A phase-space formulation of the theory of elasticity and its relaxation

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Introduction

Usual approach to nonlinear elasticity in the calcuus of variations:

The deformation $u : \Omega \to \mathbb{R}^n$ minimizes the effective energy

$$E[u] = \int_\Omega W(Du) + g(x, u) dx$$

(+ boundary data).

Where does W come from?

Experimental data,
Microscopic simulation data,
Symmetry requirements,
Physical intuition,
Fitting.

Mechanics in phase space

Key idea: **compatibility** and **equilibrium** are central,

material laws come later.

Usual approach: u_j makes $\int_\Omega [W(Du_j) - f \cdot u_j] dx$ small:

Du_j is an exact gradient (compatibility)

The stress σ_j is given by $\sigma_j = DW(Du_j)$ (material law)

Equilibrium $\operatorname{div} \sigma_j + f = 0$ is fulfilled only asymptotically

Idea: $Du_j \in L^2(\Omega; \mathbb{R}^{n\times n})$ is an exact gradient (compatibility)

$\sigma_j \in L^2(\Omega; \mathbb{R}^{n\times n})$ obeys $\operatorname{div} \sigma_j + f = 0$ (equilibrium)

Asymptotically, the pair $(Du_j(x), \sigma_j(x))$ approaches the "material set" $\mathcal{D}_{loc} \subset \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$ for almost all $x \in \Omega$.

Plan

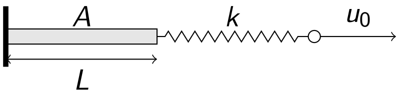
1. Elementary example: bar and spring.

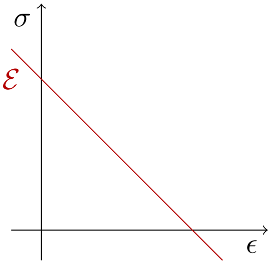
2. Finite elasticity in phase space
   Classical solutions, strong solutions, generalized solutions
   div-curl convergence, coercivity, closedness
   [SC, SM, MO, arXiv:1912.02978]

3. Linearized elasticity in phase space
   Transversality
   Relaxation
   [SC, SM, MO, ARMA 2018]

4. Related: Relaxation in stress space
   sym-div-quasiconvexity
   [SC, SM, MO, ARMA 2019]

Elementary example: bar and spring



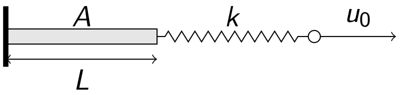


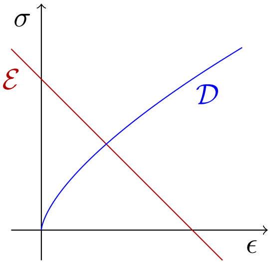
Phase space of bar $X = \{(\epsilon, \sigma)\} = \mathbb{R}^2$

Compatibility + equilibrium: $\sigma A = k(u_0 - \epsilon L)$

Constraint set $\mathcal{E} := \{(\epsilon, \sigma) : \sigma A = k(u_0 - \epsilon L)\} \subset X$

Elementary example: bar and spring





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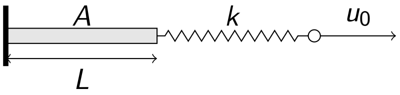
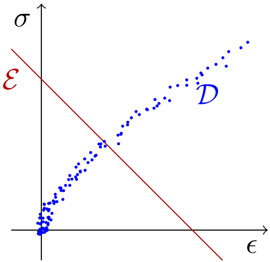
Material data set $\mathcal{D} \subset X$, e.g., $\mathcal{D} = \{(\epsilon, \epsilon^{1/3}) : \epsilon \in \mathbb{R}\}$

Classical solution set: $\mathcal{D} \cap \mathcal{E}$.

Elementary example: bar and spring





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Classical solution set: $\mathcal{D} \cap \mathcal{E}$.

