

- Define compactly supported partition of unity mapping from cells to particles

$$\sum_p W_{pc} = 1$$

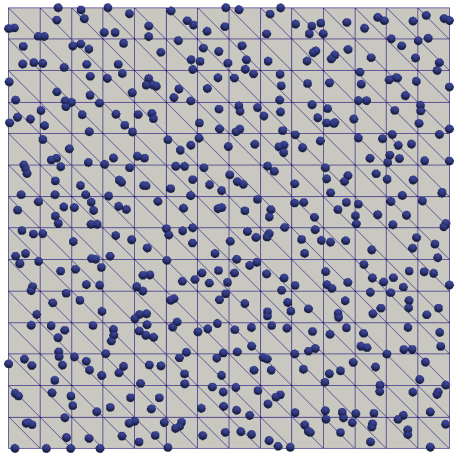
$$\|x_p - x_c\| < \epsilon \implies W_{pc} = 0$$

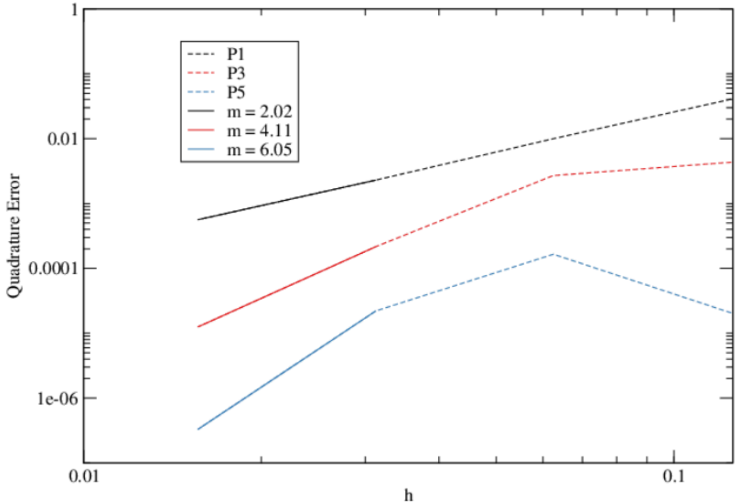
- Scatter mesh volume to particles

$$V_p^\alpha = \sum_c W_{pc} V_c^\alpha$$

$$I_p^h[\phi] := \mathbf{v}_p^\intercal \mathbf{b}_\phi^*$$

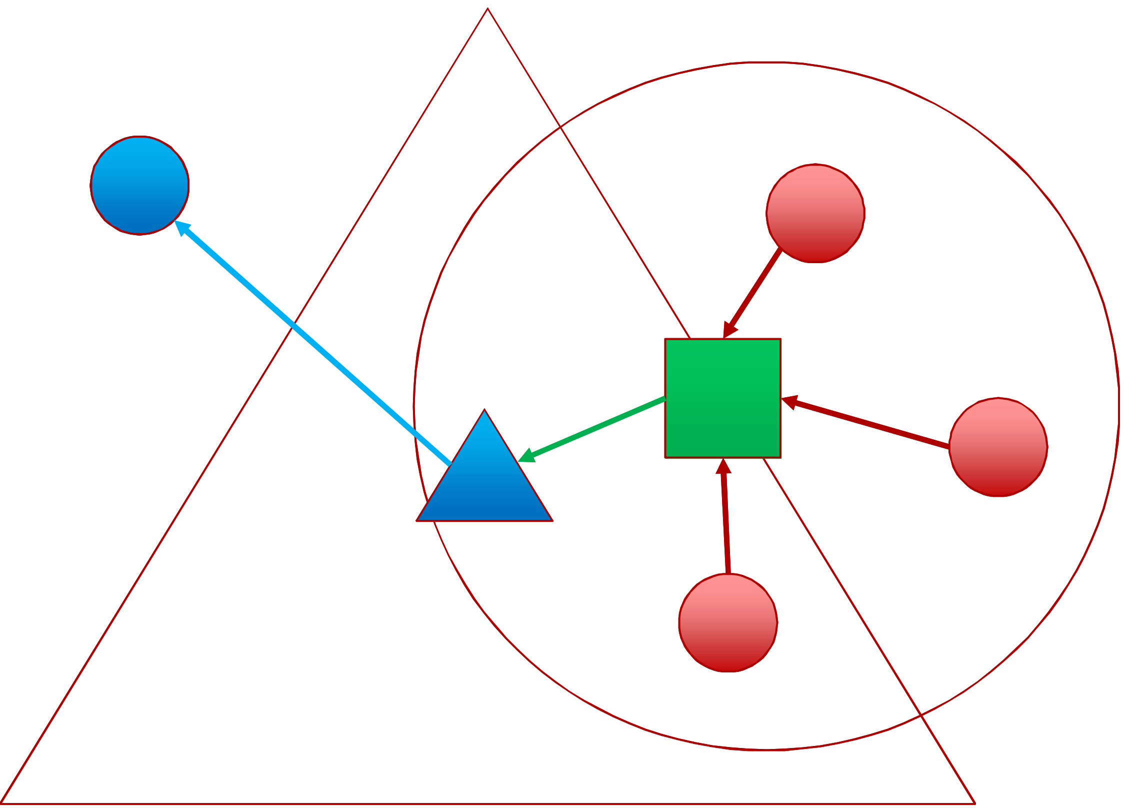
