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Mini-Workshop: Mathematical Analysis for Peridynamics

Organised by
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January 16th – January 22nd, 2011

Abstract. A mathematical analysis for peridynamics, a nonlocal elastic theory, is the subject of the mini-workshop. Peridynamics is a novel multiscale mechanical model where the canonical divergence of the stress tensor is replaced by an integral operator that sums forces at a finite distance. As such, the underlying regularity assumptions are more general, for instance, allowing discontinuous and non-differentiable displacement fields. Although the theoretical mechanical formulation of peridynamics is well understood, the mathematical and numerical analyses are in their early stages. The mini-workshop proved to be a catalyst for the emerging mathematical analyses among an international group of mathematicians.

Mathematics Subject Classification (2000): 35S11, 70G70, 70G75, 74B20.

Introduction by the Organisers

The mini-workshop *Mathematical Analysis for Peridynamics*, organised by Etienne Emmrich (Bielefeld), Max Gunzburger (Tallahassee), and Richard Lehoucq (Albuquerque), was held January 16th–January 22nd, 2011. This meeting was attended by 17 participants with broad geographic representation.

The response of materials to environments and loads occurring in practice requires an understanding of mechanics at disparate spatial and temporal scales. Such "multiscale" understanding is a fundamental challenge for next generation materials modeling. A currently popular multiscale approach couples two or more well-known models, for example, molecular dynamics and classical elasticity, each of which is useful at different scales. Although some notable successes have resulted from this type of multiscale material modeling, some issues remain unresolved, some of which stem from the inherent difficulty encountered when coupling local models to nonlocal ones.

An alternative approach is to develop a single multiscale material model that remains valid and useful over a wide range of temporal and spatial scales. Peridynamics [5], a nonlocal elastic theory, is a promising multiscale mechanical nonlinear model. The canonical divergence of the stress tensor is replaced by an integral operator that sums forces at a finite distance. As such, the underlying regularity assumptions are more general, for instance, allowing discontinuous, let alone non-differentiable, displacement fields. For example, the recent review [1] includes peridynamic applications to fracture and failure of composites, nanofiber networks, and polycrystal fracture. The article [7] studies the peridynamic model for solid mechanics. Furthermore, although peridynamics by itself is a multiscale material model and has proved to be extremely useful for simulations of singular phenomena such as fracture, peridynamics also can be used as bridge between local continuum models and nonlocal atomistic models, mitigating the difficulties one encounters when trying to directly couple the latter two types of models.

The goal of the mini-workshop is to bring together applied and computational mathematicians, and mechanicians to further the mathematical understanding of peridynamics. Although the theoretical mechanical formulation of peridynamics is well understood, the mathematical and numerical analyses are in their early stages (see [2, 3, 4, 6] for examples). Successful mathematical treatments of peridynamics are not only interesting from the mathematics point of view, but will lead to improved temporal and spatial multiscale discretization and solution algorithms, and improved understanding of the range of applicability of peridynamics. Topics of interest include:

- well posedness of the time-dependent peridynamics equation of motion; Nonlocal vector calculus, variational formulations of peridynamic models; homogenization; stochastic peridynamic models;
- analysis and development of a finite element and other discretization methods; development and analysis of efficient and robust solution methods for discretized peridynamic models; coupling peridynamics to molecular dynamics and finite element discretizations of classical elasticity;
- relationship and convergence to classical elasticity as the nonlocality vanishes; relationship with other nonlocal continuum mechanical theories.

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Mini-Workshop: Mathematical Analysis for Peridynamics

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Abstracts

Multiscale Dynamics of Heterogeneous Media in the Peridynamic Formulation

Robert Lipton
(joint work with Bacim Alali)

A methodology is presented for investigating the dynamics of heterogeneous media using the nonlocal continuum model given by the peridynamic formulation [2]. The approach presented here provides the ability to model the macroscopic dynamics while at the same time resolving the dynamics at the length scales of the microstructure. Central to the methodology is a novel two-scale evolution equation. The rescaled solution of this equation is shown to provide a strong approximation to the actual deformation inside the peridynamic material. The two scale evolution can be split into a microscopic component tracking the dynamics at the length scale of the heterogeneities and a macroscopic component tracking the volume averaged (homogenized) dynamics. The interplay between the microscopic and macroscopic dynamics is given by a coupled system of evolution equations. The equations show that the forces generated by the homogenized deformation inside the medium are related to the homogenized deformation through a history dependent constitutive relation.

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A nonlocal vector calculus and finite element methods for nonlocal diffusion and mechanics

Max Gunzburger
(joint work with Xi Chen, Qiang Du, Richard Lehoucq, Kun Zhou)

Let $\mathbf{x}$ and $\mathbf{y}$ denote points in $\mathbb{R}^d$. The *nonlocal divergence operator*

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) := -\int_\Omega \big(\boldsymbol{\nu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\nu}(\mathbf{y},\mathbf{x})\big) \cdot \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

where $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})$ is a given anti-symmetric function, maps vector functions of $\boldsymbol{\nu}(\mathbf{x},\mathbf{y})$ to scalar functions of $\mathbf{x}$. Likewise, we have the *nonlocal gradient operator* (mapping scalars to vectors)

$$\mathcal{G}\big(\eta\big)(\mathbf{x}) := -\int_\Omega \big(\eta(\mathbf{x},\mathbf{y}) + \eta(\mathbf{y},\mathbf{x})\big)\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega$$

and, in $\mathbb{R}^3$, the *nonlocal curl operator* (mapping vectors to vectors)

$$\mathcal{C}(\boldsymbol{\mu})(\mathbf{x}) := -\int_\Omega \big(\boldsymbol{\mu}(\mathbf{x},\mathbf{y}) + \boldsymbol{\mu}(\mathbf{y},\mathbf{x})\big) \times \boldsymbol{\alpha}(\mathbf{x},\mathbf{y})\, d\mathbf{y} \quad \text{for } \mathbf{x} \in \Omega.$$

One easily obtains the *nonlocal integral theorems* analogous to the Gauss and Stokes theorems of the differential calculus. For example, we have the nonlocal Gauss theorem

$$\int_\Omega \mathcal{D}(\boldsymbol{\nu})\, d\mathbf{x} = 0.$$

Adjoint operators may also be defined, e.g., the *adjoint of* $\mathcal{D}$ is given by

$$\mathcal{D}^*\big(u\big)(\mathbf{x},\mathbf{y}) = (u' - u)\boldsymbol{\alpha} \quad \text{for } \mathbf{x},\mathbf{y} \in \Omega.$$

One can then define nonlocal Green's identities such as

$$\int_\Omega u\mathcal{D}\big(\mathcal{D}^*(v)\big)\, d\mathbf{x} - \int_\Omega \int_\Omega \mathcal{D}^*(u) \cdot \mathcal{D}^*(v)\, d\mathbf{y} d\mathbf{x} = 0.$$

The nonlocal operators also satisfy identities such as

$$\mathcal{D}\big(\mathcal{C}^*(\mathbf{u})\big) = 0 \qquad \text{and} \qquad \mathcal{C}\big(\mathcal{D}^*(u)\big) = \mathbf{0}$$

that mimic similar identities of the differential calculus.

By dividing the domain Ω into the disjoint subdomains Ω_s, Ω_{c1}, and Ω_{c2}, one can define nonlocal *constrained-value problems* that mimic classical elliptic boundary-value problems with Dirichlet and Neumann boundary conditions. For example, we have the following analog of the Poisson problem:

$$\mathcal{D}\big(\mathcal{D}^*(u)\big) = f \text{ in } \Omega, \qquad u = g \text{ in } \Omega_{c1}, \qquad \mathcal{N}\big(\mathcal{D}^*(u)\big) = h \text{ in } \Omega_{c2},$$

where $\mathcal{N}$ is an appropriately defined constraint operator. Nonlocal constrained-value problems have application to nonlocal diffusion and to nonlocal mechanics through the peridynamics model.

