Nonlocal variational problems and applications to peridynamics

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Introduction

Existence of minimizers

Lower semicontinuity

Coercivity

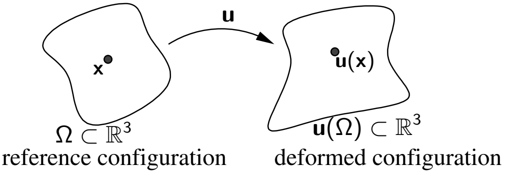
Existence

Passage nonlocal $\rightsquigarrow$ local

Relaxation

Alternative model

Classical Solid Mechanics (A.-L. Cauchy, G. Green)



Total energy of elastic deformation

$$\underbrace{\int_\Omega W(Du(x))\,\mathrm{d}x}_{\text{elastic}} - \underbrace{\int_\Omega f \cdot u\,\mathrm{d}x}_{\text{external force}}.$$

where $W : \mathbb{R}^{3\times 3} \to \mathbb{R}$ stored energy function.

Peridynamics

S.A. Silling (*J. Mech. Phys. Solids* 2000) proposed a reformulation of classical continuum mechanics:

$$\int_\Omega \int_\Omega w(x - x', u(x) - u(x'))\, \mathrm{d}x' \, \mathrm{d}x.$$

Features:

- non-local: points at a positive distance exert a force upon each other.
- absence of gradients.
- main example: $w = \dfrac{|y - y'|^p}{|x - x'|^\alpha}$ for some $p \geq 1$ and $0 \leq \alpha < n + p$. Also $K(x - x')\,|y - y'|^p$.
- Deformations with discontinuities (fracture, dislocation, cavitation...) do not require a separate treatment.

This motivates the study of functionals of the form

$$\mathcal{I}(u) = \int_\Omega \int_\Omega w(x, x', u(x), u(x'))\, \mathrm{d}x'\, \mathrm{d}x$$

for $w : \Omega \times \Omega \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ and $\Omega \subset \mathbb{R}^n$. By Fubini's theorem we can assume

$$w(x, x', y, y') = w(x', x, y', y),$$

which is the realization in this context of Newton's third law.

In this talk we will study existence, passage nonlocal $\rightsquigarrow$ local, relaxation and an alternative model.

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For existence, we will use the *direct method of Calculus of Variations* to find conditions on w for $\mathcal{I}$ to have a minimizer. The method is based on *coercivity* and *lower semicontinuity*.

How does **lower semicontinuity** work in the local case?

Necessary and sufficient condition for

$$\int_\Omega W(x, u(x))\,\mathrm{d}x$$

to be swlsc in L^p is that $W(x,\cdot)$ is convex. (L. Tonelli 1921)

Necessary and sufficient condition for

$$\int_\Omega W(x, u(x), Du(x))\,\mathrm{d}x$$

to be swlsc in $W^{1,p}$ is that $W(x,y,\cdot)$ is quasiconvex.

(C. B. Morrey 1952)

It is essential the choice of topology.

In our nonlocal case, if

$$w \approx \frac{|y - y'|^p}{|x - x'|^\alpha}$$

with $\alpha > n$ we will choose the weak topology in $W^{s,p}$ (with $s + np = \alpha$).

If

$$w \approx \frac{|y - y'|^p}{|x - x'|^\alpha}$$

with $\alpha < n$ we will choose the weak topology in L^p.

For simplicity, in this talk we will focus on the L^p case.

P. Elbau (arXiv 2011): Necessary and sufficient condition for

$$\mathcal{I}(u) = \int_\Omega \int_\Omega w(x, x', u(x), u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

to be swlsc in L^p is that for a.e. $x \in \Omega$ and all $u \in L^p(\Omega, \mathbb{R}^d)$,

$$y \mapsto \int_\Omega w(x, x', y, u(x'))\,\mathrm{d}x' \quad \text{is convex in } \mathbb{R}^d.$$

A fake proof:

$$\int_\Omega \underbrace{\boxed{\int_\Omega w(x, x', u(x), u(x'))\,\mathrm{d}x'}}_{:= F(x, u(x))} \mathrm{d}x.$$

Seems that semicontinuity for double integral holds iff $F(x, \cdot)$ is convex, i.e., for a.e. $x \in \Omega$ and all $u \in L^p(\Omega, \mathbb{R}^d)$, the function

$$y \mapsto \int_\Omega w(x, x', y, u(x'))\,\mathrm{d}x' \quad \text{is convex.}$$

$$\text{(NC)}\quad y \mapsto \int_\Omega w(x, x', y, u(x'))\,\mathrm{d}x' \text{ is convex.}$$

Strangely, condition (NC) (weaker than convexity of $w(x, x', \cdot, y')$) depends on the domain Ω.

