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SAND2019-2732C

The Conforming Reproducing Kernel Method

for an Agile Design-to-Simulation Workflow

SAND2019-XXXX

UC San Diego
JACOBS SCHOOL OF ENGINEERING
Structural Engineering

Center for Extreme Events Research

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LSTC Meshfree Workshop
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Analyst's Goal

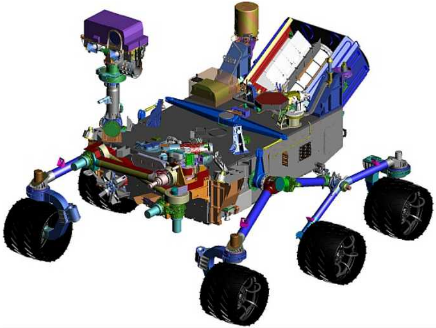
A large portion of people using the finite element method are faced with a general task:

Deliver critical engineering analyses in a timeframe consistent with project requirements

Meshing is Time Consuming

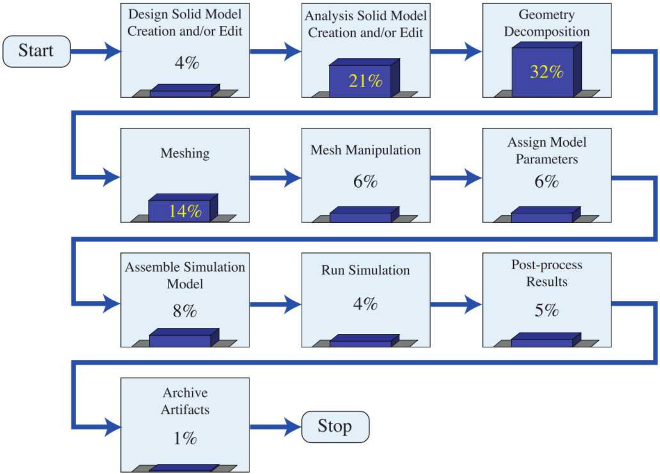
Challenging engineering analyses are common at Sandia. Goal is to have a general solution, must address the more burdensome models: *multi-body / material, complex geometries, contact, nonlinear materials, dynamic loading*

Battery Microstructure



source: https://www.nasa.gov

Engineering Analysis, Process Cost Breakdown[1,2]



[1] M. F. Hardwick, R. L. Clay, P. T. Boggs, *et al.*, "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.

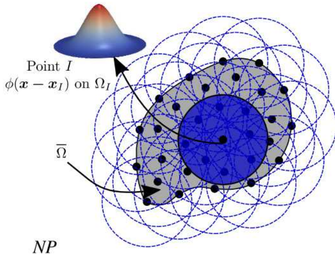
Reproducing Kernel Overview

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

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

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

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

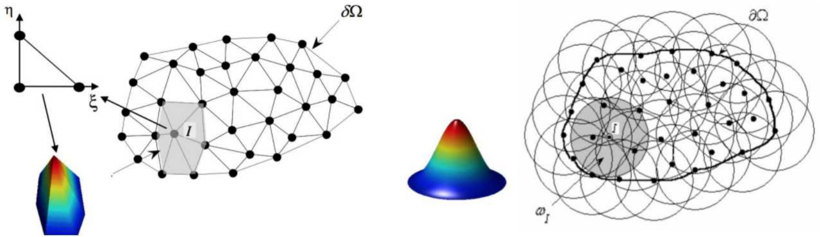


$\mathbf{b}(x)$is obtained by imposing completeness requirement: $\sum_{I=1}^{NP} \Psi_I x_I^i = x^i, \; 0 \leqslant i \leqslant n$

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

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

Meshfree Rapid D2A Challenges



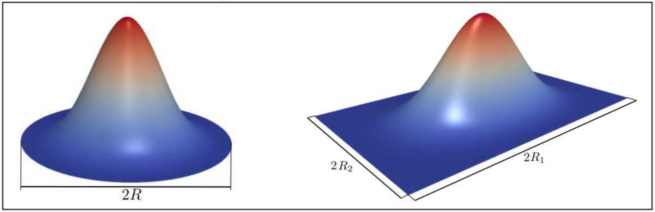
The following challenges all stem from shape functions not conforming to boundaries