$$\sum_p I_p[\phi] = \sum_c I_c[\phi] = \int_\Omega \phi \, dV, \quad \forall \phi \in \mathbf{V}_h$$





A particle divergence theorem

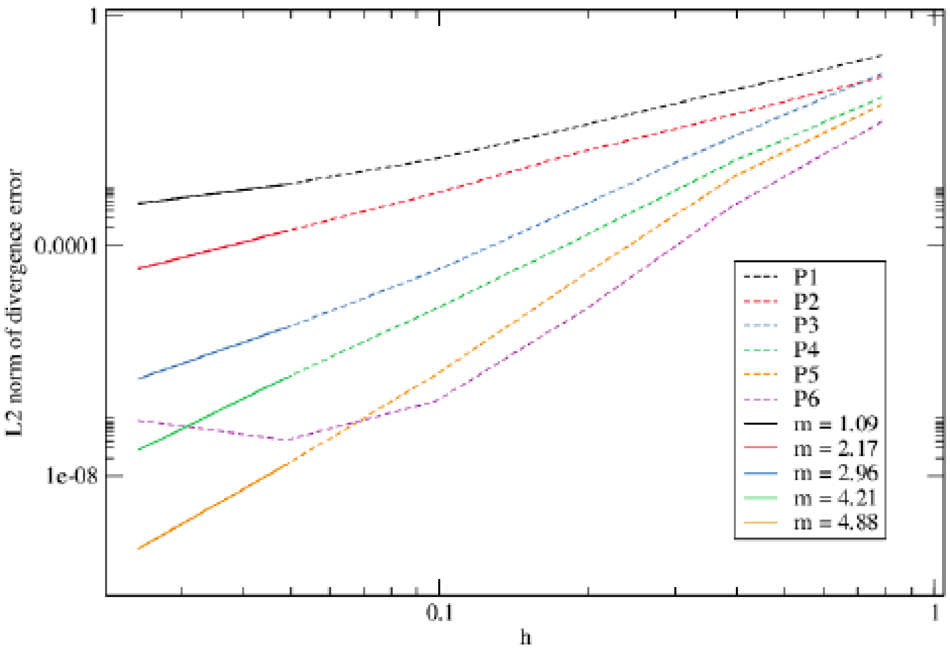
First a cartoon…



1. Solve a GMLS problem to reconstruct the fluxes at the mesh face from the surrounding particles
2. Apply the Gauss divergence theorem on the mesh to obtain a volume form from the face fluxes
3. Apply the scattering operator to distribute the cell integral of the divergence back to particles

