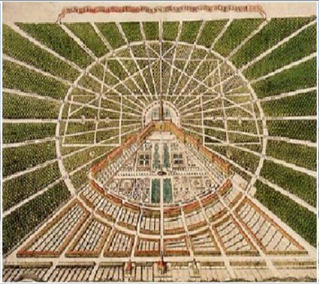
Karlsruhe Institute of Technology

Université franco-allemande
Deutsch-Französische Hochschule

Matti Schneider

Treating inelastic problems with the basic scheme

Introduction to FFT-based numerical methods for the homogenization of random materials


In memoriam

Prof. Dr. Wolfgang Seemann
31.3.1961 - 8.2.2022

Overview I

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Overview

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Linear elasticity

given:

- cell Q
- stiffness $\mathbb{C}(x)$
- strain $\bar{\varepsilon}$

sought:

- $u : Q \to \mathbb{R}^d$ (periodic)

$$\begin{aligned} \varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= \mathbb{C} : \varepsilon && \text{(material law)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)} \end{aligned}$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\texttt{eff}} : \bar{\varepsilon}$

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Linear elasticity - beyond?

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output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\texttt{eff}} : \bar{\varepsilon}$

Inelasticity?

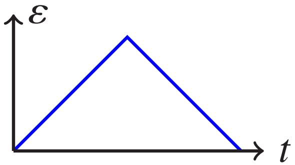
input:

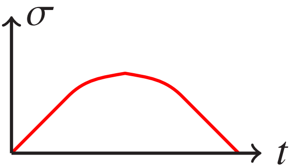
- initial state
- strain history $\varepsilon : [t_{\mathtt{start}}, t_{\text{end}}] \to \mathrm{Sym}\,(d)$

output:

- stress history $\sigma : [t_{\mathtt{start}}, t_{\text{end}}] \to \mathrm{Sym}\,(d)$

Inelasticity?

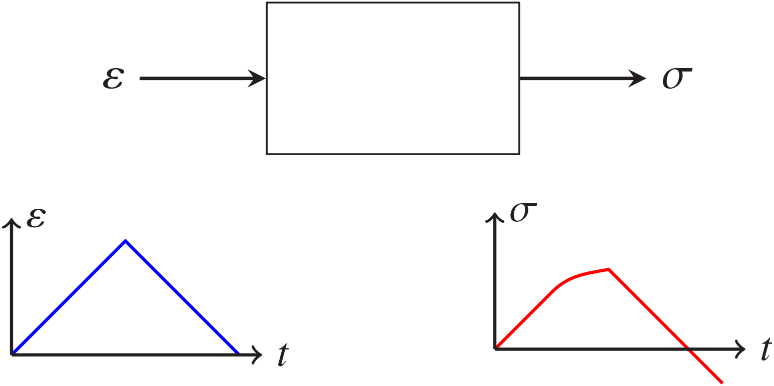




elasticity:

$$\sigma = f(\varepsilon)$$

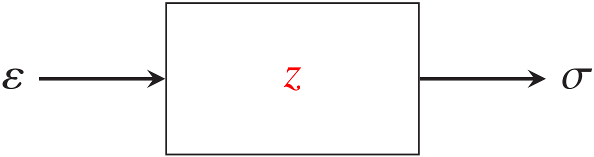
Inelasticity?

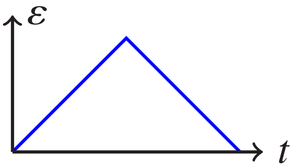


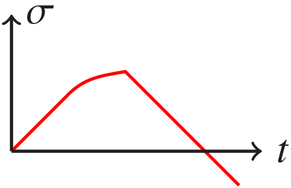
inelasticity:

$$\sigma = f(\varepsilon, z)$$
$$0 = g(\varepsilon, z, \dot{z})$$

Inelasticity?







