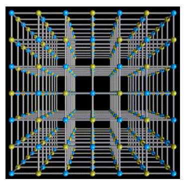
Numerical Analysis of Fracture Evolution Using Nonlocal Models



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Joint work with

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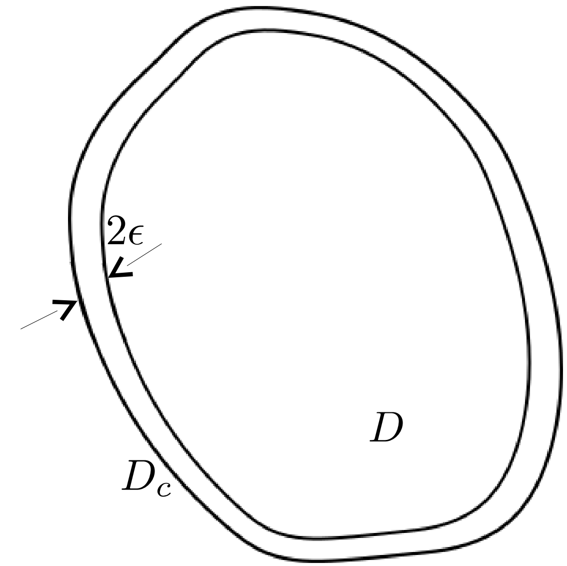
*Figure : http://www.themolecularuniverse.com/mile/mile1.htm

Peridynamics model with bond-based potential [1]

Peridynamics equation: $\rho\ddot{\mathbf{u}}(\mathbf{x},t) = -\nabla PD^{\epsilon}(\mathbf{u}(t))(\mathbf{x}) + \mathbf{b}(\mathbf{x},t)$

Strain: Linearized strain (assuming small displacement)

$$\mathrm{S}(\mathbf{y},\mathbf{x};\mathbf{u}) = \frac{\mathbf{u}(\mathbf{y})-\mathbf{u}(\mathbf{x})}{|\mathbf{y}-\mathbf{x}|}\cdot\frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}$$



Peridynamics force:

$$-\nabla PD^{\epsilon}(\mathbf{u})(\mathbf{x}) = \frac{2}{|B_\epsilon(\mathbf{0})|}\int_{B_\epsilon(\mathbf{x})}\frac{J^\epsilon(|\mathbf{y}-\mathbf{x}|)}{\epsilon|\mathbf{y}-\mathbf{x}|}\partial_S f(|\mathbf{y}-\mathbf{x}|S^2)\frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}d\mathbf{y}$$

Linear peridynamics force: $\mathsf{f}(\mathsf{r}) = \mathsf{f}'(0)\mathsf{r}$ implies $\partial_{\mathsf{S}}\mathsf{f}(|\mathbf{y}-\mathbf{x}|\mathsf{S}^2) = 2|\mathbf{y}-\mathbf{x}|\mathsf{S}\mathsf{f}'(0)$

$$-\nabla PD^{\epsilon}_l(\mathbf{u})(\mathbf{x}) = \frac{2}{|B_\epsilon(\mathbf{0})|}\int_{B_\epsilon(\mathbf{x})}\frac{J^\epsilon(|\mathbf{y}-\mathbf{x}|)}{\epsilon|\mathbf{y}-\mathbf{x}|}\left(2Sf'(0)|\mathbf{y}-\mathbf{x}|\right)\frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}d\mathbf{y}$$

Elastic constants: The limiting equation, excluding cracking zone, is elastodynamics

$$\lambda = \mu = \tfrac{1}{4}\mathsf{f}'(0)\int_0^1 \mathsf{r}^2\mathsf{J}(\mathsf{r})d\mathsf{r},\ \mathcal{G}_c = \tfrac{2}{\pi}\mathsf{f}_\infty\int_0^1 \mathsf{r}^2\mathsf{J}(\mathsf{r})d\mathsf{r}$$

