

Analysis and computation of nonlocal models

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Introduction •000000 Asymptotically compatible schemes

Fast algorithms

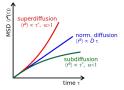
Homogenizatio

Summary

Nonlocality is ubiquitous







Anomalous diffusion



Mechanics



Image processing



Computational fluid dynamics

Nonlocality is ubiquitous

From modeling

- Biological and social models: Lévy flight, anomalous diffusion, flocking.
- ▶ Kinetic models: Boltzmann equation with fractional collision kernels.
- Data analysis: graph Laplacian, manifold learning.
- Continuum mechanics: Eringen model, Peridynamics.

From computation

- Computational fluid dynamics: SPH, vortex-blob method.
- ▶ From solving elliptic PDEs: wide stencil monotone schemes.
- ► Nonlocality naturally appears with model reduction or homogenization.

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Motivation

"Diffusion is a process where the variable under consideration (a particle density, a temperature, or a population) tends to revert to its surrounding average. "

— Luis Caffarelli

• The heat equation takes the form

$$u_t = \Delta u = \sum_{i=1}^n u_{x_i x_i} \,.$$

However, this does not help us to understand the diffusion process unless we realize that the Laplacian is the limit of an averaging process:

$$\Delta u = \lim_{r \to 0} \frac{1}{r^{n+2}} \int_{|y-x| < r} (u(y) - u(x)) dy$$

• More generally, a diffusion operator ¹ can be written as

$$\mathcal{L}u = \int K(x,y)(u(y) - u(x))dy$$

¹More rigorously, one could refer to Levy-Khintchine formula for charactering a Levy process, Beurling-Deny formula for charactering a Dirichlet form. (2) (2) (2) (2)

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A typical nonlocal elliptic operator is given by

$$\mathcal{L}_{\delta}u(x) = \int_{\mathbb{R}^n} K_{\delta}(x, y)(u(y) - u(x))dy \,,$$

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where K_{δ} is the kernel of the operator and δ is a modeling parameter.

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•
$$u: \mathbb{R}^n \to \mathbb{R}, \quad K_{\delta}(x,y) = c_{n,\delta} |y-x|^{-n-2\delta}, \qquad \qquad \mathcal{L}_{\delta} = -(-\Delta)^{\delta} \xrightarrow{\delta \to 1} \Delta$$

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• $u : \mathbb{R}^n \to \mathbb{R}, \quad K_{\delta}(x, y) = \delta^{-n-2} K(|y - x|/\delta) \chi_{|y-x| < \delta}, \qquad \qquad \mathcal{L}_{\delta} \xrightarrow{\delta \to 0} \Delta$

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$$\begin{split} \bullet & u: \mathbb{R}^n \to \mathbb{R}, \quad K_{\delta}(x,y) = c_{n,\delta} |y-x|^{-n-2\delta}, \qquad \qquad \mathcal{L}_{\delta} = -(-\Delta)^{\delta} \xrightarrow{\delta \to 1} \Delta \\ \bullet & u: \mathbb{R}^n \to \mathbb{R}, \quad K_{\delta}(x,y) = \delta^{-n-2} K(|y-x|/\delta) \chi_{|y-x|<\delta}, \qquad \mathcal{L}_{\delta} \xrightarrow{\delta \to 0} \Delta \\ \bullet & u: \mathbb{R}^n \to \mathbb{R}^n, \quad K_{\delta}(x,y) = \delta^{-n-1} \frac{(y-x) \otimes (y-x)}{|y-x|^3} \chi_{|y-x|<\delta}, \quad \mathcal{L}_{\delta} \xrightarrow{\delta \to 0} \mu \Delta + 2\mu \nabla \operatorname{div} \end{split}$$

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A typical nonlocal elliptic operator is given by

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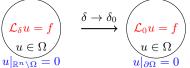
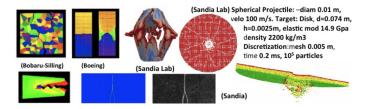


Figure: Consistency of nonlocal models with $\delta > 0$ to classical models with $\delta = \delta_0$.