inelasticity:

$$\sigma = f(\varepsilon, z)$$
$$0 = g(\varepsilon, z, \dot{z})$$

Example - vM plasticity

$$\begin{aligned} \sigma &= f(\varepsilon, z) \\ 0 &= g(\varepsilon, z, \dot{z}) \end{aligned}$$

- $z = (\varepsilon^p, p)$
- Hooke's law

$$\sigma = \mathbb{C} : (\varepsilon - \varepsilon^p)$$

- evolution

$$\dot{\varepsilon}^p = \dot{p}\,\sqrt{\frac{3}{2}}\,\frac{\text{dev}\,\sigma}{\|\text{dev}\,\sigma\|},$$

$$\sqrt{\frac{3}{2}}\,\|\text{dev}\,\sigma\| \leq \sigma_Y(p), \quad \dot{p} \geq 0, \quad \left(\sqrt{\frac{3}{2}}\,\|\text{dev}\,\sigma\| - \sigma_Y(p)\right)\dot{p} = 0$$

Example - vM plasticity

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- $z = (\varepsilon^p, p)$
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$$\sigma = \mathbb{C} : (\varepsilon - \varepsilon^p)$$

- evolution

$$\dot{\varepsilon}^p = \dot{p} \sqrt{\frac{3}{2}} \frac{\text{dev } \sigma}{\|\text{dev } \sigma\|},$$

$$\dot{p} = \max\left(0, \dot{p} + \rho\left(\sqrt{\frac{3}{2}}\|\text{dev } \sigma\| - \sigma_Y(p)\right)\right), \quad \rho > 0$$

Linear elasticity - beyond?

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given:

- cell Q
- stiffness $\mathbb{C}(x)$
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sought:

- $u : Q \to \mathbb{R}^d$ (periodic)

$$\begin{aligned} \varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= \mathbb{C} : \varepsilon && \text{(material law)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)} \end{aligned}$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$
- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\texttt{eff}} : \bar{\varepsilon}$

Upscaling inelasticity

given:

- cell Q
- functions $f(x, \varepsilon, z)$ and $g(x, \varepsilon, z, \dot{z})$
- strain history $\bar{\varepsilon}(t)$
- initial condition $z_0(x)$

sought:

- $u : Q \times [t_{\mathtt{start}}, t_{\mathrm{end}}] \to \mathbb{R}^d$ (periodic) and $z : Q \times [t_{\mathtt{start}}, t_{\mathrm{end}}] \to \mathbb{R}^K$

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\begin{aligned}
\varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)}\\
\sigma &= f(x, \varepsilon, z) && \text{(material law)}\\
0 &= g(\varepsilon, z, \dot{z}), \quad z(x, t_{\mathtt{start}}) = z_0(x) && \text{(internal evolution)}\\
\operatorname{div} \sigma &= 0 && \text{(equilibrium)}
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output:

- $\bar{\sigma}(t) = \langle \sigma(t, \cdot) \rangle_Q$

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Upscaling inelasticity

given:

- cell Q
- functions $f(x, \varepsilon, z)$ and $g(x, \varepsilon, z, \dot{z})$
- strain history $\bar{\varepsilon}(t)$
- initial condition $z_0(x)$
- time discretization $t_{\mathtt{start}} = t_0 < t_1 < \ldots < t_N = t_{\mathtt{end}}$, e.g., $\dot{z}(t_{n+1}) \approx (z_{n+1} - z_n)/(t_{n+1} - t_n)$

sought $(n \longrightarrow n+1)$:

- $u_{n+1} : Q \to \mathbb{R}^d$ (periodic) and $z_{n+1} : Q \to \mathbb{R}^K$

$$
\begin{aligned}
0 &= \operatorname{div} f(x, \bar{\varepsilon}_{n+1} + \nabla^s u_{n+1}, z_{n+1}) \\
0 &= g(\varepsilon_{n+1}, z_{n+1}, (z_{n+1} - z_n)/(t_{n+1} - t_n))
\end{aligned}
$$

output:

- $\bar{\sigma}_{n+1} = \langle \sigma_{n+1} \rangle_Q$

Fix time step, drop $n+1$

sought:

- $u : Q \to \mathbb{R}^d$ (periodic) and $z : Q \to \mathbb{R}^K$

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\begin{aligned}
0 &= \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z) \\
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\end{aligned}
$$

- PDE in u (d unknowns) $\nearrow$ non-local, sparse (after discretization)
- algebraic equation in z (K unknowns) $\nearrow$ local

Fix time step, drop $n+1$

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Option I: solve full system

sought:

- $u : Q \to \mathbb{R}^d$ (periodic) and $z : Q \to \mathbb{R}^K$

$$
\begin{aligned}
0 &= \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z) \\
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\end{aligned}
$$

- $d + K$ unknowns (at x)
- non-local, sparse (after discretization)

Option II: eliminate z

sought:

- $u : Q \to \mathbb{R}^d$ (periodic) and $z : Q \to \mathbb{R}^K$

$$\begin{aligned} 0 &= \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, z) \\ 0 &= g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n)) \end{aligned}$$

- idea: write z as implicit function of ε

$$z \quad \text{solves} \quad g(\varepsilon, z, (z - z_n)/(t_{n+1} - t_n)) = 0 \qquad \Longleftrightarrow \qquad z = h_n(\varepsilon)$$

Option II: eliminate z

sought:

- $u : Q \to \mathbb{R}^d$ (periodic) and $z : Q \to \mathbb{R}^K$

$$\begin{aligned} 0 &= \operatorname{div} f(x, \bar{\varepsilon} + \nabla^s u, h_n(\bar{\varepsilon} + \nabla^s u)) \\ z &= h_n(\bar{\varepsilon} + \nabla^s u) \end{aligned}$$

- d unknowns (at x)
- non-local, sparse (after discretization)
- “static condensation”

Option II: eliminate z

sought:

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$$

- leads to a **pseudo-elastic** problem for u
- z obtained in post-processing
- basis of user material routines

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- leads to a **pseudo-elastic** problem for u
- z obtained in post-processing
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Digression Part I

- inelasticity $\nearrow$ time steps
- move from one time step to the next
- eliminate the internal variables, update later
- we are left with solving

$$\operatorname{div} \mathsf{S}(x, \bar{\varepsilon} + \nabla^s u) = 0$$

with an **elastic** “stress function" S

$$\mathsf{S}(x, \varepsilon) \equiv f(x, \varepsilon, h_n(\varepsilon))$$

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\operatorname{div} \sigma &= 0 && \text{(equilibrium)}
\end{aligned}
$$

output:

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- $\Rightarrow \bar{\sigma} = \mathbb{C}^{\mathtt{eff}} : \bar{\varepsilon}$

Non-Linear elasticity

given:

- cell Q
- stress function S
- strain $\bar{\varepsilon}$

sought:

- $u : Q \to \mathbb{R}^d$ (periodic)

$$\begin{aligned} \varepsilon &= \bar{\varepsilon} + \nabla^s u && \text{(compatibility)} \\ \sigma &= \mathsf{S}(x, \varepsilon) && \text{(material law)} \\ \operatorname{div} \sigma &= 0 && \text{(equilibrium)} \end{aligned}$$

output:

- $\bar{\sigma} = \langle \sigma \rangle_Q$

Lippmann-Schwinger reformulation

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seek $u : Q \to \mathbb{R}^d$:

$$0 = -\text{div}\, \mathbb{S}(\cdot, \bar{\varepsilon} + \nabla^s u)$$

Lippmann-Schwinger reformulation

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seek $u : Q \to \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) = -\operatorname{div} \left[\mathsf{S}(\cdot, \bar{\varepsilon} + \nabla^s u) - \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) \right]$$