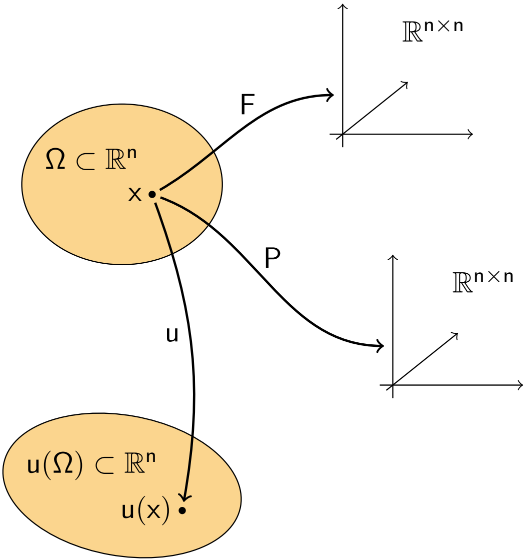
Data-driven solution: $\min\{dist(z, \mathcal{D}) : z \in \mathcal{E}\}$.

The general data-driven problem

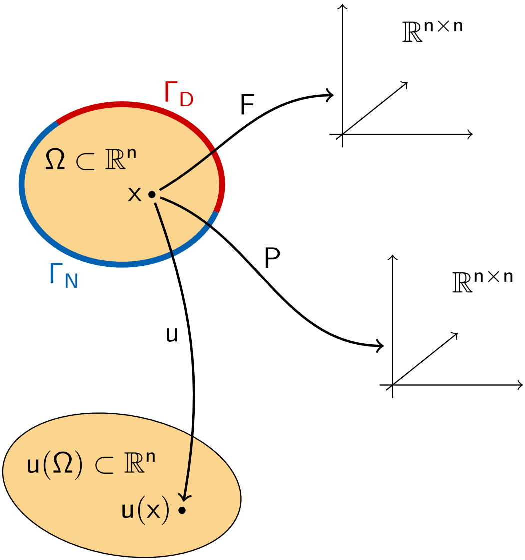
- $\boxed{\text{minimize } \text{dist}^2(z, y) \text{ over } y \in \mathcal{D},\ z \in \mathcal{E}}$
  - $\mathcal{D} = \{\text{material data}\}$
  - $\mathcal{E} = \{\text{compatibility and equilibrium}\}$
- Aim: find the compatible strain field and the equilibrated stress field **closest** to the material data set
- No material modeling, no data fitting (ideally)
- Raw material data is used (ideally, unprocessed) in calculations ('the facts, nothing but the facts . . . ')

T. Kirchdoerfer and M. Ortiz CMAME (2016, 2017).

The general data-driven problem



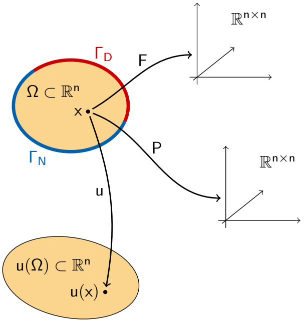
The general data-driven problem



Finite elasticity in phase space

$\Omega \subset \mathbb{R}^n$ Lipschitz, bounded, $\partial\Omega = \overline{\Gamma_D} \cup \overline{\Gamma_N}$, $\quad \mathcal{H}^{n-1}(\Gamma_D) > 0$

Phase space:
$X_{p,q}(\Omega) := \{(F,P) : F \in L^p(\Omega;\mathbb{R}^{n\times n}),\ P \in L^q(\Omega;\mathbb{R}^{n\times n})\}$
1/p+1/q=1



Constraint set $\mathcal{E} \subset X_{p,q}$:
pairs (F,P) which satisfy
i) Compatibility $\quad F = \nabla u, \quad u = g$ on Γ_D
ii) Equilibrium $\quad \operatorname{div} P = f, \quad P\nu = h$ on Γ_N
iii) Moment equilibrium $\quad FP^T = PF^T$

Material data set
$\mathcal{D} = \{(F,P) \in X_{p,q} : (F(x),P(x)) \in D_{loc} \text{ a.e.}\}$

Minimizers of the data-driven problem

Minimize

$$I((F,P),(F',P')) := \begin{cases} \int_\Omega \Big(|F(x) - F'(x)|^p + |P(x) - P'(x)|^q \Big)\, dx \\ \qquad \text{if } (F,P) \in \mathcal{E},\ (F',P') \in \mathcal{D}, \\ \infty, \qquad \text{otherwise.} \end{cases}$$

Questions:

Existence?