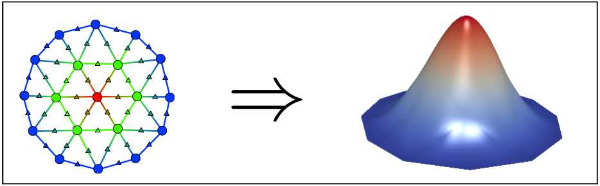
- Concave geometries
  - Visibility
  - Diffraction
- Bi-material (weak discontinuity)
  - Enriching
  - Coupling
- Essential boundaries
  - Lagrange multiplier
  - Singular kernel
  - Penalty
  - Nitsche's
  - Coupling

Conforming Window Functions

Utilize the flexibility that meshfree methods provide, supply more control where needed.

Traditional, Euclidean Windows / Kernels





New, Graph-Informed Windows / Kernels

Conforming Window Functions

The conceptual steps in creating conforming windows are:

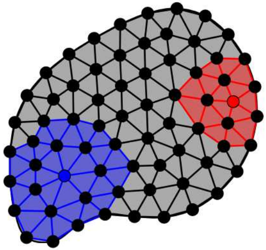
- Choose the subdivision strategy and create subdomains for each window
- Define the function space (on the subdivisions) for building the window function
- Construct the functions by specifying the coefficients of the space

The conforming window functions replace the traditional window functions and the rest of the RK or MLS method remains the same.

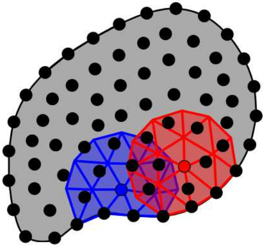
Subdivision

Many ways to subdivide. Here we choose triangulations.
RK / MLS to build approximation functions, requires overlapping kernels

- Extract "stars" from global triangulation
- Construct local, kernel specific triangulations



Example for two vertices, using star^2

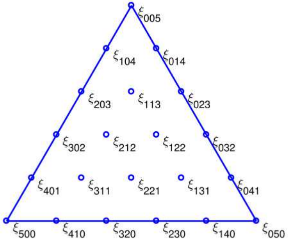


Local overlapping triangulations

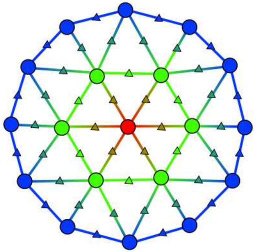
Function Space for Constructing Window Functions

Bernstein-Bézier polynomials on triangles. For example, $\mathcal{S}_5^{1,2}$ (Argyris Space, quintic, C^1 on edges, C^2 at vertices)

- Established theory for smoothly joining functions between triangles within a triangulation
- Convenient for Hermite interpolation



Domain points on a triangle



Nodal locations for a triangulation

Need function and derivative values at nodal locations for Hermite interpolation.

Setting the Coefficients

Function values and derivative for Hermite interpolation.

Modify a traditional, radial cubic B-spline window function

Traditional window function:

$$\phi(\bar{r}) = \begin{cases} 1 - 6\bar{r}^2 + 6\bar{r}^3 & \text{for } 0 \leqslant \bar{r} \leqslant \frac{1}{2} \\ 2 - 6\bar{r} + 6\bar{r}^2 - 2\bar{r}^3 & \text{for } \frac{1}{2} \leqslant \bar{r} \leqslant 1 \\ 0 & \text{otherwise,} \end{cases}$$

$\bar{r} = r(\mathbf{x})/R$, the normalized distance.