- reference material $\mathbb{C}^0$

Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : \nabla^s u = -\operatorname{div} \left[S(\cdot, \bar{\varepsilon} + \nabla^s u) - \mathbb{C}^0 : (\bar{\varepsilon} + \nabla^s u) \right]$$

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Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$\operatorname{div} \mathbb{C}^0 : \nabla^s u = -\operatorname{div} \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material $\mathbb{C}^0$
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$

Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$u = -G^0 \text{div} \left[\mathsf{S}(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material $\mathbb{C}^0$
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $G^0 = (\text{div}\ \mathbb{C}^0 : \nabla^s)^{-1}$

Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$\nabla^s u = -\nabla^s G^0 \operatorname{div} \left[\mathsf{S}(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material $\mathbb{C}^0$
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Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$\bar{\varepsilon} + \nabla^s u = \bar{\varepsilon} - \nabla^s G^0 \text{div} \left[\mathsf{S}(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material $\mathbb{C}^0$
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
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Lippmann-Schwinger reformulation

seek $u : Q \to \mathbb{R}^d$:

$$\bar{\varepsilon} + \nabla^s u = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

- reference material $\mathbb{C}^0$
- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
- $\Gamma^0 = \nabla^s (\text{div}\, \mathbb{C}^0 : \nabla^s)^{-1} \text{div}$

Lippmann-Schwinger reformulation

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seek $\varepsilon : Q \to \mathrm{Sym}(d)$:

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[S(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

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- total strain $\varepsilon = \bar{\varepsilon} + \nabla^s u$
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Nonlinear Lippmann-Schwinger equation

seek $\varepsilon : Q \to \mathrm{Sym}(d)$:

$$\varepsilon = \bar{\varepsilon} - \Gamma^0 : \left[\mathsf{S}(\cdot, \varepsilon) - \mathbb{C}^0 : \varepsilon \right]$$

Nonlinear basic scheme

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seek $\varepsilon^{k+1} : Q \to \text{Sym}(d)$:

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- conceived by Moulinec & Suquet

  [H. Moulinec and P. Suquet, Comptes Rendus de l'Académie des Sciences, 1994]

  [H. Moulinec and P. Suquet, CMAME, 1998]

- works with any discretization

Nonlinear basic scheme

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Questions:

- When does it converge?
- How to choose $\mathbb{C}^0$?

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Overview

1. From inelasticity to elasticity

2. The nonlinear basic scheme

3. Gradient descent

Gradient descent

Goal:

$$f(x) \longrightarrow \min_{x \in X}$$

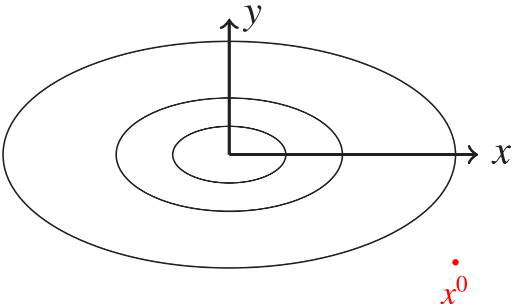
Critical point eq.:

$$\nabla f(x) \stackrel{!}{=} 0$$

Gradient descent:

$$x^{k+1} = x^k - s^k \, \nabla f(x^k)$$

s^k ... step size



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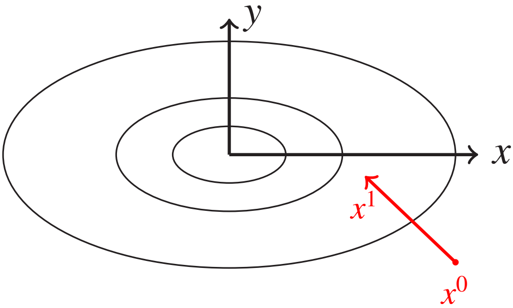