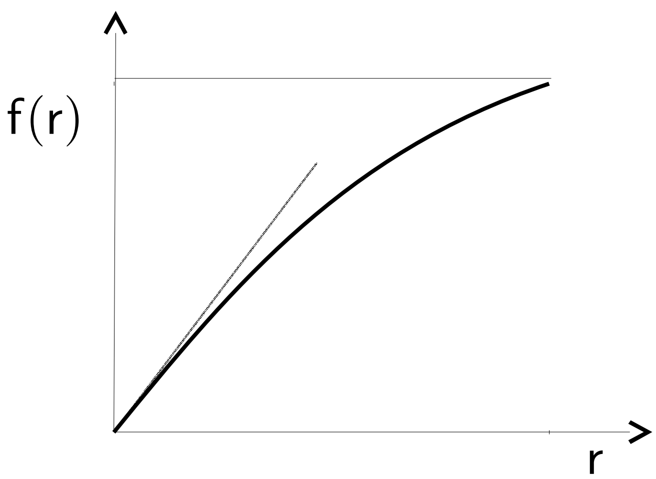
Influence function: Let $\mathsf{J}:[0,1]\to\mathbb{R}^+$ be bounded. For given ϵ

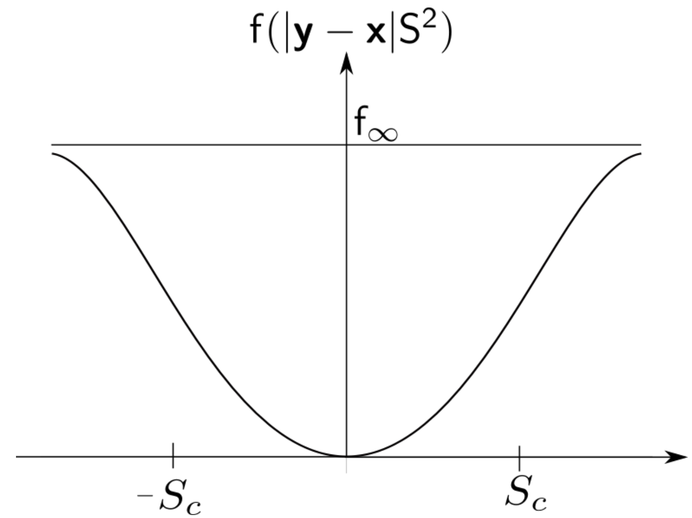
$$\mathsf{J}^\epsilon(|\mathbf{x}|) = \mathsf{J}(|\mathbf{x}|/\epsilon), \mathbf{x}\in \mathsf{B}_\epsilon(\mathbf{0})$$

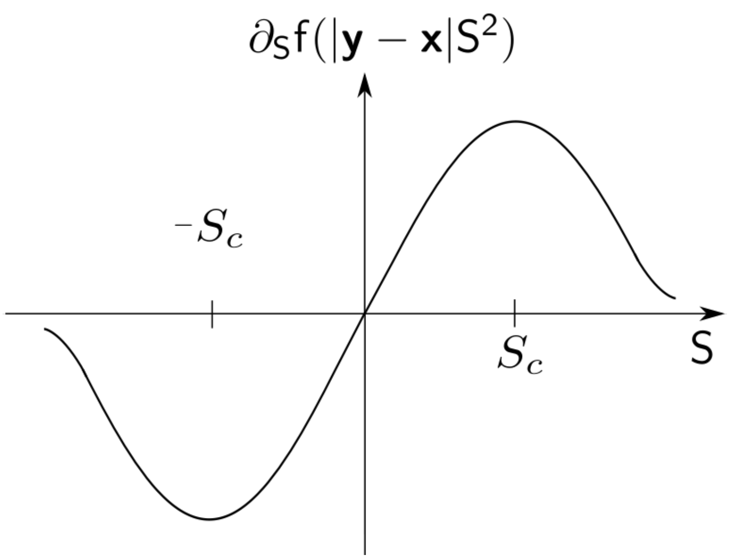
[1] Robert Lipton (2014) Dynamic brittle fracture as a small horizon limit of peridynamics Journal of Elasticity 117 no. 1 2150

Potential and peridynamics force

f: smooth, bounded far away, and linear near origin (**Lipton 2014**[1])







- Critical strain: $S_c(\mathbf{y},\mathbf{x}) = \frac{\bar{r}}{\sqrt{|\mathbf{y}-\mathbf{x}|}}$
- Weak form:

$$(\rho\ddot{\mathbf{u}}(t),\tilde{\mathbf{u}}) + a^\epsilon(\mathbf{u}(t),\tilde{\mathbf{u}}) = (\mathbf{b}(t),\tilde{\mathbf{u}}) \quad \forall \tilde{\mathbf{u}} \in L^2$$

- If strain of sufficient bonds exceed S_c, coercivity of a^ϵ is lost

[1] Robert Lipton (2014) Dynamic brittle fracture as a small horizon limit of peridynamics Journal of Elasticity 117 no. 1 2150

Existence of solution

- In **Lipton 2014**[1] existence of solution in $C^2([0,T]; L^2(D,\mathbb{R}^d))$ is shown provided initial conditions are in $L^2(D,\mathbb{R}^d)$ and body force $\mathbf{b} \in C^1([0,T]; L^2(D,\mathbb{R}^d))$.