The nonlocal operators may be related, in a distributional sense to the analogous differential operators, e.g., if we set $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = \nabla_\mathbf{y}\delta(\mathbf{y}-\mathbf{x})$ or $|\boldsymbol{\alpha}(\mathbf{x},\mathbf{y})|^2 = \frac{1}{2}\Delta_\mathbf{y}\delta(\mathbf{y}-\mathbf{x})$, where Δ denotes the differential Laplace operator, we respectively have that

$$\mathcal{D}\big(\boldsymbol{\nu}\big)(\mathbf{x}) = \nabla \cdot \boldsymbol{\nu}(\mathbf{x},\mathbf{x}) \qquad \text{or} \qquad \mathcal{D}\big(\mathcal{D}^* u(\mathbf{x})\big) = -\Delta u(\mathbf{x}).$$

One can also define weighted averages of the nonlocal operators, e.g., for a weight function $\omega(\mathbf{x},\mathbf{y})$, we have the *weighted nonlocal divergence* operator

$$\mathcal{D}_\omega(\mathbf{u})(\mathbf{x}) := \mathcal{D}\big(\omega(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{x})\big)(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega.$$

If we choose $\boldsymbol{\alpha}(\mathbf{x},\mathbf{y}) = (\mathbf{y}-\mathbf{x})/|\mathbf{y}-\mathbf{x}|$ for $\mathbf{x} \neq \mathbf{y}$ and

$$\omega(|\mathbf{x}-\mathbf{y}|) = \begin{cases} |\mathbf{y}-\mathbf{x}|\phi(|\mathbf{y}-\mathbf{x}|) & \mathbf{y} \in B_\varepsilon(\mathbf{x}) \\ 0 & \text{otherwise} \end{cases}$$

where, for $\varepsilon > 0$, $B_\varepsilon(\mathbf{x}) := \{\mathbf{y} \in \mathbb{R}^d \,:\, |\mathbf{y}-\mathbf{x}| < \varepsilon\}$, one can show that $\mathcal{D}_\omega$ is a bounded linear operators from $H^t(\mathbb{R}^d)$ to $H^{t-s}(\mathbb{R}^d)$ for $0 \le s \le 1$, where s depends on the particular choice for ϕ. Moreover, if $\mathbf{u} \in [H^1(\mathbb{R}^d)]^d$, then $\mathcal{D}_\omega(\mathbf{u}) \to \nabla \cdot \mathbf{u}$, where the convergence as $\varepsilon \to 0$ is with respect to $L^2(\mathbb{R}^d)$.

We have focused on just the nonlocal divergence operator; similar results hold for the nonlocal gradient and curl operators. See [2, 3, 4, 5] for details.

Variational formulations of nonlocal constrained-value problems can be used to define finite element approximations; see, e.g., [2] for one-dimensional examples. One important feature of nonlocal constrained-value problems is that, with appropriate choices for kernels, solutions operators effect less smoothing than elliptic differential operators. In fact, one can choose a kernel such that no smoothing occurs, i.e., the nonlocal operator maps $L(\mathbb{R}^d)$ to $L(\mathbb{R}^d)$. As a result, solutions with jump discontinuities are admissible to the variational formulation. As a consequence, discontinuous finite element approximating spaces are *conforming* and can be used to advantage to approximate solutions containing jump discontinuities. Several observations are made in [2] based on computational experimentation. First, the use of continuous finite element spaces yields optimally accurate approximations for the case of smooth solutions of the constrained-value problems, but are not appropriated for solutions with jump discontinuities. Piecewise constant approximations are not robust in the sense that whenever the cutoff radius ε is greater than the grid size, approximations fail to converge. However, discontinuous piecewise linear approximations are robust with respect the relative sizes of ε and the grid. Moreover, abrupt refinement in the neighborhood of discontinuities can be used to obtain optimally accurate approximations. A key conclusion is that finite element discretizations can be to define multiscale computational models for nonlocal diffusion and mechanics problems. Indeed, by refining the grid so that $h < \varepsilon$, where h denotes a measure of the grid size, in regions where solution singularities occur and coarsening the grid so that $\varepsilon \ll h$ in regions where the solution is smooth, one defines a single model that can resolve phenomena occurring at disparate scales; see [1] for details.

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The Cauchy problem for a non-linear peridynamic equation

Albert Erkip
(joint work with Husnu A. Erbay, Gulcin M. Muslu)

We consider the one-dimensional nonlinear nonlocal partial differential equation, arising in the peridynamic modelling of an elastic bar,

$$u_{tt} = \int_{\mathbb{R}} \alpha(y-x)w(u(y,t)-u(x,t))dy, \ x \in \mathbb{R}, \ t > 0. \tag{1}$$

Our motivation is to understand the effect of nonlinearity in this model so that the ideas can be carried over to more general peridynamic problems. This work extends some ideas in [1, 2, 3] to the nonlinear case.

We assume that $\alpha \in L^1(\mathbb{R})$ and that w is a sufficiently smooth function. These assumptions yield estimates for the operator

$$(Kv)(x) = \int_{\mathbb{R}} \alpha(y-x)w(v(y)-v(x))dy,$$

which in turn yield the local well posedness of the Cauchy problem with solution in the spaces $C^2([0,T],X)$ where X is any of the spaces $C_b(\mathbb{R})$ (continuous and bounded functions), $C_b^1(\mathbb{R})$, $L^p(\mathbb{R})$, or $W^{1,p}(\mathbb{R})$ with $1 \leq p \leq \infty$.

As an example of how our results can be modified to more general peridynamic problems, we prove:

Theorem *Consider the Cauchy problem for the equation*

$$u_{tt} = \int_{\mathbb{R}} f(u(y,t)-u(x,t), y-x)dy.$$

Assume that $f(0,\eta)=0$ and $f(\xi,\eta)$ is measurable in η for each ξ and continuously differentiable in ξ for almost all η. Moreover, suppose that for each $R>0$, there are integrable functions Λ_1^R, Λ_2^R satisfying

$$|f(\xi,\eta)| \leq \Lambda_1^R(\eta), \ |f_\xi(\xi,\eta| \leq \Lambda_2^R(\eta)$$

for almost all η and for all $|\xi| \leq 2R$. Then there is some $T>0$ such that the Cauchy problem is well posed with solution in $C^2([0,T],C_b(\mathbb{R}))$ for initial data in $C_b(\mathbb{R})$.

For the maximal life of a solution, we show that the solution can be continued as long as $\|u\,(t)\,\|_\infty$ does not blow up. When $\alpha \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$ we prove global existence for nonlinearities of the form $w(\xi) = a|\xi|^{\nu-1}\xi$ with $\nu \leq 3$ and $a > 0$. We also give sufficient conditions on the nonlinearity, that ensure blow-up in finite time.

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Viscoelastic effects in non-local elasticity

Olaf Weckner
(joint work with Nik Abdullah Nik Mohamed)

The equation of motion at time t for the material point x with density ρ in a homogeneous, infinite[1], viscoelastic, peridynamic material in one spatial dimension is given by

$$(1) \qquad \rho\,\ddot{u}(x,t) = \int_{-\infty}^{+\infty} c(x'-x)[\,u(x',t)-u(x,t)\,]dx' + \int_{-\infty}^{+\infty} d(x'-x)[\,u(x',t)-u(x,t)\,]^{\cdot}dx' + b(x,t)$$

$u(x,t)$ is the displacement field, $b(x,t)$ a given external force field, $c(\xi)=c(-\xi)$ is the so-called micromodulus function or stiffness distribution and $d(\xi)=d(-\xi)$ is the damping distribution. Additionally, we are given the initial data $u_0(x)=u(x,t=0), v_0(x)=\dot{u}(x,t=0)$. In the following we will derive an integral representation for the non-local, peridynamic solution.
1 represents an slight extension of the bond-based peridynamic material model introduced initially in [1]. The solution method outline in the following is based on [2].