Coercivity, lower semicontinuity?

Relaxation?

Approximation?

Discretization?

Many concepts of solution

$u \in W^{1,p}(\Omega;\mathbb{R}^n)$ is a **classical solution** if $(Du, T(Du)) \in \mathcal{E}$,
with $\mathcal{D}_{loc} = \{(F', P') : P' = T(F'), F' \in \mathbb{R}^{n\times n}\}$.

$(F, P) \in X_{p,q}(\Omega)$ is a **strong solution** if $(F, P) \in \mathcal{E} \cap \mathcal{D}$.

$((F, P), (F', P')) \in \mathcal{E} \times \mathcal{D} \subset X_{p,q}(\Omega) \times X_{p,q}(\Omega)$ is a **generalized solution** if it is a minimizer of I.

$((F, P), (F', P')) \in \mathcal{E} \times \mathcal{D} \subset X_{p,q}(\Omega) \times X_{p,q}(\Omega)$ is a **relaxed solution** if it is accumulation point of a minizing sequence of I.

Remark: "Strong solution" is the same as
"generalized solution and $\inf I = 0$".

Coercivity

Lemma: If $(F, P) \in \mathcal{E}$, then $\int_\Omega F \cdot P \le c\|(F, P)\|_{X_{p,q}} + c$, with c depending on the boundary data.

Proof: If $F = \nabla u$ and $\operatorname{div} P + f = 0$ in Ω, then
$\int_\Omega F \cdot P = \int_\Omega \nabla u \cdot P = \int_{\partial\Omega} u \cdot P\nu + \int_\Omega uf$.
By the boundary data, $\int_{\partial\Omega} u \cdot P\nu$ has linear growth.

Definition: We say that $\mathcal{D}_{loc}$ is (p, q)-coercive if

$$\frac{1}{c}|F|^p + \frac{1}{c}|P|^q - c \le F \cdot P \text{ for all } (F, P) \in \mathcal{D}_{loc}.$$

Theorem: If $\mathcal{D}_{loc}$ is coercive, and $\inf I < \infty$, then minimizing sequences have a weak limit (in $X_{p,q}$). The constraint set $\mathcal{E}$ is weakly closed.

Example in 2d

Let $W_2(\xi) := \frac{1}{2}|\xi|^2 + \frac{1}{4}a|\xi|^4 + g(\det\xi)$,

with $g \in C^1(\mathbb{R})$ convex, $|g'|(t) \leq b + d|t|$, $n = 2$, $0 \leq d < 2a$.

Then DW_2 generates a $(4, 4/3)$-coercive data set.

Choosing $g(t) = \frac{1}{2}\beta(t - 1 - \frac{1+2a}{\beta})^2$, W_2 is minimized by $SO(2)$.

Example in 3d

Let $W_3(\xi) := \frac{1}{2}|\xi|^2 + \frac{1}{4}a|\xi|^4 + \frac{1}{6}e|\xi|^6 + g(\det \xi)$.

with $g \in C^1(\mathbb{R})$ convex, $|g'|(t) \leq b + d|t|$, $n = 3$, $0 \leq d < 3e$.

Then DW_3 generates a $(6, 6/5)$-coercive data set.

Choosing $g(t) = \frac{1}{2}\beta(t - 1 - \frac{1+3a+9e}{\beta})^2$, W_3 is minimized by $SO(3)$.

div-curl convergence

$(F_k, P_k) \in X_{p,q}(\Omega)$ is **div-curl convergent** to (F, P) if

$F_k \rightharpoonup F$ in L^p, $P_k \rightharpoonup P$ in L^q,
$\operatorname{curl} F_k \to \operatorname{curl} F$ in $W^{-1,p}$, $\operatorname{div} P_k \to \operatorname{div} P$ in $W^{-1,q}$.

Div-curl Lemma [Murat-Tartar]:
If $(F_k, P_k) \stackrel{div-curl}{\rightarrow} (F, P)$ then $F_k P_k^T \rightharpoonup FP^T$.