Proof follows once we show that peridynamic force is Lipschitz continuous in $L^2(D,\mathbb{R}^3)$, i.e. $\exists$ constant $L > 0$ independent of $\mathbf{u}, \mathbf{v} \in L^d(D,\mathbb{R}^3)$ such that

$$||-\nabla PD^\epsilon(\mathbf{u}) - (-\nabla PD^\epsilon(\mathbf{v}))||_{L^2} \leq \frac{L}{\epsilon^2}||\mathbf{u}-\mathbf{v}||_{L^2}$$

- Existence of solution in Hölder space is shown in **Jha and Lipton 2017**[2].

Let $\gamma \in (0,1]$ and Hölder norm given by

$$||\mathbf{u}||_{C^{0,\gamma}} := \sup_{\mathbf{x}\in D}|\mathbf{u}(\mathbf{x})| + \sup_{\mathbf{x},\mathbf{y}\in D, \mathbf{x}\neq\mathbf{y}} \frac{|\mathbf{u}(\mathbf{x})-\mathbf{u}(\mathbf{y})|}{|\mathbf{x}-\mathbf{y}|}]$$

$C^{0,\gamma}$ is space of functions which have bounded Hölder norm.

$$||-\nabla PD^\epsilon(\mathbf{u}) - (-\nabla PD^\epsilon(\mathbf{v}))||_{C^{0,\gamma}} \leq \frac{L_1 + L_2(||\mathbf{u}||_{C^{0,\gamma}} + ||\mathbf{v}||_{C^{0,\gamma}})}{\epsilon^2}||\mathbf{u}-\mathbf{v}||_{C^{0,\gamma}}$$

[1] Robert Lipton (2014) Dynamic brittle fracture as a small horizon limit of peridynamics Journal of Elasticity 117 no. 1 2150

[2] Prashant K Jha and Robert Lipton (2017) Numerical analysis of nonlocal fracture models in H\"{o}lder space. arXiv preprint arXiv:1701.02818

Existence of solution

Outline of proof is as follows

1. Lipschitz continuity in Hölder space

$$||-\nabla PD^\epsilon(\mathbf{u}) - (-\nabla PD^\epsilon(\mathbf{v}))||_{C^{0,\gamma}} \leq \frac{L_1 + L_2(||\mathbf{u}||_{C^{0,\gamma}} + ||\mathbf{v}||_{C^{0,\gamma}})}{\epsilon^2} ||\mathbf{u} - \mathbf{v}||_{C^{0,\gamma}}$$

2. Local existence of fixed point $\mathsf{y}(\mathsf{t}) = \mathsf{S}(\mathsf{y}(\mathsf{t}))$ where

$$S(y(t)) = x_0 + \int_0^t F^\epsilon(y(\tau), \tau) d\tau, \qquad x_0 = (\mathbf{u}_0, \mathbf{v}_0)$$

For given initial condition x_0, we show that there exists $\mathsf{T}' > 0$, independent of initial condition, such that unique fixed point exists for $\mathsf{t} \in [-\mathsf{T}', \mathsf{T}']$.

3. Global existence of solution: For any given $\mathsf{T} > 0$, using local existence theorem for small intervals we can show the existence of unique solution for all $\mathsf{t} \in [-\mathsf{T}, \mathsf{T}]$.