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Peridynamics

• Since Silling 2000, peridynamics (PD) has found various applications



• Classical continuum theory derives local PDEs for smooth fields. PD uses an integro-differential equation to allow more singular solutions

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{b} \qquad \Leftrightarrow \qquad \rho \ddot{\mathbf{u}} = \int_{B_{\delta}(\mathbf{x})} \mathbf{f}(\mathbf{u}(\mathbf{y}) - \mathbf{u}(\mathbf{x}), \mathbf{y} - \mathbf{x}) \, d\mathbf{y} + \mathbf{b}$$

Classical continuum model

Nonlocal peridynamics model

• PD describes a nonlocal force balance law, accounting for interactions in a nonlocal neighborhood characterized by a horizon parameter δ .

Numerical challenges

- While singularities in solutions (cracks/fractures) may make peridynamics (PD) closer to reality, the added complexities also highlight the importance of understanding their mathematical properties and developing efficient and robust numerical methods, rigorous and careful validation and verification.
- In fact, the first issue encountered in the community is the consistency of the numerical simulations based on the nonlocal PD model with those based on the conventional PDE model when the latter is known to be valid, such as in cases where linear elasticity theory holds.
- Moreover, the discretization of the nonlocal operator in results in a matrix A with high density, for which fast algorithms must be considered in order to lower the cost of matrix multiplication and inversion.

Today

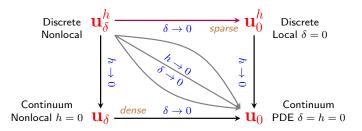
- Asymptotically compatible schemes
 - Variational methods
 - Non-variational methods
- Fast algorithms
- Homogenization and nonlocal effects

Introduction

Asymptotically compatible schemes

Asymptotically compatible (AC) ² schemes

AC schemes: discrete schemes that are convergent to nonlocal solution with a fixed δ as $h \to 0$, and to the *correct* local limit $\delta \to 0$, $h \to 0$.



Q: Why AC? robust, useful to VV and multi-scale simulations, efficient for adaptivity. Q: What schemes are AC?

²There are many existing studies on the effective discretization in limiting regimes, such as asymptotic preserving schemes for kinect equations, locking-free finite element methods for elasticity models, numerical discretization of radiative transfer in diffusive limit, etc.

AC schemes

Note that not all discretizations of linear PD models are AC. In fact, some of the most popular schemes are known not to be AC! [T-Du, 2013]

- The scheme using Riemann sum approximations of integrals is not AC.
- Finite element with piecewise constant functions is not AC.
- When δ/h is kept as a constant (to maintain sparsity/banded-structure), the above approximations may converge, but to a wrong local limit! They tend to over-estimate elastic constants, thus are incompatible to the correct local limit $\delta = 0$.
- We will discuss the way to find AC schemes for both variational and non-variational methods.

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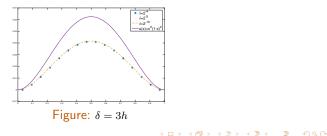
1d example

$$\mathcal{L}_{\delta}u(x) = \int_{-\delta}^{\delta} (u(x+s) - u(x))\gamma_{\delta}(|s|)ds = \int_{0}^{\delta} D^{2}u(x,s)\gamma_{\delta}(|s|)ds$$

where $D^{2}u(x,s) = u(x+s) + u(x-s) - 2u(x)$.

Direct quadrature scheme: $\mathcal{L}_{\delta,h}u(x_i) = h \sum_{j=1}^{\prime} (u_{i-j} - 2u_i + u_{i+j})\gamma_{\delta}(jh)$

It is convergent with fixed δ , but not convergent with fixed ratio δ/h .



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Variational methods

• Weak formulation needed for $-\mathcal{L}_{\delta}u = f$. Choose a test function v, then

$$-(\mathcal{L}_{\delta}u,v)=(f,v)\,.$$

Through nonlocal integration by parts

$$\begin{split} &- \iint \gamma_{\delta}(\mathbf{y} - \mathbf{x})(u(\mathbf{y}) - u(\mathbf{x}))v(\mathbf{x})d\mathbf{y}d\mathbf{x} \\ B_{\delta}[u, v] := &\frac{1}{2} \iint \gamma_{\delta}(\mathbf{y} - \mathbf{x})(u(\mathbf{y}) - u(\mathbf{x})(v(\mathbf{y}) - v(\mathbf{x}))d\mathbf{y}d\mathbf{x} \end{split}$$

• Find solution in the space \mathcal{S}_{δ}

$$\mathcal{S}_{\delta} = \{ u \in L^2 | \iint \gamma_{\delta} (\mathbf{y} - \mathbf{x}) (u(\mathbf{y}) - u(\mathbf{x}))^2 d\mathbf{y} d\mathbf{x} < \infty, u |_{\Omega_{\delta}} = 0 \}$$