Lemma: If $(F_k, P_k) \in \mathcal{D}$, $(F'_k, P'_k) \in \mathcal{E}$,
and $I((F_k, P_k), (F'_k, P'_k)) \to 0$,
then both sequences are div-curl convergent
and they have the same limit (F, P).

div-curl closed data sets

$\mathcal{D} \subset X_{p,q}(\Omega)$ is **div-curl closed** if it is closed with respect to div-curl convergence.

$\mathcal{D}_{loc} \subset \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$ is **locally div-curl closed** if $(F_k, P_k) \in \mathcal{D}_{loc}$ a.e. and $(F_k, P_k) \stackrel{div-curl}{\rightarrow} (F_*, P_*) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}$ implies $(F_*, P_*) \in \mathcal{D}_{loc}$.

Theorem: $\mathcal{D}$ is div-curl closed iff it is locally div-curl closed.

Proof: localization by blow-up, Hodge decomposition for truncation, ...

Polymonotonicity and quasimonotonicity

$T : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ is **strictly polymonotone** if there are $A : \mathbb{R}^{n\times n} \to \mathbb{R}^{\tau(n)}$, $B \in C^0(\mathbb{R}^{n\times n} \times \mathbb{R}^{n\times n}; [0,\infty))$ such that

$$(T(F+G) - T(F)) \cdot G \geq A(F) \cdot M(G) + B(F,G),$$

for all $F, G \in \mathbb{R}^{n\times n}$, with $B(F,G) > 0$ for all $G \neq 0$.
Here $M : \mathbb{R}^{n\times n} \to \mathbb{R}^{\tau(n)}$ is the vector of minors.

$T : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ (Borel, loc. bd.) is **strictly quasimonotone** if

$$\int_\omega (T(F+D\varphi) - T(F)) \cdot D\varphi \, dx \geq \int_\omega B(F, D\varphi) dx$$

for all $F \in \mathbb{R}^{n\times n}$, $\varphi \in C_c^\infty(\omega; \mathbb{R}^n)$. [cp. Zhang 1988]

Theorem: both imply that D is div-curl-closed.

Example in 2d

Let $W_2(\xi) := \frac{1}{2}|\xi|^2 + \frac{1}{4}a|\xi|^4 + g(\det \xi)$,

with $g \in C^1(\mathbb{R})$ convex, $|g'|(t) \le b + d|t|$, $b \le 2$, $0 \le d < 2a$.

Then DW_2 generates a $(4, 4/3)$-coercive, div-curl closed data set.

Choosing $g(t) = \frac{1}{2}\beta(t - 1 - \frac{1+2a}{\beta})^2$, W_2 is minimized by $SO(2)$.

Example in 3d

Let $W_3(\xi) := \frac{1}{2}|\xi|^2 + \frac{1}{4}a|\xi|^4 + \frac{1}{6}e|\xi|^6 + g(\det \xi)$.

with $g \in C^1(\mathbb{R})$ convex, $|g'(t) - g'(s)| \leq d(|t| + |s|)$, $0 \leq^d < c_* e$.

Then DW_3 generates a $(6, 6/5)$-coercive, div-curl closed data set.

Choosing $g(t) = \frac{1}{2}\beta(t - 1 - \frac{1+3a+9e}{\beta})^2$, W_3 is minimized by $SO(3)$.

Open problems

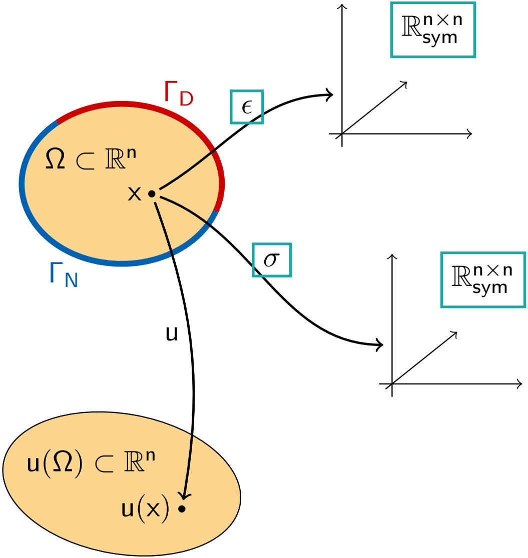
Approximation of $\mathcal{D}$: What happens if we have a sequence $\mathcal{D}_h \to \mathcal{D}$, do solutions converge to solutions? What topology is relevant?

