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ASCEND: Asymptotically compatible strong form foundations for nonlocal discretization

Marta D'Elia, David Littlewood, Stewart Silling, Jeremy Trageser, Mike Tupek, Nathaniel Trask (PI)

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185
Livermore, California 94550

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ASCEND: Asymptotically compatible strong form foundations for nonlocal discretization

Nathaniel Trask
Center for Computing Research
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185-9999
natrask@sandia.gov

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ABSTRACT

Nonlocal models naturally handle a range of physics of interest to SNL, but discretization of their underlying integral operators poses mathematical challenges to realize the accuracy and robustness commonplace in discretization of local counterparts. This project focuses on the concept of *asymptotic compatibility*, namely preservation of the limit of the discrete nonlocal model to a corresponding well-understood local solution. We address challenges that have traditionally troubled nonlocal mechanics models primarily related to consistency guarantees and boundary conditions. For simple problems such as diffusion and linear elasticity we have developed complete error analysis theory providing consistency guarantees. We then take these foundational tools to develop new state-of-the-art capabilities for: lithiation-induced failure in batteries, ductile failure of problems driven by contact, blast-on-structure induced failure, brittle/ductile failure of thin structures. We also summarize ongoing efforts using these frameworks in data-driven modeling contexts. This report provides a high-level summary of all publications which followed from these efforts.

ACKNOWLEDGMENT

The efforts of this project have followed from valuable collaborations with academic partners: John Foster's group at University of Texas Austin, Yuri Bazilevs' group at Brown University, and Yue Yu's group at Lehigh University. We also acknolwedge contributions from Xiaochuan Tian, J.S. Chen, and David Kamensky at University of California San Diego. Finally, we acknowledge many advances from this project followed from an earlier LDRD (COMPADRE: Compatible particle discretization) PI'ed by Pavel Bochev.

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SUMMARY

Nonlocal discretizations of local theories of continuum physics opt for a description using integrodifferential equations (IDEs) in place of traditional local operators such as partial differential equations (PDEs). This leads to reduced regularity requirements (e.g. solutions in L^p-spaces as opposed to Sobolev spaces) which is ideal for handling problems involving fracture or interfacial conditions. Such problems are an integral part of many applications of interest to Sandia. In 2000 Stewart Silling reformulated continuum mechanics in this nonlocal setting [31] and the resulting *peridynamic* description of mechanics has subsequently led to over 6000 publications as of this report. Nonlocality has also emerged in the recently booming field of fractional equations [26] as well as classical mesoscale physical processes involving non-local interactions (e.g. Coulombic). We consider nonlocal operators of the form

$$\mathcal{L}_\delta[u](x) = \int_{B(x,\delta)} K(x,y)\,(u(y) \pm u(x))\,dy \tag{1}$$

where $K(x,y)$ is a possibly singular problem dependent kernel and $B(x,\delta)$ is a ball of radius δ, where δ is termed the *horizon* which models the extant of nonlocality.

In this project we focus on nonlocal models which reduce to a corresponding local model $\mathcal{L}$ as δ is reduced to zero, i.e. $\lim_{\delta\to 0} \mathcal{L}_\delta = \mathcal{L}$. For example, in the linear peridynamic solid model [16] one recovers classical linear elasticity as $\delta \to 0$. More recent *correspondence models* are designed to recover classical continuum theories of finite deformation elastoplasticity [32]. For these models, the reduced regularity requirements offered by nonlocal formulations provide an effective regularization of the traditional local theory avoiding the need for enrichment strategies to handle fracture (e.g. [2, 34, 40]).

At a practical level, discretization of the nonlocal theory introduces a discretization lengthscale h, and simulation requires treatment of linear operators $\mathcal{L}_{h,\delta}[u]$. In the setting where the ratio $h/\delta = M > 0$ is fixed during grid refinement (so-called M-convergence [11]), one obtains sparse matrices amenable to efficient and scalable implementation similar to traditional finite element methods. A natural question is in what sense solutions of $\mathcal{L}_{h,\delta}$ converge to those of $\mathcal{L}$ in this limit. Until recently, popular particle-based discretizations of the theory (e.g. [33]) exhibited $O(1)$ errors for complex geometries that precluded convergence. This translates to a challenge regarding proper verification and validation of production codes, as an analyst cannot confirm whether one has achieved an accurate solution as refinement is increased.

Recent work pioneered by Xiaochuan Tian and Qiang Du has shown that for variational discretizations of nonlocal models, one may obtain *asymptotically compatible* (AC) discretizations which preserve this, and several other, important limits by working with sufficiently high order polynomial finite element spaces [35]. While theoretically important, these variational discretization pose challenges for practical engineering application. Discretizing the weak form of nonlocal models requires quadrature for a double integral involving piecewise polynomial functions against possibly singular kernels. The resulting computation leads to costly computation of geometric intersections between spheres and elements [30], and one may obtain approximations which diverge (i.e. errors of $O(1/h)$).

To avoid these computations while preserving robust accuracy, this project pursues the development of strong-form discretizations of the theory while using the generalized moving least squares (GMLS) framework for guaranteeing consistency. GMLS is a technique for estimating general linear operators from local scattered samples, possesses a rigorous mathematical theory [39, 27, 37], and has a performant Trilinos implementation stemming from the previous COMPADRE LDRD [21, 12]. This allows a fast implementation of the schemes developed here, many of which have been implemented in Peridigm (a scalable Trilinos implementation of peridynamics [29]). In the past few years, several other projects have emerged using the reproducing kernel particle method (RKPM) as an alternative means of achieving AC (e.g. [20]). It is well known that traditional RKPM and moving least squares can be shown to be identical, up to the definition of the kernel and we have shown that this is also the case for GMLS/RKPM discretizations of peridynamics [9]. They differ superficially: our AC GMLS quadrature provides an implementation in terms of quadrature weights, while AC RKPM is more naturally described by shape functions, and for a given application we adopt whichever viewpoint is more mathematically convenient.

In this report, we provide a summary of the journal papers which have been developed. The goals of this project are twofold:

1. <u>Mathematical AC foundations:</u> Develop discretizations and boundary condition treatments so that discrete nonlocal models recover local solutions as $\delta \to 0$.
2. <u>Exemplar AC problems:</u> Apply new schemes to a diverse set of application problems spanning elastoplastic dynamics, ductile/brittle fracture, thin shell theories, and fluid-structure interactions, and demonstrate for exemplar problems including the recent Sandia fracture challenge and energy storage systems.

1. MATHEMATICAL FOUNDATIONS

Two major challenges for adoption of nonlocal by non-specialists are:

1. Consistency: Discretizations should rigorously guarantee algebraic truncation error bounds of the form $|\mathcal{L}_{\delta,h}[u]-\mathcal{L}[u]| \leq C\delta^m ||u||$ for suitably defined norms. Practically, this guarantees that for a doubling of resolution, one may obtain a 2^m reduction in error and recover a well-understood local model. We primarily consider GMLS/RKPM quadrature to obtain such results for strong form discretizations.