• Galerkin approximation. Find finite dimensional solution $u_{\delta}^{h} \in W_{\delta,h} \subset S_{\delta}$ s.t.

$$B_{\delta}[u^{h}_{\delta}, v] = (f, v) \quad \forall v \in W_{\delta, h}$$

Summary

AC schemes for parameterized variational problems ³

About the spaces

- Ai) Uniform embedding: $C_1 \|u\|_{L^2} \le \|u\|_{\mathcal{S}_{\delta}} \le C_2 \|u\|_{H^1}$
- Aii) Asymptotically compact embedding: If $\{||u_{\delta}||_{S_{\delta}}\}_{\delta < \delta_0}$ is uniformly bounded, then $\{u_{\delta}\}$ is relatively compact in L^2 and each limit point is in H_0^1 .

3 About the bilinear forms

• $B_{\delta}(u,v)$ is uniformly bounded & coercive. (Nonlocal Poincaré inequality)

Consistency in a dense subspace

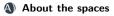
- Ci) \exists dense subspace $C_0^{\infty} \subset H_0^1$ such that $\mathcal{L}_{\delta} u \in L^2$, $\forall u \in C_0^{\infty}$
- Cii) Δ is the limit of \mathcal{L}_{δ} in C_0^{∞} , $\lim_{\delta \to 0} \|\mathcal{L}_{\delta}u \Delta u\|_{L^2} = 0 \quad \forall u \in C_0^{\infty}$

Approximation properties

- Di) Given $\delta > 0, \ \forall v \in \mathcal{S}_{\delta}, \ \inf_{v^h \in W_{\delta,h}} \{ \|v v^h\|_{\mathcal{S}_{\delta}} \} \to 0 \ \text{as} \ h \to 0,$
- Dii) $\{W_{\delta,h}, \delta \in (0, \delta_0), h \in (0, h_0)\}$ is asymptotically dense in H_0^1 , i.e., $\forall v \in H_0^1, \exists \{v_k \in W_{\delta_k, h_k}\}_{\delta_k \to 0}^{h_k \to 0}$ such that $\|v - v_k\|_{H^1} \to 0$ as $k \to \infty$.

³[T-Du, 2014]

AC schemes for parameterized variational problems ³



• Aii) Asymptotically compact embedding: If $\{||u_{\delta}||_{S_{\delta}}\}_{\delta < \delta_0}$ is uniformly bounded, then $\{u_{\delta}\}$ is relatively compact in L^2 and each limit point is in H_0^1 .

Approximation properties

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³[T-Du, 2014]

Properties Aii) and Dii)

Aii) Asymptotically compact embedding: ([Bourgain-Brezis-Mironescu, 2001]⁴)

$$\|v_{\delta}\|_{S_{\delta}} \leq C \Longrightarrow \{v_{\delta}\}$$
 is relatively compact in L^2
and each of the limit is in H_0^1

Dii) Let $W_{\delta,h} = \{$ space of p.w polynomials that contains p.w linear functions $\}$, then $\{W_{\delta,h}, \delta \in (0, \delta_0), h \in (0, h_0)\}$ is asymptotically dense in H^1 since

 $\forall v \in H^1, \exists \{v_k \in W_{\delta_k, h_k}\}$ such that $\|v - v_k\|_{H^1} \to 0$ as $k \to \infty$.

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AC schemes for parameterized variational problems

- Theorem 1. Any continuous or discontinuous conforming FEM containing all continuous linear elements is AC, thus is good for both nonlocal and local regimes.
- Theorem 2. Conforming FEM containing only piecewise constant elements is convergent if $h/\delta \rightarrow 0$.
- The framework can be applied to PD systems, uniform/unstructured-mesh & any space dimension.

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Non-variational methods

- 1. Finite difference method ([T-Du, 2013], [Du-Tao-T-Yang, 2018.])
- On uniform grid, we have the AC finite difference discretization

$$\mathcal{L}_{\delta,h}u(\boldsymbol{x}) = \int I_h^k \Big[\frac{u(\boldsymbol{x} + \mathbf{z}) + u(\boldsymbol{x} - \mathbf{z}) - 2u(\boldsymbol{x})}{W_k(\mathbf{z})} \Big] W_k(\mathbf{z}) \gamma_\delta(\mathbf{z}) d\mathbf{z}$$

where k = 0 or k = 1, and $W_0(\mathbf{z}) = |\mathbf{z}|^2$, $W_1(\mathbf{z}) = |\mathbf{z}|^2/|\mathbf{z}|_1$.