By a Lebesgue-point argument, we can prove:

Proposition. $\mathcal{I}_{\Omega'}$ is weakly lower semicontinuous in $L^p(\Omega', \mathbb{R}^d)$ for all $\Omega' \subset \Omega$ (equivalently, the function in (NC) is convex for all $\Omega' \subset \Omega$) iff for a.e. $x, x' \in \Omega$ and all $y' \in \mathbb{R}^d$, the function $w(x, x', \cdot, y')$ is convex.

How does coercivity work in the local case?

For

$$\int_\Omega W(x, u(x))\,\mathrm{d}x$$

we impose $W(x, y) \geq c\,|y|^p$.

For

$$\int_\Omega W(x, u(x), Du(x))\,\mathrm{d}x$$

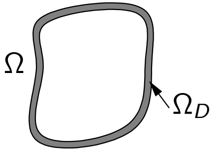
we impose $W(x, y, z) \geq c\,|z|^p$ and use boundary conditions to apply a Poincaré inequality.

- For

$$\mathcal{I}(u) = \int_\Omega \int_\Omega w(x, x', u(x), u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

we can impose $w(x, x', y, y') \geq c\,|y|^p$. But typically $\mathcal{I}$ is invariant under translations: $\mathcal{I}(u) = \mathcal{I}(u + a)$ for all $a \in \mathbb{R}^d$, so w depends on (x, x', y, y') through $(x, x', y - y')$.

- Functions in L^p do not have traces on the boundary. Dirichlet conditions are prescribed on $\Omega_D := \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \delta\}$.



- Usual assumption in engineering that $w(x, x', \cdot, \cdot) \equiv 0$ if $|x - x'| \geq \delta$.

Coercivity inequality for Dirichlet conditions:

$$\lambda \int_{\Omega} |u(x)|^p \, \mathrm{d}x \leq \int_{\Omega} \int_{\Omega \cap B(x,\delta)} |u(x) - u(x')|^p \mathrm{d}x' \, \mathrm{d}x + \int_{\Omega_D} |u(x)|^p \, \mathrm{d}x$$

F. Andreu, J. Mazón, J. Rossi & J. Toledo *SIAM J Math Anal* (2009),

B. Aksoylu & M.L. Parks *Appl Math Comput* (2011),

B. Hinds & P. Radu *Appl Math Comput* (2012).

Coercivity inequality for Neumann conditions:

$$\lambda \int_{\Omega} \left| u(x) - \fint_{\Omega} u \right|^p \mathrm{d}x \leq \int_{\Omega} \int_{\Omega \cap B(x,\delta)} \left| u(x) - u(x') \right|^p \mathrm{d}x' \, \mathrm{d}x.$$

J. Bourgain, H. Brezis & P. Mironescu *J Anal Math* (2002),

A. C. Ponce *JEMS* (2004),

F. Andreu, J. Mazón, J. Rossi & J. Toledo *J Math Pures Appl* (2008),

B. Aksoylu & T. Mengesha *Numer Funct Anal Optim* (2010),

R. Hurri-Syrjänen & A.V. Vähäkangas *J Anal Math* (2013).

Existence of minimizers in L^p

$\Omega \subset \mathbb{R}^n$. $\quad \delta > 0$. $\quad \Omega_D = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \delta\}$. $\quad p > 1$.

a) $c\, \chi_{B(0,\delta)}(x - x') \left| y - y' \right|^p \leq w(x, x', y, y') \leq a(x, x') + C\, |y|^p$
with $a \in L^1(\Omega \times \Omega)$.

b) (NC).

Let $u_0 \in L^p(\Omega_D, \mathbb{R}^d)$. Then there exists a minimizer of

$$\int_\Omega \int_\Omega w(x, x', u(x), u(x'))\, \mathrm{d}x'\, \mathrm{d}x$$

among $u \in L^p(\Omega, \mathbb{R}^d)$ such that $u = u_0$ a.e. on Ω_D.

