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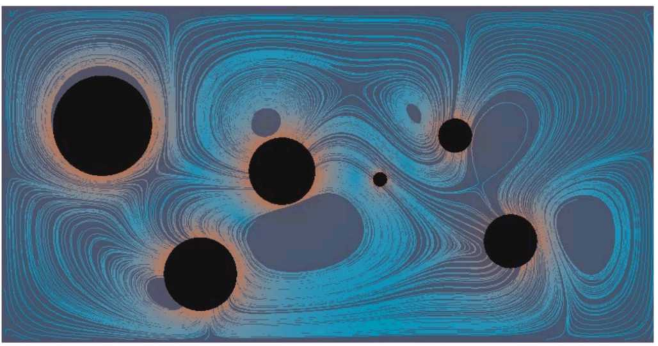

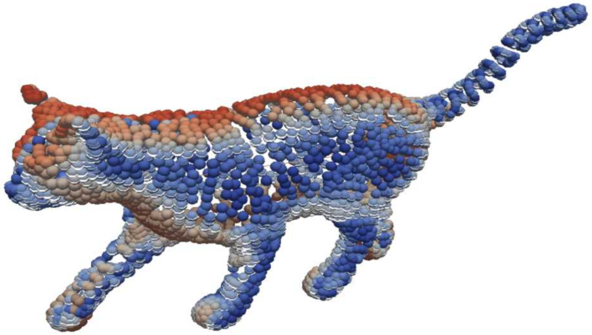

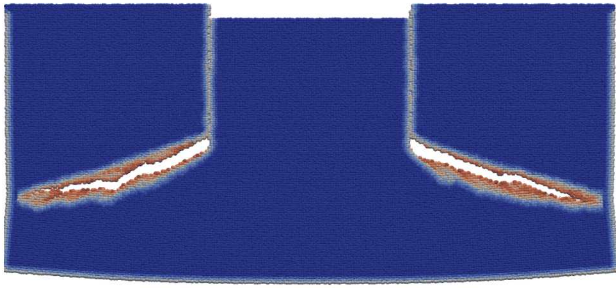

Spatially compatible meshfree discretization through GMLS and graph theory

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What does meshfree mean?

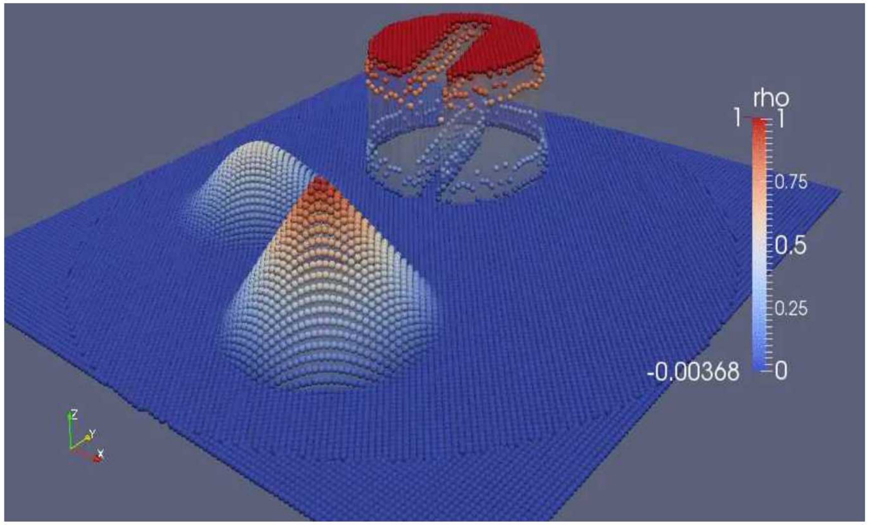
- Physics compatible FEM spaces defined via differential k-forms:
  - For a polygonal mesh in 3D

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

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

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

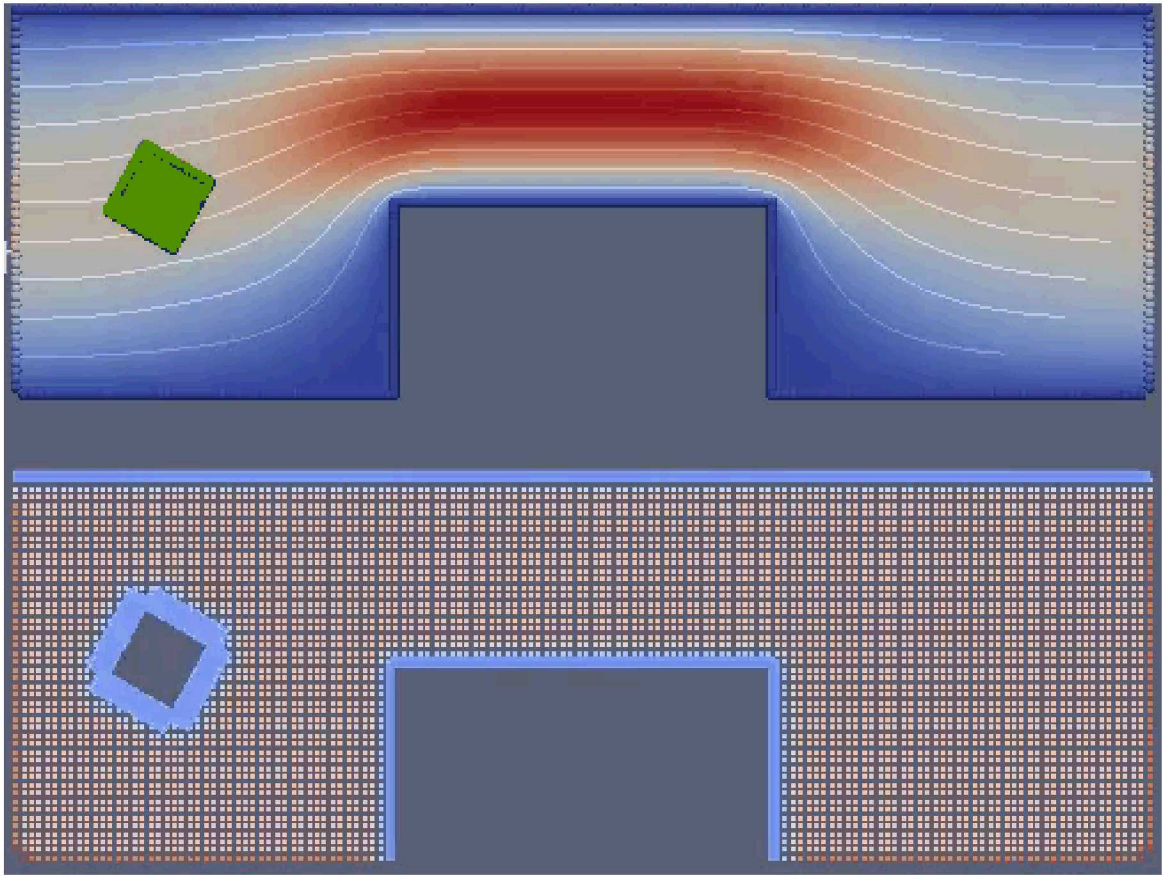
$$\textbf{Three-form:} \quad \int_C \mathbf{u} dV$$



