Mathematical and numerical analysis of peridynamic models

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Collaborators:

- Kun Zhou (who couldn't come due to visa issues)
 - 1. Linear PD bond model, Cauchy problem (ESIAM-M2AN 2011)
 - 2. Initial-boundary value problems, finite element approximation, error estimates and condition numbers (SINUM 2010)
- Max Gunzburger, Rich Lehoucq and Kun Zhou:
 - 3. Nonlocal laws and nonlocal vector calculus (Sandia preprint)
 - 4. Linear nonlocal BVPs with volumic constraints (almost done)
 - 5. Variational formulation of PD state model (in progress)
- Lili Ju, Li Tian and Kun Zhou:
 - 6. Finite element approximations to linear PD models, a posterior error analysis (in progress), adaptive methods

u: displacement $\mathbf{y} = \mathbf{x} + \mathbf{u}(\mathbf{x}, t)$

$$\mathbf{u}_{tt}(\mathbf{x}, t) = L_{\delta} \mathbf{u}(\mathbf{x}, t) + \mathbf{b}(\mathbf{x}, t)$$
$$L_{\delta} \mathbf{u}(\mathbf{x}) = c_{\delta} \int_{B_{\delta}(\mathbf{x})} \frac{(\mathbf{x}' - \mathbf{x}) \otimes (\mathbf{x}' - \mathbf{x})}{\sigma(|\mathbf{x}' - \mathbf{x}|)} (\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})) d\mathbf{x}'$$

model for a spring network



 $\boldsymbol{\sigma}$: kernel function, related to spring constants

 δ : PD horizon



• Examples: bond-based, PD fluid, PD solid, ...

Mathematical issues:

- Increasing popularity of PD based simulations demands better mathematical and numerical analysis
- Rigorous mathematical framework
 - Are all formulations used in practice well-posed?
 - Are singularities appearing from models or numerics?
- Numerical analysis
 - Stability (CFL, log dependence on mesh?)
 - Conditioning (independent of mesh?)
 - Error (uniform in δ ?)

on discretization and model parameters

Existing studies motivated our works:



Nonlocal PD & PDEs: how different/similar are they

Consider an Initial Boundary Value Problem of PD:

$$\mathbf{u}_{tt}(\mathbf{x},t) = \mathcal{L}_{\delta}\mathbf{u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t)$$

together with initial and boundary conditions.

The linear bond-based PD operator

$$\mathcal{L}_{\delta}\mathbf{u}(\mathbf{x}) = c_{\delta} \int_{B_{\delta}(\mathbf{x})} \frac{(\mathbf{x}' - \mathbf{x}) \otimes (\mathbf{x}' - \mathbf{x})}{\sigma(|\mathbf{x}' - \mathbf{x}|)} (\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})) d\mathbf{x}'$$

- PD horizon parameter δ , spherical neighborhood $B_{\delta}(\mathbf{x})$
- Kernel function $\sigma = \sigma(|\mathbf{x}' \mathbf{x}|)$
- c_{δ} a normalization constant

Nonlocal PD: boundary conditions

A simple 1-d example: equation defined on [0, π] Zhou-D. SINUM 2010 $-\delta$ 0 δ $\pi-\delta$ π $\pi+\delta$

u is odd in $(-\delta, \delta)$ and $(\pi - \delta, \pi + \delta)$:

Practical application: none, but it allows Fourier analysis (O. Weckner), offers much insight and is one of the natural extensions of its local limit: homogeneous Dirichlet BC

$$-\mathcal{L}^{o}_{\delta}u(x) = -c_{\delta} \int_{x-\delta}^{x+\delta} \frac{|x'-x|^2}{\sigma(|x'-x|)} (u(x') - u(x))dx'$$

Linear bond-based PD: assumptions/symbols

• Assumptions

 $\sigma(\mathbf{x}) > 0, \ \forall \mathbf{x} \in B_{\delta}(0)$

$$\frac{|\mathbf{y}|^2}{\sigma(|\mathbf{y}|)} \ge \rho(\mathbf{y}) \in L^1(B_{\delta}(0)) \qquad \rho \text{ non-negative}$$