References

Theoretical analysis

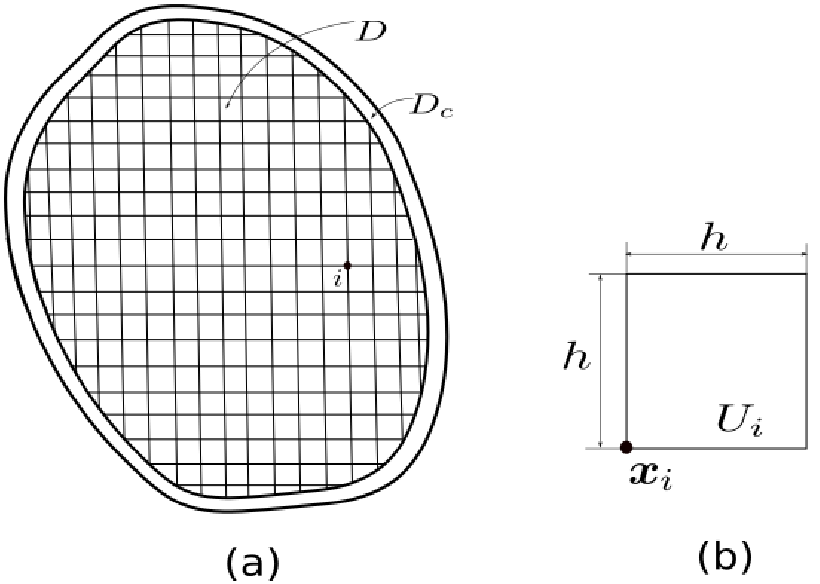
Silling & Lehoucq 2008, Lipton, Silling & Lehoucq 20016
Aksoylu & Parks 2011, Aksoylu & Unlu 2014
Du & Gunzburger, Lehoucq & Zhou 2012, Du & Zhou 2011
Lipton 2014, Lipton 2015, Mengesha & Du 2013 , Mengesha & Du 2014
Tian, Du & Gunzburger 2016, Emmrich & Puhst 2015
Emmrich & Puhst 2015 Dayal 2017

Numerical analysis and approximation

Silling & Askari 2005, Silling & Bobaru 2005, Bobaru et. al. 2009
Silling, Weckner, Askari & Bobaru 2010, Bobaru & Hu 2012
Chen & Gunzburger 2011, Du, Gunzburger, & Schiweitzer 2016
Guan & Gunzburger 2015, Tian, Du & Gunzburger 2016
Wildman & Gazonas 2014, Weckner & Emmrich 2005, Weckner 2009
Weckner & Abeyaratne 2005, Diehl, Lipton & Schiweitzer 2016

Finite difference approximation

$\mathsf{D_h = D \cap h\mathbb{Z}^d, \mathbf{x}_i = \mathbf{i}h, t^k = k\Delta t}$



$(\hat{\mathbf{u}}_i^k, \hat{\mathbf{v}}_i^k)$ satisfies

$$\frac{\hat{\mathbf{u}}_i^{k+1} - \hat{\mathbf{u}}_i^k}{\Delta t} = \hat{\mathbf{v}}_i^k$$

$$\frac{\hat{\mathbf{v}}_i^{k+1} - \hat{\mathbf{v}}_i^k}{\Delta t} = -\boldsymbol{\nabla} PD^{\epsilon}(\hat{\mathbf{u}}_h^k)(\mathbf{x}_i) + \mathbf{b}(\mathbf{x}_i, t^k)$$

where $\hat{\mathbf{u}}_h^k, \hat{\mathbf{v}}_h^k$ are piecewise constant extension of discrete solution $\hat{\mathbf{u}}_i^k, \hat{\mathbf{v}}_i^k$

$$\hat{\mathbf{u}}_h^k(\mathbf{x}) := \sum_{\mathbf{i} \in \mathbb{Z}^d, \mathbf{i}h \in D} \hat{\mathbf{u}}_i^k \chi_{U_i}(\mathbf{x})$$

[1] Prashant K Jha and Robert Lipton (2017) Numerical analysis of nonlocal fracture models in H\"{o}lder space. arXiv preprint arXiv:1701.02818

Convergence of finite difference approximation

- Error E^{k} is given by

$$E^k = ||\hat{\mathbf{u}}_h^k - \mathbf{u}(t^k)||_{L^2} + ||\hat{\mathbf{v}}_h^k - \mathbf{v}(t^k)||_{L^2}$$

- If $\mathbf{u}, \mathbf{v} \in C^2([0,T]; C^{0,\gamma}(D, \mathbb{R}^d))$ then error satisfies following (**Jha & Lipton 2017**[1])

$$\sup_{k \leq T/\Delta t} E^k = O(\Delta t + h^\gamma/\epsilon^2)$$

- Similar rate of convergence is shown for general one step time discretiztion.