Equation of motion in (k,t) space. Applying the Fourier-transform with respect to the spatial coordinate x we can equivalently characterize the nonlocal equation of motion (1) by

$$(2) \qquad \ddot{\bar{u}}(k,t) + 2D(k)\bar{u}(k,t)^{\cdot} + \omega_0^2(k)\bar{u}(k,t) = \bar{b}(k,t)/\rho$$

with

$$\omega_0^2(k) = \frac{\bar{c}(0)-\bar{c}(k)}{\rho}$$
$$2D(k) = \frac{\bar{d}(0)-\bar{d}(k)}{\rho}$$

The transformed initial conditions are

$$\bar{u}^0(k) = \mathcal{F}\{u^0(x)\}$$
$$\bar{v}^0(k) = \mathcal{F}\{v^0(x)\}$$

[1]It is physically intuitive that as the distance between a pair of particles gets very large, the interaction between them becomes negligible. In what follows we shall assume that this happens fast enough to ensure the convergence of the various infinite integrals encountered.

Equation of motion in (k,s) space. Applying the LAPLACE-transform with respect to time t we obtain

$$s^2\tilde{u}(k,s) - s\bar{u}^0(k) - \bar{v}^0(k) + 2D(k)(s\tilde{u}(k,s) - \bar{u}^0(k)) + \omega_0^2(k)\tilde{u}(k,s) = \tilde{b}(k,s)/\rho$$

which can be solved for $\tilde{u}(k,s)$

$$\tilde{u}(k,s) = \frac{\tilde{b}(k,s)/\rho + \bar{v}^0(k) + \bar{u}^0(k)(s+2D(k))}{s^2 + 2D(k)s + \omega_0^2(k)}$$

1. Integral representation of the solution

Assuming weak damping $\omega_0^2(k) > D^2(k)\,\forall k$ we find the following LAPLACE-transforms

$$\mathcal{L}^{-1}\{\frac{1}{s^2+2D(k)s+\omega_0^2(k)}\} = \frac{e^{-D(k)t}\sin(\omega_d(k)\,t)}{\omega_d(k)}$$

$$\omega_d(k) = \sqrt{\omega_0^2(k) - D^2(k)}$$

$$\mathcal{L}^{-1}\{\bar{v}^0(k) + \bar{u}^0(k)(s+2D(k))\} = \dot{\Delta}(t)\bar{u}^0(k) + \Delta(t)\left(\bar{v}^0(k) + 2D(k)\bar{u}^0(k)\right)$$

In the undamped case $D(k) = 0, \omega_d(k) = \omega_0(k)$. Next, we can use the convolution theorem of LAPLACE-transforms to obtain the solution in FOURIER (k,t) space:

$$\begin{aligned}\bar{u}(k,t) &= \int_0^t \frac{e^{-D(k)\tau}\sin(\omega_d(k)\,\tau)}{\omega_d(k)}\frac{\bar{b}(k,t-\tau)}{\rho}d\tau + \\ & e^{-D(k)t}[\bar{v}^0(k)\frac{\sin(\omega_d(k)\,t)}{\omega_d(k)} + \bar{u}^0(k)\left(\cos(\omega_d(k)\,t) - D\frac{\sin(\omega_d(k)\,t)}{\omega_d(k)}\right)]\end{aligned}$$

Finally we use the convolution theorem of FOURIER-transforms to obtain the following integral representation of the solution of equation (1) in (x,t) space.

$$\begin{aligned}u(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_0^t \frac{e^{-D(k)\tau}\sin(\omega_d(k)\,\tau)}{\omega_d(k)}\frac{\bar{b}(k,t-\tau)}{\rho}d\tau e^{ikx}dk \\ &+ \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-D(k)t}[\bar{v}^0(k)\frac{\sin(\omega_d(k)\,t)}{\omega_d(k)} \\ &+ \bar{u}^0(k)\left(\cos(\omega_d(k)\,t) - D(k)\frac{\sin(\omega_d(k)\,t)}{\omega_d(k)}\right)]e^{ikx}dk\end{aligned}$$

2. Example

Concentrating on an impact loading with no initial data

$$\begin{aligned}b(x,t) &= \hat{b}\Delta(x-x_0)\Delta(t-t_0) \leftrightarrow \bar{b}(k,t) = \hat{b}e^{-ikx_0}\Delta(t-t_0) \\ u_0(x) &= v_0(x) \equiv 0\end{aligned}$$

we obtain the GREEN's function

$$u(x,t) = \frac{\hat{b}}{2\pi\rho}\int_{-\infty}^{+\infty}\frac{e^{-D(k)(t-t_0)}\sin(\omega_d(k)\,(t-t_0))}{\omega_d(k)}e^{ik(x-x_0)}dk$$

As an example we assume that both stiffness and damping have a GAUSSian distribution

$$
\begin{aligned}
c(\xi) &= \hat{c}e^{-(\frac{\xi}{\ell_c})^2} \leftrightarrow \bar{c}(k) = \hat{c}\ell_c\sqrt{\pi}e^{-\frac{1}{4}k^2\ell_c^2} \\
d(\xi) &= \hat{d}e^{-(\frac{\xi}{\ell_d})^2} \leftrightarrow \bar{d}(k) = \hat{d}\ell_d\sqrt{\pi}e^{-\frac{1}{4}k^2\ell_d^2}
\end{aligned}
$$

Then the square of the damped oscillation frequency is given by

$$
\begin{aligned}
\frac{\omega_d^2(k)}{\hat{c}\,\ell_c/\rho} &= \sqrt{\pi}\left(1 - e^{-\frac{\kappa^2(k)}{4}}\right) - \lambda\frac{\pi}{4}\left(1 - e^{-\frac{1}{4}\eta^2\kappa^2(k)}\right)^2 \\
\kappa(k) &= k\,\ell_c \\
\eta &= \frac{\ell_d}{\ell_c} \\
\lambda &= \frac{\hat{d}\,\ell_d^2}{\hat{c}\,\ell_c\,\rho}
\end{aligned}
$$

The following plot showed the damped oscillation frequency for $\eta = 1$ so both damping and stiffness distribution have the same length-scale.

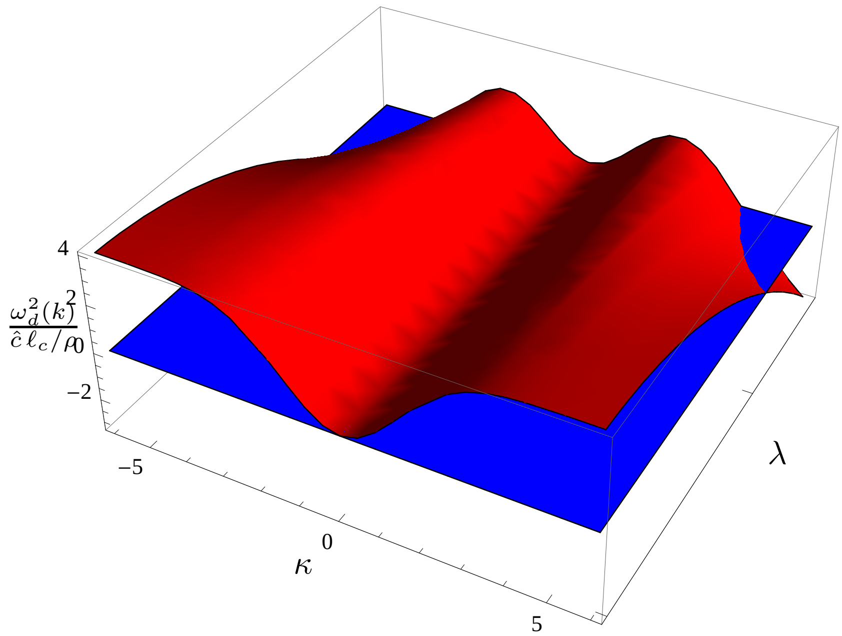

FIGURE 1. The effect of damping and wave-number on the normalized oscillation frequency

