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On plastic deformation: From physics over convex analysis to numerical simulation

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Goals of this Graduate Lecture

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3rd lecture (today)

- formulate two coupled systems (dual, primal)
- give hints for implementations

Summary - basic equations

- Stress, Displacement

$$\sigma \in \mathbb{R}_{sym}^{3 \times 3}, \quad u \in \mathbb{R}^3$$

- Strain

$$\epsilon = e + p = \frac{1}{2} (\nabla u + \nabla u^T) \in \mathbb{R}_{sym}^{3 \times 3}$$

- Yield function with hardening

$$\Phi(\sigma, \alpha, g) = \phi(\sigma + \alpha) + g \leq 0$$

- Law of equilibrium:

$$-\operatorname{div} \sigma = f$$

- Hooke's law:

$$\exists \mathbf{C} \in \mathbb{R}^{(3 \times 3) \times (3 \times 3)} : \sigma = \mathbf{C}e$$

- Maximum work

$$\dot{p} \in N_E(\sigma)$$

Summary - generalized variables

- Generalized Stress

$$\Sigma := (\sigma, \alpha, g) \in \mathbb{R}_{sym}^{3 \times 3} \times \mathbb{R}_{sym}^{3 \times 3} \times \mathbb{R}$$

- Generalized Strain

$$P := (p, a, \eta) \in \mathbb{R}_{sym,0}^{3 \times 3} \times \mathbb{R}_{sym,0}^{3 \times 3} \times \mathbb{R}_{\geq 0}$$

- Yield function with hardening

$$\Phi(\sigma, \alpha, g) = \phi(\sigma + \alpha) + g$$

defining the elastic region

$$\mathcal{E} = \{\Sigma : \Phi(\Sigma) \leq 0\}$$

- we concluded

$$a = p$$

- typical relations

$$\alpha = -k_1 p$$

$$g = -k_2 \eta$$

- We proofed in just 50 minutes

$$\dot{P} \in N_{\mathcal{E}}(\Sigma) \Leftrightarrow \Sigma \in \partial D(\dot{P})$$

- How do we couple these equations?

1st try: dual formulation

let us begin with the first ansatz: *dual formulation*

- here, we consider stress σ and displacement u as unknowns
- starting point is the line

$$\dot{P} \in N_{\mathcal{E}}(\Sigma)$$

- this is by definition

$$\langle \dot{P}, \tilde{\Sigma} - \Sigma \rangle \leq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$

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- but first, we define some (bi-)linear functions and stick them together

dual formulation – (bi-)linear functions

- for the force field f we had

$$-\operatorname{div} \sigma = f$$

- with that in mind, we define a linear functional $l(t)$

$$\langle l(t), u \rangle := - \int_{\Omega} f(t) \cdot u \, dx$$

- and a bilinear form $b(\cdot, \cdot)$

$$b(u, \sigma) := - \int_{\Omega} \epsilon(u) : \sigma \, dx$$

- this yields with integration by parts

$$b(\tilde{u}, \sigma) = \langle l(t), \tilde{u} \rangle \quad \forall \tilde{u}$$

dual formulation – more bilinear functions

from now on, we assume the Hooke tensor \mathbf{C} to be invertible and symmetric

- stress – stress mapping:

$$a(\sigma, \tilde{\sigma}) := \int_{\Omega} \sigma : \mathbf{C}^{-1} \tilde{\sigma} \, dx$$

- and for the generalized variables

$$c_1(\alpha, \tilde{\alpha}) := \int_{\Omega} \frac{1}{k_1} \alpha : \tilde{\alpha} \, dx$$

$$c_2(\mathbf{g}, \tilde{\mathbf{g}}) := \int_{\Omega} \frac{1}{k_2} \mathbf{g} \cdot \tilde{\mathbf{g}} \, dx$$

- resulting in

$$A(\Sigma, \tilde{\Sigma}) := a(\sigma, \tilde{\sigma}) + c_1(\alpha, \tilde{\alpha}) + c_2(\mathbf{g}, \tilde{\mathbf{g}})$$

dual formulation

- back to

$$\int_{\Omega} \langle \dot{P}, \tilde{\Sigma} - \Sigma \rangle dx \leq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$

- this is

$$\int_{\Omega} \dot{p} : (\tilde{\sigma} - \sigma) + \dot{a} : (\tilde{\alpha} - \alpha) + \dot{\eta} \cdot (\tilde{g} - g) dx \leq 0$$