(analogous statement for Neumann boundary conditions)

Nonlocal $\rightsquigarrow$ local

Think of $w(x,x',y,y') \approx \frac{|y-y'|^p}{|x-x'|^\alpha}$. Call $\beta := p-\alpha$. Ingredients:

- Scaling:
  $$I_\delta(u) := \frac{C_{n,\beta}}{\delta^{n+\beta}} \int_\Omega \int_{\Omega\cap B(x,\delta)} w(x-x', u(x)-u(x'))\,\mathrm{d}x'\,\mathrm{d}x.$$
- Blow-up at zero (homogenization of w):
  $$w^\circ(\tilde{x},\tilde{y}) := \lim_{t\to 0} \frac{1}{t^\beta} w(t\tilde{x}, t\tilde{y}).$$
- Density $\bar{w} : \mathbb{R}^{d\times n} \to \mathbb{R}$
  $$\bar{w}(F) := \fint_{\mathbb{S}^{n-1}} w^\circ(z, Fz)\,\mathrm{d}\mathcal{H}^{n-1}(z).$$
- Quasiconvexification: $\bar{w}^{qc} : \mathbb{R}^{d\times n} \to \mathbb{R}$ of $\bar{w}$.
  $$I(u) := \int_\Omega \bar{w}^{qc}(Du(x))\,\mathrm{d}x.$$

Pointwise limit for regular functions: If $u \in C^1(\bar{\Omega}, \mathbb{R}^d)$,

$$\lim_{\delta\to 0} I_\delta(u) = \int_\Omega \bar{w}(Du(x))\,\mathrm{d}x.$$

Proof:

$$\begin{aligned}
&\frac{C_{n,\beta}}{\delta^{n+\beta}} \int_{\Omega\cap B(x,\delta)} w(x'-x, u(x')-u(x))\,\mathrm{d}x' \\
\simeq&\frac{C_{n,\beta}}{\delta^{n+\beta}} \int_{\Omega\cap B(x,\delta)} w^\circ(x'-x, u(x')-u(x))\,\mathrm{d}x' \\
\simeq&\frac{C_{n,\beta}}{\delta^{n+\beta}} \int_{\Omega\cap B(x,\delta)} w^\circ(x'-x, Du(x)(x'-x))\,\mathrm{d}x' \\
\simeq&\frac{C_{n,\beta}}{\delta^{n+\beta}} \int_{B(0,\delta)} w^\circ(\tilde{x}, Du(x)\tilde{x})\,\mathrm{d}\tilde{x} \\
=&\bar{w}(Du(x)).
\end{aligned}$$

$$\begin{cases} I_\delta(u) = \dfrac{C_{n,\beta}}{\delta^{n+\beta}} \displaystyle\int_\Omega \int_{\Omega \cap B(x,\delta)} w(x - x', u(x) - u(x'))\,\mathrm{d}x'\,\mathrm{d}x, \\ \text{in } \mathcal{A}_\delta := \big\{u \in L^p(\Omega, \mathbb{R}^d) \colon u = u_0 \text{ in } \Omega_\delta := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \delta\}\big\} \end{cases}$$

$$\begin{cases} I(u) = \displaystyle\int_\Omega \bar{w}^{qc}(Du(x))\,\mathrm{d}x, \\ \text{in } \mathcal{A} := \big\{u \in W^{1,p}(\Omega, \mathbb{R}^d) \colon u = u_0 \text{ on } \partial\Omega\big\} \end{cases}$$

Theorem. $I_\delta \xrightarrow{\Gamma} I$ in $L^p(\Omega, \mathbb{R}^d)$ as $\delta \to 0$. Specifically,

- Compactness: If $u_\delta \in \mathcal{A}_\delta$ satisfy $I_\delta(u_\delta) \le M$ then there exists $u \in \mathcal{A}$ such that $u_\delta \to u$ in $L^p(\Omega, \mathbb{R}^d)$.
- Lower bound.
- Upper bound.

Use results by J. Bourgain, H. Brezis & P. Mironescu (2001), A. Ponce *Calc Var* (2004), B. Dacorogna *J. Funct. Anal.* (1982).

The Γ-convergence result requires the natural assumption

$$(\mathrm{NC}_\delta)\quad y \mapsto \int_{\Omega\cap B(x,\delta)} w(x, x', y, y')\,\mathrm{d}x' \text{ is convex}$$

for a.e. $x \in \Omega$, all $y' \in \mathbb{R}^d$ and all $\delta > 0$ small enough.