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Mathematical and numerical analysis of linear peridynamic models

Qiang Du
(joint work with Kun Zhou)

Peridynamics has been proposed by Silling as a new continuum materials theory which incorporates the modeling of long-range forces within a continuous body and allows a consistent atomistic to continuum coupling. In this talk, we present some mathematical and numerical analysis of some linear peridynamic models. We use some simple setting to illustrate a number of interesting properties associated with the peridynamic models. Examples include:
1) Basic questions on the well-posedness of Cauchy problems [2] and nonlocal boundary-initial value problems for time-dependent models, and nonlocal boundary value problems for the steady state models [1];
2) Spectral analysis, coercivity and Poincare inequalities and elliptic smoothing properties associated with the linear peridynamic operators and their implications;
3) Nonlocal boundary value problems for a two dimensional system that is a nonlocal analog of the conventional Navier equation with greased wall boundary conditions; Spectral analysis for the vector-valued peridynamic operator and related Korn's inequality for the special nonlocal boundary condition [1];
4) Convergence of solutions to peridynamic model to that of classical PDE models;
5) Error estimates and condition number estimates for the finite dimensional numerical approximations to the linear peridynamic models [1];
6) (Jointly with Gunzburger and Lehoucq) Application of the nonlocal vector calculus framework developed in [3] for the linearized peridynamic state solid model.

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A model for nonlocal advection

James Kamm
(joint work with Richard Lehoucq, Michael Parks)

This work describes an approach to nonlocal, nonlinear advection in one dimension, extending the usual pointwise concepts to account for nonlocal contributions to the fluxes. The spatially nonlocal operators that are considered do not involve derivatives. Instead, they involve integral operators that, in the appropriate limit, reduce to the familiar local equations. Such nonlocal models are inherently multiscale. Many classical local models, e.g., the one-way wave equation or the inviscid Burgers' equation, do not possess a length scale and, so, are scale invariant; that is, for any rescaling of space, there exists a related re-scaling of the field from which the original equation is recovered. Thus, these local models do not change their behavior as a function of the length scale to which they are applied. In contrast, nonlocal models can be constructed to have identifiable and controllable length scales, allowing them to manifest different response at different length scales; see [3] for details.

These ideas of nonlocality motivate the approach upon which peridynamics is built. Peridynamics [4, 5] is a nonlocal continuum theory developed for and successfully applied to elastic material response, including phenomena such as material failure. Instead of the usual peridynamics equations corresponding to elastic waves, here we consider a nonlocal, nonlinear advection equation. We focus on model equations that capture the fundamental character of nonlocal advection phenomena. Our ultimate goal is to develop an approach to nonlocal advection that is compatible with the peridynamics framework. As a first step, we develop a nonlocal, inviscid Burgers equation as an nonlinear example of these ideas.

The fundamental representation of advection in one dimension is given by

$$u_t + f(u)_x = 0 \quad \text{or} \quad u_t + f'(u)\, u_x = 0\,, \tag{1}$$

where the second equality holds for f differentiable in u and u differentiable in x. The simplest nonlinear case is given by a flux function quadratic in u, $f(u) = u^2/2$, yielding the well-known inviscid Burgers equation,

$$u_t + \big(u^2/2\big)_x = 0 \quad \text{or} \quad u_t + u\, u_x = 0\,, \tag{2}$$

where, again, the second form holds for u differentiable in x. This equation is a simple yet powerful model for shock phenomena, as it leads to the development of shocks in finite time for smooth-but-nontrivial initial conditions and forms a basis for exploring fundamental shock wave concepts, such as the entropy.

The literature contains several instances of what can be broadly termed “nonlocal advection.” None of these approaches, however, couches the advection operator in a manner consistent with peridynamic theory. Instead, we consider a generalization of the flux term and posit the following integro-differential equation:

$$\begin{aligned} u_t(x,t) + \int_{\mathbb{R}} \psi\bigg(\frac{u(y,t)+u(x,t)}{2}\bigg)\phi_a(y,x)\,dy &= 0\,, \qquad && (x,t) \in \mathbb{R}\times(0,\infty)\,,\\ u(x,0) &= g(x)\,, && x \in \mathbb{R}\,, \end{aligned} \tag{3}$$

where the kernel $\phi(y,x)$ (called the *micromodulus* in peridynamics) is antisymmetric in its arguments: $\phi_a(y,x) = -\phi_a(x,y)$. This equation represents a nonlocal, nonlinear conservation law for advection. Setting the kernel to the derivative of the Dirac delta distribution, i.e., $-\partial\delta(y-x)/\partial y$, it can be shown that this nonlocal equation is equivalent to its local counterpart in the sense of distributions. Moreover, for (3) on any finite interval (a,b), using the antisymmetry of the kernel and extending the (a,b) to the entire line gives the result that $\frac{d}{dt}\int_{\mathbb{R}} u(x,t)\,dx = 0$, demonstrating that $\int_{\mathbb{R}} u(x,t)\,dx = \int_{\mathbb{R}} g(x)\,dx$ is a conserved quantity.

Regularization of inviscid advection equations plays an important role in the associated physics and mathematics. We propose a regularization of the (inviscid) nonlocal advection equation (3) that is a variation of the convection-diffusion equation introduced by Ignat and Rossi [1] of the form:

$$\begin{aligned} u_t(x,t) + \int_{\mathbb{R}} \psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\phi_a(y,x)\,dy &= \epsilon\,\mathcal{L}u(x,t),\; (x,t)\in\mathbb{R}\times(0,\infty)\,, \\ u(x,0) &= g(x)\,, \qquad\qquad x\in\mathbb{R}\,, \end{aligned} \tag{4}$$

where

$$\mathcal{L}u(x,t) := \int_{\mathbb{R}} \big(u(y,t)-u(x,t)\big)\,\phi_s(y,x)\,dy\,, \qquad (x,t)\in\mathbb{R}\times(0,\infty)\,, \tag{5}$$

with the kernel ϕ_s symmetric in its arguments: $\phi_s(y,x) = \phi_s(x,y)$.

We obtain a conservative numerical scheme for 1-D inviscid nonlocal equations as an analogue of classical conservative numerical schemes. Divide the spatial domain into cells $(x_{i-1/2}, x_{i+1/2})$, each of width Δx, and let time be divided into discrete intervals (t^n, t^{n+1}) of extent Δt. We propose a nonlocal Lax-Friedrichs method of the form:

$$\overline{u}_i^{n+1} = \frac{\overline{u}_{i-1}^n + \overline{u}_{i+1}^n}{2} - \frac{\Delta t}{\Delta x}\Psi(x_{i-1/2}, x_{i+1/2}, t^n)\,, \tag{6}$$

where $\overline{u}_i^n$ denotes the value of u at t^n spatially averaged over the cell centered at x_i. We write an exact quadrature for this scheme as

$$\Psi\left(x_{i-1/2}, x_{i+1/2}, t\right) = \sum_{j=-r}^{r} \omega_j \psi\left(\frac{u_h(x_{i+j},t)+u_h(x_i,t)}{2}\right)\phi_a(x_{i+j},x_i)(\Delta x)^2\,, \tag{7}$$

with

$$\omega_j = \begin{cases} 0\,, & j=0\,,\\ 1\,, & j=\pm1,\ldots,\pm(r-1)\,,\\ 1/2\,, & j=-r,r\,. \end{cases} \tag{8}$$