- and now we use

$$\dot{\alpha} = -k_1 \dot{a}, \quad \dot{g} = -k_2 \dot{\eta}$$

- and for \dot{p} with Hooke's law

$$\epsilon(\dot{u}) = \dot{p} + \dot{e} = \dot{p} + \mathbf{C}^{-1} \dot{\sigma} \quad \Rightarrow \quad \dot{p} = \epsilon(\dot{u}) - \mathbf{C}^{-1} \dot{\sigma}$$

dual formulation

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$$\int_{\Omega} \dot{p} : (\tilde{\sigma} - \sigma) + \dot{\alpha} : (\tilde{\alpha} - \alpha) + \dot{\eta} \cdot (\tilde{g} - g) dx \leq 0$$

- and now we use

$$\dot{\alpha} = -k_1 \dot{\alpha}, \quad \dot{g} = -k_2 \dot{\eta}, \quad \dot{p} = \epsilon(\dot{u}) - \mathbf{C}^{-1} \dot{\sigma}$$

- which means

$$\int_{\Omega} \underbrace{\epsilon(\dot{u}) : (\tilde{\sigma} - \sigma)}_{-b(\dot{u}, \tilde{\sigma} - \sigma)} - \underbrace{\mathbf{C}^{-1} \dot{\sigma} : (\tilde{\sigma} - \sigma)}_{a(\dot{\sigma}, \tilde{\sigma} - \sigma)} - \underbrace{\frac{1}{k_1} \dot{\alpha} : (\tilde{\alpha} - \alpha)}_{c_1(\dot{\alpha}, \tilde{\alpha} - \alpha)} - \underbrace{\frac{1}{k_2} \dot{g} \cdot (\tilde{g} - g)}_{c_2(\dot{g}, \tilde{g} - g)} dx \leq 0$$

- therefore,

$$A(\dot{\Sigma}, \tilde{\Sigma} - \Sigma) + b(\dot{u}, \tilde{\sigma} - \sigma) \geq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$

dual formulation – time discrete

- if we approximate the time derivative by finite (implicit) differences

$$A(\dot{\Sigma}, \tilde{\Sigma} - \Sigma) + b(\dot{u}, \tilde{\sigma} - \sigma) \geq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$

- we will get

$$A(\Sigma_n - \Sigma_{n-1}, \tilde{\Sigma} - \Sigma_n) + b(u_n - u_{n-1}, \tilde{\sigma} - \sigma_n) \geq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$

- and don't forget

$$b(\tilde{u}, \sigma_n) = \langle l_n, \tilde{u} \rangle \quad \forall \tilde{u}$$

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dual formulation – solution algorithms

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- there are countless numerical schemes in literature...
- let's look at the "classical" strategy, which is the base of most schemes

dual formulation – solution algorithms

- how do we solve this problem?
- there are countless numerical schemes in literature...
- let's look at the "classical" strategy, which is the base of most schemes
- in each time step, we have to find Σ_n and u_n

$$A(\Sigma_n - \Sigma_{n-1}, \tilde{\Sigma} - \Sigma_n) + b(u_n - u_{n-1}, \tilde{\sigma} - \sigma_n) \geq 0 \quad \forall \tilde{\Sigma} \in \mathcal{E}$$
$$b(\tilde{u}, \sigma_n) = \langle l_n, \tilde{u} \rangle \quad \forall \tilde{u}$$

- we will *predict* an (incorrect) displacement and *correct* with a suitable stress until convergence
- \Rightarrow this is called *predictor-corrector* method

Predictor

let u_n^i and Σ_n^i denote the currently known iterates

- we assume that we have an elastic process (may be wrong, of course):

$$\begin{aligned}\sigma_n^{i+1} &= \mathbf{C}\epsilon(u_n^{i+1}) = \mathbf{C}\epsilon(u_n^i + u_n^{i+1} - u_n^i) \\ &= \sigma_n^i + \mathbf{C}\epsilon(u_n^{i+1} - u_n^i)\end{aligned}$$

- this implies

$$\langle l_n, \tilde{u} \rangle = b(\tilde{u}, \sigma_n^{i+1}) = b(\tilde{u}, \sigma_n^i) + \int_{\Omega} \mathbf{C}\epsilon(u_n^{i+1} - u_n^i) : \epsilon(\tilde{u}) dx$$

- this is a linear equation in u_n^{i+1} , which can be solved with common methods (no details here, sorry)

Corrector

Of course, assuming an elastic process may have been wrong!