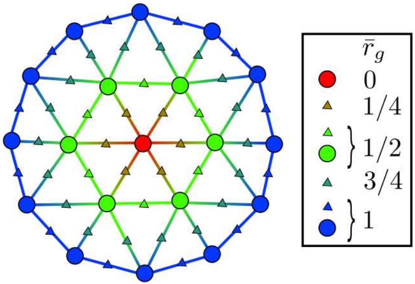
Replace $\bar{r}$ with $\bar{r}_g$, the normalized graph distance:

$$\bar{r}_g = \begin{cases} 1 & \forall\, v_I \in \mathcal{N}_b,\ \ v_0 \notin \mathcal{N}_b \\ d_g(v_0, v_I)/R_g & \text{otherwise} \end{cases}$$

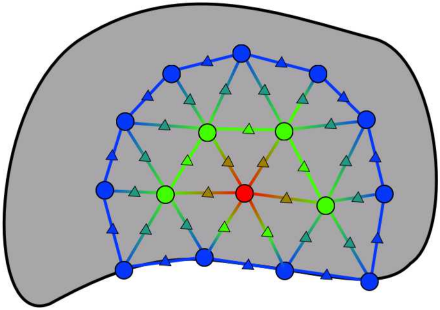
$d_g(v_0, v_I)$ is the graph distance between vertex v_I and the center v_0, R_g is the chosen graph extent (e.g. star^{R_g}), $\mathcal{N}_b$ is the set of nodal parameter locations on conforming boundaries

Normalized Graph Distances

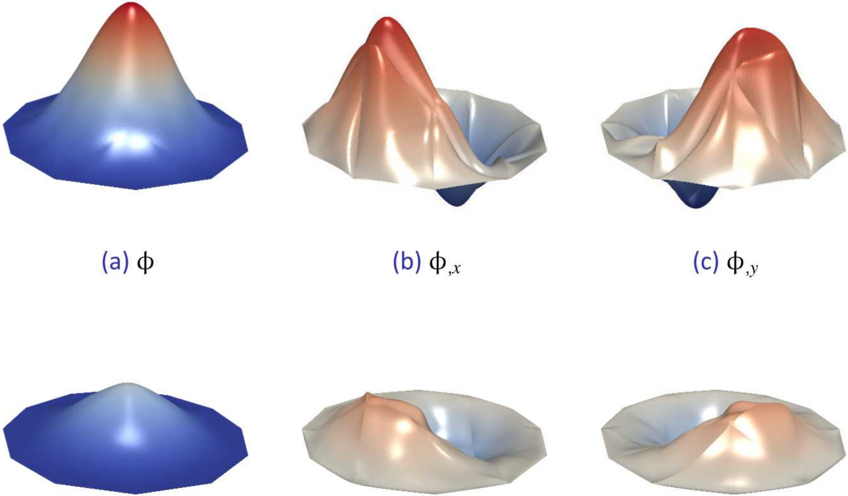
Normalized graph distances, d_g, at the $\mathcal{S}_5^{1,2}$ nodal parameter locations for a second order stars:



Away from a boundary



Near a boundary



(a) ϕ (b) $\phi_{,x}$ (c) $\phi_{,y}$

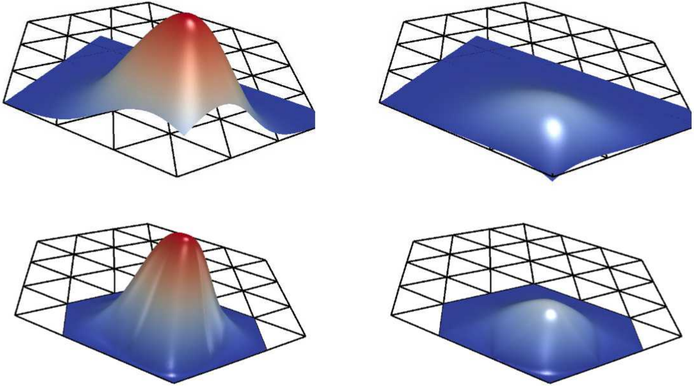
(d) Ψ (e) $\Psi_{,x}$ (f) $\Psi_{,y}$

Figure: Interior conforming windows and approximation functions

Conforming to Essential Boundary

Non-conforming at essential boundary

Conforming at essential boundary



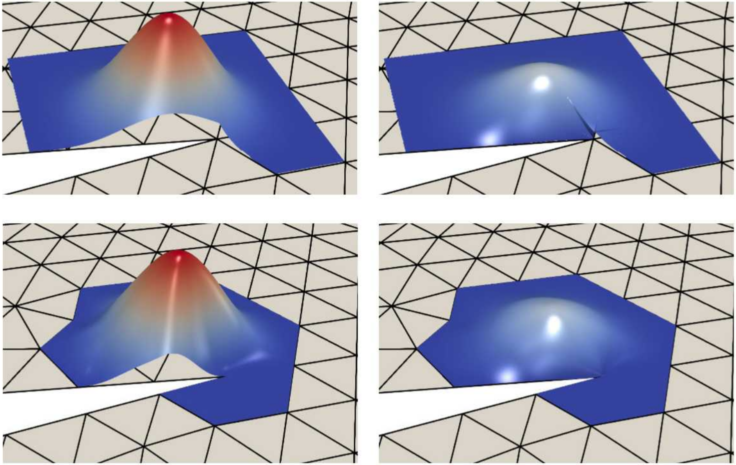
ϕ_I
(Kernel)

Ψ_I
(Shape Function)

Near Non-Convex Region

Non-conforming window with visibility check

Conforming window



ϕ_I
(Kernel)

Ψ_I
(Shape Function)

"Snap" Star

Avoid quality issues by adapting the star shape with poor quality meshes.

- Use all elements that are contained or intersect a Euclidean ball
- Use normalized Euclidean distance for nodal locations inside the ball
- Set the normalized distance for nodal location outside the ball

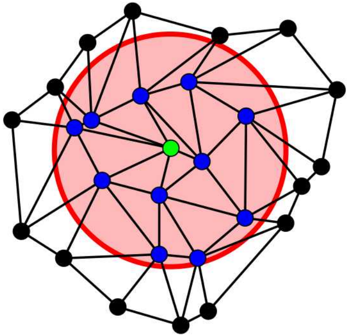


Figure: star[2]

"Snap" Star

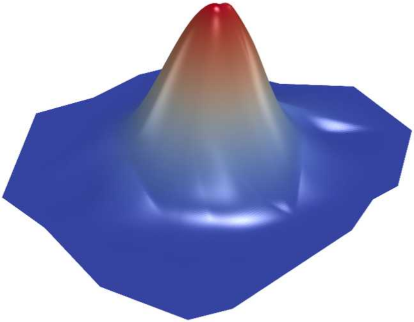


Figure: "snap" star

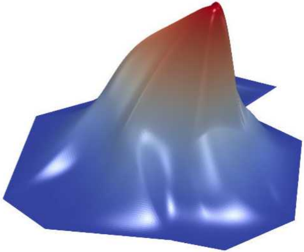


Figure: $star^2$

"Local" Star

Construct window function using local triangulations, not from a global mesh

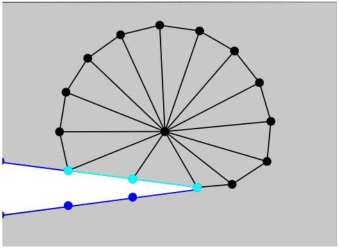


Figure: Local Triangulation

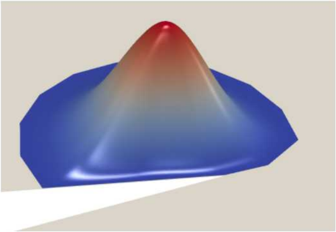


Figure: "local" star

Elasticity Patch Tests

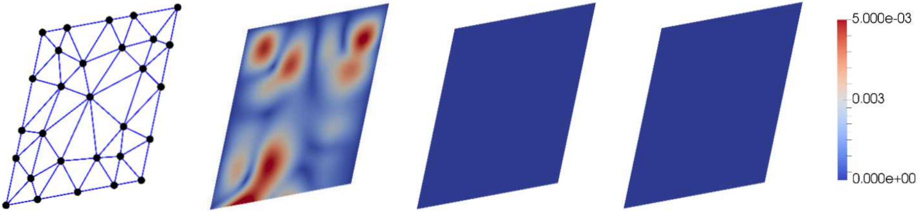


Figure: Deformed triangulation

Figure: RKPM, transformation method

Figure: RKPM, Nitsche's method

Figure: CRK, static condensation

Method	L^2	H_1
RKPM with transformation method	2.05e-03	2.44e-02
RKPM with Nitsche's method	3.85e-16	4.93e-15
Conforming window RK with static condensation	7.65e-17	1.04e-15