Approximation of $\mathcal{E}$: How do we discretize $\mathcal{E}$, for example, for numerics? How to deal with the condition $FP^T = PF^T$?

Relaxation: What if we have coercivity but no lower semicontinuity, what is the appropriate concept of relaxation?

How should we deal with the $\inf I > 0$ case?

Geometrically linear elasticity in phase space



Geometrically linear elasticity in phase space

$\Omega \subset \mathbb{R}^n$ Lipschitz, bounded, $\partial\Omega = \overline{\Gamma_D} \cup \overline{\Gamma_N}$, $\quad \mathcal{H}^{n-1}(\Gamma_D) > 0$

Phase space:
$X_{\text{Lin}} := \{(\epsilon, \sigma) : \epsilon \in L^2(\Omega; \mathbb{R}^{n\times n}_{\text{sym}}),\ \sigma \in L^2(\Omega; \mathbb{R}^{n\times n}_{\text{sym}})\}$

Constraint set: $\mathcal{E} \subset X_{\text{Lin}}$ consists of pairs (ϵ, σ) which satisfy:
i) Compatibility $\quad \epsilon = \frac{1}{2}(\nabla u + (\nabla u)^T), \quad u = g$ on Γ_D
ii) Equilibrium $\quad \operatorname{div} \sigma = f, \quad \sigma\nu = h$ on Γ_N.

Material data set:
$\mathcal{D} = \{(\epsilon, \sigma) \in X_{\text{Lin}} : (\epsilon(x), \sigma(x)) \in D_{loc} \text{ a.e.}\}$

Simplest example:
Hooke's law, $\quad \mathcal{D}_{loc} = \{(\epsilon, \sigma) \in (\mathbb{R}^{n\times n}_{\text{sym}})^2 : \sigma = \mathbb{C}\epsilon\}, \quad \mathbb{C} > 0$

Compatibility with the classical theory

Proposition: Assume $f \in L^2(\Omega; \mathbb{R}^n)$, $g \in H^{1/2}(\partial\Omega; \mathbb{R}^n)$, $h \in H^{-1/2}(\partial\Omega; \mathbb{R}^n)$,

$$\mathcal{D} = \{(\epsilon, \sigma) : \sigma(x) = \mathbb{C}\epsilon(x) \text{ a.e.}\}$$

Then, the data-driven problem

$$\min\{d(z, \mathcal{D}),\ z \in \mathcal{E}\}$$

has a unique solution. Moreover, the data-driven solution satisfies

$$\sigma = \mathbb{C}\epsilon$$

$$\operatorname{div}\sigma + f = 0$$

$$\epsilon = \frac{1}{2}(\nabla u + \nabla u^T),\ u \in W^{1,2}(\Omega; \mathbb{R}^n)$$

$$\sigma\nu = h \text{ on } \Gamma_N \ (\text{in } H^{-1/2})$$

$$u = g \text{ on } \Gamma_D \ (\text{in } H^{1/2})$$

Coercivity

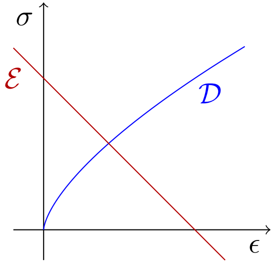
Coercivity follows from **transversality:** $\exists c > 0, b \geq 0$

$$\|y - z\| \geq c(\|y\| + \|z\|) - b \quad \forall y \in \mathcal{D}\ \forall z \in \mathcal{E}.$$

If this holds, and $I(y_h, z_h) < C$, then, up to a subsequence, $(y_h, z_h) \rightharpoonup (y, z)$ in $L^2(\Omega; \mathbb{R}^{n\times n\times n\times n} \times \mathbb{R}^{n\times n\times n\times n})$.

If $I(y_h, z_h) \to 0$ then $y_h - z_h \to 0$.

