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SAND2019-8760C

The Conforming Reproducing Kernel (CRK) Method

Recent Developments and Applications

SAND2019-XXXXXC

UC San Diego
JACOBS SCHOOL OF ENGINEERING
Structural Engineering

Center for Extreme Events Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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USNCCM

Austin, TX, July 28, 2019

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Analyst's Goal

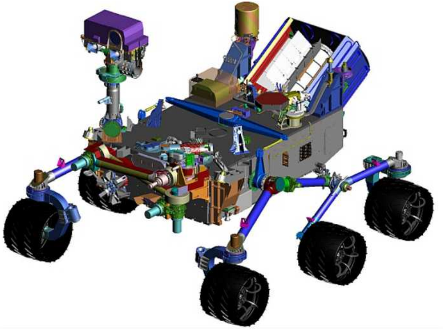
A large portion of people using the finite element method are faced with a general task:

Deliver critical engineering analyses in a timeframe consistent with project requirements

Meshing is Time Consuming

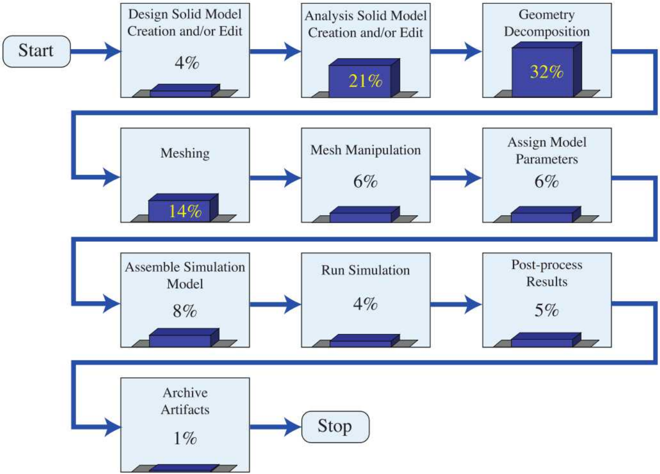
Challenging engineering analyses are common at Sandia. Goal is to have a general solution, must address the more burdensome models: *multi-body / material, complex geometries, contact, nonlinear materials, dynamic loading*

Battery Microstructure



source: https://www.nasa.gov

Engineering Analysis, Process Cost Breakdown[1,2]



[1] M. F. Hardwick, R. L. Clay, P. T. Boggs, E. J. Walsh, A. R. Larzelere, and A. Altshuler, "DART system analysis," Sandia National Laboratories, Tech. Rep. SAND2005-4647, 2005.

[2] J. A. Cottrell, T. J. Hughes, and Y. Bazilevs, *Isogeometric analysis: toward integration of CAD and FEA*. John Wiley & Sons, 2009.

Can a reproducing kernel method be used to help create an agile design-to-simulation process?

- Can it effectively handle complex, multi-body, domains?
- Will it efficiently provide quality solutions for large deformations?
- Is it compatible with rapid meshing / discretization?

Handling Complex Domains

Quick overview, for more details see:
J. J. Koester and J.-S. Chen, "Conforming window functions for meshfree methods," *Computer Methods in Applied Mechanics and Engineering*, vol. 347, pp. 588–621, 2019

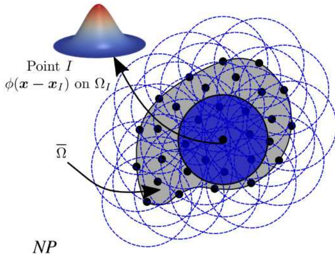
Reproducing Kernel Overview

Approximate solutions are constructed over a point cloud. Shape functions are constructed as the product of a *kernel function* and a *correction function*

$$u^h(x) = \sum_{I=1}^{NP} \Psi_I d_I; \qquad \Psi_I = C(x; x - x_I)\phi_a(x - x_I)$$