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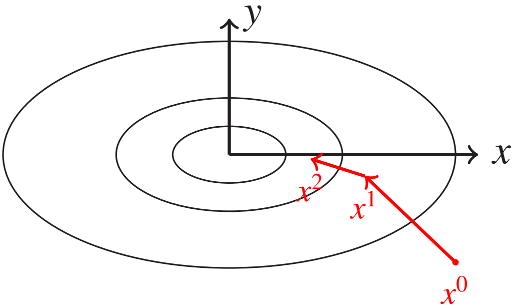

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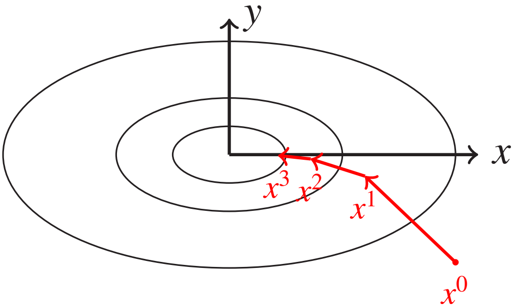

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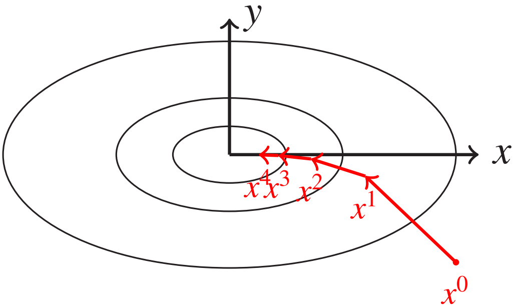


Projected gradient descent

Goal:

$$f(x) \longrightarrow \min_{x \in A \subseteq X}$$

Critical point eq.:

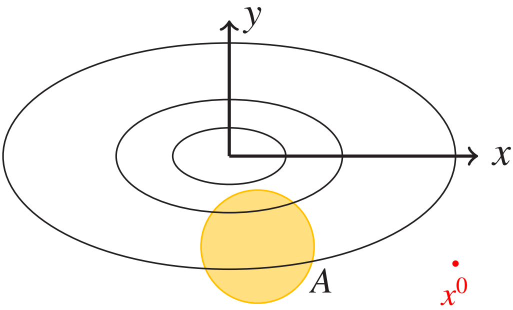
$$x \overset{!}{=} P_A(x - s\,\nabla f(x))$$

Gradient descent:

$$x^{k+1} = P_A(x^k - s^k\,\nabla f(x^k))$$

s^k … step size

$z = P_A(y)$ realizes $\min_{z \in A} \|y - z\|$



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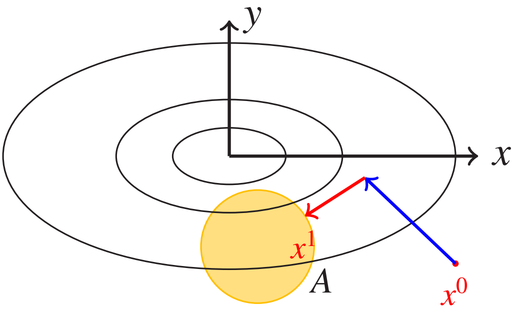

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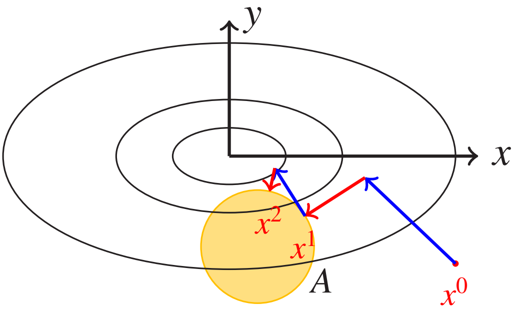