[1] Prashant K Jha and Robert Lipton (2017) Numerical analysis of nonlocal fracture models in H\"{o}lder space. arXiv preprint arXiv:1701.02818

Convergence of finite difference approximation

Outline of proof:

1. Comparing exact solution $(\mathbf{u}(\mathsf{t}^\mathsf{k}), \mathbf{v}(\mathsf{t}^\mathsf{k}))$ with its piecewise constant projection $(\tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k})$ given by

$$\tilde{\mathbf{u}}_h^k(\mathbf{x}) = \sum_{\mathbf{x}_i \in D \cap (h\mathbb{Z}^d)} \chi_{U_1}(\mathbf{x}) \tilde{\mathbf{u}}_i^k, \qquad \tilde{\mathbf{u}}_i^k = \frac{1}{h^d} \int_{U_i} \mathbf{u}(\mathbf{y}, t^k) d\mathbf{y}$$

We can show $||\mathbf{u}(\mathsf{t}^\mathsf{k}) - \tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2} = \mathsf{O}(\mathsf{h}^\gamma)$.

2. Comparing $(\tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k})$ with piecwise constant extension $(\hat{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \hat{\mathbf{v}}_\mathsf{h}^\mathsf{k})$ of discrete approximate solution.

(1) Writing eridynamics equation for $(\tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k})$ involving consistency error.

(2) Estimating consistency error term. One of the error term is as follows

$$|| - \boldsymbol{\nabla} PD^\epsilon(\mathbf{u}(t^k)) - (-\boldsymbol{\nabla} PD^\epsilon(\tilde{\mathbf{u}}_h^k))||_{L^2} \leq \frac{L}{\epsilon^2} ||\mathbf{u}(t^k) - \tilde{\mathbf{u}}_h^k)||_{L^2} \leq \frac{L}{\epsilon^2} C h^\gamma$$

(3) By substracting peridynamics equation corresponding to $(\tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \tilde{\mathbf{v}}_{\mathsf{kh}})$ and $(\hat{\mathbf{u}}_\mathsf{h}^\mathsf{k}, \hat{\mathbf{v}}_\mathsf{h}^\mathsf{k})$, we get bounds on $||\hat{\mathbf{u}}_\mathsf{h}^\mathsf{k} - \tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2} + ||\hat{\mathbf{v}}_\mathsf{h}^\mathsf{k} - \tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2}$

3. $\mathsf{E}^\mathsf{k} \leq ||\mathbf{u}(\mathsf{t}^\mathsf{k}) - \tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2} + ||\mathbf{v}(\mathsf{t}^\mathsf{k}) - \tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2} + ||\tilde{\mathbf{u}}_\mathsf{h}^\mathsf{k} - \hat{\mathbf{u}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2} + ||\tilde{\mathbf{v}}_\mathsf{h}^\mathsf{k} - \hat{\mathbf{v}}_\mathsf{h}^\mathsf{k}||_{\mathsf{L}^2}$

One dimensional model

Objective:

- To see if we can improve the rate of convergence h^γ/ϵ^2 where $\gamma \in (0,1]$.
- Rate of convergence of nonlinear peridynamics to elastodynamics.

We show in **Jha & Lipton 2017**[1] that if $u \in C^2([0,T]; C^4(D,\mathbb{R}))$ then solution of nonlinear peridynamic converges to the elastodynamic solution, i.e.

$$u^\epsilon \to u \qquad \text{in } H_0^1(D)$$

at the rate ϵ uniformly in time $t \in [0,T]$.

We follow the quadrature based FE approximation in **Tian & Du 2014**[2] and **Tian, Du & Gunzburger 2016**[3]. Let $\mathcal{I}_h[u]$ is given by

$$\mathcal{I}_h[u](x) = \sum_{i, x_i \in D} u(x_i)\phi_i(x)$$

[1] Prashant K. Jha and Robert Lipton (2017) Numerical convergence of nonlinear nonlocal continuum models to local elastodynamics. arXiv:1707.00398
[2] X. Tian and Qiang Du (2014) Asymptotically compatible schemes and applications to robust discretization of nonlocal models. SIAM Journal on Numerical Analysis, 52(4):1641–1665.
[3] X. Tian, Qiang Du and Max Gunzburger (2016) Asymptotically compatible schemes for the approximation of fractional laplacian and related onlocal diffusion problems on bounded domains. Advances in Computational Mathematics, 42(6):1363–1380.

