Dirichlet's principle and well posedness of steady state solutions in peridynamics

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Work supported by NSF - DMS award 0908435

January 19, 2011

The steady state peridynamic model

Consider the "elliptic" nonlocal model:

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

where

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

- Ω is an open bounded subset of $\mathbb{R}^n$
- $\Gamma \subset \mathbb{R}^n \backslash \Omega$ denotes a "collar" domain surrounding Ω which has nonzero volume
- $\mu(x, x')$ is nonegative, $\mu(x, x') = \mu(x', x)$.

Remark: The integral operator is defined on the boundary Γ as well.

Notation

$\alpha : \Omega \cup \Gamma \times \Omega \cup \Gamma \to \mathbb{R}^n$, $u : \Omega \cup \Gamma \to \mathbb{R}^n$, $f : \Omega \cup \Gamma \times \Omega \cup \Gamma \to \mathbb{R}^n$

(i) Generalized nonlocal gradient

$$\mathcal{G}(u)(x,x') := (u(x') - u(x))\alpha(x,x'), \quad x, x' \in \Omega,$$

(ii) Generalized nonlocal divergence

$$\mathcal{D}(f)(x) := \int_{\Omega\cup\Gamma} (f(x,x')\alpha(x,x') - f(x',x)\alpha(x',x))dx', \quad x \in \Omega,$$

(iii) Generalized nonlocal normal component

$$\mathcal{N}(f)(x) := -\int_{\Omega\cup\Gamma} (f(x,x')\alpha(x,x') - f(x',x)\alpha(x',x))dx', \quad x \in \Gamma.$$

Note: For the given peridynamic model we will use $\mu = \alpha^2$

Useful nonlocal calculus identities

Gunzburger & Lehoucq:

- $\mathcal{L}u = \mathcal{D}(\mathcal{G}(u))$
- For $u, v \in L^2(\Omega \cup \Gamma)$

$$\int_\Omega v\mathcal{D}(\mathcal{G}(u))dx + \int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(u)\mathcal{G}(v)dx'dx = \int_\Gamma v\mathcal{N}(\mathcal{G}(u))dx.$$

- For $u, v \in L^2(\Omega \cup \Gamma)$, $v = 0$ over Γ

$$\int_\Omega (\mathcal{L}u)v\,dx = -\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(v)\cdot\mathcal{G}(u)dx'dx.$$

Nonlocal boundary conditions

Dirichlet Problem:

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

Neumann Problem:

$$\begin{cases} \mathcal{L}u = b, & x \in \Omega \\ \displaystyle\int_\Gamma (u' - u)\mu(x, x')dx' = g, & x \in \Gamma, \end{cases}$$

where $u' = u(x')$, $u = u(x)$.

Set up for the Dirichlet's principle. Spaces

Introduce the inner product

$$\langle u, v\rangle_\mu = \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma}(u(x') - u(x))(v(x') - v(x))\mu(x, x')dx'dx + (u, v)_{L^2(\Omega\cup\Gamma)},$$

The space

$$\mathcal{W} := \{w \in L^2(\Omega)|\ \langle w, w\rangle_\mu < \infty, w = 0 \text{ on } \Gamma\},$$

endowed with the norm

$$\|w\|_{\mathcal{W}} = \langle w, w\rangle_\mu^{1/2}.$$

is a Banach space whenever μ is nonnegative and symmetric.

The energy functional

The energy functional associated with the peridynamic problem (PD) is given by:

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

for u in the class of admissible functions

$$\mathcal{A} = \{w \in L^2(\Omega) \, | u = g + u_0, \text{ for some } u_0 \in \mathcal{W}\},$$

Convention: $\mathcal{A}$ will also be denoted by $g + \mathcal{W}$.

The Nonlocal Dirichlet's Principle

Theorem

Let $\mu(x, x')$ be nonnegative and symmetric.