A meshfree method uses only zero-forms as degrees of freedom

- Easy to push points around if you don't care about preserving a mesh
- Exchange nice mathematical setting to get more descriptive models
  - No Stokes theorems, no natural bilinear forms

Why meshfree? Large deformation problems



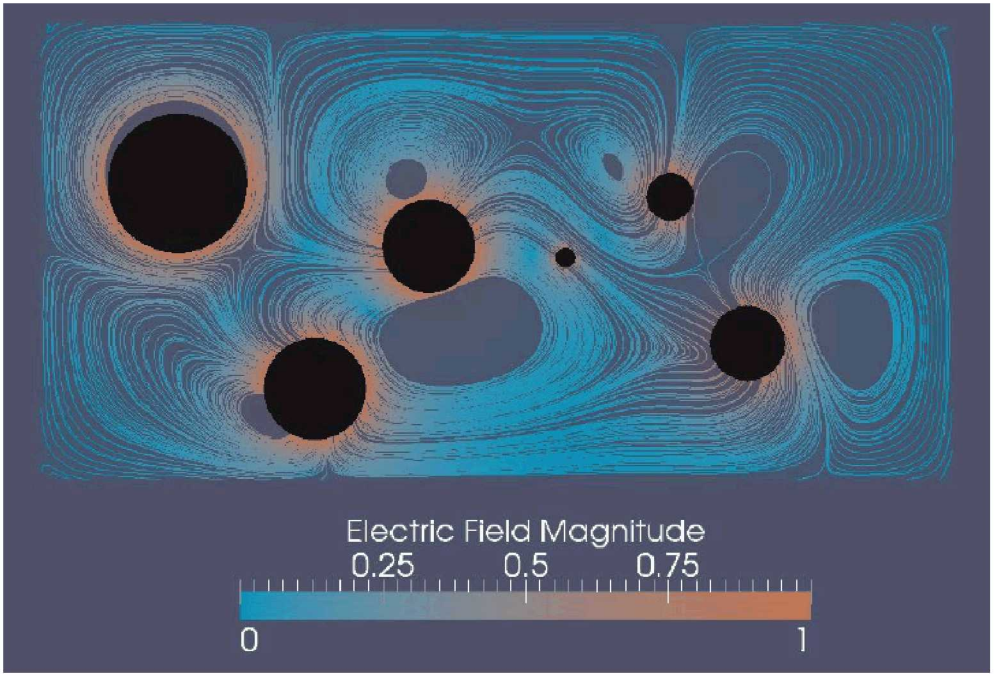
$$\begin{cases} -\nabla^2 \mathbf{u} + \nabla p = \mathbf{f} \\ \nabla \cdot \mathbf{u} = 0 \\ \mathbf{u}|_{\partial\omega} = \mathbf{U} + (x - \mathbf{X}) \times \Omega \\ \int_{\partial\omega} \sigma \cdot d\mathbf{A} = 0 \end{cases}$$

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

Hu, W., Trask, N., Hu, X.,Pan,W.
A spatially adaptive high-order meshless method for fluid–structure interactions.
Computer Methods in Applied Mechanics and Engineering (2019)

Trivial treatment of large deformation problems – no remeshing + remap

Why meshfree? Large deformation problems



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

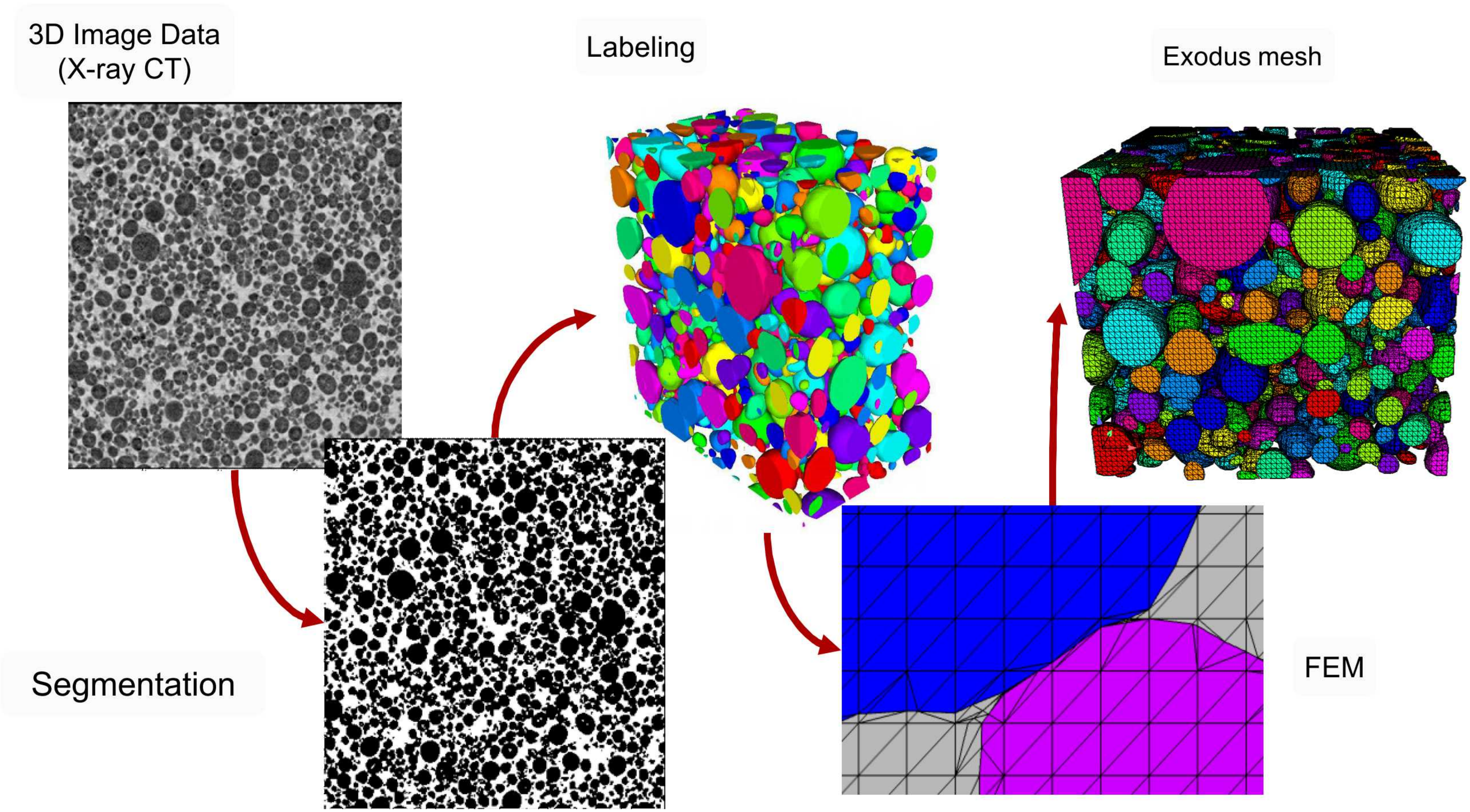
$$-l_c^2\nabla^4\phi + \nabla^2\phi = -\frac{\rho_e(\phi)}{\epsilon}$$