- now we have u_n^{i+1} given and try to find a Σ_n^{i+1}
- we set the so-called *trial stress*

$$\Sigma^{trial} := \Sigma_{n-1} + \left[\mathbf{C}\epsilon(u_n^{i+1} - u_{n-1}), 0, 0 \right]^T$$

- and if we plug this in

$$A(\Sigma^{trial} - \Sigma_n^{i+1}, \tilde{\Sigma} - \Sigma_n^{i+1}) \leq 0$$

one can show (due to lack of time, this person is not me) that this forms a suitable pair

$$(\Sigma_n^{i+1}, u_n^{i+1})$$

if the inequality is solved for Σ_n^{i+1}

Corrector

- it was a quadratic optimization, so again, there are efficient methods for solving
- but σ_n^{i+1} may (again) violate the first equation

$$(\tilde{u}, \sigma_n^{i+1}) = \langle I_n, \tilde{u} \rangle \quad \forall \tilde{u}$$

- so we keep repeating the predictor–corrector algorithm until both (in-)equalities are fulfilled
- under some elliptic assumptions on \mathbf{C} , the algorithm will converge

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- so we keep repeating the predictor–corrector algorithm until both (in-)equalities are fulfilled
- under some elliptic assumptions on \mathbf{C} , the algorithm will converge
- problem: the algorithm is slow in practice

2nd try: primal formulation

- in the second lecture, we proofed

$$\dot{P} \in N_{\mathcal{E}}(\Sigma) \Leftrightarrow \Sigma \in \partial D(\dot{P})$$

- D was the dissipation function of the yield function:

$$D(\dot{P}) := \sup_{\Sigma \in \mathcal{E}} \{\dot{P} : \Sigma\}$$

- D can be expressed directly for Von Mises

$$D(\dot{P}) = \begin{cases} \sigma_0 \|\dot{P}\|_F & \|\dot{P}\|_F \leq \eta \\ \infty & \text{else} \end{cases}$$

- and for Tresca flow rule

$$D(\dot{P}) = \begin{cases} \sigma_0 \|\dot{P}\|_2 & \|\dot{P}\|_2 \leq \eta \\ \infty & \text{else} \end{cases}$$

2nd try: primal formulation

- the formulation

$$\Sigma \in \partial D(\dot{P})$$

is defined by

$$D(\tilde{P}) \geq D(\dot{P}) + \Sigma : (\tilde{P} - \dot{P}) \quad \forall \tilde{P}$$

- which is

$$D(\tilde{P}) \geq D(\dot{P}) + \sigma : (\tilde{p} - \dot{p}) + \alpha(\tilde{a} - \dot{a}) + g \cdot (\tilde{\eta} - \dot{\eta}) \quad \forall \tilde{P}$$

- again, we use $\alpha = -k_1 a$, $g = -k_1 \eta$ and $a = p$!
- for σ , we use

$$\sigma = \mathbf{C}e = \mathbf{C}(\epsilon(u) - p)$$

2nd try: primal formulation

- we had

$$D(\tilde{P}) \geq D(\dot{P}) + \sigma : (\tilde{p} - \dot{p}) + \alpha(\tilde{a} - \dot{a}) + g \cdot (\tilde{\eta} - \dot{\eta}) \quad \forall \tilde{P}$$

- with $\alpha = -k_1 a$, $g = -k_1 \eta$ and $a = p$!
- fand

$$\sigma = \mathbf{C}e = \mathbf{C}(\epsilon(u) - p)$$

- and therefore

$$\int_{\Omega} D(\tilde{P}) dx \geq \int_{\Omega} D(\dot{P}) + \mathbf{C}(\epsilon(u) - p) : (\tilde{p} - \dot{p}) - k_1 p : (\tilde{p} - \dot{p}) - k_2 \eta \cdot (\tilde{\eta} - \dot{\eta}) dx \quad \forall \tilde{P}$$

2nd try: primal formulation

- and therefore

$$\int_{\Omega} D(\tilde{P}) dx \geq \int_{\Omega} D(\dot{P}) + \mathbf{C}(\epsilon(u) - p) : (\tilde{p} - \dot{p}) - k_1 p : (\tilde{p} - \dot{p}) - k_2 \eta \cdot (\tilde{\eta} - \dot{\eta}) dx \quad \forall \tilde{P}$$

- now, use also that

$$-\operatorname{div} \sigma \cdot (\tilde{u} - \dot{u}) = f \cdot (\tilde{u} - \dot{u})$$