(i) *Assume u solves the nonlocal peridynamics problem*

$$\text{(PD)} \qquad \begin{cases} \mathcal{L}(u)(x) = b(x), & x \in \Omega \\ u(x) = g(x), & x \in \Gamma. \end{cases}$$

Then

$$\mathcal{F}[u] \leq \mathcal{F}[v]$$

for every $v \in \mathcal{A}$.

(ii) *Conversely, if $u \in \mathcal{A}$ satisfies $\mathcal{F}[u] \leq \mathcal{F}[v]$ for every $v \in \mathcal{A}$, then u solves the above nonlocal peridynamics problem.*

Proof:

(i) If $w \in \mathcal{A}$, then $u - w = 0$ over Γ. Integration by parts yields:

$$\begin{aligned} 0 &= \int_{\Omega} (Lu - b)(u - w)dx \\ &= -\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(u)\cdot\mathcal{G}(u-w)dx'dx - \int_{\Omega} b(u-w)dx \end{aligned}$$

By Cauchy-Schwarz we obtain:

$$\frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(u)\cdot\mathcal{G}(u)dx'dx + \int_{\Omega} budx \\ \leq \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(w)\cdot\mathcal{G}(w)dx'dx + \int_{\Omega} bwdx$$

(ii) Fix $v \in \mathcal{W}$ and write

$$i(\tau) := \mathcal{F}[u + \tau v],$$

where $\tau \in \mathbb{R}$. Since $u + \tau v \in \mathcal{A}$ for each τ, the scalar function $i(\cdot)$ has a minimum at zero. Thus $i'(0) = 0$, $\left(' = \frac{d}{d\tau}\right)$, provided the derivative exists. Now we have

$$i(\tau) = \int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \frac{1}{2}\mathcal{G}(u)\cdot\mathcal{G}(u) + \tau\mathcal{G}(u)\cdot\mathcal{G}(v) + \frac{\tau^2}{2}\mathcal{G}(v)\cdot\mathcal{G}(v)dx'dx \\ + \int_\Omega b(u + \tau v)dx$$

Hence, after integration by parts we obtain:

$$0 = i'(0) = \int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \mathcal{G}(u)\cdot\mathcal{G}(v)dx'dx + \int_\Omega vbdx = \int_\Omega (\mathcal{L}u - b)vdx$$

A particular kernel

Assumption A. For every $x' \in \mathcal{H}_x$, there exists a constant $C_0 > 0$ such that $\mu(x, x') \geq C_0$. In other words, for all $x \in \Omega \cup \Gamma$ we have:

$$C_0 \chi_\delta(x, x') \leq \mu(x, x'),$$

where $\chi_\delta(x, x') = \begin{cases} 1, & |x - x'| \leq \delta \\ 0, & |x - x'| > \delta. \end{cases}$

Remark: The prototype kernel

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

satisfies this assumption for all $\beta > 0$.

Prototype kernel:

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

where $\beta \geq 0$.

- $\beta \geq n \implies$ strong singularity; work in the framework of Nikolskii spaces $H^{(\beta-n)/2}(\Omega)$
- $\beta < n \implies$ weak singularity; work with L^2 spaces (with weights?)

More "elliptic" properties of $\mathfrak{L}$

Proposition

The operator $\mathfrak{L}$ admits the following properties:

(a) *If $u \equiv$ constant then $\mathfrak{L}u = 0$.*

(b) *Let $x \in \Omega \cup \Gamma$. For any maximal point x_0 that satisfies $u(x_0) \geq u(x)$, we have $-\mathfrak{L}u(x_0) \geq 0$. Similarly, if x_1 is a minimal point such that $u(x_1) \leq u(x)$, then $-\mathfrak{L}u(x_1) \leq 0$.*

(c) *$\mathfrak{L}u$ is a positive semidefinite operator, i.e. $\langle -\mathfrak{L}u, u \rangle \geq 0$.*

(d) $\displaystyle\int_{\Omega\cup\Gamma} -\mathfrak{L}u(x)dx = 0.$

(e) Weak mean-value inequality.