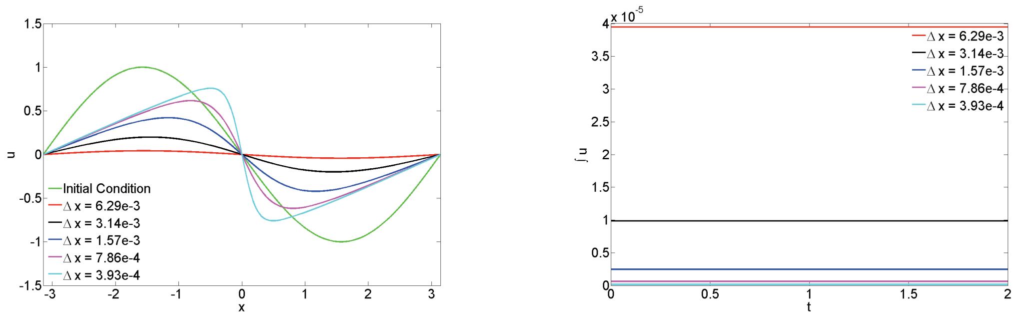
We apply this method to a nonlocal Burgers equation of the form

$$u_t(x,t) + \frac{1}{2}\int_{-\pi}^{\pi}\left(\frac{u(y,t)+u(x,t)}{2}\right)^2\phi_a(y,x)\,dy = 0\,,\; x\in[-\pi,\pi)\,, \tag{9}$$

with periodic boundary conditions and the kernel given by

$$\phi_a(y,x) = \frac{1}{\varepsilon^2}\begin{cases} -1\,, & -\varepsilon < y-x < 0\,,\\ 0\,, & 0 = y-x\,,\\ 1\,, & 0 < y-x < \varepsilon\,. \end{cases} \tag{10}$$

We set $u(x,0) = -\sin x$, which leads to shock formation for the local Burgers equation. Preliminary results for the solution of (9), with $\varepsilon = 0.05$, for $N = 1000, 2000, 4000, 8000$, and 16000 nodes, are shown in Fig. 1. The plot in Fig. 1(a) suggests that the dissipation of this numerical method strongly damps the solution structure, while Fig. 1(b) shows that the method is indeed conservative.



(a) $u(x, 2)$ for various Δx, $\varepsilon \approx 5 \times 10^{-2}$

(b) $\int_{-\pi}^{\pi} u(x, t)\, dx$ for various Δx, $\varepsilon \approx 5 \times 10^{-2}$

Figure 1. For the initial conditions and mesh refinements described in the text, Fig. (a) shows the computed results at $t = 2$, and Fig. (b) shows the time-dependent value of $\int_{-\pi}^{\pi} u(x, t)\, dx$.

The development described here comprises the first steps toward a mathematical approach for nonlocal advective phenomena consistent with peridynamics theory. Further details can be found in the report of Parks et al. [2]

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Computational peridynamics

Michael L. Parks

Peridynamics is a nonlocal extension of classical continuum mechanics suitable for modeling discontinuous phenomena, especially fracture [2, 3]. Whereas classical continuum mechanics is governed by familiar partial differential equations, peridynamics is governed by an integro-differential equation. A specific class of peridynamic models takes the form $d^2\mathbf{u}/dt^2 = \mathcal{L}(\mathbf{u})$, along with boundary conditions, where

$$\mathcal{L}(\mathbf{u}) := -\int_{\Omega \cup \mathcal{B}\Omega} \mathbf{C}(\mathbf{x}, \mathbf{x}')\, [\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})]\, d\mathbf{x}', \tag{1}$$

with $\Omega \subset \mathrm{R}^d$ a bounded domain and $\mathcal{B}\Omega$ its nonlocal boundary, and $\mathbf{C}$ a symmetric kernel function supported only over spherical regions of radius δ about $\mathbf{x}$. We discuss the impact of this nonlocal formulation upon the computational structure of the problem, reviewing discretization techniques and solution methods. We also survey the state-of-the-art in computational peridynamics, discussing available codes and showing demonstration problems, as well as highlighting current research directions.

We highlight several peridynamic numerical simulations, including fracture in fiber-reinforced composites, Taylor impact tests in aluminum, failure in nanofiber networks, hard sphere impact on a brittle disk, and dynamic brittle fracture in glass, and fragmentation of a cylinder. These simulation results were produced by a family of peridynamic codes: EMU, PDLAMMPS, and Peridigm. All of these codes utilize the so-called "EMU" numerical method: a discretization of the strong form of the operator utilizing a midpoint quadrature rule in space combined with a central difference in time [4].

We then discuss development and discretization of the weak form of the peridynamic operator (1). The weak form of (1) takes the form

$$a(\mathbf{u},\mathbf{v}) = \frac{1}{2}\int_{\Omega\cup\mathcal{B}\Omega}\int_{\Omega\cup\mathcal{B}\Omega} \mathbf{C}(\mathbf{x},\mathbf{x}')\,[\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x})]\,[\mathbf{v}(\mathbf{x}') - \mathbf{v}(\mathbf{x})]\; d\mathbf{x}'\; d\mathbf{x}.$$

Our main purpose is to investigate the conditioning of the peridynamic operator as a function of the horizon δ as a first step to developing preconditioning strategies useful for computational peridynamics at extreme scales. We report a spectral equivalence result [1] bounding the condition number of the discrete nonlocal operator K as $\kappa(K) \leq \mathcal{O}(\delta^{-2})$. Computational results in the $h \ll \delta$ regime (where h is the mesh spacing) demonstrate this bound is descriptive, and that there is at most weak h-dependance.

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Global existence and blow-up results for some problems in nonlinear nonlocal elasticity

Husnu A. Erbay
(joint work with Nilay Duruk, Saadet Erbay, Albert Erkip)

We study the initial-value problem for a general class of nonlinear nonlocal wave equations arising in nonlocal elasticity. The model involves a convolution integral operator with a general kernel function whose Fourier transform is nonnegative. We show that some well-known examples of nonlinear wave equations, such as Boussinesq-type equations, follow from the present model for suitable choices of the kernel function. We establish global existence of solutions of the model assuming enough smoothness on the initial data together with some positivity conditions on the nonlinear term. Furthermore, conditions for finite time blow-up are provided.

This presentation summarizes the results obtained in [1, 2, 3]. In those studies three different problems which model longitudinal, transverse and anti-plane shear motions, respectively, were considered. The equations are of the form

$$u_{tt} = (\beta * (u + g(u)))_{xx}, \ x \in \mathbb{R}, \ t > 0$$

for longitudinal motion,

$$u_{1tt} = (\beta * (u_1 + g_1(u_1, u_2)))_{xx}, \ x \in \mathbb{R}, \ t > 0$$
$$u_{2tt} = (\beta * (u_2 + g_2(u_1, u_2)))_{xx}, \ x \in \mathbb{R}, \ t > 0$$

for transverse motion and

$$w_{tt} = \left(\beta * \frac{\partial F}{\partial w_x}\right)_x + \left(\beta * \frac{\partial F}{\partial w_y}\right)_y, \ (x, y) \in \mathbb{R}^2, \ t > 0$$

for anti-plane shear motion. Note that, in the first two equations, u, u_1 and u_2 represent strains and the functions $g(u)$ and $g_i(u_1, u_2)$ $(i = 1, 2)$ represent the nonlinear parts of the strain energy functions. Also the functions $g_i(u_1, u_2)$ $(i = 1, 2)$ satisfy the exactness condition

$$\frac{\partial g_1}{\partial u_2} = \frac{\partial g_2}{\partial u_1}.$$

In the third equation w is the out-of-plane displacement and the nonlinear function F is the strain energy function corresponding to the anti-plane motion with $F(0) = 0$. For isotropic solids $F = F(w_x^2 + w_y^2)$. The kernel β is assumed to be an integrable function whose Fourier transform, $\widehat{\beta}(\xi)$, satisfies

$$0 \le \widehat{\beta}(\xi) \le C(1 + |\xi|^2)^{-r/2} \text{ for all } \xi,$$

where C is a positive constant and $r \ge 2$. The number r is closely related to the smoothness of β and, consequently, as the decay rate r gets larger the regularizing effect of the nonlocal behavior increases.

