Variational principles in nonlinear mechanics using convex optimization and automated numerical tools

Jeremy Bleyer



Habilitation à Diriger des Recherches November, 22nd 2024

About me Curriculum



Teaching

pprox 120 hours/year



Teaching

pprox 120 hours/year



MEALOR II Summer school: *physics and mechanics of brittle and ductile fracture* collective open-access book



PhD students

Academic/Industrial



Others

2023 = acting scientific director of a European executive master on Digital Twins for Infrastructures and Cities



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Outline

1 Context

- **(2)** Conic programming for non-smooth optimization
- **3** Applications to limit analysis in civil engineering
- **4** Structural optimization
- **(5)** Risk-averse formulation of material behavior
- **6** Conclusions & perspectives

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Introduction

Nothing takes place in the world whose meaning is not that of some maximum or minimum. (Leonhard Euler)

Collapse

Thresholds

Optimization



Masonry dome [Zessin, 2015]



Membrane wrinkling [shellbuckling.com]



Vault [P. Block group, ETH]



Landslides [geologypage.com]



Mayonnaise drips [Coussot et al, 2005]



Topology interlocking assembly [M. Pauly group, EPFL]

But also: finance, power networks, image processing, supply chain, machine learning, etc.

Differentiable case

 $\inf_{u\in V}J(u)$

variational equality: $D_u J(u, v) = 0 \quad \forall v \in V$

e.g. potential energy:
$$J(u) = \int_{\Omega} \psi(\nabla u) \, \mathrm{d}\Omega - \int_{\Omega} f u \, \mathrm{d}\Omega$$



VI arise in presence of inequality constraints or non-smooth objective functions



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Obstacle problem

$$\inf_{u \in V} \int_{\Omega} \frac{1}{2} \|\nabla u\|_{2}^{2} d\Omega - \int_{\Omega} f u d\Omega$$

s.t. $u \ge g$ on Ω

e.g. PETSc bound-constrained solvers





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Motivation

non-smooth optimization problems entail rich physics, exhibit high modeling expressiveness and can now be solved efficiently using appropriate algorithms

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Non-smooth optimization as conic programming Linear programming

$$\min_{x} \quad c^{\mathsf{T}}x \\ \text{s.t.} \quad Ax = b \\ x > 0$$

Non-smooth optimization as conic programming Conic programming

$$\begin{array}{ll} \min_{x} & \boldsymbol{c}^{\mathsf{T}}\boldsymbol{x} \\ \text{s.t.} & \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \\ & \boldsymbol{x} \in \mathcal{K} \end{array}$$

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where \mathcal{K} is a product of elementary cones e.g.:

- positive orthants \mathbb{R}^{m}_{+} ;
- Lorentz quadratic cones: $Q_m = \{z = (z_0, \overline{z}) \in \mathbb{R}^+ \times \mathbb{R}^{m-1} \text{ s.t. } \|\overline{z}\|_2 \le z_0\}$
- semi-definite cones \mathcal{S}_m^+ , the cone of positive semi-definite m imes m symmetric matrices;
- power cones, exponential cones, etc.

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The magic cone family [Juditsky & Nemirovski, 2021]

very large modelling power of convex functions and constraints

$$F(\mathbf{x}) = \min_{\mathbf{y}} \quad \mathbf{c}^{\mathsf{T}}\mathbf{x} + \mathbf{d}^{\mathsf{T}}\mathbf{y}$$

s.t. $\mathbf{b}_{l} \leq \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{y} \leq \mathbf{b}_{u}$
 $\mathbf{y} \in \mathcal{K}_{1} \times \ldots \times \mathcal{K}_{p}$

(conic representation)

Solvers

interior-point algorithms, very efficient and robust (20-30 iterations)

Jeremy Bleyer (Laboratoire Navier)

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The dolfinx optim package

```
prob = MosekProblem(domain, name="Obstacle problem")
u = prob.add_var(V, bc=bc, lx=g)
J = QuadraticTerm(ufl.grad(u), degree)
prob.add_convex_term(J)
prob.add_obj_func(-ufl.dot(f, u) * ufl.dx)
prob.optimize()
```

Obstacle problem

$$\begin{split} \inf_{u \in V} & \int_{\Omega} \frac{1}{2} \| \nabla u \|_2^2 \, \mathrm{d}\Omega - \int_{\Omega} f u \, \mathrm{d}\Omega \\ \mathrm{s.t.} & u \geq g \text{ on } \Omega \end{split}$$



- Domain-Specific Language based on UFL for convex functions and their composition
- Mosek interior-point solver
- pre-defined convex primitives
 - AbsValue, LinearTerm, QuadraticTerm, QuadOverLin, etc.
 - vectors: L1Norm, L2Norm, LinfNorm, LpNorm, etc.
 - matrices: SpectralNorm, NuclearNorm, FroebeniusNorm, LambdaMax, etc.
- composability through convex-preserving transformations