If μ satisfies (A) and u is a **nonnegative** solution of $\mathcal{L}u(x) = 0$ then:

$$u(x) \geq \frac{1}{|\mathcal{H}_x|} \int_{\mathcal{H}_x} u(y)dy$$

(f) Maximum and minimum principle (Rossi)

Assume that $u \in C(\Omega)$ solves (PD) with $f = 0$. If

$$u(x_0) = \max_{x \in \Omega \cup \Gamma} u(x)$$

then $x_0 \in \Gamma$. Similarly, if

$$u(x_0) = \max_{x \in \Omega \cup \Gamma} u(x)$$

then $x_0 \in \Gamma$.

Lemma

(Nonlocal Poincaré's Inequality - Rossi, Aksoylu &Parks) If $u \in L^p(\Omega)$, $p > 1$, $m \geq 1$, and $\mathcal{G}$ is as defined in (3), then there exist $\lambda_{Pncr} = \lambda_{Pncr}(\Omega, \Gamma, \delta, m) > 0$ and $C_g > 0$ such that the following inequality holds:

$$\lambda_{Pncr} \|u\|_{L^p(\Omega)} \leq \|\mathcal{G}(u)\|_{L^p(\Omega \cup \Gamma \times \Omega \cup \Gamma)} + C_g.$$

Wellposedness of the system (PD)

Theorem

With $\mathcal{F}[u]$ defined as before and μ satisfying assumption (A) we have that

$$inf\{\mathcal{F}[u] : u \in \mathcal{A}\}$$

attains its minimum, and furthermore this minimizer is unique. Hence, there exists a unique solution to (PD) in $\mathcal{A}$ for every f, g in $\mathcal{A}$.

Existence of solutions

Follows from **convexity** of $\mathcal{F}$ and **coercivity** of $\mathcal{F}$.
First note that since $\mathcal{F}[u] \geq 0$ for $u \in L^2(\Omega)$, we have that

$$inf\{\mathcal{F}[u] : u \in \mathcal{A}\} = m \geq 0.$$

Let $\{u_\nu\}$ be a minimizing sequence so that $\mathcal{F}[u_\nu] \to m$. Thus there exists $M > 0$ such that $\mathcal{F}[u_\nu] < M$. We will show that the sequence u_ν is bounded in L^2 (**coercivity.**).

$$\begin{aligned} M &> \frac{1}{2}\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma}[\mathcal{G}(u_\nu)]^2 dx' dx + \int_\Omega b(x) u_\nu(x) dx \\ &\geq \tfrac{1}{2}\|\mathcal{G}(u_\nu)\|^2_{L^2(\Omega\cup\Gamma\times\Omega\cup\Gamma)} - \tfrac{\varepsilon}{2}\|b\|^2_{L^2(\Omega)} - \tfrac{1}{2\varepsilon}\|u_\nu\|^2_{L^2(\Omega)}, \end{aligned}$$

Existence contd.

By the nonlocal Poincaré's inequality we have:

$$M > C_1\|u_\nu\|^2_{L^2(\Omega)} + C_2\|g\|^2_{L^2(\Gamma)} - C_3\|b\|^2_{L^2(\Omega)}$$

Thus, we can find $\gamma > 0$ such that

$$\|u_\nu\|_{L^2(\Omega)} \leq \gamma.$$

Therefore, we may extract a subsequence $\{u_\nu\}$ and find $\bar{u} \in L^2(\Omega)$ such that $u_\nu \to \bar{u}$ in $L^2(\Omega)$. By Mazur's Lemma we can find a sequence of convex combinations of u_ν, denoted by $\bar{u}_\nu \to \bar{u}$ in $L^2(\Omega)$, hence