If $\mathcal{D}$ is linear at infinity, then transversality holds.



Abstract data convergence

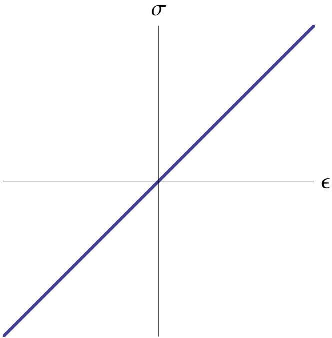
Def.: A sequence (y_h, z_h) in $X_{\text{Lin}} \times X_{\text{Lin}}$ is said to converge to $(y, z) \in X_{\text{Lin}} \times X_{\text{Lin}}$ in the data topology, $(y_h, z_h) \xrightarrow{\Delta} (y, z)$, if

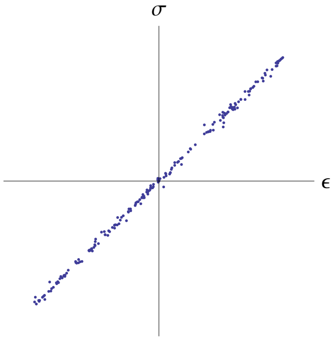
$$y_h \rightharpoonup y, \quad z_h \rightharpoonup z \quad \text{and} \quad y_h - z_h \to y - z.$$

Corresponding notion of
$\Gamma(\Delta)$-convergence for functionals $F : X_{\text{Lin}} \times X_{\text{Lin}} \to [0, \infty]$
Kuratowski $K(\Delta)$-convergence for subsets of $X_{\text{Lin}} \times X_{\text{Lin}}$.

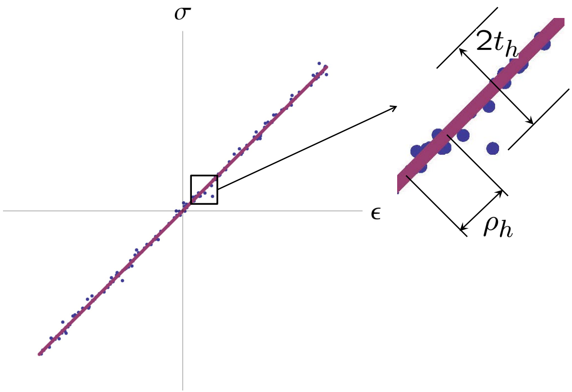
Concept of relaxation! (Γ-limit of constant sequence)

Sampled local material data sets





Convergence of sampled data sets



t_h uniform approximation

ρ_h fine approximation

Relaxation and approximation

Theorem: Let $\mathcal{E} \subset X_{\mathrm{Lin}}$ be weakly sequentially closed, $\mathcal{D} = \{z : z(x) \in D_{loc} \text{ a.e.}\}$, $\bar{\mathcal{D}} \subset X_{\mathrm{Lin}}$. Suppose:

i) (Relaxation) $\bar{\mathcal{D}} \times \mathcal{E} = K(\Delta)-\lim_{h\to\infty}(\mathcal{D} \times \mathcal{E})$.

ii) (Fine approximation)
$\exists\ \rho_h \downarrow 0 \quad d(\xi, \mathcal{D}_{loc,h}) \leq \rho_h \quad \forall \xi \in \mathcal{D}_{loc}$;

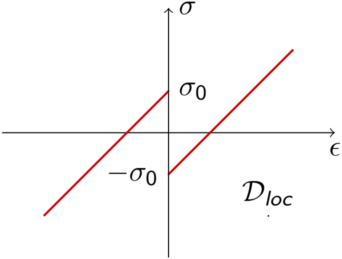
iii) (Uniform approximation)
$\exists\ t_h \downarrow 0 \quad d(\xi, \mathcal{D}_{loc}) \leq t_h \quad \forall \xi \in \mathcal{D}_{loc,h}$.

iv) (Transversality) $\exists c > 0,\ b \geq 0$

$$\|y - z\| \geq c(\|y\| + \|z\|) - b \quad \forall y \in \mathcal{D}\ \forall z \in \mathcal{E}.$$

Then, $\bar{\mathcal{D}} \times \mathcal{E} = K(\Delta)-\lim_{h\to\infty}(\mathcal{D}_h \times \mathcal{E})$.