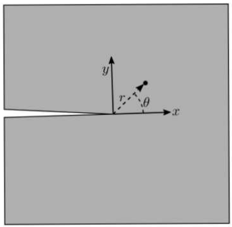
- Weak Kronecker-Delta $\rightarrow$ Kinematically Admissible Approximations
- Interpolatory along boundary: $u^h(\mathbf{x}_I) = d_I \rightarrow$ *directly impose essential boundaries* (like FEM)

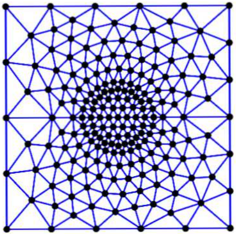
Panel with a Re-entrant Corner

An elastic plate with an edge crack

- $E = 3.E7$, $\nu = 0.3$
- Mode I loading
- Exact displacement along edges (except re-entrant edges)
- Plane strain
- $\lambda = 0.5$
- $Q = 1/3$

$$\sigma_{xx} = \lambda r^{\lambda-1} \left[(2 - Q(\lambda+1)) \cos((\lambda-1)\theta) - (\lambda-1)\cos((\lambda-3)\theta) \right]$$
$$\sigma_{yy} = \lambda r^{\lambda-1} \left[(2 + Q(\lambda+1)) \cos((\lambda-1)\theta) + (\lambda-1)\cos((\lambda-3)\theta) \right]$$
$$\sigma_{xy} = \lambda r^{\lambda-1} \left[(\lambda-1) \sin((\lambda-3)\theta) + Q(\lambda+1)\sin((\lambda-1)\theta) \right]$$





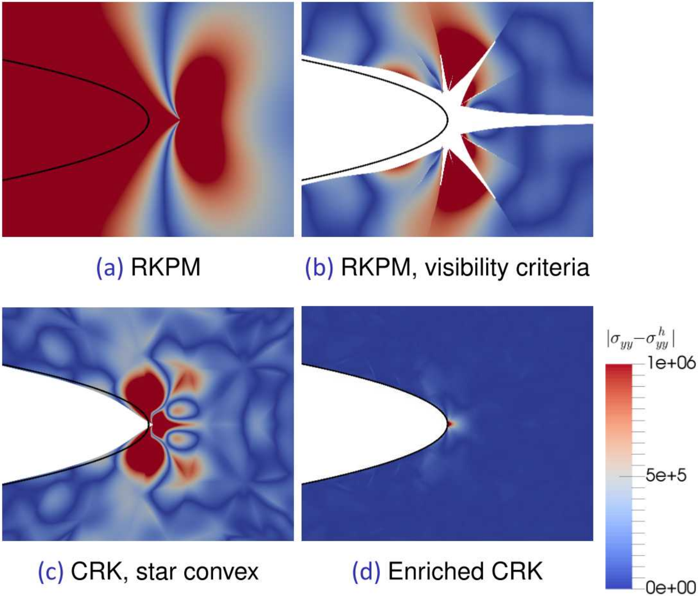
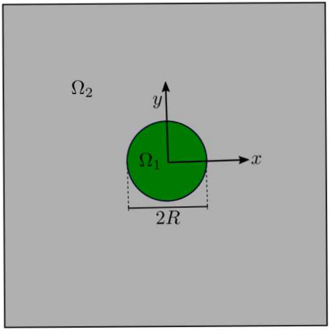


Figure: Error in σ_{yy} near the crack tip. Nodal spacing $h_1 = 0.02$.