$$C(x; x - x_I) = \sum_{i=0}^{n} b_i(x)(x - x_I)^i \equiv \mathbf{H}^T(x - x_I)\mathbf{b}(x)$$

$$\mathbf{H}^T(x - x_I) = [\,1, x - x_I, (x - x_I)^2, ..., (x - x_I)^n]$$

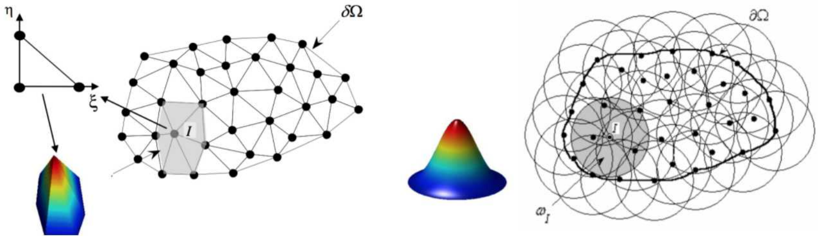


$\mathbf{b}(x)$is obtained by imposing completeness requirement: $\sum_{I=1}^{NP} \Psi_I x_I^i = x^i, \; 0 \leqslant i \leqslant n$

$$\mathbf{b}(x) = \mathbf{H}^T(0)\mathbf{M}^{-1}(x) \qquad \text{where} \qquad \mathbf{M}(x) = \sum_{I=1}^{NP} \mathbf{H}(x - x_I)\mathbf{H}^T(x - x_I)\phi_a(x - x_I)$$

- **Kernel function: compact support, determines smoothness**
- Correction function: provides completeness

Meshfree Challenges

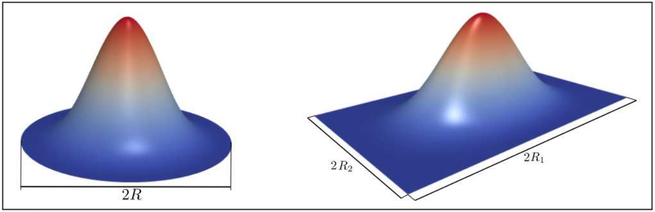


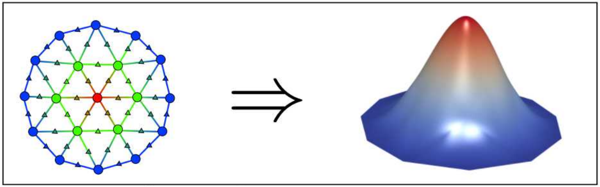
The following challenges all stem from shape functions not conforming to boundaries

- Concave geometries
  - Visibility
  - Diffraction
- Bi-material (weak discontinuity)
  - Enriching
  - Coupling
- Essential boundaries
  - Lagrange multiplier
  - Singular kernel
  - Penalty
  - Nitsche's
  - Coupling

Conforming Window Functions

Traditional, Euclidean Windows / Kernels





New, Graph-Informed Windows / Kernels

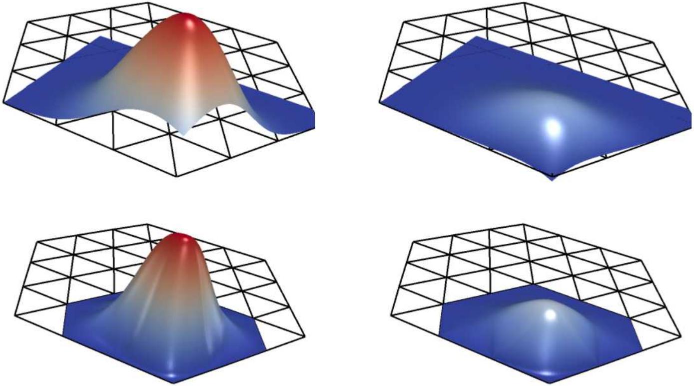
- Mesh is used to inform RK functions about boundaries
- RK functions are not local to elements, reducing the connection between mesh and approximation quality

Conforming to Boundaries / Interfaces

Define kernel functions using, smooth spline spaces on triangles or tetrahedra (Bernstein-Bézier polynomials).