$$\lim_{\nu\to\infty} \mathcal{F}[\bar{u}_\nu] \leq m.$$

By Fatou's lemma

$$\mathcal{F}[\bar{u}] \leq \lim_{\nu\to\infty} \mathcal{F}[\bar{u}_\nu],$$

hence, from the above inequalities we have that $\bar{u}$ is a minimizer since

$$\mathcal{F}[\bar{u}] \leq m.$$

Uniqueness of solutions

Let $\bar{u}, \bar{v} \in L^2(\Omega)$ be minimizers of $\mathcal{F}$ with $\bar{u} \neq \bar{v}$. Set

$$\bar{w} = \frac{\bar{u} + \bar{v}}{2} \in L^2(\Omega).$$

By the strict convexity of the integrand, we have

$$m \leq \mathcal{F}[\bar{w}] \leq \frac{1}{2}\mathcal{F}[\bar{u}] + \frac{1}{2}\mathcal{F}[\bar{v}] = m.$$

Hence $\bar{w}$ is a minimizer of $\mathcal{F}$. This implies that

$$\frac{1}{2}\mathcal{F}[\bar{u}] + \frac{1}{2}\mathcal{F}[\bar{v}] - \mathcal{F}[\bar{w}] = 0.$$

Thus

$$\int_{\Omega\cup\Gamma}\int_{\Omega\cup\Gamma} \frac{\mathcal{G}[\bar{u}]^2}{2} + \frac{\mathcal{G}[\bar{v}]^2}{2} - \mathcal{G}[\bar{w}] dx' dx = 0.$$

Again, by strict convexity, the integrand is strictly positive – contradiction!!

Fick diffusion in peridynamics models

Consider the nonlocal flux that satisfies a nonlocal Fourier's law:

$$\mathcal{Q}[u](x, x') = -a\mathcal{G}[u](x, x'),$$

The nonlocal conservation law:

$$u_t = -\mathcal{D}(\mathcal{Q}).$$

We obtain the nonlocal peridynamic diffusion law

$$u_t = \mathcal{D}(a\mathcal{G}(u)) = a\mathcal{L}u.$$

Hyperbolic diffusion in peridynamics

Assum that the flux $\mathcal{Q}$ is given by the Cattaneo-Vernotte equation

$$\mathcal{Q}_t + a\mathcal{Q} = -\mathcal{G}(u).$$

Differentiate the conservation law $u_t = -\mathcal{D}(\mathcal{Q})$ with respect to time:

$$u_{tt} = -\mathcal{D}(\mathcal{Q}_t).$$

Substituted into the above equation yields:

$$u_{tt} = -\mathcal{D}(-\mathcal{G}(u) - a\mathcal{Q}) = \mathcal{D}(\mathcal{G}(u)) + \mathcal{D}(a\mathcal{Q}) = \mathcal{L}u - au_t.$$

or

$$u_{tt} - \mathcal{L}u + au_t = 0.$$

Importance of hyperbolic diffusion (classical case)

Consider the classical heat and damped wave equations:

$$\begin{cases} v_t - \Delta v = 0 \text{ in } \mathbb{R}^n \\ v|_{t=0} = v_0 \text{ in } \mathbb{R}^n. \end{cases} \qquad \begin{cases} u_{tt} - \Delta u + u_t = 0 \text{ in } \mathbb{R}^n \\ (u, u_t)|_{t=0} = u_0 + u_1 \text{ in } \mathbb{R}^n. \end{cases}$$

- hyperbolic diffusion is important in unsteady heat conduction (the second sound of helium)
- the long time behavior of u with initial conditions (u_0, u_1) can be very well approximated by the long time behavior of v with initial condition $v_0 = u_0 + u_1$ (Abstract Diffusion Phenomenon - JDE)

Questions and future directions

1. physical interpretation of the exponent β in μ;
2. what if μ depends on time? OR the horizon changes with space (different phases of the material)
3. weakly singular kernels ($0 < s < n$): Harnack's inequality
4. obtain regularity results via Calculus of Variations techniques
5. wellposedness and regularity for time dependent models (diffusion, elasticity,..)
6. nonlinear local problems: very difficult since there is no gain in "smoothness" (higher integrability or more derivatives for the solution)
7. wellposedness in weighted spaces