• A key property of the discretization is the *quadratic exactness*

$$\mathcal{L}_{\delta,h} \boldsymbol{x}^{\boldsymbol{\alpha}} = \mathcal{L}_{\delta} \boldsymbol{x}^{\boldsymbol{\alpha}}, \ |\boldsymbol{\alpha}| \leq 2.$$

- The scheme satisfies discrete maximum principle (DMP). We have uniform convergence rates $O(h^{k+1})$.
- DMP is lost when going to higher order interpolation ($k \ge 2$).

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Non-variational methods

- 2. Meshfree method ([Leng-T-Foster-Trask, 2019])
- Reproducing kernel (RK) approximations ([Liu, 1995]) are meshfree methods that construct shape functions from sets of scattered data.
 - Function approximation:

$$u(\boldsymbol{x}) pprox u^{RK}(\boldsymbol{x}) = \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}(\boldsymbol{x}) u(\boldsymbol{x}_{\boldsymbol{k}}),$$

► Shape function:

$$\Psi_{\boldsymbol{k}}(\boldsymbol{x}) = C(\boldsymbol{x}, \boldsymbol{x} - \boldsymbol{x}_{\boldsymbol{k}}) \boldsymbol{\phi}_{\boldsymbol{a}}(\boldsymbol{x} - \boldsymbol{x}_{\boldsymbol{k}}),$$

Reproducing condition:

$$\sum_{oldsymbol{k}\in\mathbb{Z}^d}\Psi_{oldsymbol{k}}(oldsymbol{x})oldsymbol{x}_{oldsymbol{k}}^{oldsymbol{lpha}}=oldsymbol{x}^{oldsymbol{lpha}},\quad |oldsymbol{lpha}|\leq p,$$

$$\blacktriangleright \ \mathcal{L}_{\delta} u^{RK}(\boldsymbol{x_i}) = \sum_{\boldsymbol{k}} u(\boldsymbol{x_k}) \int \gamma_{\delta}(|\boldsymbol{y} - \boldsymbol{x_i}|) (\Psi_{\boldsymbol{k}}(\boldsymbol{y}) - \Psi_{\boldsymbol{k}}(\boldsymbol{x_i})) d\boldsymbol{y}$$

• RK collocation method: $-r^h \mathcal{L}_{\delta} u^{RK} = r^h f$ (r^h restricts the function value to the nodes)

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Non-variational methods

2. Meshfree method ([Leng-T-Foster-Trask, 2019])

• $p \ge 2$ preserves *quadratic exactness* naturally. For p = 1, it turns out we also have *quadratic exactness* because of

$$\sum_{\mathbf{k}\in\mathbb{Z}^d}\Psi_{\mathbf{k}}(\boldsymbol{x})\boldsymbol{x}_{\mathbf{k}}^{\boldsymbol{\alpha}} = \boldsymbol{x}^{\boldsymbol{\alpha}} + c, \quad |\boldsymbol{\alpha}| = 2$$

• DMP is lost for all cases. However, we can show the stability of method for p = 1 on bounded domains with rectangular grids. Using *Fourier analysis*, we could show the equivalence of the RK collocation scheme with a RK Galerkin scheme.

 \bullet We have the uniform convergence rates ${\cal O}(h^2)$ for the RK collocation scheme with p=1.

• It is ongoing work (with Leng-Foster-Trask) to extend the analysis to the PD models.

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Fast algorithms

Our next goal is to develop fast algorithm for the nonlocal operator:

$$\mathcal{L}u = \int K(\boldsymbol{x}, \boldsymbol{y})(u(\boldsymbol{y}) - u(\boldsymbol{x}))d\boldsymbol{y}$$

or a sum of the form

$$\sum_{i=1}^N w_{i,j}(u(x_j) - u(x_i))$$

- Direct evaluation of such sums at N target points requires $O(N^2)$ operations
- Algorithms which reduce the cost to O(N^α) (1 ≤ α < 2), O(N log(N))··· are referred to as *fast summation methods*⁵.
- Fast evaluate of the operator is critical in solving time-dependent problems or iterative methods for solving static problems.