Non-conforming at essential boundary

Conforming at essential boundary



ϕ_I
(Kernel)

Ψ_I
(Shape Function)

Elasticity Patch Tests

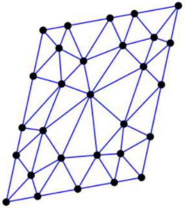


Figure: Deformed triangulation

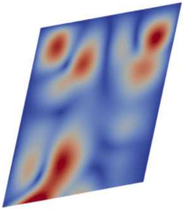


Figure: RKPM, transformation method

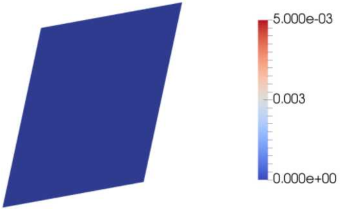


Figure: CRK, static condensation

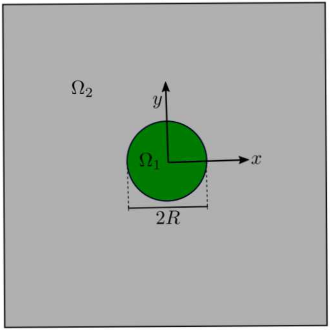
Method	L^2	H_1
RKPM with transformation method	2.05e-03	2.44e-02
Conforming window RK with static condensation	7.65e-17	1.04e-15

- Weak Kronecker-Delta $\rightarrow$ Kinematically Admissible Approximations
- Interpolatory along boundary: $u^h(\mathbf{x}_I) = d_I \rightarrow$ *directly impose essential boundaries* (like FEM)

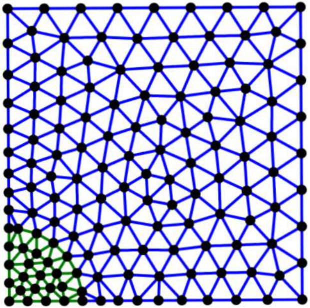
Panel with an Inclusion

An elastic panel with an inclusion

- (4x4) panel, $R = 1$ for inclusion
- Inclusion: $E = 10.E4$, $\nu = 0.3$
- Panel: $E = 10.E3$, $\nu = 0.3$



- Tension in x direction
- Exact displacement on symmetry planes
- Exact traction on other edges



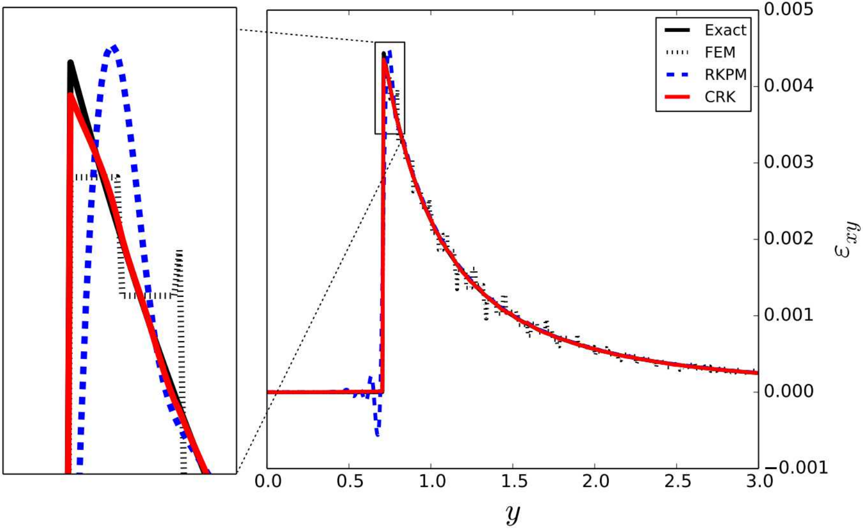


Figure: ε_{xy} near the material interface.