(can be relaxed to include negative part, see for example D-G-L-Z 2011 for an illustration of sign-changing kernels)

$$\tau_{\delta} := c_{\delta} \int_{B_{\delta}(0)} \frac{|\mathbf{x}|^4}{\sigma(|\mathbf{x}|)} d\mathbf{x} < \infty$$

(necessary for well-defined elastic modulus)

Linear bond-based PD: symbols

• Fourier symbol: consider $u(x) = \sum u_k^o \sin(kx)$

$$u_k^o = \frac{2}{\pi} \int_0^\pi u(x) \sin(kx) dx$$

$$-\mathcal{L}_{\delta}^{o}u(x) = \sum_{k} \eta_{\delta}(k)u_{k}^{o}\sin(kx)$$
$$\eta_{\delta}(k) = c_{\delta} \int_{-\delta}^{\delta} (1 - \cos(ky)) \frac{|y|^{2}}{\sigma(|y|)} dy$$

In comparison $-u''(x) = \sum_{k}^{o} k^2 u_k^o \sin(kx)$

Nonlocal BVP for Linear bond-based PD

• Natural spaces for PD operator L_{δ} : for any s

$$M^{so}_{\sigma} = \left\{ u : \|u\|^2_{M^{so}_{\sigma}} = \sum_k \eta^s_{\delta}(k) u^{o2}_k < \infty \right\}$$

are generalized energy spaces, in particular, s=1

$$\|u\|_{M^o_{\sigma}} = \left[-\frac{2}{\pi} (\mathcal{L}^o_{\delta} u, u)\right]^{\frac{1}{2}} = \left\{\sum_k \eta_{\delta}(k) u_k^{o2}\right\}^{1/2}$$

 M_{σ}^{-so} : the dual space of M_{σ}^{so}

Nonlocal BVP for Linear bond-based PD

• L_{δ} is an self-adjoint operator: M_{σ}^{o} to M_{σ}^{-o}

And an isometry: by the Riemann Lemma

$$\lim_{k \to \infty} \int_{-\delta}^{\delta} \rho(|y|) \cos(ky) dy = 0$$

$$\begin{cases} \eta_{\delta}(k) \ge \inf_{k\ge 1} c_{\delta} \int_{-\delta}^{\delta} (1 - \cos(ky))\rho(y) dy > 0 \\ 0 \le \tau_{\delta} k^2 - \eta_{\delta}(k) \le \frac{k^4 \delta^2 \tau_{\delta}}{12} . \end{cases}$$

 $\longrightarrow H^1_{\alpha} \hookrightarrow M^o_{\sigma} \hookrightarrow L^2_{\alpha}$

Nonlocal BVP for Linear bond-based PD

• If in addition
$$\frac{|\mathbf{y}|^2}{\sigma(|\mathbf{y}|)} \in L^1(B_{\delta}(0))$$

 $0 < \inf_{k \ge 1} \eta_{\delta}(k) \le \eta_{\delta}(k) \le 4c_{\delta} \int_0^{\delta} \frac{y^2}{\sigma(y)} dy$
 $\longrightarrow M_{\sigma}^{2o} = M_{\sigma}^o = L_o^2$

1.0

*L*² theory: Emmrich/Weckner, Alali/Lipton

the corresponding linear bond-based PD models no longer have smoothing effect

• Other kernels:

$$\begin{aligned} \sigma(|y|) &\geq \gamma_1 |y|^{3+\alpha} \longrightarrow 0 \leq \eta_\delta(k) \leq C_1^\delta(\alpha)^2 k^\alpha \\ \alpha \in (0,2) \qquad \qquad H_o^{\alpha/2} \hookrightarrow M_\sigma^o \end{aligned}$$

$$\sigma(|y|) \leq \gamma_2 |y|^{3+\beta} \longrightarrow \eta_\delta(k) \geq C_2^\delta(\beta)^2 k^\beta$$
$$\beta < 2 \qquad \qquad M_\sigma^o \hookrightarrow H_o^{\beta/2}$$

• Elliptic regularity:

$$-\mathcal{L}^o_\delta u = f$$

Theorem: (Zhou-D. SINUM 2010) For $\alpha = \beta$, $C_2^{\delta}(\beta)^2 k^{\beta} \leq \eta_{\delta}(k) \leq C_1^{\delta}(\beta)^2 k^{\beta} \qquad \beta \in (0,2)$ For $f \in H_o^m$, $m \geq -\alpha$, we have $u \in H_o^{m+\beta}$ which implies "smoothing effect" of the PD model

The dependence on horizon is *explicitly* estimated.