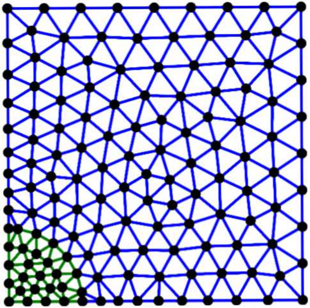
Panel with an Inclusion

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



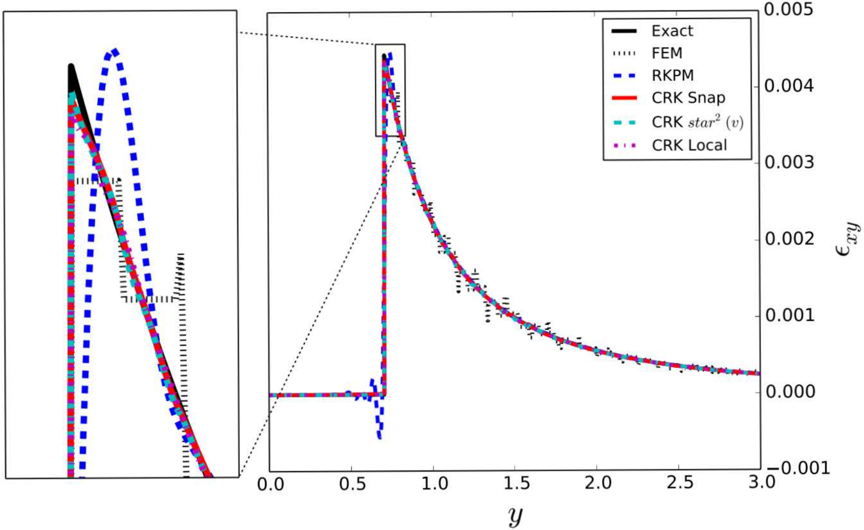


Figure: ε_{xy} near the material interface.

Results Comparison

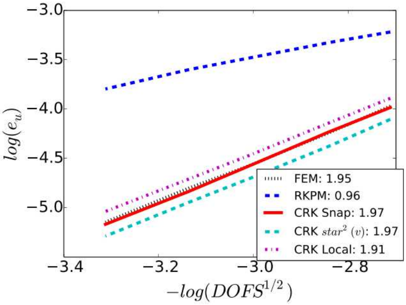


Figure: Convergence in $\mathbf{u}$

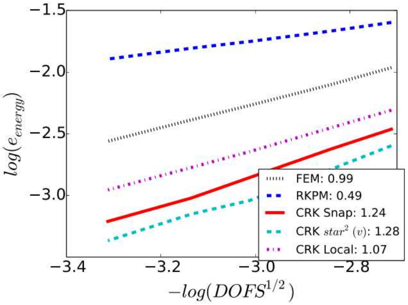


Figure: Convergence in energy

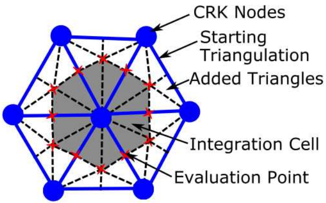
3D Implementation and Examples

Simplification of Conforming Kernel Implementation

Require integration points to be nodal locations (i.e. Hermite interpolation locations) of the kernel function space

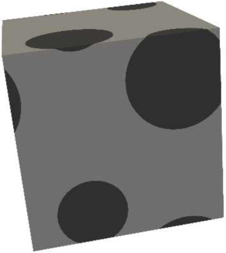
- *No construction of Bernstein-Bézier spaces required.* Values are explicitly set at the integration points, implied elsewhere.
- Pairs well with integration using smoothed gradients[3]

Example for Stabilized Conforming Nodal Integration (SCNI) with boundary edge integration using trapezoid rule.

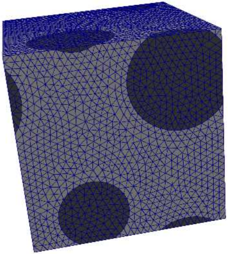


[3] J.-S. Chen, C.-T. Wu, S. Yoon, *et al.*, "A stabilized conforming nodal integration for Galerkin mesh-free methods," *International Journal for Numerical Methods in Engineering*, vol. 50, no. 2, pp. 435–466, 2001.