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

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

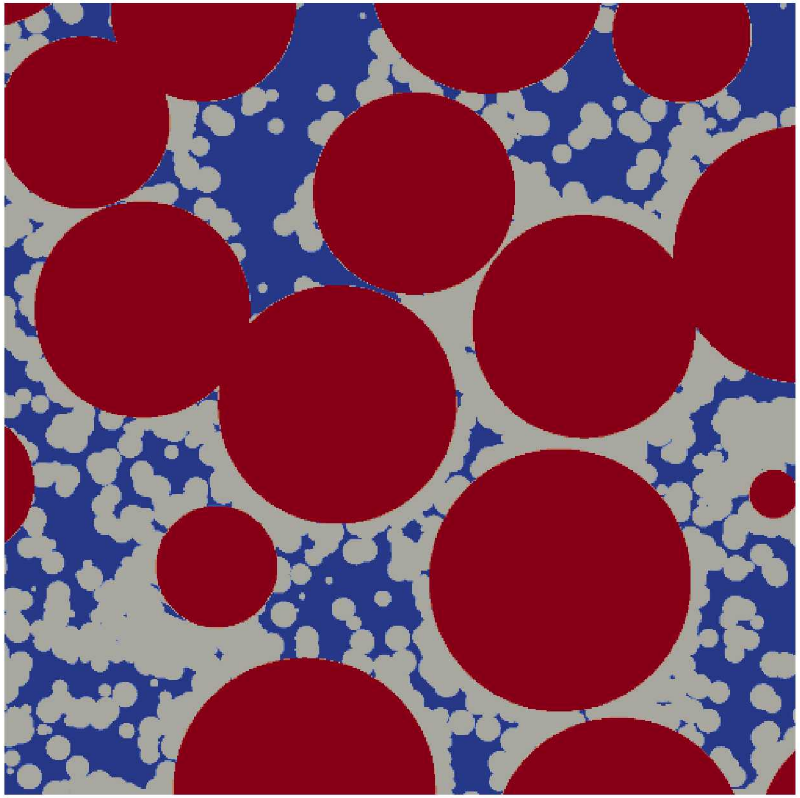
Compatible meshfree discretization: A framework for physics compatible discretization of multiphysics problems that mimics robustness of mimetic methods

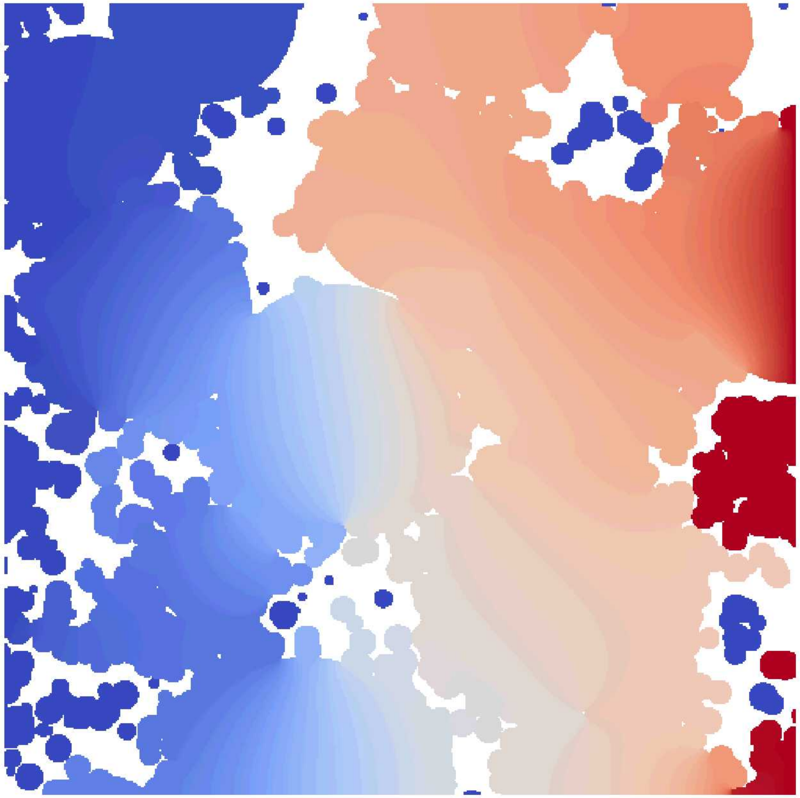
Why meshfree? Automatic geometry discretization



- For engineering problems **meshing constitutes 60-70% of time to solution** (SAND-2005-4647), which cannot be improved by moving to larger computers
  - Automating geometry discretization is fundamental to developing large throughput workflows based on either experimental data or UQ/optimization

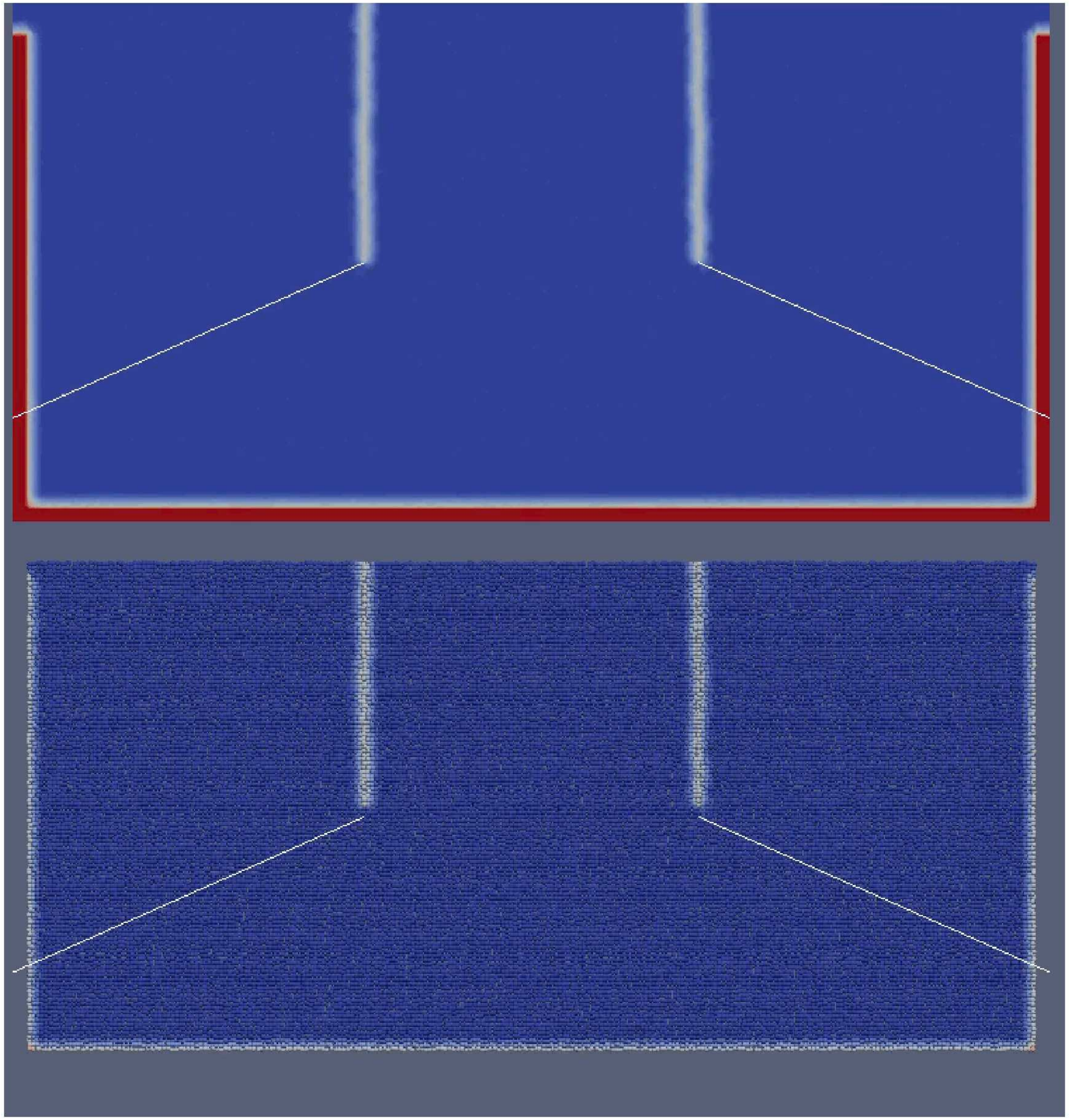
Why meshfree? Automatic geometry discretization