⁵Classical fast summation methods include FFT (for translation-invariant kernel with uniform discretization), FMM ([Greengard-Rokhlin 1987]), *H*-matrices ([Hackbusch, 1999])

The kernel $K({m x},{m y})$

- () Non-radial symmetric kernels (such as the kernel with variable nonlocal interaction $\delta(x)$)
 - * FFT-based methods are exact, but fail to work if symmetry is broken.
- **2** Type I singularity: point singularity (x = y).

Example:
$$K(\boldsymbol{x}, \boldsymbol{y}) = rac{1}{|\boldsymbol{y} - \boldsymbol{x}|^2}$$

 \ast The classical FMM and $\mathcal H\text{-matrices}$ techniques are approximate. They deal with point singularity. 6

* The main idea is to take advantage of the smooth far field interaction (off-diagonal blocks of the matrix are low-rank)

3 Type *II* singularity: co-dimension 1 singularity.

Example: nonlocal model with finite interaction distance.

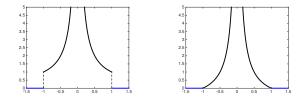
 $K(\boldsymbol{x}, \boldsymbol{y}) = \chi(|\boldsymbol{y} - \boldsymbol{x}| < 1)$

⁶[Lin-Lu-Ying,2001], [Ho-Ying, 2016], [Zhao-Hu-Cai⊨Karmiadakis,201≩] = ೨९९८

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The peridynamics kernel

* The graphs for the typical peridynamics kernels in practice are



* It contains both Type I singularity and Type II singularity ⁷.

* The existing fast algorithms fail to work ([T-Engquist, 2019]).

⁷The non-smooth truncation of kernels also appears as the retarded potentials raised in time domain boundary integral equations, where the potentials are discontinuous functions defined in space-time.

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The splitting of singularities

In practice, the kernel γ contains both Type *I* singularity and Type *II* singularity. We thus propose to split the kernel into two and deal with them separately.

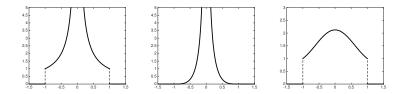


Figure: The kernel $\gamma(s)$ (left) splits into $\kappa(s)$ (middle) and $p(s)\chi(|s| < 1)$ (right).

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The hierarchical subdivision of $\boldsymbol{\Omega}$

Let $L = \log_2(n)$, then from level 1 to L, the computation domain $\Omega = [0, 1]^d$ is hierarchically subdivided into panels. Each panel in the *i*th level can be represented by one of the cubes $\prod^d [\frac{k_j}{2^i}, \frac{k_j + 1}{2^i}]$, $0 \le k_j \le 2^i - 1$.

This forms a tree structure. (In 1d, this forms a binary tree, in 2d a quadtree, and in 3d an octree.)

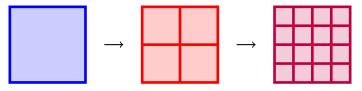
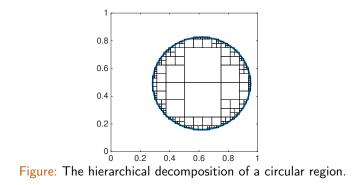


Figure: The hierarchical subdivision of $[0, 1]^2$.



A fast algorithm for the Type II singularity

Step 1. Initialization step. For each x_i , decompose the domain of integration $\{|\boldsymbol{y} - \boldsymbol{x}_i| < \delta(\boldsymbol{x}_i)\} \cap \Omega \text{ using the panels.}$



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Asymptotically compatible schemes

Summary

A fast algorithm for the Type *II* singularity

Step 2. Compute the the partial sums for each tree node. For a given vector $\{u(\boldsymbol{x}_i)\}_{i=1}^N$, we assign the value $u(\boldsymbol{x}_i)$ to a leaf node. Then traverse the tree bottom to top, we assign each parent node the value of the sum of all its children.

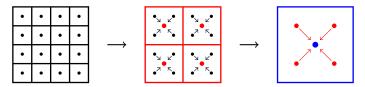


Figure: A 2d example of the process of computing partial sums.

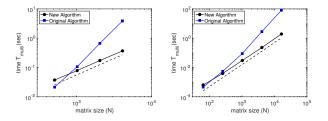
Step 3. For each x_i , use (1) and (2) to calculate the summation $\sum_{j \in \mathcal{N}(x_i)} u(x_i)$.