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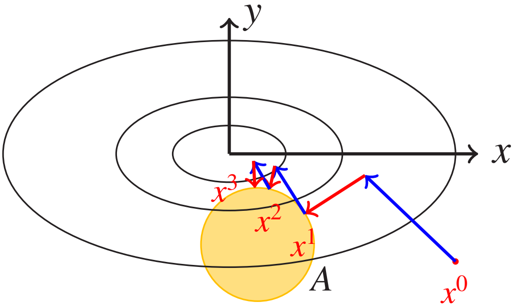

Application to hyperelasticity

- X contains $\varepsilon : Q \to \mathrm{Sym}(d)$ with inner product

$$(\varepsilon_1, \varepsilon_2)_{L^2} = \langle \varepsilon_1 : \varepsilon_2 \rangle_Q$$

- $f(\varepsilon) = \langle w(\cdot, \varepsilon) \rangle_Q$ for elastic energy, $\mathsf{S} = \partial w / \partial \varepsilon$
- constraint set

$$A = \left\{ \varepsilon \,\middle|\, \varepsilon = \bar{\varepsilon} + \nabla^s u \quad \text{for some periodic} \quad u : Q \to \mathbb{R}^d \right\}$$

- any critical point of $f(\varepsilon) \longrightarrow \min_{\varepsilon \in A}$ satisfies

$$\mathrm{div}\, \mathsf{S}(\cdot, \varepsilon) = 0$$

for some u with $\varepsilon = \bar{\varepsilon} + \nabla^s u$

Projected gradient descent?

$$x^{k+1} = P_A(x^k - s^k \nabla f(x^k))$$

- $\nabla f(x) =?$
- $P_A =?$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$f(\varepsilon) = \langle w(\cdot, \varepsilon)\rangle_Q$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$f(\varepsilon) = \frac{1}{|Q|} \int_Q w(x, \varepsilon)\, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$f(\varepsilon + s\,\xi) = \frac{1}{|Q|} \int_Q w(x, \varepsilon + s\,\xi)\, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$\frac{d}{ds} f(\varepsilon + s\,\xi)\Big|_{s=0} = \frac{d}{ds} \frac{1}{|Q|} \int_Q w(x, \varepsilon + s\,\xi)\, dx\Big|_{s=0}$$

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$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$\frac{d}{ds} f(\varepsilon + s\,\xi)\Big|_{s=0} = \frac{1}{|Q|} \int_Q \frac{d}{ds} w(x, \varepsilon + s\,\xi)\Big|_{s=0} \, dx$$

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$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$\frac{d}{ds} f(\varepsilon + s\,\xi)\Big|_{s=0} = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$(\nabla f(\varepsilon), \xi)_{L^2} = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$\frac{1}{|Q|} \int_Q \nabla f(\varepsilon) : \xi \, dx = \frac{1}{|Q|} \int_Q \frac{\partial w}{\partial \varepsilon}(x, \varepsilon) : \xi \, dx$$

Gradient?

implicit characterization:

$$(\nabla f(x), v)_X = \frac{d}{ds} f(x + sv)\Big|_{s=0} \quad \text{for all} \quad v$$

our case:

$$\nabla f(\varepsilon) = \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon)$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\xi = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \xi\|_{L^2}^2 \quad \text{among} \quad \xi \in A$$

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our case:

$$\bar{\varepsilon} + \nabla^s u = P_A(\varepsilon) \quad \text{minimizes} \quad \|\varepsilon - \bar{\varepsilon} - \nabla^s u\|_{L^2}^2 \quad \text{among} \quad \bar{\varepsilon} + \nabla^s u \in A$$

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i.e.,

$$\frac{d}{ds}\|\varepsilon - \bar{\varepsilon} - \nabla^s(u + sv)\|_{L^2}^2\Big|_{s=0} \stackrel{!}{=} 0 \quad \text{for all} \quad v : Q \to \mathbb{R}^d$$

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i.e.,

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i.e.,

$$\langle(\varepsilon - \bar{\varepsilon} - \nabla^s u) : \nabla^s v\rangle_Q \overset{!}{=} 0 \quad \text{for all} \quad v : Q \to \mathbb{R}^d$$