- Meshfree methods operate **directly on the degrees of freedom available in experiment**
- Placing a particle at each voxel of the CT scan is sufficient to obtain a high-fidelity simulation without human-in-the-loop meshing process

Why meshfree? Fracture mechanics

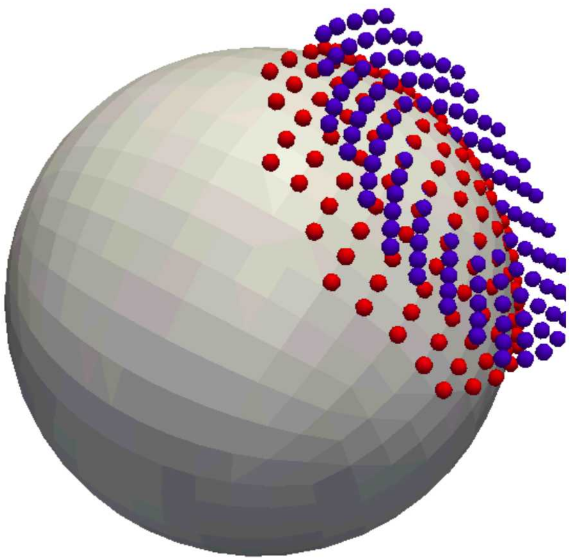


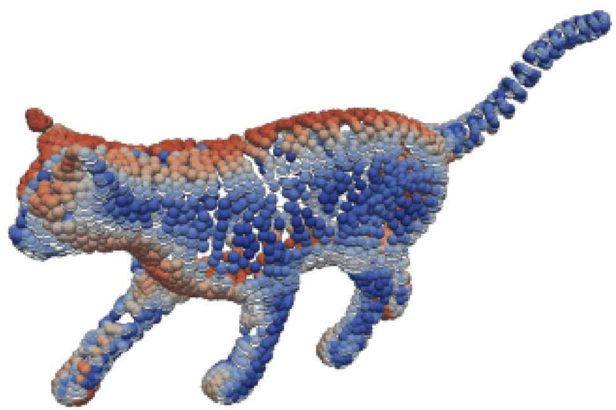
Automatic treatment of topology changes:
No need to reconnect elements, manage mesh quality, etc. as topology evolves as a function of solution

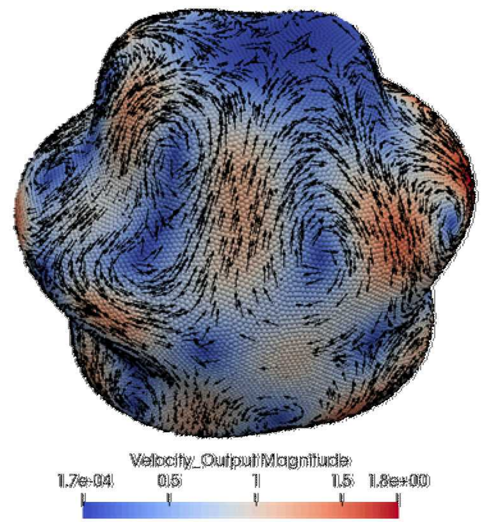
Trask, N., et al.
"An asymptotically compatible meshfree quadrature rule for nonlocal problems with applications to peridynamics." *Computer Methods in Applied Mechanics and Engineering* 343 (2019): 151-165.

Why meshfree? Differential geometry on evolving manifolds

To solve surface PDE, one may learn mapping between local charts and tangent space to access metric tensor, curvature, surface differential operators, etc.