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Complexity of the algorithm

* The complexity of the algorithm ([T-Engquist, 2019]) is given as

$$\begin{cases} O(N \log N) & \text{for } d = 1; \\ O(N^{2-1/d}) & \text{for } d \ge 2. \end{cases}$$



* For further complexity reduction in higher dimensions, it would be natural to use different geometries than boxes, for example, curvelets [Candes-Donoho,2000] in 2d deals efficiently with line discontinuities.

Homogenization and nonlocal effects ⁸

- The PD community claimed that nonlocal interactions necessarily appear in a homogenized model of heterogeneous system ([Silling, 2014]), but rigorous mathematical theory remains largely missing.
- The classical homogenization theory shows that nonlocal effects could be induced by homogenization, such as [Bensoussan-Lions-Papanicolaou, 1978], [Tartar, 1989].
- Numerical homogenization also connects to nonlocal effects, such as the projection-based method [Dorobantu-Engquist,1998], or generalized FEM based on subspace decomposition [Gallistl-Peterseim,2016].
- Here we the model of wave propagation to illustrative the origin of nonlocality through homogenization.

⁸See [Du-Engquist-T, 2019].

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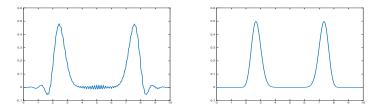
Homogenization of wave equation

• Consider wave propagation through a periodic medium

$$\partial_t^2 u^\epsilon(x,t) = \operatorname{div}\left(A(x/\epsilon)\nabla u^\epsilon\right)$$

• The classical homogenization theorem give a non-dispersive effective model

 $\partial_t^2 u^0(x,t) = \operatorname{div}(\bar{A}\nabla u^0(x,t))\,,$



• u^0 is an $O(\epsilon)$ approximation of u^{ϵ} only for finite time ([Bensoussan-Lions-Papanicolaou, 1978], [Lin-Shen, 2019]).

Dispersive effective model

• [Santosa-Symes, 1991] were the first that gave a dispersive effective model by using Bloch wave expansion.

• Loosely speaking, their model is of the form $\partial_t^2 u = \bar{L}^{\epsilon} u$, with $\bar{L}^{\epsilon} \approx \Delta + \epsilon^2 (\Delta)^2$, and the effective model is an $O(\epsilon)$ approximation when time scale $t \sim O(\epsilon^{-2})$. The equation is actually ill-posed due to the $(\Delta)^2$ term, although it can be made well-posed by a classical Boussinesq trick.

• To get an $O(\epsilon)$ approximation for all time $t \in (0, \infty)$, it is necessary for \bar{L}^{ϵ} to be a nonlocal operator.

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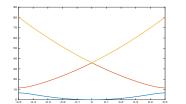
Bloch wave analysis

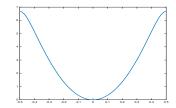
• Consider the eigenvalue problem for $-\operatorname{div}(A(x)\nabla)$:

 $-{\rm div}\left(A(x)\nabla u(x)\right)=\lambda u\,.$

For any real vector $k \in \mathbb{R}^d$, there exists eigenfunctions $\{\psi_m(x,k) = e^{2\pi i k \cdot x} \phi_m(x,k)\}_{m=0}^{\infty}$ and eigenvalues $\{\lambda_m(k)\}_{m=0}^{\infty}$.

• For the ϵ -problem, $\psi_m^{\epsilon}(x,k) := \psi_m(x/\epsilon,\epsilon k), \quad \lambda_m^{\epsilon}(k) = \frac{1}{\epsilon^2}\lambda_m(\epsilon k).$





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Bloch wave analysis

 \bullet The solution u^ϵ with initial condition $u^\epsilon(x,0)=f(x)$ is written as the expansion:

$$u^{\epsilon}(x,t) = \sum_{m=0}^{\infty} \int_{Z/\epsilon} \hat{f}_m(k) \psi^{\epsilon}_m(x,k) e^{\pm it\sqrt{\lambda^{\epsilon}_m(k)}} dk \,.$$

 \bullet First observation: for smooth initial condition, the higher eigenmodes $m\geq 1$ could be neglected. By defining

$$u_0^{\epsilon}(x,t) = \int_{Z/\epsilon} \hat{f}_0(k) \psi_0^{\epsilon}(x,k) e^{\pm it \sqrt{\lambda_0^{\epsilon}(k)}} dk \,,$$

we have $\|u^{\epsilon}(\cdot,t) - u_0^{\epsilon}(\cdot,t)\| = O(\epsilon)$ for $t \in (0,\infty)$.