2. Boundary conditions: Typical engineering problems require imposition of physical quantities as boundary conditions, such as tractions and fluxes for Neumann problems or displacements for Dirichlet problems. Nonlocal methods require non-physical volumetric conditions, and we require nonlocal boundary conditions which enforce physical ones without impacting the AC property. Traditional peridynamic discretization suffer from *surface effects* where improper imposition of non-physical boundary conditions manifest as artificial softening/hardening of material near boundaries [19, 10, 22, 28]. While remedies in literature alter the nonlocal model, we show that proper choice of boundary condition and quadrature are sufficient to avoid this problem.

3. Stability: A rigorous stability analysis is challenging for strong form discretizations lacking a variational principle. We consider a full error analysis for strong-form discretization in a simplified setting, as well as demonstrate preliminary extensions to variational settings.

In what follows, we summarize papers generated in this project which remedy these theoretical deficiencies of nonlocal discretizations. These results will form the foundation for applications in the second half of the report.

1.1. Asymptotically compatible quadrature via GMLS

Trask, Nathaniel, Huaiqian You, Yue Yu, and Michael L. Parks. "An asymptotically compatible meshfree quadrature rule for nonlocal problems with applications to peridynamics." Computer Methods in Applied Mechanics and Engineering 343 (2019): 151-165.

Idea: The quadrature for evaluation of nonlocal operators may be replaced with an optimization problem to obtain quadrature weights guaranteeing consistency. This replaces the geometrically intensive quadrature problem with an algebraic one requiring the local inversion of small matrices at each particle.

Impact: This quadrature idea forms the foundation for the project, and a lightweight software library has been developed to evaluate the quadrature weights. An attractive feature of this is that the traditional quadrature weights used may be replaced with a call to this lightweight library to obtain a set of AC quadrature weights, allowing one to easily update legacy peridynamic codes with minor alteration.

Mathematical contribution: Truncation error analysis establishing algebraic convergence rate of order $m+1-|\alpha|$, where m is order of polynomial reproduction and α is order singularity in

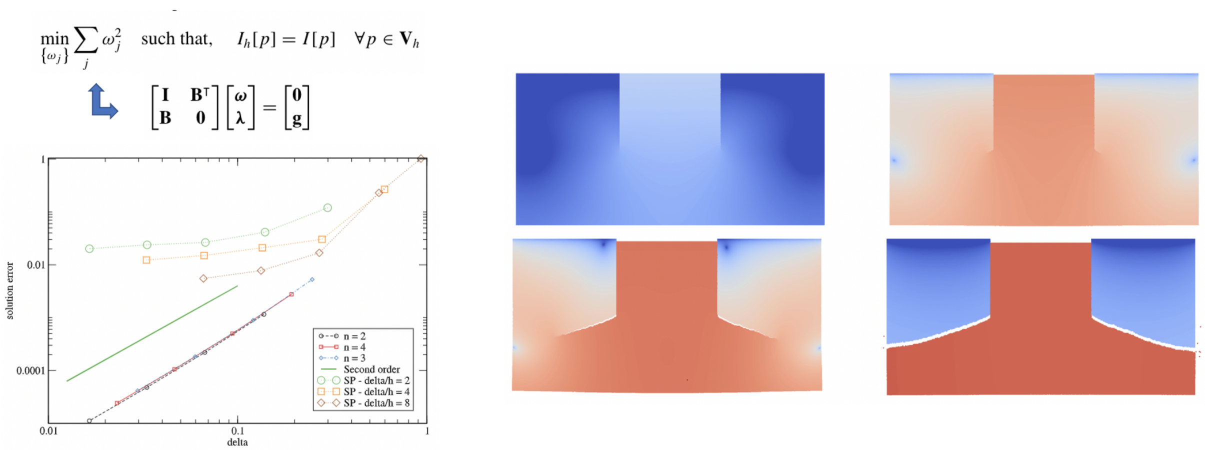


Figure 1-1 Summary of results from [38]. ***Top left:*** **Prohibitively expensive geometric quadrature problem replaced with efficient optimization problem requiring inexpensive linear solves.** ***Bottom left:*** **AC convergence demonstrated, avoiding $O(1)$ errors in typical peridynamics codes.** ***Right:*** **Technique easily incorporated into peridynamic workflows with bond-breaking fracture models to obtain AC treatment of traction-free fracture surfaces.**

nonlocal kernel. Empirical demonstration of AC property, including AC solution for problems with fracture consistent with traction-free condition at fracture surface.

1.2. Asymptotically compatible boundary condition treatment

Yu, Yue, Huaiqian You, and Nathaniel Trask. "An asymptotically compatible treatment of traction loading in linearly elastic peridynamic fracture." Computer Methods in Applied Mechanics and Engineering 377 (2021): 113691.

Idea: An AC nonlocal extension may be defined by performing polynomial extrapolation of the solution normal to the boundary in a manner consistent with the local boundary condition. For fracture mechanics problems, this allows extensions of the AC traction free condition introduced in [38] to treat inhomogeneous traction loading, allowing simulation of pressure-driven fracture.

Impact: Treatment of inhomogeneous traction boundary conditions without introducing "surface effects". First treatment of general engineering boundary conditions which preserves AC property, including for material interfaces and evolving free surfaces generated dynamically during fracture. Extensive comparisons to experiment demonstrate applicability and predictivity of approach to non-trivial engineering problems.

Mathematical contribution: Modified nonlocal dilitation to correct for boundary effect in kinematic constraint. Proof of consistency in both continuous and discrete setting. Proof of well-posedness/invertibility of correction tensor. Proof of patch test for classes of boundaries. Construction of quadrature for linear peridynamic solid model with polynomial reproduction guarantees. Analysis of geometric conditions under which AC fails to hold. Empirical validation of results for analytic solutions with free-surface, pressure loadings, and heterogeneous material properties, along with study of dynamic crack growth for: bifurcating crack in soda glass,

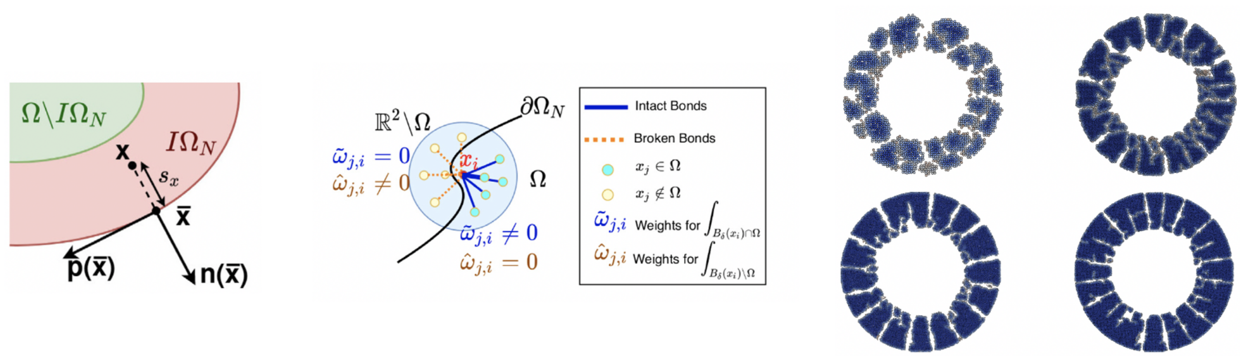


Figure 1-2 Summary of results from [42]. ***Left:*** **Local boundary conditions are used to define an extension operator into nonlocal boundary region. Analysis supports well-posedness and consistency for continuous model.** ***Center:*** **Application of AC quadrature from [38] provides consistent treatment of traction loading for smooth boundaries, and good accuracy near problematic corners.** ***Right:*** **Application to a suite of problems in traction-driven fracture provide predictions consistent with experiment, with AC leading to converged fragments as resolution is increased.**

V-notched glass under impact, and fragmenting cylinder (with experimental comparison where possible).