Formally…

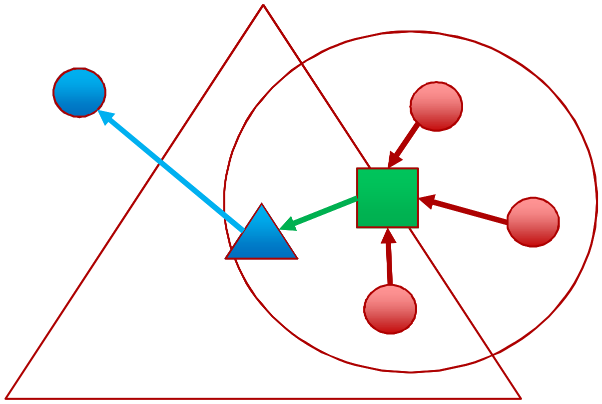
$$
\begin{aligned}
DIV_h\,\mathbf{F} &= I_p[\nabla\cdot\mathbf{F}] \\
&= \sum_c W_{pc} I_c[\nabla\cdot\mathbf{F}] \\
&= \sum_{c,f\in\partial c} W_{pc} I_f[\mathbf{F}]
\end{aligned}
$$



To obtain point value of div(F) at particles:

$$I_p[d] = DIV_h\mathbf{F}$$

$$\mathbf{M}\vec{d} = \mathbf{D}\vec{\mathbf{F}}$$



Solving a conservation law

$$\partial_t u = -\nabla \cdot \mathbf{F}$$

$$\begin{aligned}\frac{d}{dt} I_p[u] &= -\, I_p[\nabla \cdot \mathbf{F}] \\ &= -\sum_c W_{pc} I_c[\nabla \cdot \mathbf{F}] \\ &= -\sum_{c, f \in \partial c} W_{pc} I_f[\mathbf{F}]\end{aligned}$$

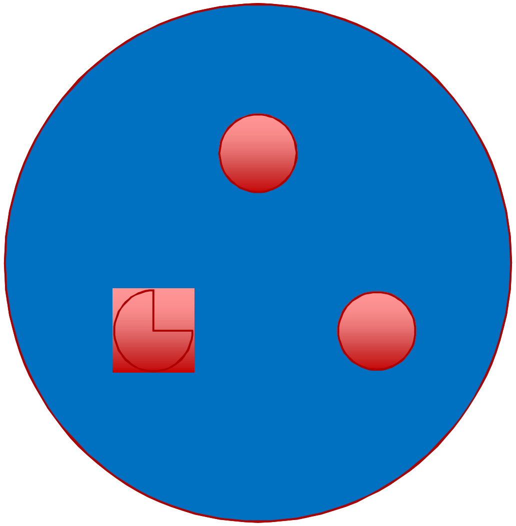
Discrete conservation principle:

$$\begin{aligned}\frac{d}{dt} \sum_p I_p[u] &= -\sum_{p, c, f \in \partial c} W_{pc} I_f[\mathbf{F}] \\ &= \sum_{f \in \partial\Omega} \int_f \mathbf{F}\end{aligned}$$