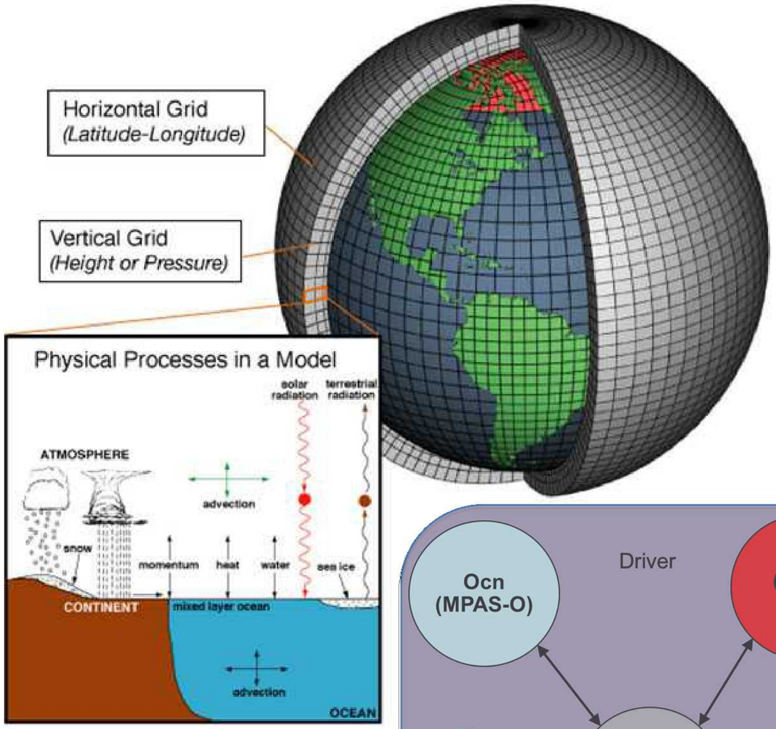


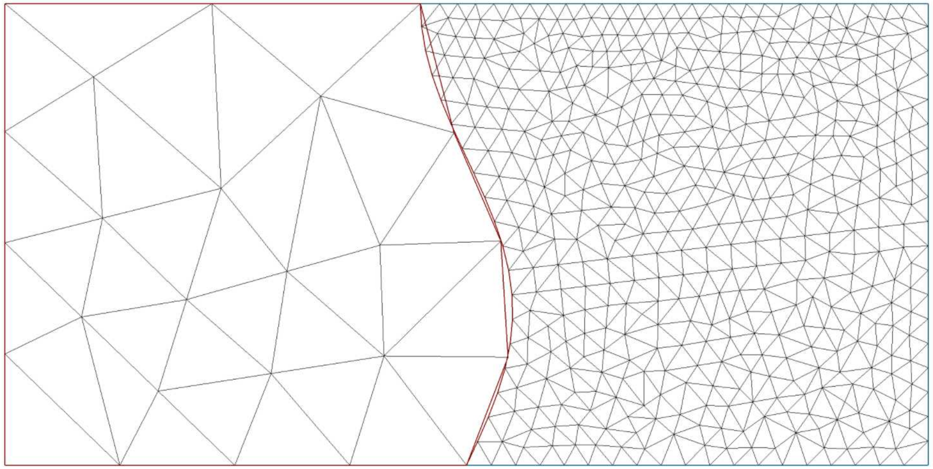


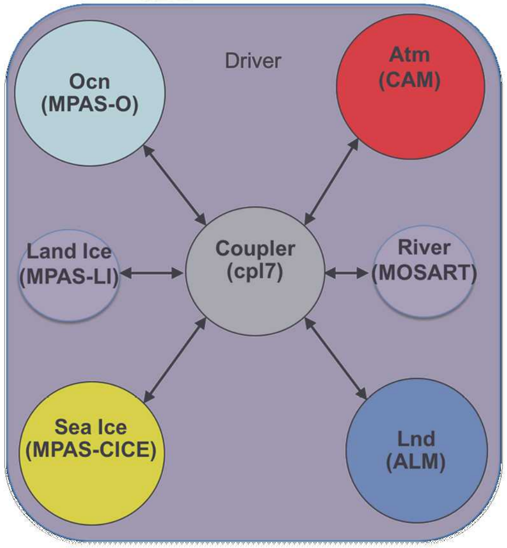
$$\begin{cases} \mu_m \left(-\boldsymbol{\delta}\mathbf{d}\mathbf{v}^\flat + 2K\mathbf{v}^\flat\right) - \gamma\mathbf{v}^\flat - \mathbf{d}p & = & -\mathbf{b}^\flat \\ -\boldsymbol{\delta}\mathbf{v}^\flat & = & 0. \end{cases}$$

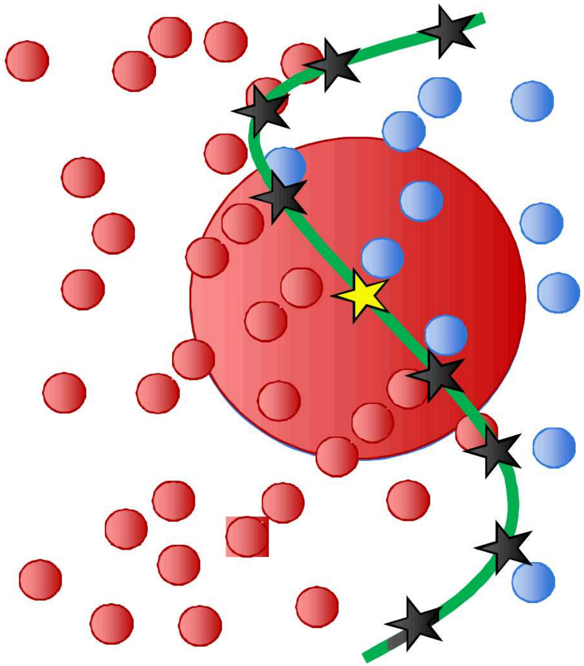
Trask, Nathaniel, and Paul Kuberry. "Compatible meshfree discretization of surface PDEs."*Computational Particle Mechanics*(2019): 1-7.
Gross, B. J., Trask, N., Kuberry, P.,&Atzberger, P. J. (2019).Meshfree Methods on Manifolds for Hydrodynamic Flows on Curved Surfaces:A Generalized Moving Least-Squares (GMLS) Approach.*arXiv preprint arXiv:1905.10469*.

Why meshfree? Code couplers for E3SM









Outline

- Generalized moving least squares (GMLS)
  - An approximation theory framework for generating meshfree methods with rigorous accuracy guarantees
- Conservative meshless discretization
  - How can we construct conservative schemes if we don't have access to discrete Stokes theorems?
- Meshfree discretizations of nonlocal mechanics
  - Can we construct a meshfree discretization framework for integral operators for fracture mechanics?
- Meshfree machine learning
  - For scientific machine learning applications, can we use scattered data approximation theory to build learning frameworks appropriate for unstructured scientific data?

Generalized moving least squares (GMLS)

Given $u \in V$, a framework for estimating operators $\tau \in V^*$ by finding an optimal reconstruction over a subspace $P \subset V$ which best matches unstructured samples

$$\Lambda := \{\lambda_i(u)\}_i$$

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

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

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

Example:

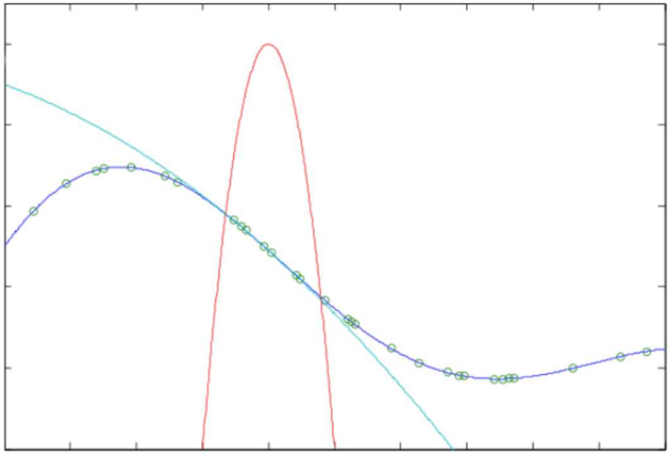
Approximate point evaluation of derivatives:

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

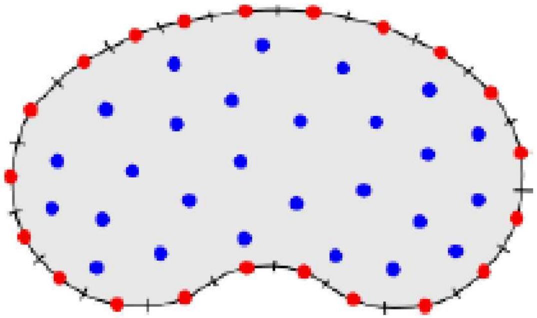
Reconstruction space $P = \pi_m$

Sampling functional $\lambda_j = \delta_{x_j} \in V^*$

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



Preliminaries: Quasi-uniform point clouds



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

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

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

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

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

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

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

Classical MLS: quasi-interpolants [Wendland04]

Definition 1. ***Local polynomial reproduction:*** *A process defining* $\forall x_i \in X$ *an approximation* $u(x) = \sum_j \phi_j u(x_j)$ *Is a local polynomial reproduction if there exist* $C_1, C2 > 0$.