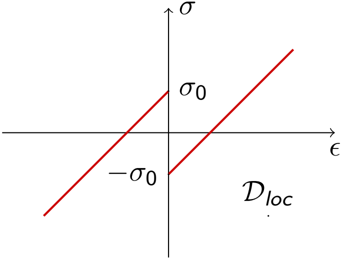
Relaxation: The two-well problem in 1d

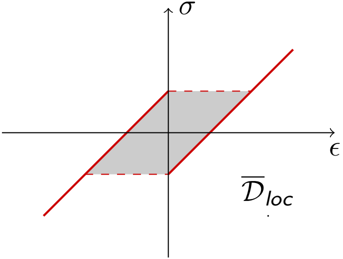


$$\begin{aligned}\mathcal{D}_{loc} &= \{(\epsilon, \mathbb{C}\epsilon + \sigma_0), \epsilon \leq 0\} \cup \{(\epsilon, \mathbb{C}\epsilon - \sigma_0), \epsilon \geq 0\},\\ &= \{(\mathbb{C}^{-1}\sigma - \epsilon_0, \sigma) : \sigma \leq \sigma_0\} \cup \{\mathbb{C}^{-1}\sigma + \epsilon_0, \sigma) : \sigma \geq -\sigma_0\},\end{aligned}$$

$(\mathbb{C} > 0,\ \sigma_0 \geq 0, \epsilon_0 := \mathbb{C}^{-1}\sigma_0)$.

Relaxation: The two-well problem in 1d





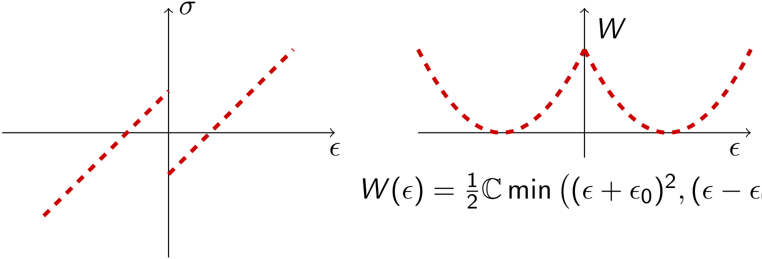
$$\begin{aligned}\mathcal{D}_{loc} &= \{(\epsilon, \mathbb{C}\epsilon + \sigma_0), \epsilon \leq 0\} \cup \{(\epsilon, \mathbb{C}\epsilon - \sigma_0), \epsilon \geq 0\}, \\ &= \{(\mathbb{C}^{-1}\sigma - \epsilon_0, \sigma) : \sigma \leq \sigma_0\} \cup \{\mathbb{C}^{-1}\sigma + \epsilon_0, \sigma) : \sigma \geq -\sigma_0\},\end{aligned}$$

$$\bar{\mathcal{D}}_{loc} = \mathcal{D}_{loc} \cup \{(\mathbb{C}^{-1}\sigma + \mu\epsilon_0, \sigma), |\mu| \leq 1, |\sigma| \leq \sigma_0\}$$

$(\mathbb{C} > 0,\ \sigma_0 \geq 0, \epsilon_0 := \mathbb{C}^{-1}\sigma_0)$.

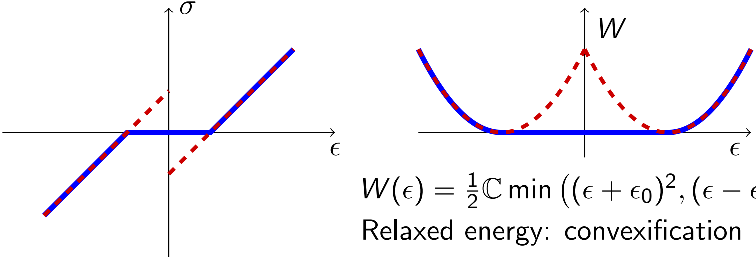
Then, $\bar{\mathcal{D}} \times \mathcal{E} = K(\Delta) - \lim_{h\to\infty} \mathcal{D} \times \mathcal{E}$.