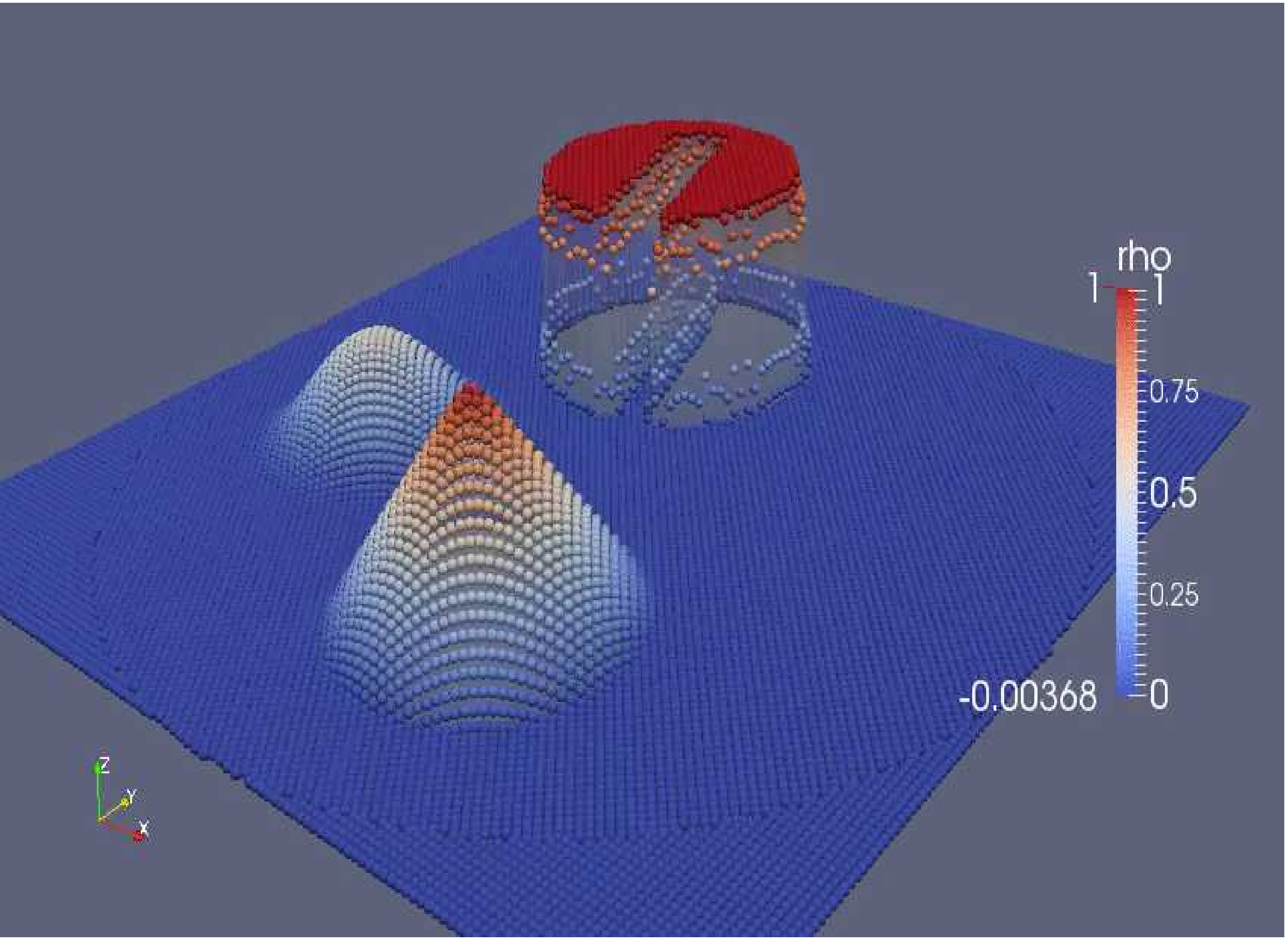
Example:
Leveques spinning disk

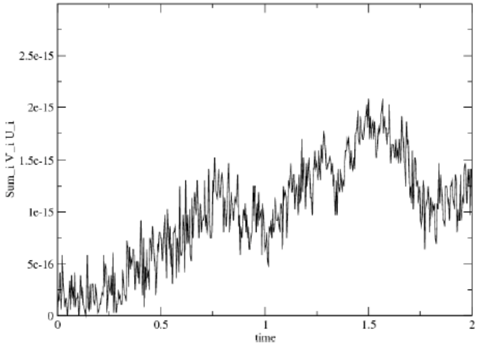
$$F = -\mathbf{v} u$$

$$\mathbf{v} = \left\langle \frac{1}{2} - y, x - \frac{1}{2} \right\rangle$$



Leveque’s spinning disk in Lagrangian frame





Disclaimer:
Careful with GCL

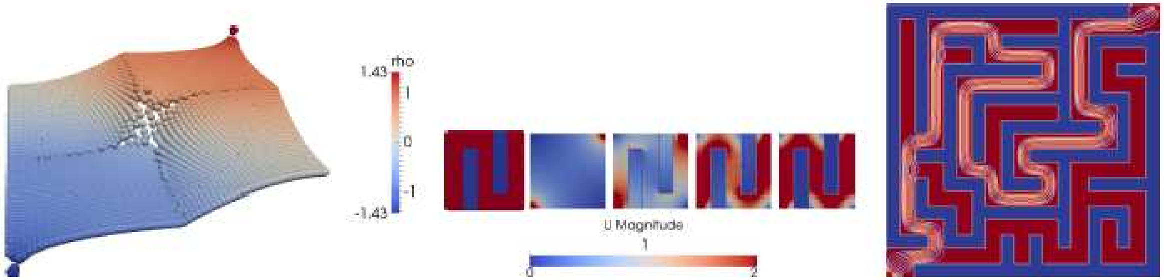
Key Idea:
Preprocess moments on static mesh, scatter moments as particles move

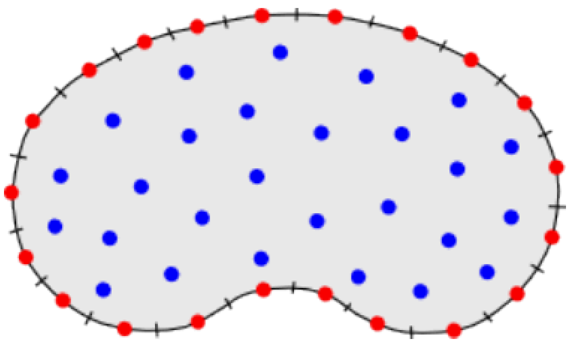
Truly meshfree methods for conservation laws

Need metric information from somewhere
– we get it by applying some ideas from combinatorial Hodge theory

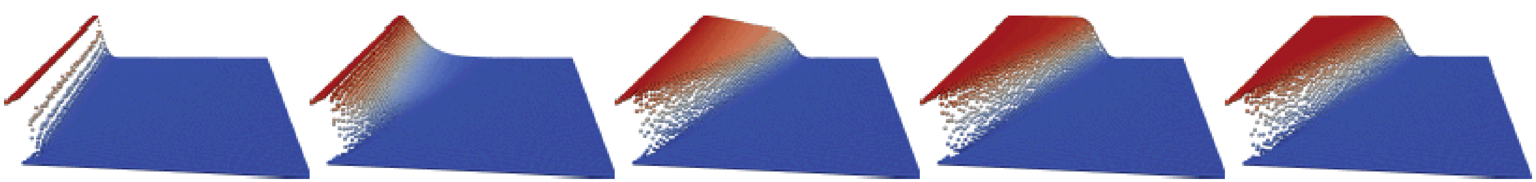
Darcy flow

Jumps in permissivity $\frac{\kappa_1}{\kappa_2} \in \{1, 10, 100, \infty\}$





Singularly perturbed steady advection-diffusion



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

Conclusions

- Some research snapshots of the discretizations + applications we're currently interested in
  - Locally compatible schemes
    - Stable solution of div-grad, curl-curl, Stokes, Darcy
  - Globally compatible schemes
    - Constructing discrete notions of conservation on point clouds
      - Hybrid particle/mesh, pure meshfree
    - Moving beyond div-grad to full de Rham complex
  - Meshfree for surface PDE
    - Using GMLS to parameterize diffeomorphism to tangent space on local patches
    - Couple bulk-manifold transport problems, topology optimization
  - Strong form discretizations of Lagrangian solid mechanics
    - Locally compatible discretizations of elastic materials
    - Discretizations of non-local mechanics for fracture problems