By a Lebesgue-point argument, this is equivalent to saying that $w(x, x', \cdot, y')$ is convex. Hence $w^\circ(\tilde{x}, \cdot)$ is convex and $\bar{w}$ is convex, so no quasiconvexification of $\bar{w}$ is needed.

A more serious problem will arise.

Relaxation

The *relaxation* $\mathcal{I}^*$ of a functional $\mathcal{I}$ is the *lower semicontinuous envelope* in the appropriate topology:

$$\mathcal{I}^*(u) = \sup\left\{ I(u) : I \text{ lsc}, \ I \leq \mathcal{I} \right\}.$$

Also

$$\mathcal{I}^*(u) = \inf\left\{ \liminf_{j\to\infty} \mathcal{I}(u_j) : u_j \to u \right\}.$$

How does relaxation work in the local case?

The relaxation of

$$\int_\Omega W(x, u(x))\,\mathrm{d}x$$

in the weak topology of $L^p(\Omega, \mathbb{R}^d)$ is

$$\int_\Omega W^c(x, u(x))\,\mathrm{d}x,$$

where $W^c(x, \cdot)$ is the convexification of $W(x, \cdot)$. L.C. Young 1931.

The relaxation of

$$\int_\Omega W(x, u(x), Du(x))\,\mathrm{d}x$$

in the weak topology of $W^{1,p}(\Omega, \mathbb{R}^d)$ is

$$\int_\Omega W^{qc}(x, u(x), Du(x))\,\mathrm{d}x,$$

where $W^{qc}(x, y, \cdot)$ is the quasiconvexification $W(x, y, \cdot)$.

B. Dacorogna *J Funct Anal* (1982).

In our nonlocal case, we will focus on the weak topology of L^p.

In the simplest case $w = f(y - y')$, recall that

$$\mathcal{I}(u) = \int_\Omega \int_\Omega f(u(x) - u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

is swlsc iff f is convex. If f is not convex, we are tempted to think that the relaxation $\mathcal{I}^*$ is

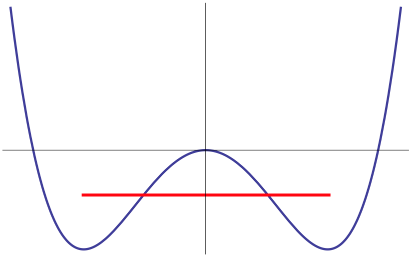
$$\int_\Omega \int_\Omega f^c(u(x) - u(x'))\,\mathrm{d}x'\,\mathrm{d}x,$$

where f^c is the convexification of f. This turns out *not* to be the case.

We suspect that $\mathcal{I}^*$ does not admit an integral representation of the form

$$\int_\Omega \int_\Omega W(x, x', u(x), u(x'))\,\mathrm{d}x'\,\mathrm{d}x.$$

Example. Let $w = f(y - y')$ with f =blue graph.



Then $\mathcal{I} \geq C$, even though f takes values both above and below C.

Moreover, if $\mathcal{I}^*$ admitted an integral representation of the form

$$\int_\Omega \int_\Omega g(u(x) - u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

then g =red graph. So the relaxed energy density g would be neither above nor below f.

A new model is needed

In Solid Mechanics, the model

$$\int_\Omega \int_\Omega w(x - x', u(x) - u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

is wrong. Let's see why.

Start with

$$\mathcal{I}(u) = \int_\Omega \int_\Omega w(x, x', u(x), u(x'))\,\mathrm{d}x'\,\mathrm{d}x$$

and apply familiar conditions in Solid Mechanics.

a) $\mathcal{I}$ is frame-indifferent iff $w = w(x, x', |y - y'|)$.

b) $\mathcal{I}$ is homogeneous and isotropic iff $w = w(|x - x'|, y, y')$.

Let the material be frame-indifferent, homogeneous and isotropic: $w = w(|x - x'|, |y - y'|)$. We do the nonlocal $\rightsquigarrow$ local passage. Recall the process $w \rightsquigarrow w^\circ \rightsquigarrow \bar{w} \rightsquigarrow W$. W.l.o.g., $w = w^\circ$.

$$\begin{aligned}\bar{w}(F) &= \fint_{\mathbb{S}^{n-1}} w(z, Fz)\,\mathrm{d}\mathcal{H}^{n-1}(z) = \fint_{\mathbb{S}^{n-1}} w(|z|, |Fz|)\,\mathrm{d}\mathcal{H}^{n-1}(z)\\ &= \fint_{\mathbb{S}^{n-1}} w(1, |Fz|)\,\mathrm{d}\mathcal{H}^{n-1}(z).\end{aligned}$$