Results Comparison

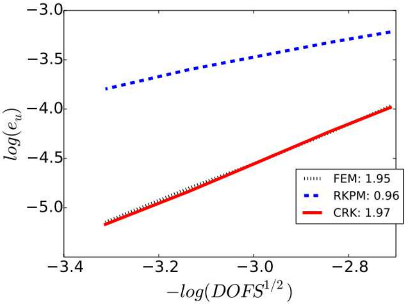


Figure: Convergence in $\mathbf{u}$

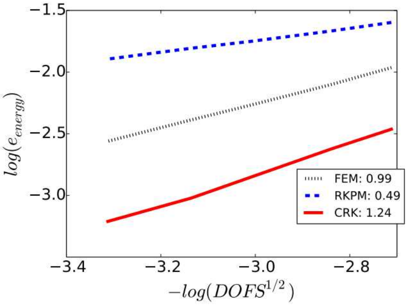


Figure: Convergence in energy

Efficient, Quality Solutions for Large Deformations

Domain integration and addressing nearly incompressible materials

For more details, see:

G. Moutsanidis, J. Koester, M. Tupek, Y. Bazilevs, and J.-S. Chen, "Treatment of near-incompressibility in meshfree and immersed-particle methods," *Computational Particle Mechanics*, 2019

Overview of Integration

The *smoothed gradient*[3] operator is commonly used:

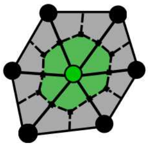
$$\widetilde{\nabla} f(\Omega_L) = \frac{1}{V_L} \int_{\Omega_L} \nabla f \, d\Omega, = \frac{1}{V_L} \int_{\Gamma_L} f \mathbf{n} \, d\Gamma$$

where Ω_L is the smoothing volume surrounding corresponding to a material point L with boundary Γ_L, volume V_L and outward facing surface normal $\mathbf{n}$.

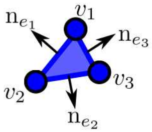
- Improved efficiency
- Consistent, passes patch test

but, can have

- Low energy modes
- Pressure oscillations for nearly incompressible materials



Example Nodal Domain (SCNI)

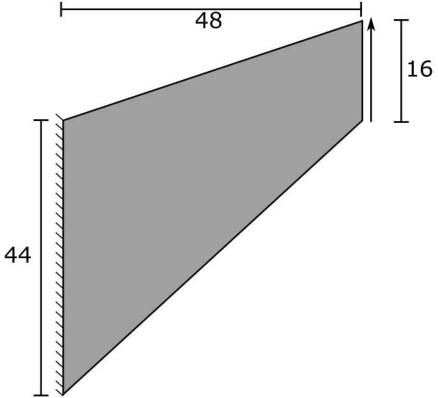


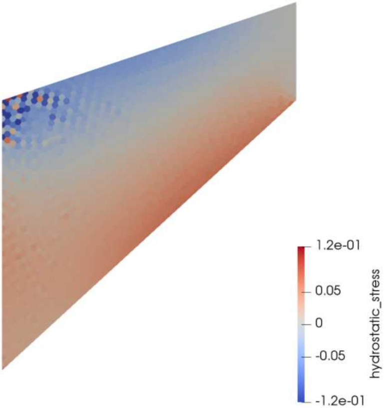
Example Smoothing Cell

[3] J.-S. Chen, C.-T. Wu, S. Yoon, and Y. You, "A stabilized conforming nodal integration for Galerkin mesh-free methods," *International Journal for Numerical Methods in Engineering*, vol. 50, no. 2, pp. 435–466, 2001.

Example Pressure Oscillations

Cook's membrane problem. Neo Hookean, $E = 1000$, $\nu = 0.499$. SCNI





Proposed $\overline{\mathbf{F}}$-Based Method

An $\overline{\mathbf{F}}$ method is proposed to address low energy modes and pressure oscillations in nearly incompressible problems.