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i.e.,

$$-\langle \operatorname{div}\,(\varepsilon - \bar{\varepsilon} - \nabla^s u) \cdot v \rangle_Q \overset{!}{=} 0 \quad \text{for all} \quad v : Q \to \mathbb{R}^d$$

Projector?

implicit characterization:

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i.e.,

$$\text{div}\ \nabla^s u \stackrel{!}{=} \text{div}\ (\varepsilon - \bar{\varepsilon})$$

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i.e.,

$$u = (\operatorname{div} \nabla^s)^{-1} \operatorname{div} \varepsilon$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$\bar{\varepsilon} + \nabla^s \, (\text{div} \, \nabla^s)^{-1} \, \text{div} \, \varepsilon = P_A(\varepsilon)$$

Projector?

implicit characterization:

$$z = P_A(x) \quad \text{minimizes} \quad \|x - z\|_X^2 \quad \text{among} \quad z \in A$$

our case:

$$P_A(\varepsilon) = \bar{\varepsilon} + \Gamma : \varepsilon \quad \text{with} \quad \Gamma \equiv \nabla^s\,(\mathrm{div}\,\nabla^s)^{-1}\,\mathrm{div}\,.$$

Projected gradient descent?

$$\varepsilon^{k+1} = P_A(\varepsilon^k - s^k \nabla f(\varepsilon^k))$$

- $\nabla f(\varepsilon) = ?$
- $P_A(\varepsilon) = ?$

Projected gradient descent?

$$\varepsilon^{k+1} = P_A(\varepsilon^k - s^k \nabla f(\varepsilon^k))$$

- $\nabla f(\varepsilon) = \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon)$
- $P_A(\varepsilon) = \bar{\varepsilon} + \Gamma : \varepsilon$ with $\Gamma \equiv \nabla^s \, (\mathrm{div} \, \nabla^s)^{-1} \, \mathrm{div}$

Projected gradient descent?

$$\varepsilon^{k+1} = P_A\left(\varepsilon^k - s^k \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k)\right)$$

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Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} + s^k \, \Gamma : \left(\frac{1}{s^k} \, \varepsilon^k - \frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) \right) \quad \text{with} \quad \Gamma \equiv \nabla^s \, (\mathrm{div} \, \nabla^s)^{-1} \, \mathrm{div}$$

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- suppose $s^k \equiv s^0$
- define $\mathbb{C}^0 \equiv \frac{1}{s^0}\, \mathrm{Id}$
- associated $\Gamma^0 \equiv s^0\, \Gamma$
- write $\mathsf{S} = \partial w / \partial \varepsilon$

Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - s^k \, \Gamma : \left(\frac{\partial w}{\partial \varepsilon}(\cdot, \varepsilon^k) - \frac{1}{s^k} \, \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s \, (\text{div} \, \nabla^s)^{-1} \, \text{div}$$

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Projected gradient descent?

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Projected gradient descent?

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left(S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right) \quad \text{with} \quad \Gamma \equiv \nabla^s \, (\text{div} \, \nabla^s)^{-1} \, \text{div}$$

- suppose $s^k \equiv s^0$
- define $\mathbb{C}^0 \equiv \frac{1}{s^0} \, \text{Id}$
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- write $S = \partial w / \partial \varepsilon$

Projected gradient descent!

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$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left(S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right)$$

- hyperelastic basic scheme ≡ projected gradient descent

[M. Kabel, T. Böhlke, MS, Comput Mech, 2014]

So what?