Connection to DE and standard Sobolev spaces

-u'' = fODE π $u(0) = u(\pi) = 0$ $-\delta \quad 0 \quad \delta \qquad \pi - \delta \quad \pi \quad \pi + \delta$ $-\mathcal{L}^{o}_{\delta}\mathcal{U}=f$ PD u is odd in $(-\delta, \delta)$ and $(\pi - \delta, \pi + \delta)$: $0 \le \tau_{\delta} k^2 - 2\eta_{\delta}(k) \le \frac{k^4 \delta^2 \tau_{\delta}}{12}$ Notice that

When $\tau_{\delta} \to 2$ we have $u^o_{\delta} - u \to 0$ in M^{2o}_{σ}

Convergence in conventional norms follows from space equivalence Peridynamics Are these effects due to the special 1-d BC?

u is odd in
$$(-\delta, \delta)$$
 and $(\pi - \delta, \pi + \delta)$:

No, the results are similar when using other (more conventional) nonlocal BCs

For example,

- for scalar equation, same results were shown in any dim with general nonlocal volumic constraints (D-G-L-Z [4]);
 Null kernel + compactness, similar to works of Rossi
- similar results can be shown in higher dim for linear PD bond system (Zhou-D. SINUM 2010) and state (D-G-L-Z [5])

Linear bond-based PD: I(nonlocal)BVP

$$\begin{cases} \mathbf{u}_{tt}(\mathbf{x},t) = L_{\delta}\mathbf{u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t), \ t \in (0,T) \\ \mathbf{u}(\mathbf{x},0) = \mathbf{g}(\mathbf{x}), \quad \{t=0\} \\ \mathbf{u}_{t}(\mathbf{x},0) = \mathbf{h}(\mathbf{x}), \quad \{t=0\} \end{cases}$$

$$\mathcal{L}_{\delta}\mathbf{u}(\mathbf{x}) = c_{\delta} \int_{B_{\delta}(\mathbf{x})} \frac{(\mathbf{x}' - \mathbf{x}) \otimes (\mathbf{x}' - \mathbf{x})}{\sigma(|\mathbf{x}' - \mathbf{x}|)} (\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})) d\mathbf{x}'$$

The operator has a non-diagonal tensor kernel

A nonlocal BC for a square: $\mathbf{u} = \sum_{k,l=1}^{\infty} \begin{pmatrix} u_{kl} \sin(kx_1) \cos(lx_2) \\ v_{kl} \cos(kx_1) \sin(lx_2) \end{pmatrix}$

Alternatingly odd in one direction, even in the other

Linear bond-based PD: I(nonlocal)BVP

Alternatingly odd and even in variables: a strange BC?

Not totally. Again, it is a natural nonlocal analog of the Navier equation with the well-known greased wall BC and allows a block diagonalization via Fourier

$$\begin{cases} \mathbf{u}_{tt} = \mu \triangle \mathbf{u} + 2\mu \nabla \nabla \cdot \mathbf{u} + \mathbf{b}, \\ \mathbf{u}(0, \mathbf{x}) = \mathbf{g}(\mathbf{x}), \quad \mathbf{u}_t(0, \mathbf{x}) = \mathbf{h}(\mathbf{x}), \\ u_1(\mathbf{x}) = \frac{\partial}{\partial n} u_2(\mathbf{x}) = 0, \quad x_2 \in \{0, \pi\} \\ u_2(\mathbf{x}) = \frac{\partial}{\partial n} u_1(\mathbf{x}) = 0, \quad x_1 \in \{0, \pi\} \end{cases}$$