One dimensional model

Let $\hat{u}_i^{\epsilon,k}$ denote the approximate displacement at $x_i = ih \in D, i \in \mathbb{Z}$ and $t^k = k\Delta t$. It satisfies

$$\frac{\hat{u}_i^{\epsilon,k+1} - 2\hat{u}_i^{\epsilon,k} + \hat{u}_i^{\epsilon,k-1}}{\Delta t^2} = -\nabla PD^\epsilon(\hat{u}_h^{\epsilon,k})(x_i) + b(t^k, x_i)$$

with initial condition as $\hat{u}_i^{\epsilon,0} = u_0(x_i)$. For initial condition on velocity, we use

$$\frac{\hat{u}_i^{\epsilon,1} - \hat{u}_i^{\epsilon,-1}}{2\Delta t} = v_0(x_i)$$

and use above to start the time iteration for $k = 0$.

$\hat{u}_h^{\epsilon,k}$ is the extension of discrete set $\hat{u}_i^{\epsilon,k}$ using linear interpolation functions ϕ_i. It is given by

$$\hat{u}_h^{\epsilon,k}(x) = \sum_{i\in\mathbb{Z}, ih\in[0,1]} \hat{u}_i^{\epsilon,k}\phi_i(x)$$

Consistency error and stability

We approximate the peridynamic force $-\nabla PD^{\epsilon}(u)$ by $-\nabla PD^{\epsilon}(\mathcal{I}_h[u])$. Consistency error satisfies

$$\sup_{i, x_i \in D} |-\nabla PD^{\epsilon}(\mathcal{I}_h[u])(x_i) - (-\nabla PD^{\epsilon}(u)(x_i))| = O(h/\epsilon)$$

← comparing this with $O(h^{\gamma}/\epsilon^2)$

$$\sup_{i, x_i \in D} |-\nabla PD^{\epsilon}(\mathcal{I}_h[u])(x_i) - \mathbb{C} u_{xx}(x_i)| = O(\epsilon) + O(h/\epsilon)$$

← rate of convergence to elastodynamics depends on h/ϵ.

Stability: For linear peridynamics, we obtain following stability condition, for Central difference scheme

$$\Delta t \leq \frac{h}{\sqrt{\mathbb{C} + 2f'(0)\frac{Mh^2}{\epsilon^2}}} \quad \text{where} \quad \mathbb{C} = \frac{2f'(0)}{\epsilon^2} \int_0^1 J(|z|) z dz$$

Numerical verification: h-convergence

- For fixed ϵ we expect the rate of convergence to be $O(h)$.

$u_0(x) = a\exp[-(0.5-x)^2/\beta], v_0(x) = 0$
$a = 0.005, \beta = 10^{-5}$, time domain $= [0, 1.7]$