- integrated by parts

$$\int_{\Omega} \mathbf{C}(\epsilon(u) - p) : (\epsilon(\tilde{u}) - \epsilon(\dot{u})) dx = \int_{\Omega} \sigma : (\epsilon(\tilde{u}) - \epsilon(\dot{u})) dx = \int_{\Omega} f \cdot (\tilde{u} - \dot{u}) dx$$

primal formulation

- subtracting the last two (in-)equalities leads to

$$\begin{aligned} - \int_{\Omega} f \cdot (\tilde{u} - \dot{u}) \, dx \geq & \int_{\Omega} D(\dot{P}) - D(\tilde{P}) - \mathbf{C}(\epsilon(u) - p) : ((\epsilon(\tilde{u}) - \epsilon(\dot{u})) - (\tilde{p} - \dot{p})) \\ & - k_1 p : (\tilde{p} - \dot{p}) - k_2 \eta \cdot (\tilde{\eta} - \dot{\eta}) \, dx \quad \forall \tilde{P}, \tilde{u} \end{aligned}$$

- then, we set $w = (u, p, \eta)$ and define new (!) (bi-)linear function that represent

$$- \langle l(t), \tilde{w} - \dot{w} \rangle \geq j(\dot{w}) - j(\tilde{w}) - a(w, \tilde{w} - \dot{w}) \quad \forall \tilde{w}$$

- or rearranged

$$a(w, \tilde{w} - \dot{w}) + j(\tilde{w}) - j(\dot{w}) \geq \langle l(t), \tilde{w} - \dot{w} \rangle \quad \forall \tilde{w}$$

primal formulation – time discrete

- like before, we replace the time derivative by an implicit finite difference

$$\alpha(\Delta w_n, \tilde{w} - \Delta w_n) + j(\tilde{w}) - j(\Delta w_n) \geq \underbrace{\langle I_n, \tilde{w} - \Delta w_n \rangle}_{\text{contains part of } \alpha} \quad \forall \tilde{w} \quad (1)$$

with

$$\Delta w_n = w_n - w_{n-1}$$

- now we can use a result from convex optimization

primal formulation – time discrete

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$$a(\Delta w_n, \tilde{w} - \Delta w_n) + j(\tilde{w}) - j(\Delta w_n) \geq \underbrace{\langle I_n, \tilde{w} - \Delta w_n \rangle}_{\text{contains part of } a} \quad \forall \tilde{w} \quad (1)$$

with

$$\Delta w_n = w_n - w_{n-1}$$

- now we can use a result from convex optimization

Theorem

Solving the inequality (1) for Δw_n is equivalent to minimizing

$$L(\Delta w_n) := \frac{1}{2}a(\Delta w_n, \Delta w_n) + j(\Delta w_n) - \langle I_n, \Delta w_n \rangle$$

primal formulation – summary

Theorem

Solving the inequality (1) for Δw_n is equivalent to minimizing

$$L(\Delta w_n) := \frac{1}{2}a(\Delta w_n, \Delta w_n) + j(\Delta w_n) - \langle I_n, \Delta w_n \rangle$$

- to compute the increment, we have to minimize a strictly convex function
- we get uniqueness and existence of solution for free
- but: L is not smooth everywhere!
- so classical minimizing algorithms won't work, we need special solvers

Summary

- we have seen two different formulations:
- primal:
 - starting from $\Sigma \in \partial D(\dot{P})$
 - resulting in a convex minimization problem
 - efficient solvers are available (ask me 😊)
- dual:
 - starting from $\dot{P} \in N_{\mathcal{E}}(\Sigma)$
 - leading to optimization inequalities
 - algorithms are mostly of predictor-corrector type
 - but easy to implement

Summary - overall

We did it!

- we have seen the engineering approach of plasticity
- we considered different elastic regions
- we have seen hardening rules
- an important theorem from convex analysis was proofed
- different approaches of solving the complete system were given
- Slides can be found here:

<https://www.math.tu-dresden.de/~jaap/>

- contact me for the simulations, programs, etc.

Sources

- plasticity theory:
 - Weimin Han & B. Daya Reddy, Plasticity, Mathematical Theory and Numerical Analysis, Second Edition, Springer Science+Business Media, LLC 2013
- convex analysis/optimization
 - Ivar Ekeland & Roger Temam, Convex Analysis and Variational Problems, North-Holland Publishing Company, 1973