You, Huaiqian, XinYang Lu, Nathaniel Trask, and Yue Yu. "An asymptotically compatible approach for Neumann-type boundary condition on nonlocal problems." ESAIM: Mathematical Modelling and Numerical Analysis 54, no. 4 (2020): 1373-1413.

Idea: Formal mathematical analysis of extensional boundary condition with numerical verification.

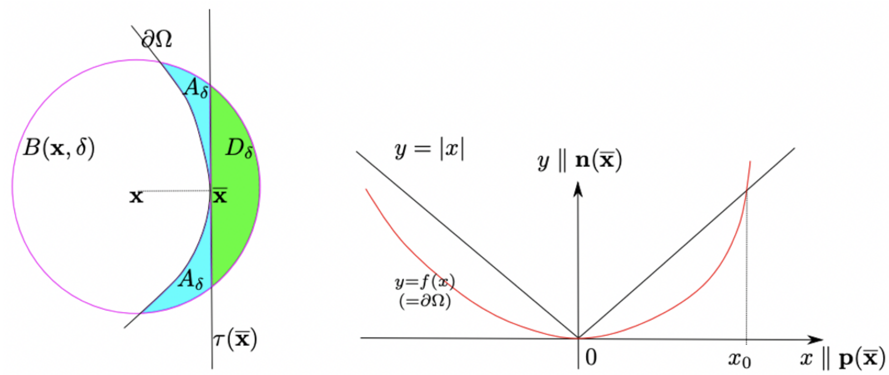
Impact: Establishes rigorous well-posedness results for nonlocal diffusion problem with extensional boundary condition. Theoretical justification for more general application to linear elasticity in [42].

Mathematical contribution: Well-posedness theory. Establishment of asymptotic compatibility in L_2 and L_∞, pointwise convergence rates, and maximum principle under appropriate geometric/regularity restrictions in variational setting. Fundamental embedding, compactness and Poincare inequality results which may be applied more broadly. Empirical study confirming results hold with strong-form discretization.

D'Elia, Marta, Xiaochuan Tian, and Yue Yu. "A physically consistent, flexible, and efficient strategy to convert local boundary conditions into nonlocal volume constraints." SIAM Journal on Scientific Computing 42, no. 4 (2020): A1935-A1949.

M. D'Elia, Y. Yue, On the prescription of boundary conditions for nonlocal Poisson's and peridynamics models, submitted, 2021, arXiv:2107.04450.

Idea: As an alternative to polynomial extension, D'Elia considered another class of extension operators obtained by solving the limiting local PDE in the boundary region. The first [14] considers diffusion problems, while the second [15] considers extensions to linear elasticity.



Theorem 3.10. *Suppose u_δ is the weak solution of (2.5) and u_0 is the weak solution of (2.1), then*

$$\lim_{\delta\to 0} ||u_\delta - u_0||_{L^2(\Omega)} = 0.$$

Lemma 4.1. *For $u \in C(\overline{\Omega}) \cap C(\partial\Omega_{D\delta} \backslash \partial\Omega_D)$ and u bounded on $\partial\Omega_{D\delta}$, assuming that u satisfies $L_\delta u \leq 0$ for all $x \in \Omega\backslash\Omega_{N\delta}$ and $L_{N\delta} u \leq 0$ for all $x \in \Omega_{N\delta}$, we have*

$$\sup_{\mathbf{x}\in\overline{\Omega}\cup\partial\Omega_{D\delta}} u(\mathbf{x}) \leq \sup_{\mathbf{x}\in\partial\Omega_{D\delta}} u(\mathbf{x}). \tag{4.4}$$

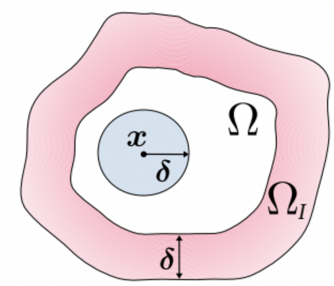
Theorem 4.5. *Suppose $f \in C(\overline{\Omega})$, u_δ solves the nonlocal problem (4.2) and u_0 is the solution to the corresponding local problem (4.3), then for sufficiently small δ there exists a constant C independent of δ such that*

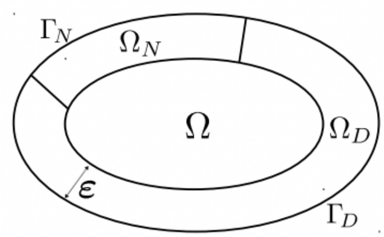
$$\sup_{\mathbf{x}\in\Omega} |u_\delta(\mathbf{x}) - u_0(\mathbf{x})| \leq C\delta^2. \tag{4.22}$$

h	$\delta/h = 4$				$\delta/h = 3.5$			
	$\|\|u_\delta - u_0\|\|_\infty$	order	$\|\|u_\delta - u_0\|\|_2$	order	$\|\|u_\delta - u_0\|\|_\infty$	order	$\|\|u_\delta - u_0\|\|_2$	order
2^{-3}	7.43×10^{-2}	–	1.91×10^{-2}	–	5.45×10^{-2}	–	1.46×10^{-2}	–
2^{-4}	1.52×10^{-2}	2.29	4.01×10^{-3}	2.26	1.13×10^{-2}	2.27	3.10×10^{-3}	2.24
2^{-5}	3.30×10^{-3}	2.20	9.12×10^{-4}	2.13	2.40×10^{-3}	2.24	6.97×10^{-4}	2.15
2^{-6}	7.42×10^{-3}	2.15	2.17×10^{-4}	2.06	5.60×10^{-4}	2.11	1.66×10^{-4}	2.07
2^{-7}	1.74×10^{-4}	2.09	5.32×10^{-5}	2.03	1.31×10^{-4}	2.09	4.04×10^{-5}	2.03

Table 5: Convergence to the local solution in the case with corner.