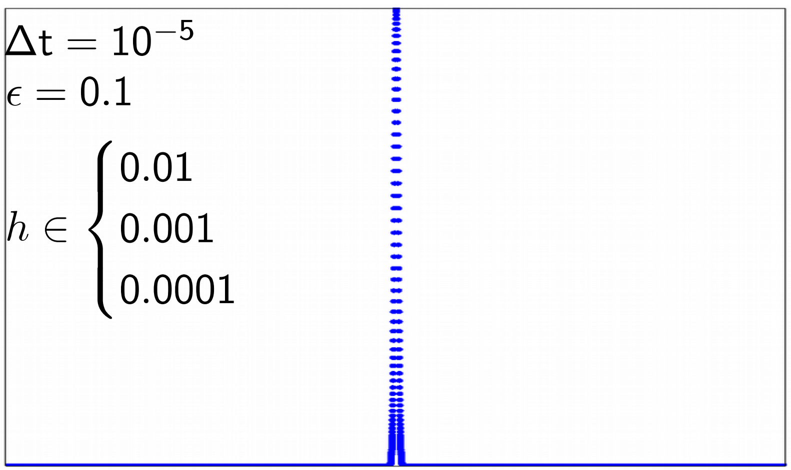


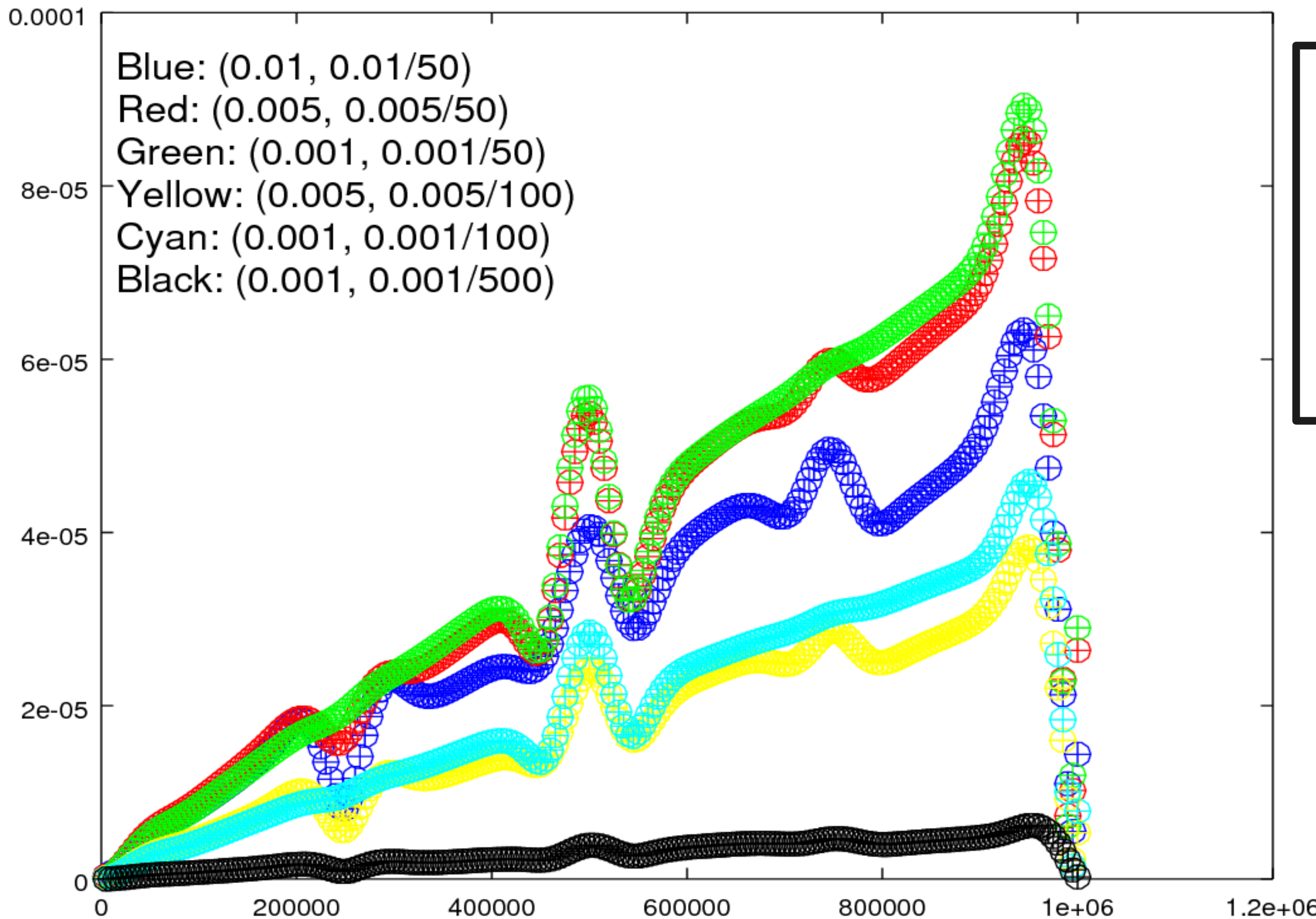
Table: LPD refers to linear peridynamics and NPD refer to nonlinear peridynamics. Superscript "1" corresponds to L^2 norm and "2" corresponds to sup norm.

Time step	LPD^1	NPD^1	LPD^2	NPD^2
6000	1.6416	1.6419	1.4204	1.4204
51500	1.3098	1.3106	1.3312	1.3331
104000	1.1504	1.1482	1.5155	1.5557
147000	1.1364	1.1262	1.6027	1.5215
165000	1.2611	1.2632	1.5496	1.6055

- Similar results have been observed for multiple simulations.

Numerical verification: m-convergence

$u_0(x) = a\exp[-(0.25-x)^2/\beta - (0.75-x)^2/\beta], v_0(x) = 0, a = 0.001, \beta = 0.003.$
Let $\Delta t = 10^{-6}$, time domain is $[0,1]$.



h has to decrease at faster rate for decreasing ϵ to reduce the error between peridynamic and elastodynamic solution.

Plot of time step k vs $||u_{peri} - u_{elasto}||_{L^2}$. "+" corresponds to LPD and "o" corresponds to NPD.