With $\overline{\mathbf{F}}$ methods, a multiplicative split is used to decompose the deformation gradient

$$\mathbf{F} = \mathbf{F}^{dil}\,\mathbf{F}^{dev}$$

$$\text{with } \det\mathbf{F} = J = \det\mathbf{F}^{dil}, \quad \det\mathbf{F}^{dev} = 1, \quad \mathbf{F}^{dev} = J^{-1/3}\mathbf{F}, \quad \mathbf{F}^{dil} = J^{1/3}\mathbf{I}$$

The volumetric part of $\mathbf{F}$ is replaces with a projected value

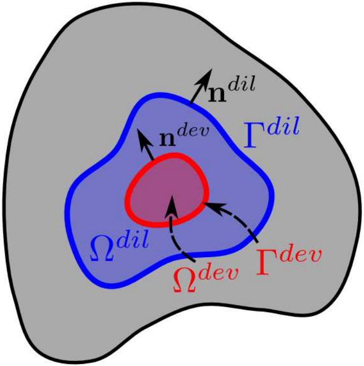
$$\overline{\mathbf{F}} = \overline{\mathbf{F}}^{\,dil}\,\mathbf{F}^{dev},$$

where

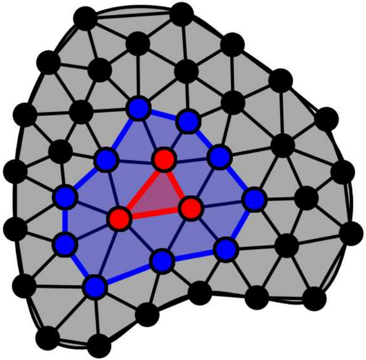
$$\overline{\mathbf{F}}^{\,dil} = \pi(\mathbf{F}^{dil}) = \overline{J^{1/3}}\,\mathbf{I},$$

New Projection for $\overline{\mathbf{F}}$

For the proposed method, the smoothed gradient operator is used and two different domains are considered for each material point, a smaller domain Ω_L^{dev} provides the deviatoric portion and a larger domain Ω_L^{dil} provides the dilatational portion.



Nested smoothing domains



Meshed domains

New Projection for $\overline{\mathbf{F}}$

For $\overline{\mathbf{F}}$ at material point L, we have

$$\overline{\mathbf{F}}_L = \overline{\mathbf{F}}_L^{dil}\, \mathbf{F}_L^{dev},$$

with the deviatoric part coming from the smoothed deformation gradient of the smaller cell,

$$\mathbf{F}_L^{dev} = \widetilde{\mathbf{F}}(\Omega_L^{dev}),$$

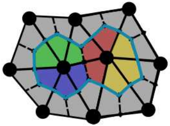
and the dilatational part coming from the smoothed deformation gradient of the larger cell,

$$\overline{\mathbf{F}}_L^{dil} = \overline{J^{1/3}}(\Omega_L^{dil})\, \mathbf{I},$$

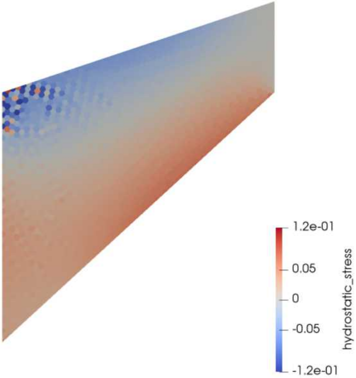
$$\bar{J}(\Omega_L^{dil}) = \frac{1}{V^{dil}} \sum_{c \in C} V_c J_c,\;\; V^{dil} = \sum_{c \in C} V_c,$$

where C is the collection of cells/elements in the volumetric domain. This allows J to be computed one time for every cell then aggregated as needed for $\bar{J}$