Figure 1-3 Summary of results from [42]. ***Top:*** **Analysis of extensional boundary condition on nonlocal boundary region is performed by bounding error in terms of δ.** ***Middle:*** **Analysis results establishing: asymptotic compatibility in L_2, a maximum principle supporting extensions to L_∞, and pointwise convergence estimates establishing 2^{nd}-order convergence with respect to δ confirmed by numerical experiment (*Bottom*).**





$$
\begin{cases}
-\Delta u_l = s, & \boldsymbol{x} \in \Omega, \\
-\nabla u_l \cdot \mathbf{n} = g_l, & \boldsymbol{x} \in \Gamma_N, \\
u_l = v_n, & \boldsymbol{x} \in \Gamma_D,
\end{cases}
$$

THEOREM 4.1. *Let* $\varepsilon_0 \in (0,\infty)$, *and let* $\mathcal{U}_l := \{u_l \in C^4(\overline{\Omega}) : u_l$ *solves* (3.3) *for* $\varepsilon \in (0,\varepsilon_0]\}$ *be a family of solutions of* (3.5). *Then, for all* $u_l \in \mathcal{U}_l$,

$$
e_E \leq C\varepsilon^2 \|D^{(4)} u_l\|_{\infty,\overline{\Omega}}\,, \tag{4.2}
$$

where C *is a positive constant independent of* ε *and* u_l, *and* $D^{(4)}$ *indicates the fourth derivative operator.*

Neumann approach: energy and L^2 *norm of the difference between local and discretized nonlocal solutions for* $h = 2^{-12}$ *and decreasing values of* ε.

ε	$e_{E,h}$	Rate	$e_{0,h}$	Rate
2^{-2}	9.99e-02	-	7.50e-02	-
2^{-3}	2.29e-02	2.12	1.55e-02	2.27
2^{-4}	5.48e-03	2.06	3.50e-03	2.15
2^{-5}	1.34e-03	2.03	8.28e-04	2.08

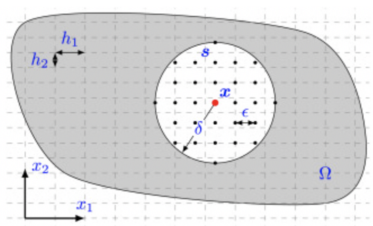
Figure 1-4 Summary of results from [14, 15].

Impact: A complete theory of boundary conditions providing AC with few geometric restrictions, and which generalizes naturally to different PDEs.
Mathematical contribution:

1.3. Complete error analysis for AC strong form discretizations

Leng, Yu, Xiaochuan Tian, Nathaniel Trask, and John T. Foster. "Asymptotically compatible reproducing kernel collocation and meshfree integration for nonlocal diffusion." SIAM Journal on Numerical Analysis 59, no. 1 (2021): 88-118.

Leng, Yu, Xiaochuan Tian, Nathaniel A. Trask, and John T. Foster. "Asymptotically compatible reproducing kernel collocation and meshfree integration for the peridynamic Navier equation." Computer Methods in Applied Mechanics and Engineering 370 (2020): 113264



Theorem 4.10 Asymptotic Compatibility

Assume the local exact solution $\boldsymbol{u}^0$ is sufficiently smooth, i.e., $\boldsymbol{u}^0 \in C^4\left(\overline{\Omega_{2\delta}}; \mathbb{R}^{\mathrm{d}}\right)$. For any $\delta \in (0, \delta_0]$, $\boldsymbol{u}^{\delta,h}$ is the numerical solution of the collocation scheme Eq. (28), *then,*

$$\|\boldsymbol{u}^0 - \boldsymbol{u}^{\delta,h}\|_{L^2(\Omega;\mathbb{R}^{\mathrm{d}})} \leq C\left(h_{\max}^2 + \delta^2\right).$$

Figure 1-5 Summary of results from [25, 24]. ***Left:*** **Assuming a Cartesian nodal layout allows one to work with a Fourier interpolant, allowing a dual interpretation of the strong-form scheme in terms of a variational one.** ***Right:*** **Analysis allows a complete error analysis establishing asymptotic compatibility.**

Idea: This academic alliance funded aspect of the project establishes AC convergence of the strong-form discretized scheme for diffusion [24] and linear elasticity [25]. For collocation, this requires assumptions of continuity and Cartesian particle grids to work with Fourier series interpolants which may be used to recast collocation scheme as a Galerkin one.
Impact: First rigorous analysis of strong-form AC discretizations of nonlocal mechanics problems amenable to large scale implementation, unlike traditional AC variational method which guarantee convergence but are prohibitively expensive and generally implemented in only one-dimensional toy problems.
Mathematical contribution: Coercivity of an energy norm over L_2 (Thm. 2.1). Discrete coercivity by linking collocation scheme with Galerkin via Fourier analysis (Thm. 4.1). Positive-definiteness of Fourier symbol of peridynamic operator (Lemmas 4.2,4.3). Convergence to nonlocal solution (Thm. 4.8) and local solution (i.e. asymptotic compatibility) (Thm 4.10,5.6). Empirical confirmation of analysis.

1.4. Efficient asymptotically compatible variational principles

(In preparation:) *Pasetto, Marco, Kamensky, David, Tian, Xiaochuan, D'Elia, Marta, Trask, Nathaniel* "Efficient optimization-based inexact quadrature for variational discretization of nonlocal problems" In unpublished work together with Pasetto and Kamensky at UCSD, we have extended the optimization based quadrature to treat variational problems. For the bilinear form associated with the diffusion problem

$$a(u,v) = \int_{\Omega'} \int_{\Omega'} K(x,y)\,(u(y) - u(x))\,(v(y) - v(x))\,dydx, \tag{2}$$

we consider discrete quadrature of the form

$$a_h(u,v) = \sum_{e \in \mathcal{T}} \sum_{i \in \mathcal{X}_1} \sum_{j \in \mathcal{X}_2} K(x_i, x_j)\left(u(x_j) - u(x_i)\right)\left(v(x_j) - v(x_i)\right)\omega_{j,i}\omega_i \tag{3}$$

where $\mathcal{T}$ is a potentially unstructured polygonal mesh and $\mathcal{X}$ is a set of nodes. The scalar quantities ω_i and $\omega_{j,i}$ are quadrature weights for the outer and inner integrals of $a(u,v)$, respectively. The challenge in deriving exact quadrature for this problem is that one must perform costly geometric intersections between $supp(K)$ and the elements $e \in \mathcal{T}$. However, if one only aims to enforce exact integration of global polynomials then a tractable local optimization problem is obtained similar to our previous work with strong form discretizations. This work demonstrates the feasibility and accuracy of this approach for simple diffusion problems and will be submitted for review in the coming fiscal year.

Impact: The use of the optimization-based quadrature rule for the computation of the inner integral in Eq.(2) allows an efficient $O(N)$ construction of the stiffness matrix for variational problems, allowing implementation in non-academic production codes.
Mathematical contribution: We prove, in the simplified case of one-dimensional domain and delta=h, that our integration approach converges linearly when used in conjunction with a C0 linear finite element approximation. We demonstrate empirically second order convergence in two-dimensions (See Figure 1-6).

2. APPLICATION PROBLEMS

In the remainder of this report, we demonstrate how these mathematical advances may be used to develop new schemes for multiphysics problems which provide accuracy while maintaining a scalable implementation. For example, problems in fluid-structure interaction require treatment of interface coupling between fluid and solid models which our boundary condition framework may treat appropriately. For these problems, due to the physical complexity of incorporating nonlinear constitutive models, fracture, and multiphysics, we focus on empirically demonstrating convergence with respect to reference analytic solutions and experiment, rather than developing formal mathematical theory.