For $\mathbf{u} = \sum_{k,l=1}^{\infty} \begin{pmatrix} u_{kl} \sin(kx_1) \cos(lx_2) \\ v_{kl} \cos(kx_1) \sin(lx_2) \end{pmatrix}$

Let
$$M_{\delta,kl} = c_{\delta} \int_{B_{\delta}(0)} \frac{1 - \cos(k\xi_1 + l\xi_2)}{\sigma(|\boldsymbol{\xi}|)} \begin{pmatrix} \xi_1^2 & \xi_1\xi_2 \\ \xi_1\xi_2 & \xi_2^2 \end{pmatrix} d\boldsymbol{\xi} .$$
$$-\mathcal{L}_{\delta} \mathbf{u} = \sum_{k,l=1}^{\infty} \begin{pmatrix} \sin(kx_1)\cos(lx_2) & 0 \\ 0 & \cos(kx_1)\sin(lx_2) \end{pmatrix} M_{\delta,kl} \begin{pmatrix} u_{kl} \\ v_{kl} \end{pmatrix}$$

Local limit
$$M_{0,kl} = \begin{pmatrix} (2\mu + \lambda)k^2 + \mu l^2 & (\mu + \lambda)kl \\ (\mu + \lambda)kl & \mu k^2 + (2\mu + \lambda)l^2 \end{pmatrix}$$

$$\mu = \lambda = \lim_{\delta \to 0} \frac{c_\delta}{2} \int_{P_{\delta}(0)} \frac{\xi_1^2 \xi_2^2}{\sigma(|\boldsymbol{\xi}|)} d\boldsymbol{\xi} = \lim_{\delta \to 0} \frac{\tau_\delta}{16}$$

$$\delta \to 0 \ 2 \ J_{B_{\delta}(0)} \ \sigma(|\boldsymbol{\xi}|) \quad \delta \to \delta$$

The matrix symbols commute (!) and

$$M_{\delta,kl} \leq c_{\delta} \left(\int_{B_{\delta}(0)} \frac{1 - \cos(k\xi_{1} + l\xi_{2})}{\sigma(|\boldsymbol{\xi}|)} |\boldsymbol{\xi}|^{2} d\boldsymbol{\xi} \right) \mathbf{I}$$
$$= c_{\delta} \left(\int_{B_{\delta}(0)} \frac{1 - \cos(k\xi_{1})\cos(l\xi_{2})}{\sigma(|\boldsymbol{\xi}|)} |\boldsymbol{\xi}|^{2} d\boldsymbol{\xi} \right) \mathbf{I}$$
$$\leq c_{\delta} \left(\int_{B_{\delta}(0)} \frac{(k^{2} + l^{2})}{2\sigma(|\boldsymbol{\xi}|)} |\boldsymbol{\xi}|^{4} d\boldsymbol{\xi} \right) \mathbf{I} \leq \frac{\tau_{\delta}}{2\mu} M_{0,kl}$$

The difference between the two symbols is

$$\begin{split} Z_{kl} &= \frac{c_{\delta}}{24} \int_{B_{\delta}(0)} \frac{(k\xi_1 + l\xi_2)^4}{\sigma(|\boldsymbol{\xi}|)} \boldsymbol{\xi} \otimes \boldsymbol{\xi} \cos(\theta) \, d\boldsymbol{\xi} \\ |Z_{kl}| &\leq \frac{\tau_{\delta}}{24} \delta^2 (k^2 + l^2)^2 \mathbf{I} \\ \text{Leads to order of convergence for small } \delta \end{split}$$

Define energy spaces accordingly M_{σ}^{soe}

Theorem: (Zhou-D. SINUM 2010) Well-posedness of IBVP in $C([0,T], M_{\sigma}^{oe}) \cap H^1(0,T; L_{oe}^2)$ and convergence to local limit

For system, the PD bond operator is not of a diagonal form, one can utilize the symmetry in the tensor and variables to achieve diagonalization, which helps establishing the analytical framework

Finite dimensional approximation

Internal approximations: dense subspace

- Truncated Fourier spaces
- Conforming finite element of piecewise polynomials of degree *m*