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A non-local p-laplacian

Julio D. Rossi
(joint work with Fuensanta Andreu, José M. Mazón, Julián Toledo)

We report the results in [1]. We have two main goals. As a first goal, we study the following nonlocal nonlinear diffusion problem with homogeneous Neumann boundary condition

$$\begin{cases} u_t(t,x) = \displaystyle\int_\Omega J(x-y) g\left(\frac{x+y}{2}\right) |u(t,y)-u(t,x)|^{p-2}(u(t,y)-u(t,x))\,dy, \\ u(x,0) = u_0(x), \end{cases}$$

where $g \in L^\infty(\mathbb{R}^N)$, $g \geq 0$ *a.e.* in $\mathbb{R}^N$, $1 \leq p < +\infty$, $\Omega \subset \mathbb{R}^N$ is a bounded smooth domain and the kernel J satisfies

(HJ) $J : \mathbb{R}^N \to \mathbb{R}$ is a nonnegative continuous radial function with compact support, $J(0) > 0$ and $\int_{\mathbb{R}^N} J(z)dz = 1$.

As a second goal, we also study the local counterpart, that is, the following local diffusion equation with homogeneous Neumann boundary condition

$$\begin{cases} u_t = \operatorname{div}\left(g|\nabla u|^{p-2}\nabla u\right), & \text{in }]0,T[\times\Omega, \\ g|\nabla u|^{p-2}\nabla u \cdot \eta = 0, & \text{on }]0,T[\times\partial\Omega, \\ u(x,0) = u_0(x), & \text{in } \Omega, \end{cases}$$

where η is the unit outward normal on $\partial\Omega$.

We prove that these two problems are related in the following way: solutions of the nonlocal problem converge to solutions of the local one when the kernel J is rescaled in a suitable way.

In these two problems we deal with a non-homogeneous diffusion coefficient, given by the function g, that we assume to be bounded and nonnegative, but we include here the case in which g vanishes in a subset of Ω that can even have positive measure. In this case we face new technical difficulties since we lost the coercivity of the associated functional in the usual Sobolev or Lebesgue spaces. These difficulties are overcome using weighted Sobolev or Lebesgue spaces with appropriate hypothesis on g that involve weights in Muckenhoupt's A_p classes.

Observe that for homogeneous diffusion, $g = 1$, the operator in the local problem is given by $\operatorname{div}\left(g|\nabla u|^{p-2}\nabla u\right) = \operatorname{div}(|\nabla u|^{p-2}\nabla u) = \Delta_p u$, that is, the well-known p-Laplacian of u. Also note that when $p = 2$ both problems become linear. In the case $g = 1$ the study of such problems has been done in [2] for the nonlocal problem while the local problem is a well known classical problem. Moreover, in this case, it is proved in [2] that under an appropriate rescaling of the kernel J, the solutions of the rescaled nonlocal problems, when the scale parameter (that measure the size of the support of J) tends to zero, converge to the solutions of the local problem.

One of the main results of [1] is to prove a similar convergence result where g can vanish in a subset of Ω of positive measure. This fact turns the whole issue more involved since the nonlocal problem, in contrast with what happens in general for the local one, takes into account the part of the domain where the diffusion coefficient g is null, that is, this part of the domain plays a role in the nonlocal diffusion case.

The case $p = 1$ is somehow different from the case $p > 1$. In fact, for $p = 1$ we need to work in weighted BV spaces (that is, weighted bounded variation spaces), an issue that forces us to introduce some delicate results from measure theory.

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Dirichlet's principle and wellposedness of steady state solutions in peridynamics

Petronela Radu

(joint work with Brittney Hinds)

This talk is concerned with Dirichlet's principle in the nonlocal setting of a peridynamic model with boundary conditions imposed on a nonzero volume collar surrounding the domain. The integration by parts technique used is adapted from the classical case and is based on nonlocal versions of the Green and Gauss identities available in [3]. The nonlocal energy functional associated with this "elliptic" type system exhibits a weakly singular kernel and its coercivity is shown by employing a nonlocal Poincare's inequality. The well-posedness of this steady state diffusion system follows from the existence and uniqueness of minimizers for the energy.

Consider the following nonlocal "elliptic" boundary value problem

$$\begin{cases} \mathcal{L}(u)(x) = b(x), & x \in \Omega, \\ u(x) = g(x), & x \in \Gamma, \end{cases} \tag{1}$$

where

$$\mathcal{L}(u)(x) := 2 \int_{\Omega \cup \Gamma} (u(x') - u(x))\mu(x, x')\, dx', \tag{2}$$

Ω denotes an open bounded subset of $\mathbb{R}^n$, and $\Gamma \subset \mathbb{R}^n \backslash \Omega$ denotes a "collar" domain surrounding Ω which has nonzero volume. The kernel $\mu(x, x')$ denotes a positive, symmetric function of its arguments, with a singularity around $x = x'$ which records the interaction of $x \in \Omega$ with its neighboring points x' from the horizon of x. To account for the interaction of x with points outside the domain Ω, as in the case when $x \in \partial\Omega$, we allow x' to belong to the collar domain Γ which contains the horizons $\mathcal{H}_x$ as x moves along $\partial\Omega$.

The prototype kernel $\mu(x, x')$ encountered in peridynamics models has the form

$$\mu(x, x') = \begin{cases} \frac{1}{|x - x'|^\beta}, & \text{for } |x - x'| < \delta, \\ 0, & \text{for } |x - x'| \geq \delta, \end{cases} \tag{3}$$

where $\beta > 0$. With this form for μ the natural framework to study regularity properties of the operator $\mathcal{L}$ for $\beta > n$ is that provided by fractional Sobolev spaces (see [1]). For $\beta < n$ the kernel is *weakly singular* and the derivation of classical regularity results can not be done following standard techniques. An important factor in this analysis is played by the Poincaré's inequality where L^2 bounds of the nonlocal gradient do not imply higher integrability for the function, as they do in the classical case.

We show that the minimizers of the energy functional associated with the above problem

$$\mathcal{F}[u] = \frac{1}{2} \int_{\Omega \cup \Gamma} \int_{\Omega \cup \Gamma} (u(x') - u(x))^2 \mu(x, x') dx' dx + \int_\Omega b(x) u(x) dx, \tag{4}$$

satisfy (1) and conversely, any solution of (1) is a minimizer for $\mathcal{F}$. This result then enables us to prove the wellposedness of the system (1) by showing existence and uniqueness of minimizers with direct methods of Calculus of Variations. As in the classical setting the existence of minimizers relies on convexity and coercivity properties of the integrand. For our functional, the convexity is immediate since the integrand is quadratic, and this ensures the necessary weakly lower semicontinuity. The coercivity property requires the use of the aforementioned nonlocal Poincaré type inequality which is proven in [2].

From discussions with other participants in the workshop several problems surfaced regarding future directions in the mathematical theory of peridynamics. Establishing elliptic-type properties (such as maximum principle, Harnack inequality) is one immediate goal of the authors; also, the derivation of regularity results is yet another important direction as these results will provide a valuable contribution in numerical computations of peridynamic models.