2.1. AC strong form discretizations of elastoplastic correspondence models

Behzadinasab, Masoud, Nathaniel Trask, and Yuri Bazilevs. "A Unified, Stable and Accurate Meshfree Framework for Peridynamic Correspondence Modeling—Part I: Core Methods." Journal of Peridynamics and Nonlocal Modeling 3.1 (2021): 24-45.

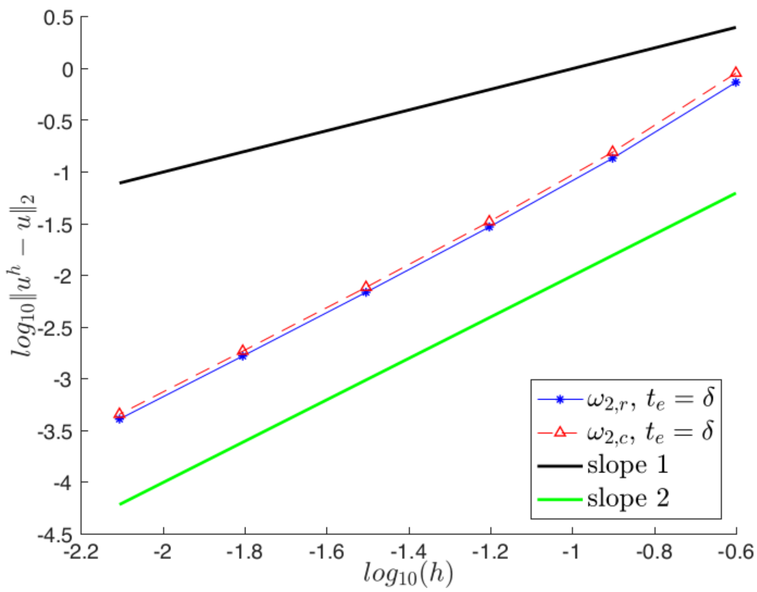


Figure 1-6 Summary of results from unpublished work on variational schemes. Convergence behavior for a manufactured 2D sinusoidal solution on uniform quadrilateral discretizations on a unit square. A 4x4 Gauss quadrature is employed for the outer integration, while 64 GMLS quadrature points were placed symmetrically within the integration ball for the inner integration. The ratio between delta and element size was taken equal to 2. For $K(x,y)$ both constant and singular kernels were considered.

Behzadinasab, M., Foster, J.T. and Bazilevs, Y., 2020. A unified, stable and accurate meshfree framework for peridynamic correspondence modeling. Part II: wave propagation and enforcement of stress boundary conditions. arXiv e-prints, pp.arXiv-2004.

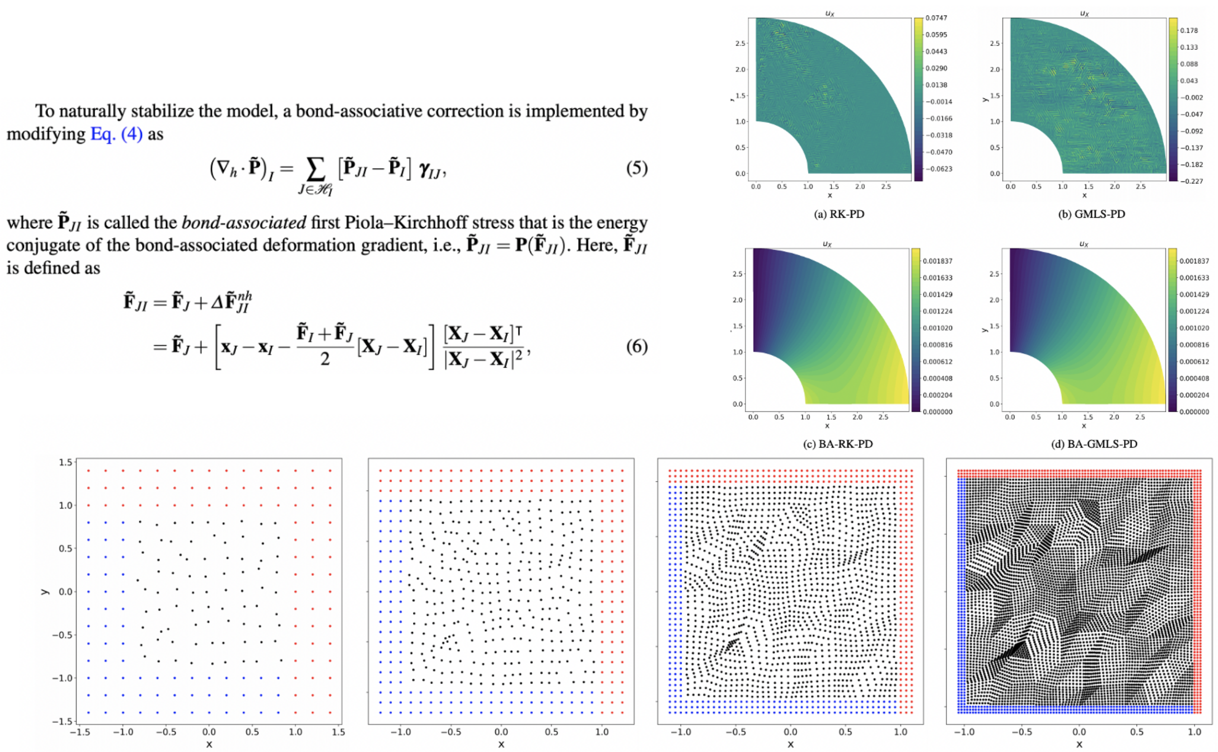
Idea: Peridynamic correspondence models are ideal for large deformation elastoplasticity, as they allow use of classical stress/strain closures. Naive application of AC quadrature to these problems however leads to an unstable scheme, and we introduce the *bond-associative* stabilization proposed in [6, 5] to achieve a scheme that is both stable and convergent.

Impact: While the analysis performed to this point in the project is focused on easily analyzed small-deformation linear theory, this provides the foundation for considering realistic large deformation problems. The scheme developed here serves as the foundation for further developments below to: shell theory, blast-on-structure FSI, and our submission to the Sandia fracture challenge.

2.2. Asymptotically compatible Kirchhoff-Love shell for brittle/ductile failure of thin structures

Behzadinasab, M., Alaydin, M., Trask, N. and Bazilevs, Y., 2021. A general-purpose, inelastic, rotation-free Kirchhoff-Love shell formulation for peridynamics. arXiv preprint arXiv:2107.13062.