Assume for simplicity that $\bar{w}$ is quasiconvex, hence $W = \bar{w}$ (and ignore the fact that we needed the assumption that $w(\tilde{x}, \cdot)$ is convex, so $\bar{w}$ is already convex). Thus, a quasiconvex W is *retrievable* in this model iff

$$W(F) = \fint_{\mathbb{S}^{n-1}} W(|Fz| I)\,\mathrm{d}\mathcal{H}^{n-1}(z) \qquad \forall F \in \mathbb{R}^{n\times n}_+.$$

Hence W is determined by the values of matrices multiple of the identity: only one degree of freedom!

W retrievable: $$W(F) = \fint_{\mathbb{S}^{n-1}} W(|Fz|I) \, \mathrm{d}\mathcal{H}^{n-1}(z).$$

There are *very few* retrievable W.

Examples:

- $|F|^2$ is retrievable, but no other squared norm is retrievable.
- $|F|^p$ is not retrievable for $p \neq 2$.
- $\det F$ is not retrievable.

The essence of this bug is that the quantity $u(x') - u(x)$ does not discretize (or *delocalize*) the gradient but an average of directional derivatives:

$$\begin{aligned}\int_{\Omega \cap B(x,\delta)} w(x' - x, u(x') - u(x)) \, \mathrm{d}x' &\simeq \int_{B(0,\delta)} w(\tilde{x}, Du(x)\, \tilde{x}) \, \mathrm{d}\tilde{x} \\ &\simeq C_{n,\beta,\delta} \fint_{\mathbb{S}^{n-1}} w(z, Du(x)\, z) \, \mathrm{d}\mathcal{H}^{n-1}(z).\end{aligned}$$

New model

Based on T. Mengesha & D. Spector 15 and T. Mengesha & Q. Du 15, we adopt the model

$$\mathcal{I}(u) = \int_\Omega W(\mathcal{G}u(x))\,\mathrm{d}x$$

where $W : \mathbb{R}^{n\times n} \to \mathbb{R}$ is a typical stored-energy function in hyperelasticity, and $\mathcal{G}u$ is a *nonlocal gradient*:

$$\mathcal{G}u(x) = \int \frac{u(x) - u(x')}{|x - x'|} \otimes \frac{x - x'}{|x - x'|}\,\rho(x - x')\,\mathrm{d}x'.$$

In essence, this new model amounts to replacing

$$\int\int w(\cdots)\,\mathrm{d}x'\,\mathrm{d}x \qquad \text{with} \qquad \int W\left(\int(\cdots)\right)\mathrm{d}x'\,\mathrm{d}x.$$

Functional setup

$$\mathcal{G}u(x) = \int \frac{u(x) - u(x')}{|x - x'|} \otimes \frac{x - x'}{|x - x'|} \, \rho(x - x') \, \mathrm{d}x'.$$

The natural functional space is

$$\{ u \in L^p : \mathcal{G}u \in L^p \} .$$

The properties of this function space depend on ρ.

For simplicity, we choose ρ leading to a known space. We follow T. Shieh & D. Spector 15, 17. For $s \in (0, 1)$, the choice $\rho(t) = t^{-n-s+1}$ gives rise to $L^{s,p}(\mathbb{R}^n)$: the Bessel potential spaces, hence

$$\mathcal{G}u(x) = D^s(x) = \int_{\mathbb{R}^n} \frac{u(x) - u(x')}{|x - x'|^{n+s}} \otimes \frac{x - x'}{|x - x'|} \, \mathrm{d}x'.$$

The advantage of this space is that we know the continuous and compact inclusions into L^q.

Current work: develop an existence theory for W polyconvex.

This entails:

- Definition of nonlocal divergence div^s: Q. Du, M. Gunzburger, R. Lehoucq, K. Zhou 13.
- Nonlocal integration by parts: T. Mengesha & D. Spector 15, T. Mengesha & Q. Du 15:

$$\int D^s u \, \phi = - \int u \operatorname{div}^s \phi \, .$$

- Nonlocal Piola's identity: $\operatorname{div}^s \operatorname{cof} D^s u = 0$.
- Weak continuity of the determinant: if $u_j \rightharpoonup u$ in $L^{s,p}$ then $\det D^s u_j \rightharpoonup \det D^s u$ in L^1.