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A probabilistic interpretation of nonlocal diffusion

Nathanial Burch
(joint work with Richard B. Lehoucq)

We present the nonlocal diffusion equation,

$$u_t(x,t) = \frac{1}{\lambda}\int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y, \tag{1}$$

as the master equation for a Markovian continuous time random walk (CTRW), i.e., a compound Poisson process

$$Y_t = \sum_{k=1}^{N_t} R_k. \tag{2}$$

In (1) and (2), ϕ is a symmetric probability density function, $\lambda > 0$ is the mean wait-time, N_t is a Poisson process with intensity $1/\lambda$, and $R_k \overset{iid}{\sim} \phi$ are independent of N_t. We review the results of [1], which demonstrates a relationship of (1) with the fractional diffusion equation

$$v_t(x,t) = -(-\Delta)^{\alpha/2} v(x,t), \tag{3}$$

under suitable assumptions on ϕ. In turn, we show that the underlying process of (1) converges in distribution to that of (3), i.e.,

$$Y_t \overset{d}{\to} S_t^\alpha,$$

where S_t^α is a α-stable process.

Following [1, 5], we augment (1) with volume constraints so to restrict the nonlocal diffusion to a bounded domain. In [2], we explore the relationship of these so-called nonlocal boundary value problems to fractional diffusion restricted to a bounded domain. The work in [3] demonstrates that the nonlocal boundary value problems are the master equations for Markovian CTRWs restricted to a bounded domain (and with appropriate boundary conditions). This is achieved by comparing numerical solutions of the former to kernel density estimates from simulations of the latter.

We then incorporate non-Markovian effects via the memory kernel Λ in

$$u_t(x,t) = \int_0^t \Lambda(t-t')\int_{\mathbb{R}} \big(u(y,t') - u(x,t')\big)\phi(x-y)\,\mathrm{d}y\,\mathrm{d}t'. \tag{4}$$

The master equation (4) includes (1) and the nonlocal Cattaneo-Vernotte equation

$$u_t(x,t) + \frac{\tau}{2}u_{tt}(x,t) = \frac{1}{\beta}\int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\phi(x-y)\,\mathrm{d}y, \tag{5}$$

as special cases. Augmenting (4), in particular (5), with volume constraints, as expected, are shown in [3] to be the master equations for non-Markovian CTRWs on bounded domains.

The equation (1) also arises from a special case of the Lévy-Khintchine decomposition of an infinitely divisible distribution.

Theorem: Let $b = 0$, $c = 0$, and ν be such that

$$\nu(-x) = \nu(x) \quad \text{and} \quad \int_{\mathbb{R}} (1 \wedge |x|^2)\nu(x)\,\mathrm{d}x < \infty.$$

Then, there is a Lévy process L_t (compound Poisson and square-integrable martingale processes) such that the characteristic function of L_t satisfies

$$\varphi_{L_t}(\xi) = \exp\left(t\left(\int_{|x|\geq\delta} \left(e^{i\xi x} - 1\right)\nu(x)\,\mathrm{d}x + \int_{|x|<\delta} \left(e^{i\xi x} - 1\right)\nu(x)\,\mathrm{d}x\right)\right)$$

and, hence, the master equation is

$$u_t(x,t) = \int_{\mathbb{R}} \big(u(y,t) - u(x,t)\big)\nu(x-y)\,\mathrm{d}y.$$

We split into the following cases:

(a) $\int_{\mathbb{R}} \nu(x)\,\mathrm{d}x < \infty$, a.s. a finite number of steps on every compact interval, the process has finite activity, no smoothing;

(b) $\int_{\mathbb{R}} \nu(x)\,\mathrm{d}x = \infty$, a.s. an infinite number of steps on every compact interval, the process has infinite activity, (fractional) smoothing;

 (i) $\int_{\mathbb{R}} |x|\nu(x)\,\mathrm{d}x < \infty$, sample paths have finite variation;

 (ii) $\int_{\mathbb{R}} |x|\nu(x)\,\mathrm{d}x = \infty$, sample paths have infinite variation.

Thus, we have established a relationship between the smoothing of the operator in [4] and the activity of the underlying stochastic process.

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Coarse-graining atomistic models at finite temperature

Frédéric Legoll
(joint work with X. Blanc, C. Le Bris, C. Patz)

We consider atomistic systems at finite temperature, modelled within the framework of statistical mechanics. Macroscopic quantities are defined as averages of some functions, the so-called observables, that depend on all the variables in the system, over the Boltzmann measure:

$$\langle \Phi \rangle = \frac{\displaystyle\int_{\mathbb{R}^N} \Phi(X) \exp(-\beta V(X))\, dX}{\displaystyle\int_{\mathbb{R}^N} \exp(-\beta V(X))\, dX}, \tag{1}$$

where Φ is the observable of interest, β is proportional to the inverse of the temperature, and $V(X)$ is the potential energy of the system, depending on the vector $X \in \mathbb{R}^N$, that represents all the atom positions.

For simple one-dimensional chains of atoms, we first show how to compute the average length of the system when we impose an external force, in the thermodynamic limit. The observable $\Phi(X)$ is thus proportional to $X_N - X_0$, and we compute the limit of (1) when $N \to \infty$. Conversely, we also show how to compute the internal force, when the elongation of the system is prescribed. See [1, 3] for more details. These results are obtained using standard tools of probability theory, such as the law of large numbers and large deviation principles, that characterize the behaviour of a sum of independent identically distributed random variables $\frac{1}{N}\sum_{i=1}^N Y_i$, when $N \to \infty$.

It turns out that, in the bulk limit $N \to \infty$, the two relations we have obtained (elongation as a function of the force and vice-versa) are inverse one to each other, and thus represent the macroscopic constitutive law, parameterized by the temperature.

We next turn to dynamics, when the evolution of the system is modelled by the overdamped Langevin equation:

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\beta^{-1}}\, dW_t,$$

where W_t is a standard N-dimensional Brownian motion. In addition, the last atom of the chain is submitted to an external, time dependent, force. Upon assuming that this force varies on a slow time scale compared to the intrinsic timescale of the system (i.e. time to return to thermal equilibrium), we show that, at the macroscopic scale, the system evolves quasi-statically. This result is obtained using approximation tools developed in [2].

Numerical results illustrate the obtained results.

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Connecting peridynamic models and coupling local and nonlocal systems

Pablo Seleson
(joint work with Max Gunzburger and Michael L. Parks)

The peridynamics (PD) theory was proposed as a reformulation of classical continuum mechanics in [1] where a model for pairwise interactions called *bond-based* PD was presented. However, the bond-based PD model can only represent materials having a Poisson's ratio of $\nu = 1/4$. As an approach for generalizing PD to the representation of materials with a general Poisson's ratio, a PD model with similar structure to the embedded-atom model (EAM) in molecular dynamics was proposed also in [1]; we refer to it as the *EAM-like* PD model. Another PD model of interest is the so called *prototype microelastic brittle* (PMB) which was presented in [2] for the purpose of simulating fracture dynamics in brittle materials. However, a framework for general deformations in PD was first proposed in [3] under the *state-base* PD formulation; a model called *linear peridynamic solid* (LPS) is introduced in [3] as well. We derive relations between state-based and bond-based PD constitutive models, i.e., EAM-like, PMB, and LPS, and present a hierarchy of models as illustrated in Figure 1.

The connections established in this work between PD models are possible by using nonstandard influence functions in state-based PD; influence functions are nonnegative scalar-valued functions $\underline{\omega}\langle\cdot\rangle : \mathbb{R}^d \to \mathbb{R}$, defined over some neighborhood, mapping PD bonds to scalar values. This motivates to study of the role of influence functions in PD. We can describe some of the properties that influence functions may have as follows:

- Allow for a bond-breaking mechanism.
- Impose a cutoff radius for the nonlocal model.
- Modulate the strength of nonlocal interactions.