Idea: We can take the correspondence models and use our previous work using GMLS for surface PDEs [36, 18] to formulate correspondence models for a recent Kirchoff-Love shell developed by



To naturally stabilize the model, a bond-associative correction is implemented by modifying Eq. (4) as

$$(\nabla_h \cdot \tilde{\mathbf{P}})_I = \sum_{J \in \mathscr{H}_I} \left[\tilde{\mathbf{P}}_{JI} - \tilde{\mathbf{P}}_I\right] \boldsymbol{\gamma}_{IJ}, \tag{5}$$

where $\tilde{\mathbf{P}}_{JI}$ is called the *bond-associated* first Piola–Kirchhoff stress that is the energy conjugate of the bond-associated deformation gradient, i.e., $\tilde{\mathbf{P}}_{JI} = \mathbf{P}(\tilde{\mathbf{F}}_{JI})$. Here, $\tilde{\mathbf{F}}_{JI}$ is defined as

$$\begin{aligned}\tilde{\mathbf{F}}_{JI} &= \tilde{\mathbf{F}}_J + \Delta\tilde{\mathbf{F}}^{nh}_{JI} \\ &= \tilde{\mathbf{F}}_J + \left[\mathbf{x}_J - \mathbf{x}_I - \frac{\tilde{\mathbf{F}}_I + \tilde{\mathbf{F}}_J}{2}[\mathbf{X}_J - \mathbf{X}_I]\right] \frac{[\mathbf{X}_J - \mathbf{X}_I]^{\intercal}}{|\mathbf{X}_J - \mathbf{X}_I|^2},\end{aligned} \tag{6}$$

Figure 2-1 Summary of results from [9, 7]. ***Top left:*** **To stabilize correspondence models to zero-energy modes, we require a** ***bond-associative*** **correspondence model [6, 5].** ***Top right:*** **Application of AC quadrature alone to classical correspondence models yields an unstable result, and we require both the bond-associative stabilization and AC quadrature to achieve a convergent result.** ***Bottom:*** **These results hold for severely deformed meshes as well, making this scheme an ideal candidate for large-deformation problems.**

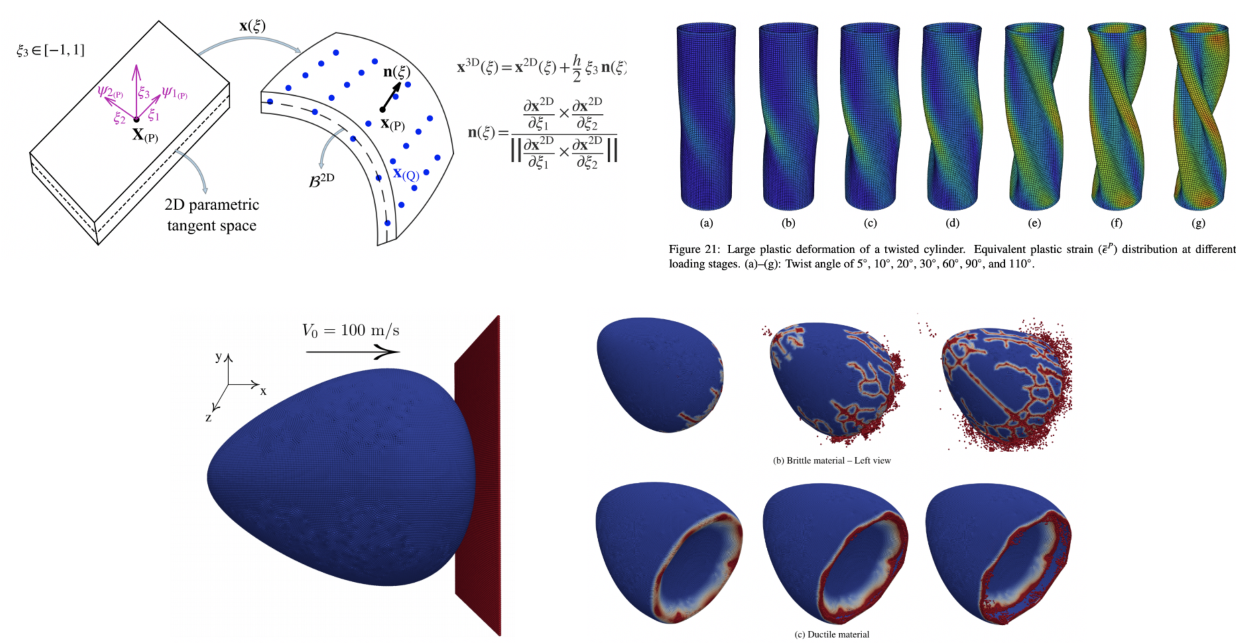


Figure 2-2 Summary of results from [4]. ***Top left:*** **Estimator from our previous work for metric tensor [36, 18] admits simplification for shell dynamics, as mapping between surface and tangent space may be naturally handled by posing reference configuration in tangent space estimated with PCA.** ***Top right:*** **Stabilized correspondence modeling developed in [9, 7] serves as foundation for large deformation elastoplasticity with accuracy comparable to isogeometric finite elements (IGA).** ***Bottom:*** **Unlike IGA, the peridynamic framework allows a simple treatment of fracture, and we demonstrate both brittle and ductile models for several benchmarks.**

Bazilevs [1]. The bond-associative stabilization and AC quadrature translate a bridge between the accuracy offered by methods like IGA and the fracture modeling of peridynamics.
Impact: This is a major step for extending peridynamic shells to a robust and accurate method for thin structures. While some works have developed peridynamic models for shells, this is the first grounded in differential geometry and providing an AC limit. Fracture of thin structures is an important problem with broad implications and this work marks a major development for developing peridynamics into a reliable design tool.

2.3. Asymptotically compatible blast-on-structure FSI

Behzadinasab, M., Moutsanidis, G., Trask, N., Foster, J.T. and Bazilevs, Y., 2021. Coupling of IGA and Peridynamics for Air-Blast Fluid-Structure Interaction Using an Immersed Approach. arXiv preprint arXiv:2108.11265.

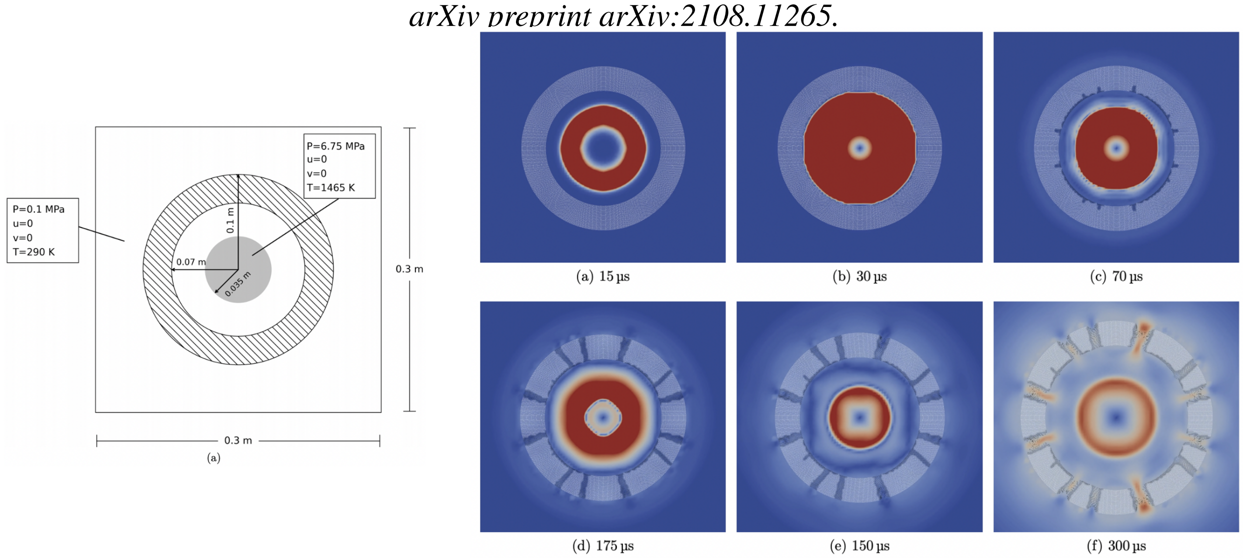


Figure 2-3 Summary of results from [8]. Incorporation of AC bond-associative correspondence models into an immersogeometric scheme for FSI allows simulation of blast-on-structure loading. Shown here a shock detonates within a cylinder, leading to fragmentation.