Data relaxation vs. relaxation of the energy



$$W(\epsilon) = \frac{1}{2}\mathbb{C}\min\left((\epsilon+\epsilon_0)^2, (\epsilon-\epsilon_0)^2\right)$$

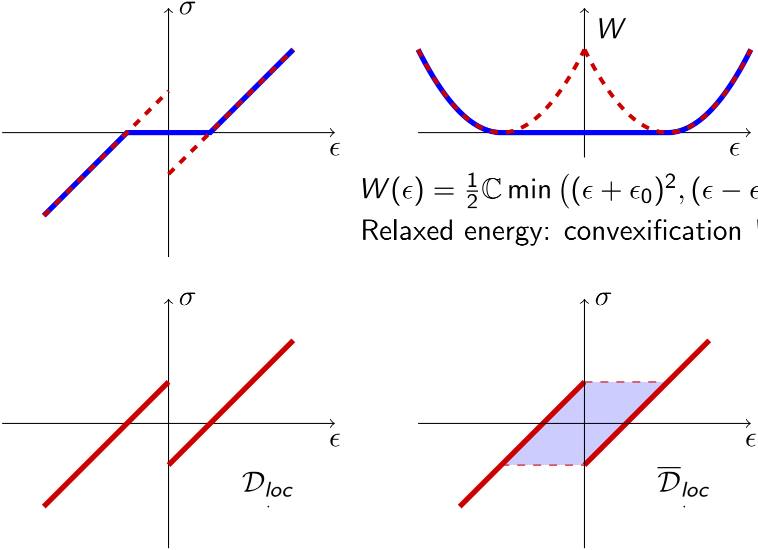
Data relaxation vs. relaxation of the energy



$W(\epsilon) = \frac{1}{2}\mathbb{C}\,\mathrm{min}\left((\epsilon+\epsilon_0)^2,(\epsilon-\epsilon_0)^2\right)$

Relaxed energy: convexification W^{**}

Data relaxation vs. relaxation of the energy



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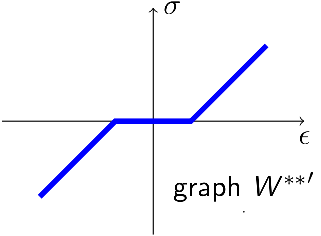
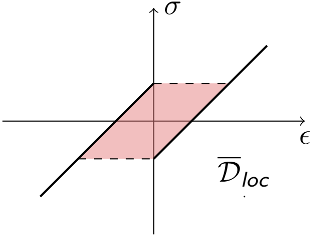
Relaxed energy: convexification W^{**}

Data relaxation and hysteresis





The general two well problem with equal moduli

Fix $\mathbb{C} > 0$ and $b \in \mathbb{R}^{n\times n}_{\mathrm{sym}}$. Let $\mathcal{D}_{loc} := \mathcal{D}^+_{loc} \cup \mathcal{D}^-_{loc}$,

$$\mathcal{D}^+_{loc} := \{(\mathbb{C}^{-1}\sigma + b, \sigma) : \sigma \in \mathbb{R}^{n\times n}_{\mathrm{sym}},\ \sigma\cdot b \geq -\mathbb{C}b\cdot b\},$$
$$\mathcal{D}^-_{loc} := \{(\mathbb{C}^{-1}\sigma - b, \sigma) : \sigma \in \mathbb{R}^{n\times n}_{\mathrm{sym}},\ \sigma\cdot b \leq \mathbb{C}b\cdot b\}.$$

..... then there is a (somewhat long) formula for $\bar{\mathcal{D}}_{loc}$, and

$$\bar{\mathcal{D}} \times \mathcal{E} = K(\Delta)\!-\!\lim_{h\to\infty} \mathcal{D} \times \mathcal{E}.$$

- Phase-space formulation
  of continuum mechanics
- Possible application:
  Data-driven simulation (no model!)
- Existence for finite elasticity
  via div-curl-convergence and quasimonotonicity
- Approximation and Relaxation
  for infinitesimal elasticity
- Example: geometrically linear
  two-well problem