Generally speaking, the smaller the support of the influence function, the more local the PD model, so that even for a fixed horizon we can obtain local and nearly local interactions. An illustration of this effect is shown in Figure 2 for one-dimensional wave propagation using p-dependent influence functions for which the interactions between further particles become weaker for larger values of p, with p a parameter. For $p = 20$, the results are effectively those obtained for a classical local model.

In addition to establishing connections between PD models and generalizing the role of influence functions in state-based PD, we investigate a domain decomposition approach for nonlocal multimaterial systems with variable interaction ranges, for the case of static problems involving scalar fields. We study analytically and

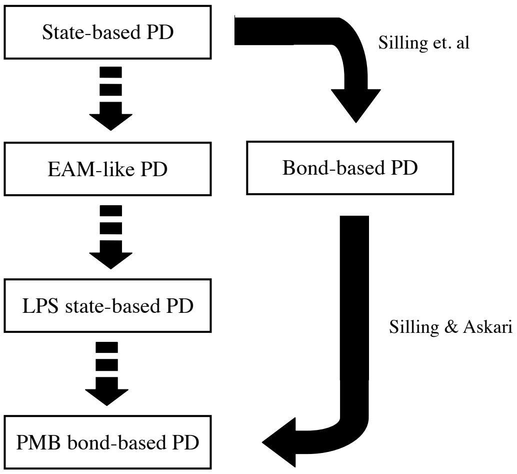
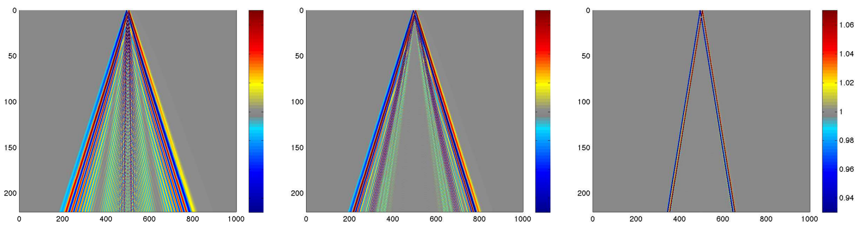


FIGURE 1. Relationships between peridynamics (PD) models. In Silling et al. [3], it was shown that bond-based PD is a special case of the state-based PD model. We demonstrate that the EAM-like PD model is an instance of the state-based PD model. Furthermore, we derive the LPS model [3] from the EAM-like PD model (*cf.* [5]), and the PMB model, presented in Silling & Askari [2], from the LPS model (*cf.* [4]). This establishes a partial taxonomy of PD constitutive models.



(a) $p = 0$ (b) $p = 3$ (c) $p = 20$

FIGURE 2. Density evolution of one-dimensional peridynamic models, for the evolution of an initial pulse, using a p-dependent influence function. The x-axis represents the reference configuration and the y-axis time (from top to bottom); the colors represent density. We observe less dispersion for higher values of p, where dispersion is numerically manifested as broadening of the lines.

numerically differences between local and nonlocal systems and show convergence of the nonlocal model to its local counterpart, in the limit where the horizons corresponding to the nonlocal interactions become very small. Particularly, we focus on the coupling of local and nonlocal models and derive appropriate transmission conditions.

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Variational theory for nonlocal boundary value problems

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(joint work with Burak Aksoylu)

Motivated by the scalar peridynamics equations, we develop a variational theory for the nonlocal linear boundary value problem $\mathcal{L}u = b \quad \text{on } \Omega$, where $\mathcal{L}$ is the nonlocal operator given by

$$\mathcal{L}(u)(x) := -\int_{\overline{\overline{\Omega}}} C(x - x')\,(u(x') - u(x))\,dx'$$

and u satisfying some volume constraints. The domain $\Omega \subset \mathbb{R}^d$ is assumed to be bounded with nonlocal boundary, $\mathcal{B}\Omega \subset \mathbb{R}^d \setminus \Omega$, and $\overline{\overline{\Omega}} = \Omega \cup \mathcal{B}\Omega$. The variational theory will enable us prove well-posedness results for the weak formulation of nonlocal boundary value problems with Dirichlet and Neumann boundary conditions. Our results are applicable when C is radial, locally integrable, compactly supported and $C(r) > 0$ on $[0, \delta)$.

The linear operator $\mathcal{L} : L^2(\Omega) \to L^2(\Omega)$, being of convolution type, is bounded and self adjoint. Thus given a closed subspace V of $L^2(\overline{\overline{\Omega}})$, proving a nonlocal Poincaré type inequality of the form

$$(\mathcal{L}u, u)_{L^2(\overline{\overline{\Omega}})} \geq \lambda \|u\|^2_{L^2(\overline{\overline{\Omega}})}, \quad \text{for all } u \in V,$$

for some $\lambda > 0$, is sufficient for the equation $\mathcal{L}u = b$ to have a unique variational solution in V corresponding to $b \in L^2(\Omega)$. Indeed in this case the solution is the minimizer of the quadratic functional $E(u) = (\mathcal{L}u, u)_{L^2} - (b, u)_{L^2}$ over V.

Clearly stated our achievements are the following.

Theorem 1: Given the closed subspace $V_D := \{v \in L^2(\overline{\overline{\Omega}}) : v = 0 \text{ on } \mathcal{B}\Omega\}$ where $|\mathcal{B}\Omega| > 0$ and $\overline{\overline{\Omega}}$ is connected, the variational problem: given $b \in L^2(\overline{\overline{\Omega}})$ find $u \in V_D$ such that $(\mathcal{L}u, v) = (b, v)$ for all $v \in V_D$ has a unique solution which satisfies the inequality

$$\|u\|_{L^2} \leq \Lambda \|b\|_{L^2},$$

for some constant $\Lambda = \Lambda(\delta) > 0$.

The nonlocal Poincaré's inequality corresponding to V_D follows from a slightly modified argument of [4].

Similarly, using a nonlocal Poincaré's inequality proved in [3] a well posedness for the variational problem corresponding to the closed space $V_N := \{v \in L^2(\overline{\overline{\Omega}}) : \int_{\overline{\overline{\Omega}}} v dx = 0\}$ can be established. The kernel C will be taken from a restricted class, namely $C(r) = \gamma(r/\delta)$ where γ is a nonnegative, radial and compactly supported such that $\gamma(r)r^{d-1} \in L^1_{loc}([0,\infty))$ and satisfying the moment condition

$$\int_0^\infty \gamma(r)r^{d+1}\; dr = 1.$$

Theorem 2: For C in the above class, the variational problem: given $b \in L^2(\overline{\overline{\Omega}})$ find $u \in V_N$ such that $(\mathcal{L}u, v) = (b, v)$ for all $v \in V_N$ has a unique solution which satisfies the inequality

$$\|u\|_{L^2} \leq \Lambda \|b\|_{L^2},$$

for some constant $\Lambda = \Lambda(\delta) > 0$.

Finally we can quantify (asymptotically) the smallest and largest eigenvalues of the operator $\mathcal{L}$ in terms δ.

Corollary [Spectral equivalence]: For C in the above class, there exist $\delta_0 > 0$, $\underline{\lambda} = \underline{\lambda}(\overline{\overline{\Omega}}, \delta_0)$ and $\overline{\lambda} = \overline{\lambda}(\gamma, d)$ such that for all $0 < \delta < \delta_0$ and $u \in V_D$ or $u \in V_N$, we have

$$\underline{\lambda}\, \delta^{d+2}\, \|u\|^2_{L^2(\overline{\overline{\Omega}})} \leq a(u,u) \leq \overline{\lambda}\delta^d \|u\|^2_{L^2(\overline{\overline{\Omega}})}. \tag{1}$$

The spectral equivalence (1) leads to a remarkable conditioning result, namely that the condition number of the discretized operator can be bounded independently from the mesh size; $\kappa(K) \leq c\delta^{-2}$, where K is a stiffness matrix. See [2] for a special case and see [5] for an estimate involving the mesh size.

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