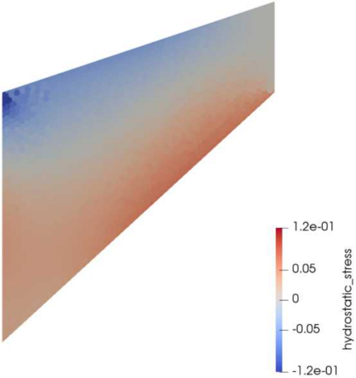
Cook's Membrane $\nu = 0.49999$



Volumetric domains: union of 2 nodal domains
Deviatoric domains: 4 per volumetric domain



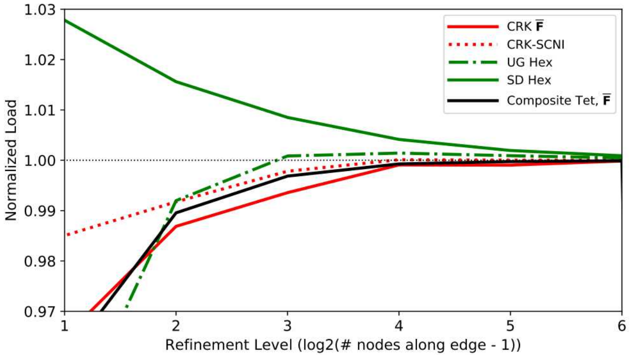
Original SCNI



Proposed $\overline{\mathbf{F}}$ Method

Cook's Membrane $\nu = 0.499$

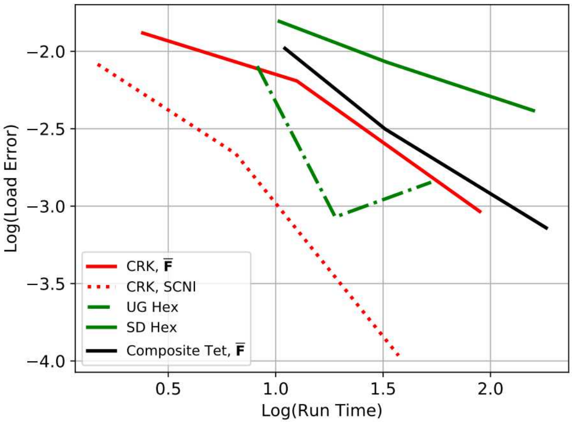
Tip load for a given displacement, normalized by a refined composite tet solution



- UG Hex: Single integration point, hourglass control (Flanagan, Belytschko)
- SD Hex: Fully integrated deviatoric, averaged volumetric response ($\overline{\mathbf{F}}$)
- Composite Tet: 12 sub tets, 10 nodes, averaged volumetric response ($\overline{\mathbf{F}}$)

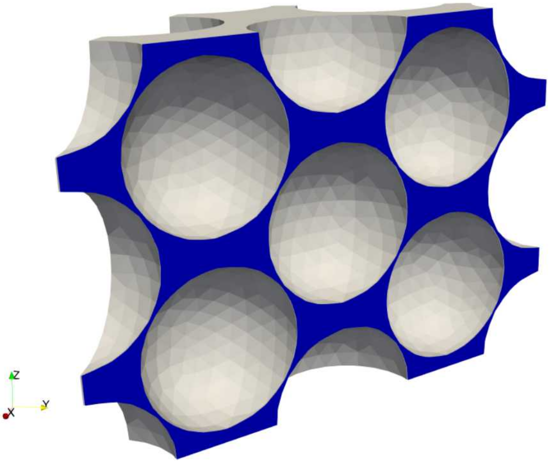
Cook's Membrane $\nu = 0.499$

Error in applied load for a given displacement for three mesh refinements.
True load estimated using a highly refined solution with the composite tet.