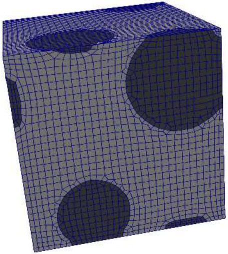
3D Example: Carbon Black Rubber



Domain

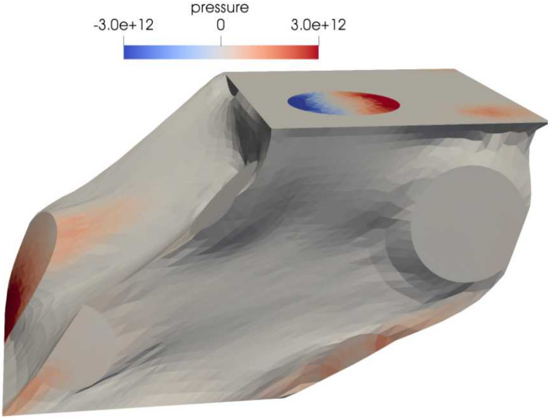


Example Tet Mesh

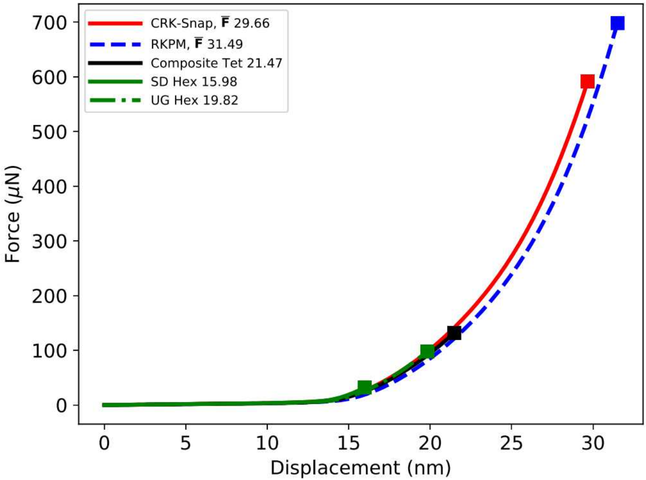


Example Hex Mesh

3D Example: Carbon Black Rubber

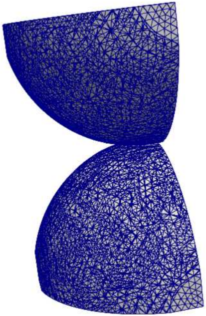


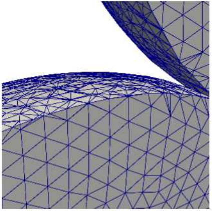
3D Example: Carbon Black Rubber



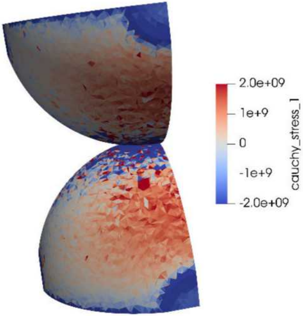
3D Example: CDFEM Spheres

The Conformal Decomposition Finite Element Method (CDFEM)[4] details a robust procedure for generating tetrahedral meshes of complicated geometries but mesh quality is often too low for structural analyses.





Mesh of Two Spheres

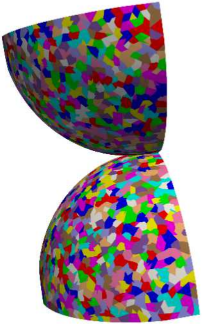


RKPM results

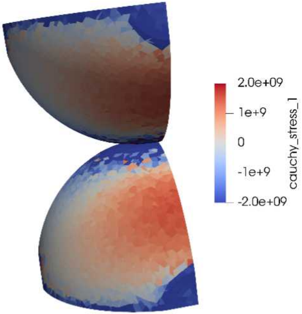
[4] S. A. Roberts, H. Mendoza, V. E. Brunini, *et al.*, "A verified conformal decomposition finite element method for implicit, many-material geometries," *Journal of Computational Physics*, vol. 375, pp. 352–367, 2018.

3D 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.

Agile Design-to-Simulation Framework

Goal: *Improving the Analyst's Response Time*
Approach: *Utilize the flexibility that meshfree methods provide, supply more control where needed*

Conforming window functions to handle boundary / geometry challenges of meshfree methods.

Global triangulation:

- Method to aggregate elements
- Less connection between element and solution quality
- Provides data structure similar to FEM, helps with efficiency

Local triangulations: Handles boundary challenges while maintaining more of the meshfree nature of the methods.

Future Work: Better classification for element aggregation. Extend to handle material separation.