Idea: Bazilevs has previously used an immersogeometric framework to couple local RKPM structure models to an IGA model of compressible flow [3], and we extend this to allow a peridynamic respresentation of the solid phase. This application builds upon advances in nonlocal boundary conditions made earlier in the project to ensure proper coupling.
Impact: While peridynamics has been used recently for fluid structure interaction (e.g. [13, 17], this marks the first application of AC discretizations. Here, AC translates to a highly accurate prediction as verified by comparison to IGA. The ability to reliably performed blast-on-structure loading maps onto many important problems at SNL.)

2.4. Machine learning of nonlocal operators

You, Huaiqian, Yue Yu, Nathaniel Trask, Mamikon Gulian, and Marta D'Elia. "Data-driven learning of nonlocal physics from high-fidelity synthetic data." Computer Methods in Applied Mechanics and Engineering 374 (2021): 113553.

H. You, Y. Yu, S. Silling, M. D'Elia, Data-driven learning of nonlocal models: from high-fidelity simulations to constitutive laws, accepted in AAAI Spring Symposium: MLPS, 2021, arXiv:2012.04157.

Idea: One may fit a nonlocal model to data by parameterizing a nonlocal kernel and performing optimization to find kernel which will generate a governing equation consistent with data. As shown in [41], well-posedness theory for sign changing kernels can be used to constrain fit to models guaranteed to be solvable.

Impact: While this LDRD predominantly adopts the viewpoint of pursuing nonlocal models as a regularizer of local ones, nonlocal models are well-known to emerge when treating both homogenized multiscale systems and systems with long-range interactions. In these settings, $\delta > 0$ and the AC limit is not taken. Typically such nonlocal models have a kernel assumed arbitrarily and their use is justified a posteriori by showing agreement with data. The purpose of this line of research is to show that nonlocality may emerge naturally from data if a machine learning model is offered the choice between local and nonlocal models.

2.5. Peridynamic failure kinetics

Silling, Stewart A. "Kinetics of Failure in an Elastic Peridynamic Material." Journal of Peridynamics and Nonlocal Modeling 3 (2021): 1-23.

Idea: We discovered that nonlocality over space in continuum mechanics results in different notions of material instability from the local theory. In particular, a peridynamic material model that has a downward-sloping branch (Figure 2-4) is unstable, but unstable waveforms grow at a bounded rate over time. This is in contrast to the local theory, in which instability grows at an unbounded rate.

Impact: This discovery provides a new way to model material failure making use of unstable material models. For example, a bar undergoing tensile strain at an initially constant rate, develops a crack at a finite rate over time, resulting in an apparent rate effect on the material strength (Figure 2-4).

2.6. Macroscopic uses of dispersion

Silling, Stewart A. "Propagation of a Stress Pulse in a Heterogeneous Elastic Bar." Journal of Peridynamics and Nonlocal Modeling (2021), accepted.

Idea: Nonlocality in peridynamics results in dispersion of stress waves (wave velocity is dependent on the wavelength). We applied this feature of the theory to predict the attenuation (decay) of a stress pulse due to impact on a heterogeneous medium. The theory, with a material

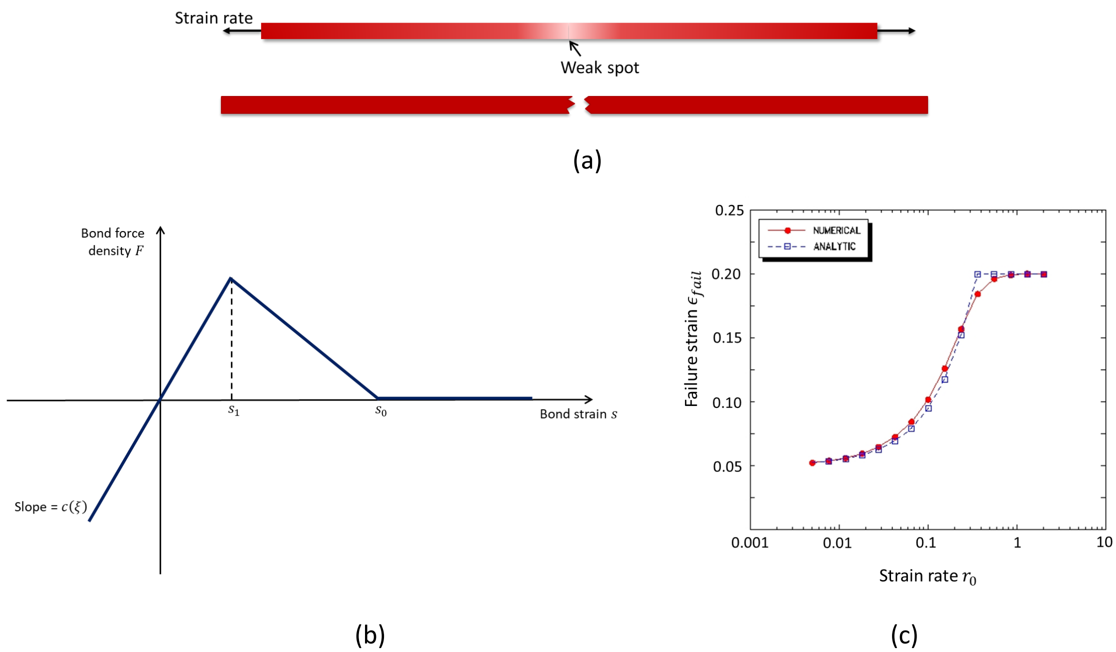
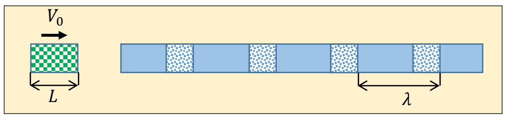


Figure 2-4 Rate effect on material strength with an unstable material model. (a): Bar undergoing an initially constant rate of strain. (b): Material model for bond response containing an unstable branch. (c): Apparent failure strain in the bar as a function of the initial strain rate.