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

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

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

Theorem 2. *Consider the GMLS process with* $\tau = \delta_x$, $\lambda_j(u) = u(x_j)$, *and* $V = \Pi_m$. *If* Ω *is compact and satisfies a cone condition, and* X *is quasi-uniform, then there exists a constant* $C > 0$ *such that* $supp(W) = C\, h_X$ *where the GMLS problem is solvable and forms a local polynomial reproduction.*

Classical MLS: derivative approximation [Mirzaei12]

Definition 1. ***Local polynomial reproduction:*** *A process defining* $\forall x_i \in X$ *an approximation* $D^\alpha u(x) = \sum_j \phi_j u(x_j)$ *Is a local polynomial reproduction if there exist* $C_1, C2 > 0$.

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

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

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

Theorem 2. *Consider the GMLS process with* $\tau(u) = D^\alpha u(x)$, $\lambda_j(u) = u(x_j)$, *and* $V = \Pi_m$. *If* Ω *is compact and satisfies a cone condition, and* X *is quasi-uniform, then there exists a constant* $C > 0$ *such that* $supp(W) = C\, h_X$ *where the GMLS problem is solvable and forms a local polynomial reproduction.*

An abstract error analysis framework

Basic technique:

$$
\begin{aligned}
|\tau_{\mathbf{x}}(u) - \tau^h_{\mathbf{x}}(u)| &\leq |\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}(p)| + |\tau_{\mathbf{x}}(p) - \tau^h_{\mathbf{x}}(u)|, \quad (\forall p \in P) \\
&\leq |\tau_{\mathbf{x}}(u) - \tau_{\mathbf{x}}(p)| + |\tau^h_{\mathbf{x}}(p - u)|, \\
&\leq |\tau_{\mathbf{x}}(u - p)| + \left| \sum_{i=1}^{N_p} \lambda_i(u - p)\, a^i_{\tau_{\mathbf{x}}} \right| \\
&\leq |\tau_{\mathbf{x}}(u - p)| + \max_{i \in I_{\mathbf{x}}} |\lambda_i(u - p)| \sum_{i \in I_{\mathbf{x}}} |a^i_{\tau_{\mathbf{x}}}|.
\end{aligned}
$$

← **reconstruction property**

← **GMLS definition**

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

Holds for any target functional and approximation space:

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

A general abstract framework

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

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

  - Ex: Solving different PDES

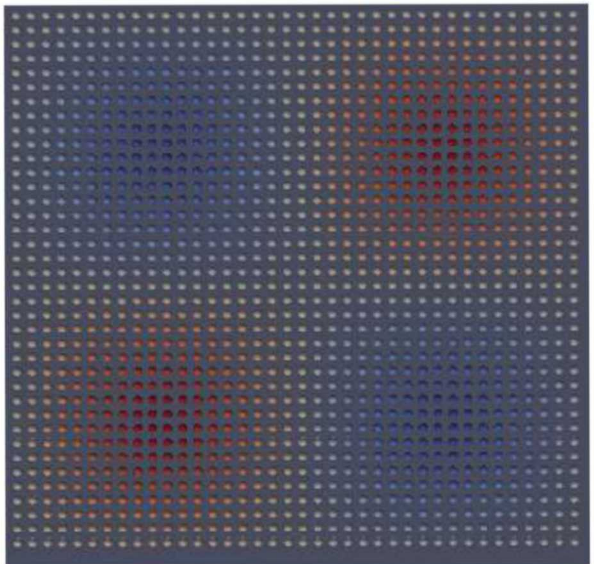
$$\tau(u) = div(u) \qquad \tau(u) = \int_{B(x)} K(x,y)u(y) - u(x)dy \qquad \tau(u) = \int_{\partial\Omega} \sigma(u)\cdot d\mathbf{A}$$

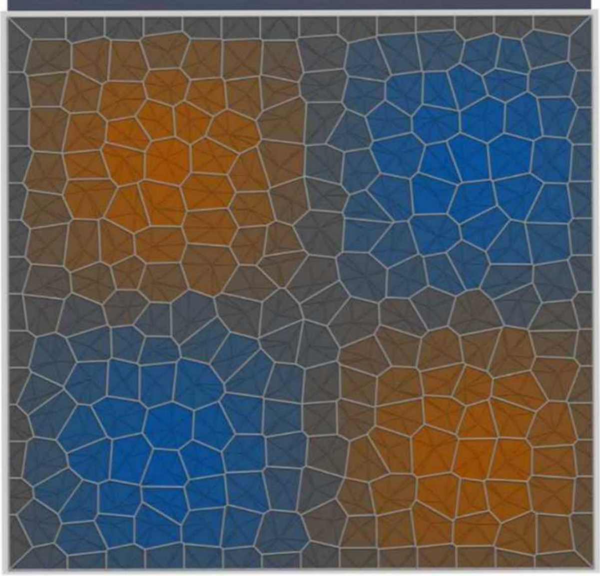
  - Ex: Handling divergence/curl constraints in saddle point problems

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

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

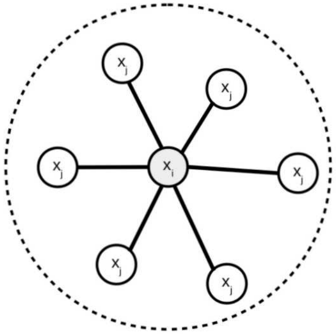
Solving PDEs with or without a mesh

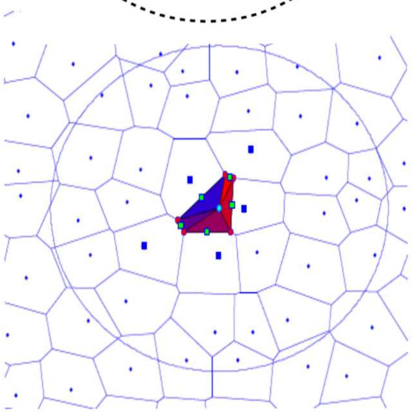


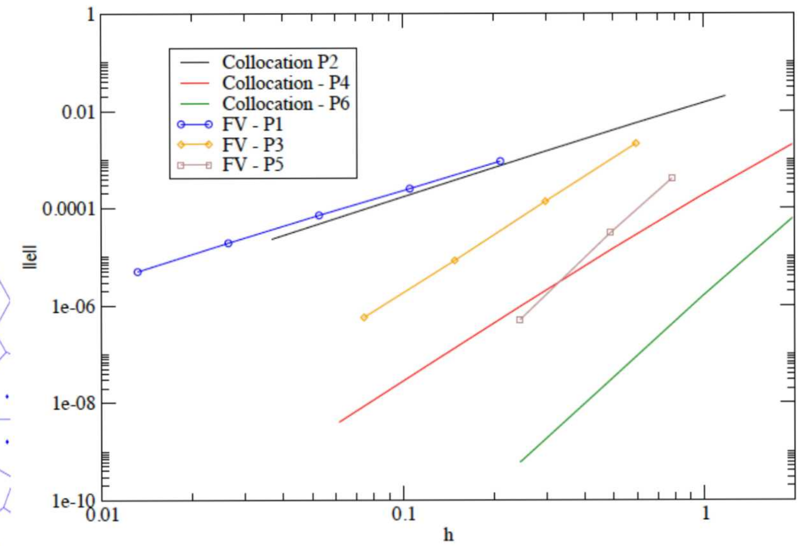


To generate mesh free schemes for $\nabla^2 \phi = f$:

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







Meshfree foundations for scientific machine learning

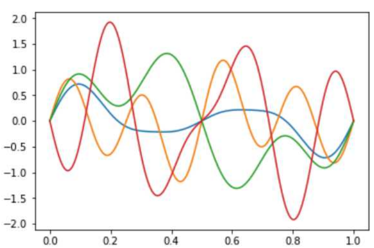
- Develop a mathematical framework for scientific machine learning (SciML) tasks
  - Data-driven model development
  - Surrogate models for optimization and UQ
  - Machine learning tools for solving numerical PDE
  - Numerical homogenization of multiscale physics
  - Development of closure models from multifidelity data
- Need tools appropriate for SciML setting
  - Augment small-data regime with domain expertise
  - Need to handle unstructured data characteristic of scientific computation (e.g. unstructured meshes vs. Cartesian grids)

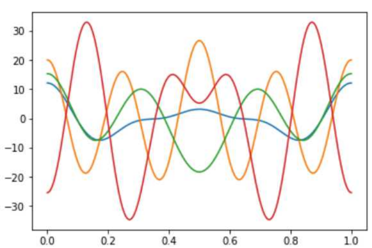
Operator regression: Problem statement

Given a collection of functions $u_i \in V$, a functional $\tau_x \in V^*$, and a domain Ω can we infer τ_x from observations of the form

$$\{u_i(x), \tau_x[u_i]\}_{i=1}^{N}?$$

Example:





$$\left\{ \;\cdot\;, \;\cdot\; \right\} \Longrightarrow \tau_x = \frac{\partial u}{\partial \hat{x}}\bigg|_{\hat{x}=x}$$

Operator regression: Problem statement

Given a collection of functions $u_i \in V$, a functional $\tau_x \in V^*$, and a domain Ω can we infer τ_x from observations of the form

$$\{u_i(x), \tau_x[u_i]\}_{i=1}^N?$$

Introduce a parametrized family of operators $\mathcal{L}_\xi \in V^*$ with hyperparameter ξ and solve the ℓ_2-optimization problem

$$\mathcal{L} = \underset{\xi}{argmin} \sum_i ||\tau_x[u_i] - \mathcal{L}_\xi[u_i]||_{V^*}^2$$

We present learning frameworks corresponding to choice of parameterization:

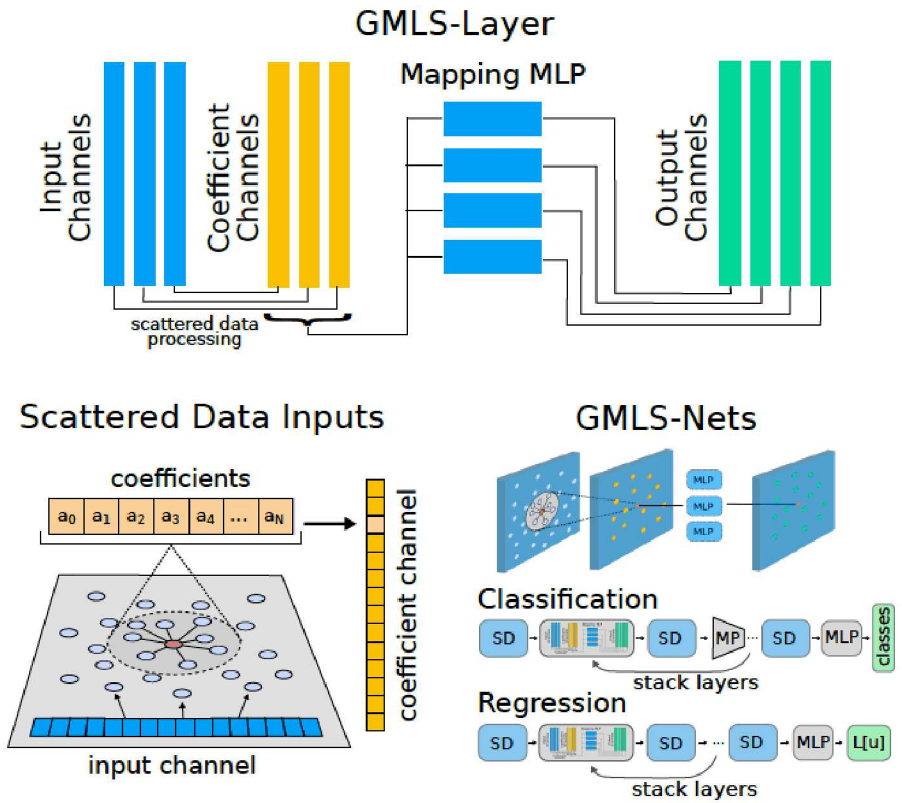
- **GMLS-Nets:** Use meshfree approximation theory to regress operators characterized by scattered samples of data
- **Fourier regression:** Characterize operators via parameterization of Fourier symbol
- **Nonlocal operator regression:** Characterize nonlocal operators via parameterization of nonlocal kernel

GMLS-Nets: SciML architecture for unstructured data

w/ Ravi Patel (SNL), Paul Atzberger (UCSB)

Sandia National Laboratories

- Assume a basis Φ, so that $p \in P \to p = a^{\intercal}\Phi$
- GMLS thus provides an *optimal local encoding* of data in terms of the coefficient a, providing a low-dimensional encoding that may e.g. exploit physics
- Traditionally, GMLS estimates $\tau(u) = a^{\intercal}\tau(\Phi)$, assuming one has knowledge of how the target functional. Instead we seek an operator $q_{\xi} : a \to \mathbb{R}$, and use gradient descent to tune ξ to match data
- Functionally identical to convolutional networks - we get a stencil that reproduces the operator, but no restriction on e.g. Cartesian data, collar region, etc.

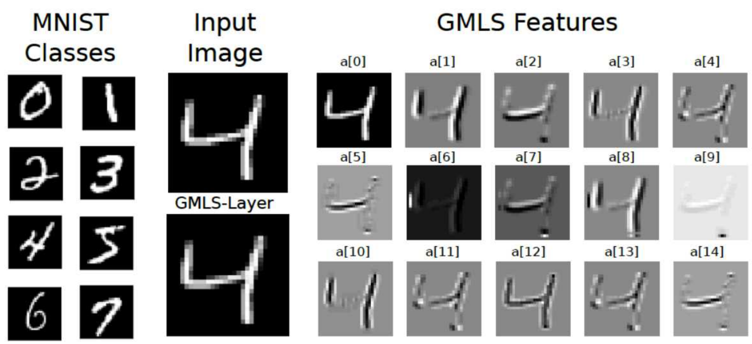


Recently submitted to neuroIPS (https://arxiv.org/pdf/1909.05371.pdf)

Open-source software: code and training sets publically available for:

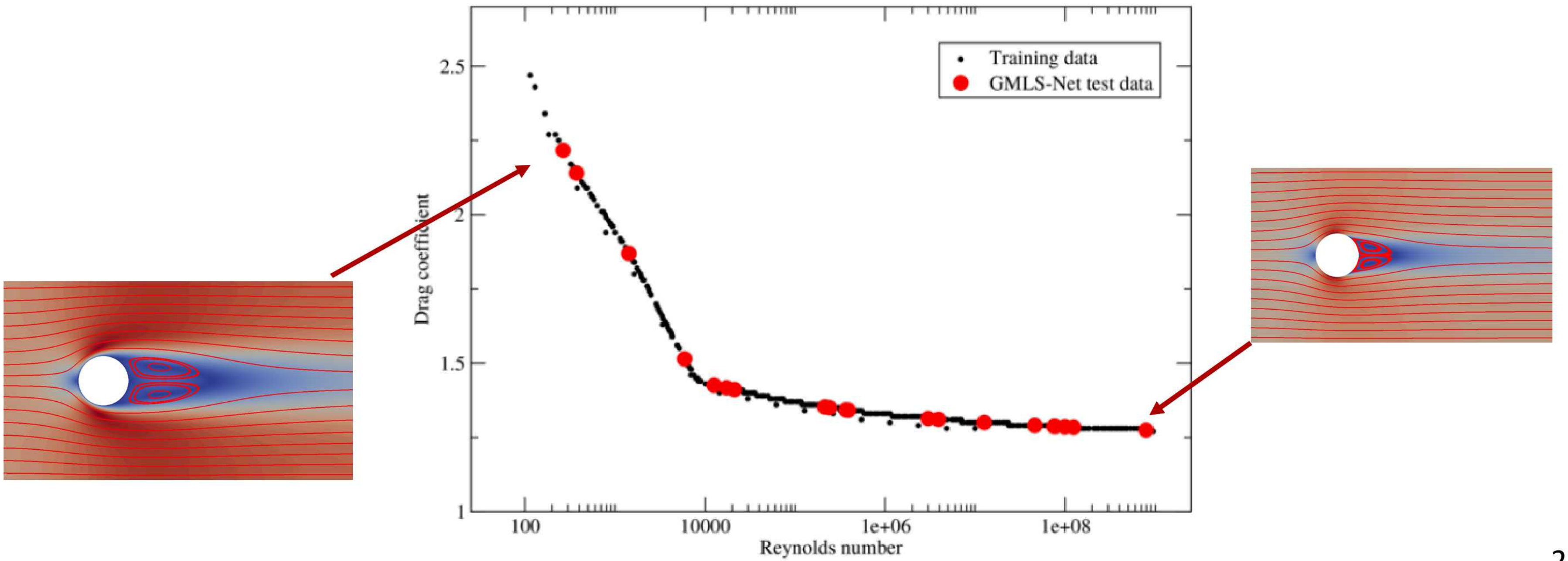
- Tensorflow (https://github.com/rgp62/gmls-nets)
- PyTorch (https://github.com/atzberg/gmls-nets)

GMLS-Nets: results



Case	Conv-2L	Hybrid-2L	GMLS-2L
MNIST	98.52%	98.41%	96.87%

- Provides similar performance to convNets on MNIST due to similar feature extraction capability
- Generalizes convNets to unstructured scientific data:
    - Prediction of drag from cell center velocity field taken from FV data
    - No pressure/viscosity information: drag characterizated entirely by flow

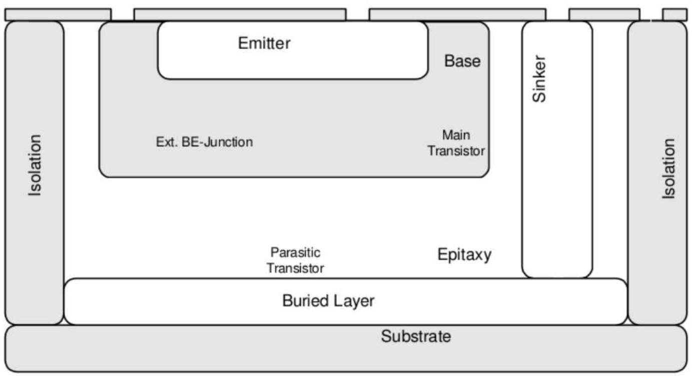


Data driven circuit models

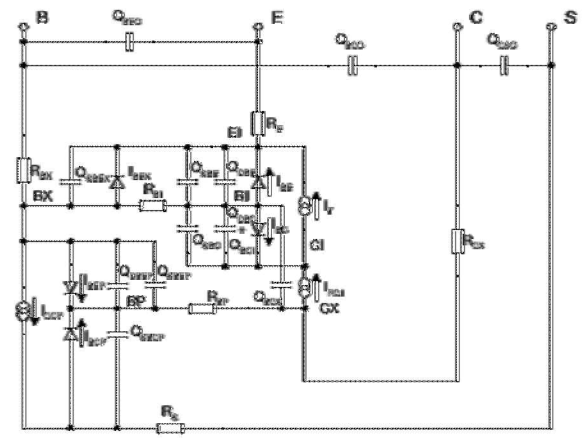
w/ P.Bochev

When analyzing systems consisting of large numbers of components, costly first principle PDE models are often abandoned in favor of efficient ODE-based network models

PDE-based drift-diffusion model



Circuit compact model



As an example, circuit models are empirically generated in a process that takes ***~10 years*** to develop for typical components and has no means to incorporate radiation effects.

Can we leverage physics from PDE model to inform an automatically generated compact model?

Data driven circuit models

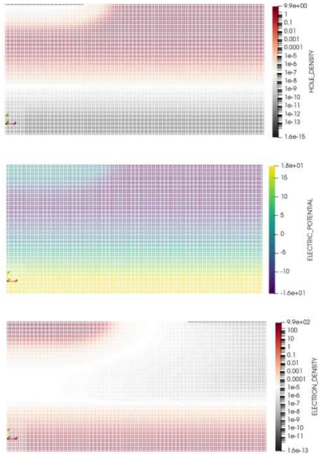
w/ P. Bochev

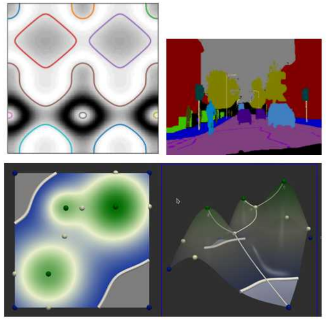
Physics Priming (PP)
Perfunctory TCAD

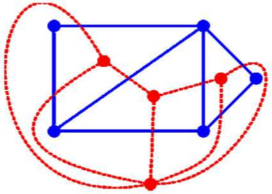
Region Recognition (RR)
ML + TDA

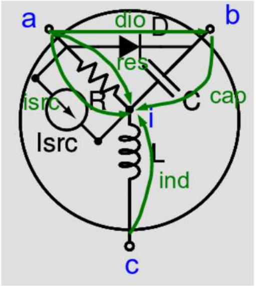
Topology Tailoring (TT)

Interaction Identification (II)
(seeded w/ established CMs)









Train and Adapt
(using available experimental data)

Simulate high fidelity physics.

Identify significant regions (ML+ Topological Data Analysis)

Identify interactions between significant regions.

Prescribe electronics components to physical interactions.

Generate **positive feedback** in the machine learning process (supervised training).