$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left(S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right)$$

- reference material ≡ inverse step size

$$\mathbb{C}^0 \equiv \frac{1}{s^0} \, \mathrm{Id}$$

- s^0 large ⇒ instability
- s^0 small ⇒ $f(\varepsilon^{k+1}) < f(\varepsilon^k)$ (unless critical)

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$$\varepsilon^{k+1} = \bar{\varepsilon} - \Gamma^0 : \left(S(\cdot, \varepsilon^k) - \mathbb{C}^0 : \varepsilon^k \right)$$

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Université franco-allemande Deutsch-Französische Hochschule

KIT Karlsruhe Institute of Technology

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- import knowledge from **optimization**, e.g., on convergence

  ↗ [MS, CMAME, 2017]

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- α_+-Lipschitz condition

$$\|\mathsf{S}(x,\xi_1) - \mathsf{S}(x,\xi_2)\| \leq \alpha_+ \|\xi_1 - \xi_2\| \quad \text{for all} \quad x \in Q \quad \text{and} \quad \xi_1, \xi_2 \in \mathrm{Sym}(d)$$

- monotone S (convex w)

$$(\mathsf{S}(x,\xi_1) - \mathsf{S}(x,\xi_2)) : (\xi_1 - \xi_2) \geq 0 \quad \text{for all} \quad x \in Q \quad \text{and} \quad \xi_1, \xi_2 \in \mathrm{Sym}(d)$$

- choose $\mathbb{C}^0 = \alpha_+ \, \mathrm{Id}$ and obtain logarithmic convergence

$$f(\varepsilon^k) - \min f(\varepsilon^*) \leq \frac{2\alpha_+ \|\varepsilon^0 - \varepsilon^*\|^2}{k+4}$$

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- choose $\mathbb{C}^0 = (\alpha_+ + \alpha_-)/2 \; \mathrm{Id}$ and obtain linear convergence

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On the conditions

- if $S \in C^1$ in ε

$$\alpha_+\text{-Lipschitz} \quad \Longleftrightarrow \quad \lambda \leq \alpha_+ \quad \forall x, \xi \; \forall \lambda \in \mathtt{Eig}\left(\frac{\partial S}{\partial \varepsilon}(x, \xi)\right)$$

$$\alpha_-\text{-strongly convex} \quad \Longleftrightarrow \quad \lambda \geq \alpha_- \quad \forall x, \xi \; \forall \lambda \in \mathtt{Eig}\left(\frac{\partial S}{\partial \varepsilon}(x, \xi)\right)$$

- maximum/minimum slopes of algo tangent
- estimated on-line
- theory does not cover porosity/softening

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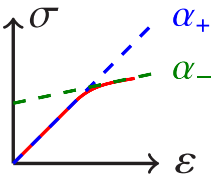

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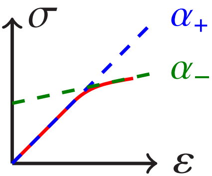

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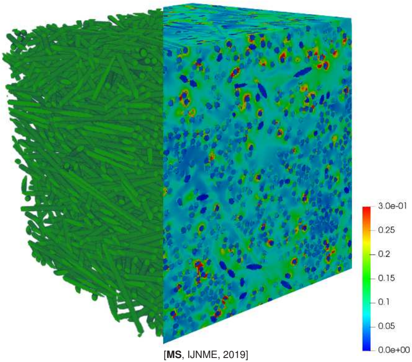
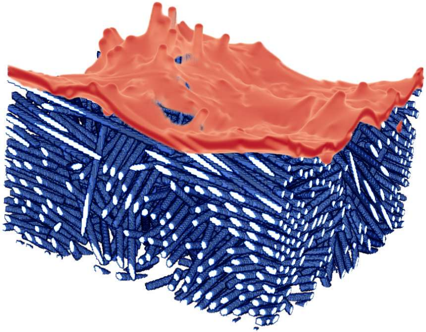
Digression Part III

- basic scheme ≡ projected gradient descent
- provides **intuition**
- import insights from optimization, e.g., Nesterov's book
- projected gradient descent ++ ≡ basic scheme ++ (tomorrow)

The end



[**MS**, IJNME, 2019]



[Ernesti-**MS**-Böhlke, CMAME, 2020]

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