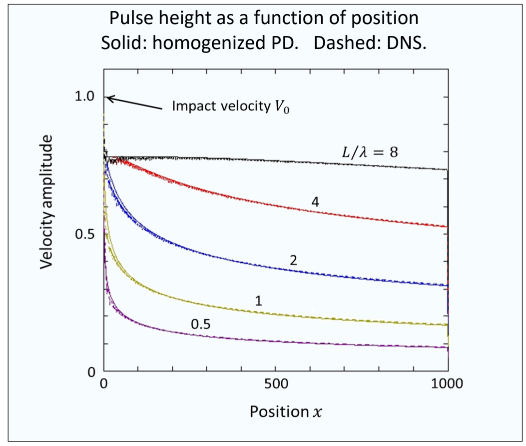


Figure 2-5 Attenuation of a stress pulse due to impact on a heterogeneous medium. Left: Impact of a projectile on an elastic bar with microstructure. Right: Amplitude of the stress pulse decays as it propagates. The peridynamic model accurately reproduces the results of direct numerical simulation (DNS).

model that is designed to create the appropriate dispersion characteristics, allows a nonlocal *homogeneous* medium to reproduce the response of a local *heterogeneous* material (Figure 2-5). **Impact:** The propagation and attenuation of stress waves in heterogeneous media is a problem of fundamental importance in the replacement of conventional materials by additively manufactured materials. The new method provides a way to analyze this problem without the introduction of dissipative terms in a mathematical model, which was the previous state of the art.

2.7. Coarse graining molecular dynamics

Silling, Stewart A., Marta D'Elia, Yue Yu, Huaiqian You, and Muge Fermen-Coker, "Peridynamic Model for Single-Layer Graphene Obtained from Coarse Grained Bond Forces." (2021), submitted.

Idea: Deriving a continuum model or a model with a reduced number of degrees of freedom from molecular dynamics (MD) is a problem that has attracted much effort. In our work, we develop a new approach that takes advantage of the nonlocal nature of both MD and peridynamics. By starting with a definition of the peridynamic degrees of freedom as the spatial average of MD displacements, the evolution equation for the new DOFs is rigorously shown to be the nonlocal peridynamic equation of motion (Figure 2-6). Furthermore, the averaging procedure produces the peridynamic bond forces that appear in the equation of motion. These are used to calibrate a peridynamic continuum material model.

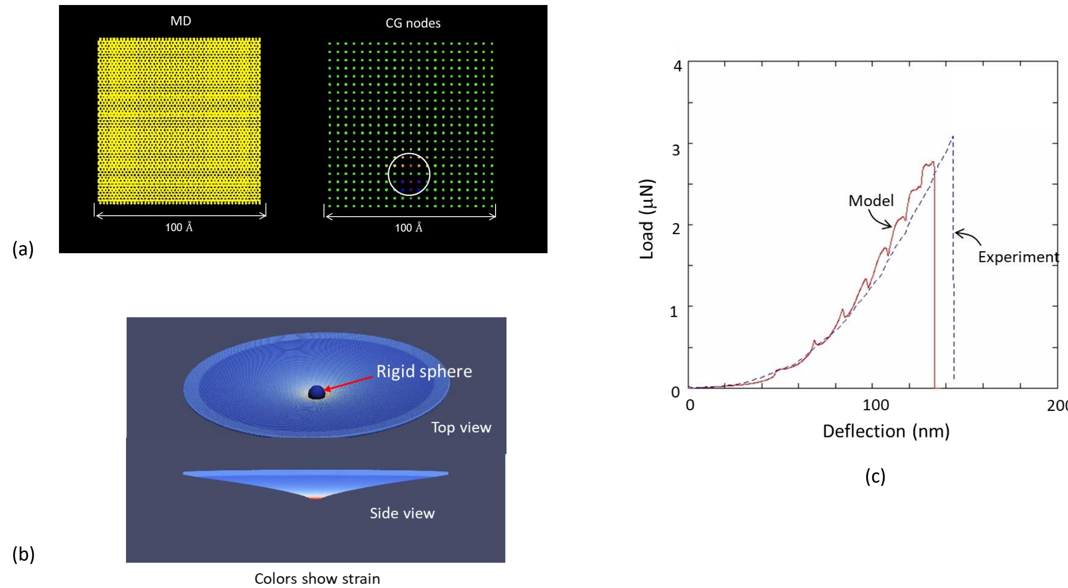


Figure 2-6 Coarse graining of MD into peridynamics. (a): MD mesh for graphene and coarse grained nodes. (b): Peridynamic continuum membrane model for deflection by a nanoscale probe. (c): Comparison of model results for probe force vs. deflection with experimental data [23].

Impact: We demonstrated that a material model derived with this method produces a practical simulation method for length scales much greater than the MD length scale. For example, the method accurately reproduces the deformation and rupture of graphene sheets by an atomic force microscope probe.

2.8. Nonlocality in mixtures and porous media

Song, Xiaoyu, and Stewart A. Silling. "On the peridynamic effective force state and multiphase constitutive correspondence principle." Journal of the Mechanics and Physics of Solids 145 (2020): 104161.

Idea: Nonlocality in a continuum model can help to incorporate the small length scales present in mixtures. In this work, a peridynamic modeling approach was developed to represent the behavior of multiphase media in which the constituent materials can have different velocities and displacements. The method helps to reproduce features of localization that occur in nonlinear poroelastic media (Figure 2-7). It can be applied to the coupling between fluid pressure and fracture in saturated or unsaturated porous media.

Impact: The method is applicable to geological media in which a fluid phase affects the response of a solid phase, possibly leading to mechanical failure. Applications include geological sequestration of carbon dioxide, nuclear waste safety, and the aging of structural materials such as concrete.

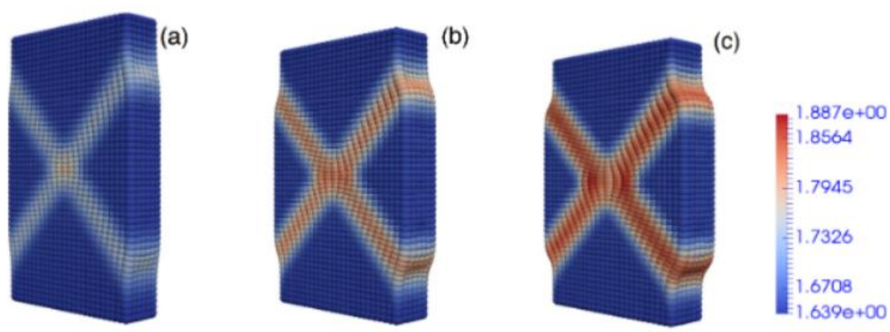


Figure 2-7 Formation of a shear band predicted by an elastic-plastic peridynamic model for multiphase medium (solid and fluid). The bar is compressed from the top and bottom at strains of (a) 0.03, (b) 0.0525, and (c) 0.075. Colors indicate specific volume.

3. CONCLUSION

This report has provided a high-level summary of the major results and papers which followed from the ASCEND LDRD project. The unifying premise of this project is that the continuum theory of nonlocal mechanics is overall sound, but the mathematical theory underpinning discretization has lagged behind. The mathematical develops and consequently enabled application work marks major advances over the current state of the art for these classes of models.

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