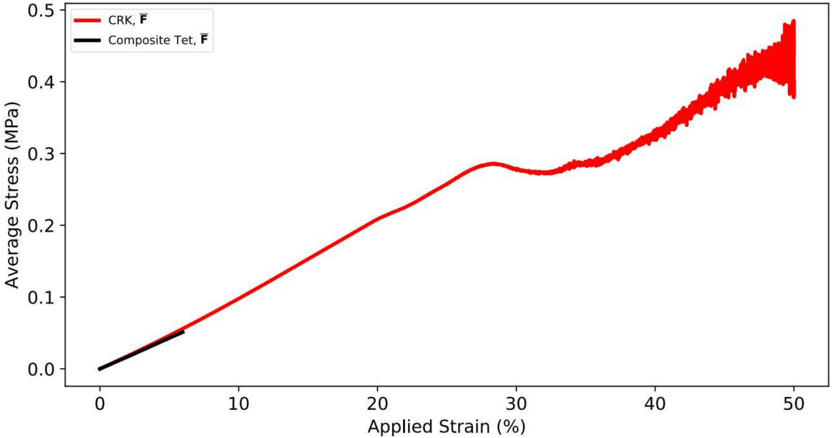


Example: Elastomeric Foam

Cube with 65% porosity, BCC voids. Gent Model: G = 0.950 MPa, K = 920 MPa



Example: Elastomeric Foam



Pairing with Automated Meshing

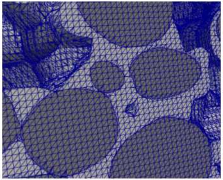
Low Quality Meshes

Generating subdivisions of complex geometries is often faced with many challenges

- Small features need to be removed
- Scanned systems may be represented with STLs, requiring extra processing

Challenging to get a mesh of quality elements. However, many methods exist that readily produce meshes with low quality elements. E.g. Conformal Decomposition Finite Element Method (CDFEM)[4]

Lithium Ion Battery



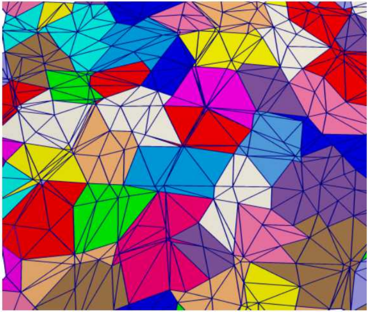
CDFEM Mesh, Close-Up

[4] S. A. Roberts, H. Mendoza, V. E. Brunini, and D. R. Noble, "A verified conformal decomposition finite element method for implicit, many-material geometries," *Journal of Computational Physics*, vol. 375, pp. 352–367, 2018.

Addressing Low Quality Meshes

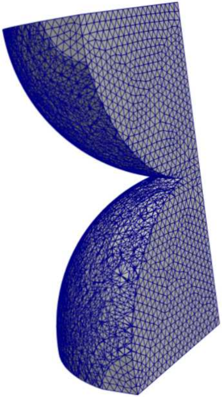
A method is being developed to work with low quality meshes. In short, use mesh only as a guide.

- **Decimate** by selecting a subset of vertices to be nodes carrying DOFs
- **Aggregate** elements into better shaped integration cells.

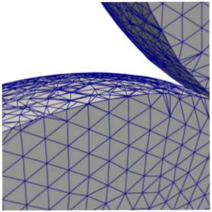


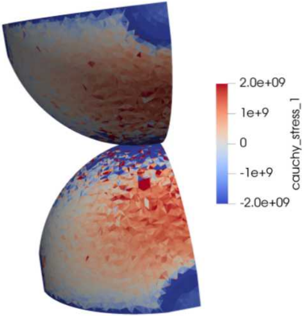
Example of clusters

Example: CDFEM Spheres



Mesh of Two Spheres

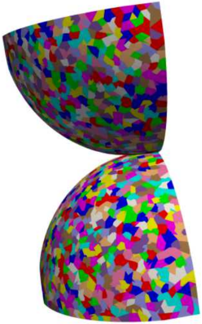




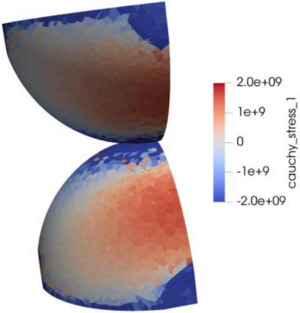
RKPM results

Example: CDFEM Spheres

Use mesh only as a guide. Select a subset of vertices to be nodes carrying DOFs. Aggregate elements into better shaped integration cells.