Finite element approximation using linear interpolation

Using weak formulation and applying finite element approximation, we can further improve the rate of convergence of error. Consider following

$$(\ddot{\mathbf{u}}(t), \tilde{\mathbf{u}}) + a^\epsilon(\mathbf{u}(t), \tilde{\mathbf{u}}) = (\mathbf{b}(t), \tilde{\mathbf{u}}) \qquad \tilde{\mathbf{u}} \in L^2_0(D, \mathbb{R}^d)$$
$$(\ddot{\mathbf{u}}_l(t), \tilde{\mathbf{u}}) + a^\epsilon_l(\mathbf{u}_l(t), \tilde{\mathbf{u}}) = (\mathbf{b}(t), \tilde{\mathbf{u}}) \qquad \tilde{\mathbf{u}} \in L^2_0(D, \mathbb{R}^d)$$

where

$$a^\epsilon(\mathbf{u}, \mathbf{v}) = \frac{2}{\epsilon^{d+1}\omega_d} \int_D \int_D J^\epsilon(|\mathbf{y}-\mathbf{x}|) f'(|\mathbf{y}-\mathbf{x}| S(\mathbf{u})^2) |\mathbf{y}-\mathbf{x}| S(\mathbf{u}) S(\mathbf{v}) d\mathbf{x} d\mathbf{x}$$
$$a^\epsilon_l(\mathbf{u}, \mathbf{v}) = \frac{2}{\epsilon^{d+1}\omega_d} \int_D \int_D J^\epsilon(|\mathbf{y}-\mathbf{x}|) f'(0) |\mathbf{y}-\mathbf{x}| S(\mathbf{u}) S(\mathbf{v}) d\mathbf{x} d\mathbf{x}$$

$$S(\mathbf{u}) = \frac{\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x})}{|\mathbf{y}-\mathbf{x}|} \cdot \frac{\mathbf{y}-\mathbf{x}}{|\mathbf{y}-\mathbf{x}|}$$

Energy is defined as

$$e^\epsilon(\mathbf{u}(t)) = \frac{1}{2}\rho ||\dot{\mathbf{u}}(t)||_{L^2} + a^\epsilon(\mathbf{u}(t), \mathbf{u}(t))$$

Finite element approximation using linear interpolation

- a_l^ϵ is coercive and bounded. If displacement field is such that $S(\mathbf{u}) \leq C < S_c$ for all $|\mathbf{y} - \mathbf{x}| \leq \epsilon$, we can show the coercivity of a^ϵ.

- For linear peridynamics, following **Baker 1976**[1], **Grote & Schötzau 2009**[2], **Karaa 2012**[3], **Guan & Gunzburger 2015**[4], we can obtain the condition on Δt.

- We can show the stability of semi-discrete scheme for linear Peridynamics and under the assumption of $S(\mathbf{u}) < S_c$ for nonlinear peridynamics.

- Using bound on energy, we can show for any $t_1 > t_2, t_1, t_2 \in [0, T]$, we have

$$||u_h(t_1) - u_h(t_2)||_{L^2} \leq |t_1 - t_2| \left[\sup_{t \in [0,T]} e^\epsilon(u_h(t)) \right]$$

- If exact solution $(\mathbf{u}(t), \mathbf{v}(t)) \in H_0^2(D, \mathbb{R}^d)$ then error $E^k = ||\hat{\mathbf{u}}^k - \mathbf{u}(t^k)||_{L^2}$ satisfies

$$\sup_k E^k = O(\Delta t + h^2/\epsilon^2)$$

[1] G. A. Baker (1976) Error estimates for finite element methods for second order hyperbolic equations. SIAM journal on numerical analysis, 13(4):564–576.

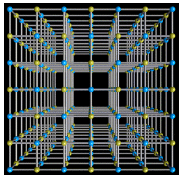
[2] M. J. Grote and D. Sch\"otzau (2009) Optimal error estimates for the fully discrete interior penalty dg method for the wave equation. Journal of Scientific Computing, 40(1):257–272.

[3] S. Karaa (2012) Stability and convergence of fully discrete finite element schemes for the acoustic wave equation. Journal of Applied Mathematics and Computing, 40(1-2):659–682.

[4] Q. Guan and M. Gunzburger (2015) Stability and accuracy of time stepping schemes and dispersion relations for a nonlocal wave equation. Numerical Methods for Partial Differential Equations, 31(2):500–516.

Future works

- Numerical analysis of state-based nonlinear model
- Nonlocal in time, i.e. damage models
- Numerical implementation of state-based and damager models



Thank you!