Galerkin-Ritz $u_n = \operatorname{argmin}_{v_n \in V_n} \{ \frac{1}{2} \| v_n \|_{M^o_\sigma}^2 - (v_n, f)_{L^2} \}$

+ A priori error estimates for nonlocal BVP/IBVP

One-d nonlocal BVP: error estimates

For smooth solutions

(Zhou-D 2010 SINUM)

Theorem:
$$C_2^{\delta}(\beta)^2 k^{\beta} \leq \eta_{\delta}(k) \leq C_1^{\delta}(\beta)^2 k^{\beta}$$

Fourier spectral with n modes $f \in H_o^m$, $m \geq -\beta$
 $\|u - u_n\|_{\alpha} \leq C_2^{\delta}(\beta)^{-2} n^{-m-\beta+\alpha} \|f\|_m$ $\alpha \leq m+\beta$

Theorem: $C_2^{\delta}(\beta)^2 k^{\beta} \leq \eta_{\delta}(k) \leq C_1^{\delta}(\alpha)^2 k^{\alpha}$, $0 \leq \beta \leq \alpha \in (0,2)$ FEM with conforming elements of degree *m* (continuity not required for $\alpha < 1$), if $f \in H_o^{m'-\alpha}$, $0 \leq m' \leq m+1$, $s \in [0, \beta/2]$ $\|u - u_n\|_s \leq c_s C_1^{\delta}(\alpha)^{1+s'} C_2^{\delta}(\beta)^{-3-s'} h^{m'-\alpha/2+(\beta-\alpha/2)s'} \|f\|_{m'-\beta}$

$$\sigma(y) = |y|^3 \qquad ||u - u_n||_0 \le O(h^{m' - \alpha/2} \delta^{-1 + \alpha/2})$$

Peridynamics Numerics: Chen-Gunzburger 2010

Finite Element Stiffness Matrix $A^o = ((\phi_i, \phi_j)_{M^o_{\sigma}})$

Theorem: (Zhou-D. 2010 SINUM) Finite element with conforming elements of degree *m*, quasi-uniform mesh

$$0 < cC_2^{\delta}(\beta)^2 h \le \lambda_1 \le \lambda_n \le cC_1^{\delta}(\alpha)^2 h^{1-\alpha}$$

 $\operatorname{cond}(A^o) \le c(C_1^{\delta}(\alpha)/C_2^{\delta}(\beta))^2 h^{-\alpha}$

$$\mathsf{Eg} \quad \sigma(y) = |y|^2 \qquad \operatorname{cond}(A^o) \le c \min\{\delta^{-2}, h^{-2}\}$$

Estimates/numerical observation $\operatorname{cond}(A^o) \leq c\delta^{-2}$ Aksoylu-Parks 2009 Eg $\sigma(|y|) = |y|^3 \operatorname{cond}(A^o) \leq c \min\{h^{-\alpha}\delta^{\alpha-2}, h^{-2}\}$

Estimates/numerical observation Seleson-Parks-Gunzburger-Lehoucq 2009

Same type estimates hold for more general scalar diffusion equation with volumic constraints, but dependence not so precise (D-G-L-Z [4])

Linear peridynamic model

- The discussion so far is for linear problems with a special, but nonlocal, type of BC.
- Still, similar results holds for Cauchy problems (D.-Zhou ESIAM-M2AN)
- Similar results for other nonlocal BVPs (see D-G-L-Z [4])
- For systems: fewer results, but they set PD apart from existing studies of other nonlocal/integral equations; simultaneous diagonalization may not be valid in general, but can still be a helpful tool (well-posedness for state models of PD solid, D-G-L-Z, [5])

PD state of solids via nonlocal calculus

- Notation: ⊗ Kronecker (tensor) product
 - Frobenius (scalar) product

Bond

Points

Х

• y

 $\Omega \subset \mathbb{R}^d$ a given material domain

D-G-L-Z [3]: nonlocal vector calculs

- Point functions $\mathbf{u} \colon \Omega \to \mathbb{R}^r$ Inner product: $(\mathbf{u}_1, \mathbf{u}_2) = \int_{\Omega} \mathbf{u}_1(\mathbf{x}) \cdot \mathbf{u}_2(\mathbf{x}) d\mathbf{x}$
- Two-point (bond) functions $\mathbf{v} \colon \Omega \times \Omega \to \mathbb{R}^m$ Inner product: $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle = \int_{\Omega} \int_{\Omega} \mathbf{v}_1(\mathbf{x}, \mathbf{y}) \cdot \mathbf{v}_2(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$