Aggregated Elements



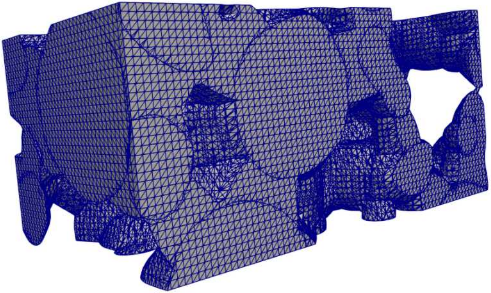
CRK Prediction

≈1000x time step advantage over a linear tet on the CDFEM mesh.

More robust. Higher solution quality.

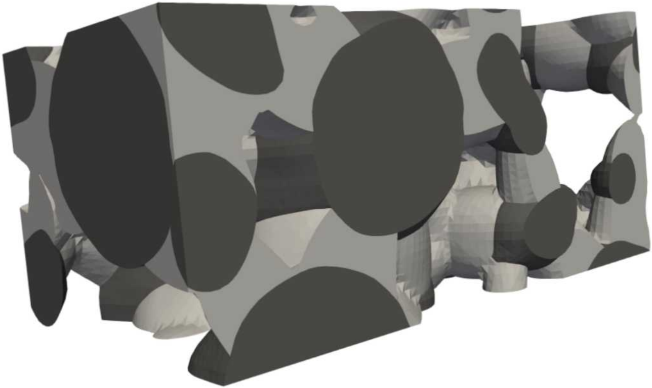
Lithium Ion Battery

CDFEM mesh with 821,437 elements and 173,917 nodes, aggregated to give 50,000 cells, each containing one node and two subcells. Loaded in compression.



Initial Mesh

Lithium Ion Battery



$\approx$200x time step advantage over a linear tet. Ran to completion

Agile Design-to-Simulation

Goal: *Improving the analyst's response time via a reproducing kernel-based agile design-to-simulation framework*

Effectively handle complex, multi-body, domains?

$\rightarrow$ Conforming window method was developed

Will it efficiently provide quality solutions for large deformations?

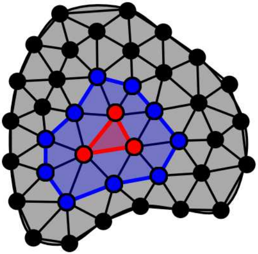
$\rightarrow$ An $\overline{\mathbf{F}}$ method was proposed

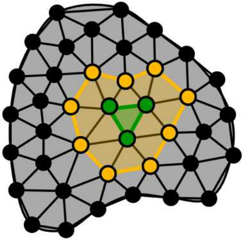
Compatible with rapid meshing / discretization?

$\rightarrow$ Use mesh only as a guide (aggregate elements, select subset of node)

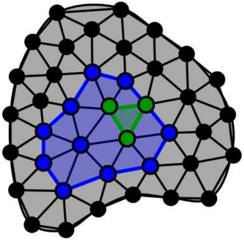
- G. Moutsanidis, J. Koester, M. Tupek, Y. Bazilevs, and J.-S. Chen, "Treatment of near-incompressibility in meshfree and immersed-particle methods," *Computational Particle Mechanics*, 2019
- J. J. Koester and J.-S. Chen, "Conforming window functions for meshfree methods," *Computer Methods in Applied Mechanics and Engineering*, vol. 347, pp. 588–621, 2019

Backup: Projection for $\overline{\mathbf{F}}$





Outward (new dil domain)



Inward (share dil domain)