• Second observation: u_0^ϵ can be further simplified by replacing $\hat{f}_0(k)$ and ψ_0^ϵ with the Fourier transform $\hat{f}(k)$ and the Fourier mode $e^{2\pi i k \cdot x}$ respectively:

$$\bar{u}^{\epsilon}(x,t) = \int_{Z/\epsilon} \hat{f}(k) e^{2\pi i k \cdot x} e^{\pm i t \sqrt{\lambda_0^{\epsilon}(k)}} dk \,,$$

then $\|u_0^{\epsilon}(\cdot,t) - \bar{u}^{\epsilon}(\cdot,t)\| = O(\epsilon)$ for $t \in (0,\infty)$.

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Nonlocal effective equation

• If $\hat{f}(k) \subset Z/\epsilon$, then

$$\bar{u}^{\epsilon}(x,t) = \int \hat{f}(k) e^{2\pi i k \cdot x} e^{\pm i t \sqrt{\lambda_0^{\epsilon}(k)}} dk \,,$$

• \bar{u}^{ϵ} satisfies

$$\partial_t^2 \bar{u}^{\epsilon}(x,t) = \bar{L}^{\epsilon} u = \int \gamma^{\epsilon} (y-x)(u(y)-u(x))dy,$$

and

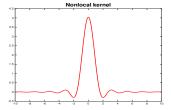
$$\int \gamma^{\epsilon}(s)(1-e^{2\pi ik\cdot s})ds = \lambda_0^{\epsilon}(k)$$

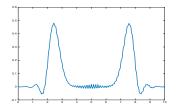
• Since $\lambda_0^{\epsilon}(k) = \frac{1}{\epsilon^2} \lambda_0(\epsilon k)$, then we have $\gamma^{\epsilon}(s) = \frac{1}{\epsilon^3} \gamma(\frac{s}{\epsilon})$

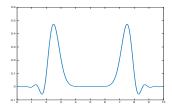
 \bullet In general $\lambda_0^\epsilon(k)$ is not a polynomial of k, we have \bar{L}^ϵ to be a nonlocal operator. 9

⁹[Peetre, 1959]

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Summary

- We presented some numerical analysis of a class of nonlocal models such as those represented by nonlocal diffusion or the peridynamic model of continuum mechanics.
- There is a class of robust discretization of parameterized nonlocal models called the AC schemes (variational and non-variational). We also discussed a new FMM type fast algorithm type method for kernels that exhibit singularities on codimension 1 sets.
- We used wave propagation to illustrate how nonlocality could be originated from homogenization of heterogeneous materials.
- The mathematical framework contains nonlocal calculus of variations and asymptotically compatible schemes that may have broad applications. Indeed, many concepts can be related to fractional calculus (for anomalous diffusion and Levy processes), nonlocal means (for imaging analysis) graph calculus/diffusion maps, SPH/RKPM (for numerical approximations),
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[1] X. Tian and Q. Du, Analysis and comparison of different approximations to nonlocal diffusion and linear peridynamic equations, SIAM J. Numer. Anal., 51: 3458-3482, 2013.

[2] X. Tian and Q. Du, Asymptotically compatible schemes and applications to robust discretization of nonlocal models, SIAM J. Numer. Anal. 52:1641-1665, 2014. (to appear in March 2020 SIGEST section of SIAM Review)

[3] Q. Du, Y. Tao, X. Tian and J. Yang. Asymptotically compatible numerical approximations of multidimensional nonlocal diffusion models and nonlocal Green's functions, IMA J. Numer. Anal., 39(2),607-625, 2018.

[4] Y. Leng, X. Tian and J. Foster. Super-convergence of reproducing kernel approximation, Comput. Methods Appl. Mech. Eng., 352(1):488-507, 2019.

[5] Y. Leng, X. Tian, N. Trask and J. Foster, Asymptotically compatible reproducing kernel collocation and meshfree integration for nonlocal diffusion, 2019.

[6] X. Tian and B. Engquist, Fast algorithm for computing nonlocal operators with finite interaction distance, to appear in Comm. Math. Sci., 2019.

 [7] Q. Du, B. Engquist and X. Tian, Multiscale Modeling, Homogenization and Nonlocal Effects: Mathematical and Computational Issues, to appear in Math. Comput., 2019. (Special issue on Celebrating 75 Years of Mathematics of Computation). Thank you!