PD state solid via nonlocal calculus

- Nonlocal point gradient and its adjoint $\mathcal{G}(\eta)(\mathbf{x}) = -\int_{\Omega} \left(\eta(\mathbf{x}, \mathbf{y}) + \eta(\mathbf{y}, \mathbf{x}) \right) \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y}) \, d\mathbf{y}$ $\mathcal{G}^*(\mathbf{v})(\mathbf{x}, \mathbf{y}) = \left(\mathbf{v}(\mathbf{y}) - \mathbf{v}(\mathbf{x}) \right) \cdot \boldsymbol{\alpha}(\mathbf{x}, \mathbf{y})$
- Weighted gradient and adjoint $\mathcal{G}_{\omega}(u)(\mathbf{x}) = \mathcal{G}(\omega(\mathbf{x}, \mathbf{y})u(\mathbf{x}))(\mathbf{x})$



$$\mathcal{G}^*_{\omega}(\mathbf{v})(\mathbf{x}) = \int_{\Omega} \mathcal{G}^*(\mathbf{v})(\mathbf{x}, \mathbf{y}) \,\omega(\mathbf{x}, \mathbf{y}) \, d\mathbf{y}$$

Linear state-based PD solid

dilatation $\hat{\theta} = \mathcal{G}_w^*(\mathbf{u})$ Volumic strain

isotropic part of the extension scalar state

$$\underline{e}^i = \mathcal{G}_w^*(\mathbf{u}) \, |\mathbf{y} - \mathbf{x}| / d$$

deviatoric part $\underline{e}^d = \mathcal{G}^*(\mathbf{u}) - \mathcal{G}^*_w(\mathbf{u}) |\mathbf{y} - \mathbf{x}|/d$

• Energy: $E(\mathbf{u})$

$$\int_{\Omega} \frac{k(\mathbf{x}) \hat{\theta}^2}{2} d\mathbf{x} + \int_{\Omega} \int_{\Omega} \frac{\eta(\mathbf{x})}{2} \underline{\omega}(\mathbf{x}, \mathbf{y}) (\underline{e}^d)^2 d\mathbf{y} d\mathbf{x} - \int_{\Omega} \mathbf{u} \cdot \mathbf{b} d\mathbf{x}$$
$$|\mathbf{u}|^2 \qquad \qquad U(\Omega): \text{Energy space with bounded } |\mathbf{u}|$$
$$\mathcal{Z} = \{\mathbf{u}: |\mathbf{u}| = 0\}$$

 $U_0(\Omega):\, {f v}\in U(\Omega)\,$ with homogenous volumic constraint

Linear state-based PD solid

Well-posedness: (D-G-L-Z [5])

For a Hilbert space $U(\Omega)$ with a Poincare on $U_0(\Omega)$, the nonlocal BVP for the linear state-based peridynamic solids is well-posed provided that $\eta(\mathbf{x}) \ge \eta_0 > 0$ and $k(\mathbf{x}) \ge k_0 > 0$ for $\mathbf{x} \in \Omega$.

An example: when ω is square integrable and we have a uniformly positive definite acoustic tensor P₀, the energy space is L^2 , thus the linear PD state model is well-posed with a L^2 well-defined homogeneous volumic constraint.

Summary: linear peridynamic model

- Linear problems provide foundation to nonlinear problems, and for linear PD setting, there are many open questions.
- Results are dependent on micromodulus functions, we may see "smoothing" vs "no-smoothing". Even for the latter case, interests might be on the horizon dependence of the regularity
- Ongoing works: for nonlinear PD, studying steady states; for linear PD, speed of propagation, material stability; for fem, characterizing mesh dependence, a posterior estimates/adaptivity; for nonlocal calculus, application to shape analysis/geometry; ...