Convexity-preserving operations:

- sum $f_1(x) + f_2(x)$
- supremum sup $\{f_1(x), f_2(x)\}$
- partial minimization
- Legendre-Fenchel transform

$$f^*(s) = \sup_{x} s^{\mathsf{T}} x - f(x)$$

• inf-convolution

$$(f \Box g)(x) = \inf_{\substack{x_1, x_2 \\ \text{s.t.}}} f(x_1) + g(x_2)$$

• perspective

(

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e.g. **perspective** function $persp_f(t, x) = tf(x/t)$

$$tf(\mathbf{x}/t) = \min_{\mathbf{y}} \quad \mathbf{c}^{\mathsf{T}}\mathbf{x} + \mathbf{d}^{\mathsf{T}}t\mathbf{y}$$

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Data transformation

• inf-convolution

$$(f \Box g)(x) = \inf_{\substack{x_1, x_2 \\ \text{s.t.}}} f(x_1) + g(x_2)$$

• . . .

 $\begin{array}{ll} \boldsymbol{x} \mapsto \begin{pmatrix} \boldsymbol{t} \\ \boldsymbol{x} \end{pmatrix} & \boldsymbol{c} \mapsto \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{c} \end{pmatrix} \\ \boldsymbol{A} \mapsto \begin{bmatrix} -\boldsymbol{b}_l & \boldsymbol{A} \\ -\boldsymbol{b}_u & \boldsymbol{A} \end{bmatrix} & \boldsymbol{B} \mapsto \begin{bmatrix} \boldsymbol{B} \\ \boldsymbol{B} \end{bmatrix} \\ \boldsymbol{b}_l \mapsto \begin{pmatrix} \boldsymbol{0} \\ \mathsf{None} \end{pmatrix} & \boldsymbol{b}_u \mapsto \begin{pmatrix} \mathsf{None} \\ \boldsymbol{0} \end{pmatrix} \end{array}$

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Limit analysis [Hill, Drucker, 1950] & Yield design [Salençon, 1983]

Goal: find the maximum collapse load $F^+ = \lambda^+ F$ that a structure can sustain under a convex plasticity domain G

Static approach = limit load maximization:

$$egin{aligned} \lambda^+ &= \max_{\lambda, \sigma} & \lambda \ & ext{ s.t. } & \sigma \in \mathcal{S}_{\mathsf{ad}}(\lambda) & (\mathsf{equilibrium}) \ & \sigma(x) \in \mathcal{G}(x) & orall x \in \Omega \end{aligned}$$



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Dual kinematic approach = plastic dissipation minimization:

$$\begin{split} \lambda^{+} &= \min_{\boldsymbol{u} \in \mathcal{U}_{ad}} \quad \int_{\Omega} \pi_{G}(\boldsymbol{\varepsilon}) \, \mathrm{d}\Omega \\ &\text{s.t.} \quad \int_{\Omega} \boldsymbol{F} \cdot \boldsymbol{u} \, \mathrm{d}\Omega = 1 \qquad \qquad \pi_{G}(\boldsymbol{\varepsilon}) = \sup_{\boldsymbol{\sigma} \in G} \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \end{split}$$

exclusively non-smooth ! conic programming perfectly suited for that, impossible with standard Newton approach

Cohesive frictional soils 3D Mohr-Coulomb plasticity criterion

3D Mohr-Coulomb support function

$$\sigma \in G \Leftrightarrow \sigma_I - a\sigma_{III} \leq \frac{2c\cos\phi}{1+\sin\phi} \qquad \pi_G(\varepsilon) = \begin{cases} c\cot a \phi \operatorname{tr} \varepsilon & \text{if } \operatorname{tr}(\varepsilon) \geq \sin\phi \sum_I |\varepsilon_I| \\ +\infty & \text{otherwise} \end{cases}$$

Conic representation (SDP) of $\pi_G(\varepsilon)$

$$\pi_{G}(\varepsilon) = \min_{\substack{\mathbf{Y}_{1}, \mathbf{Y}_{2} \\ \text{s.t.}}} \frac{2c\cos\phi}{1+\sin\phi} \operatorname{tr}(\mathbf{Y}_{1})$$

s.t. $\varepsilon = \mathbf{Y}_{1} - \mathbf{Y}_{2}$
 $a\operatorname{tr}(\mathbf{Y}_{1}) = \operatorname{tr}(\mathbf{Y}_{2})$
 $\mathbf{Y}_{1} \succeq 0, \mathbf{Y}_{2} \succeq 0$



Civil engineering applications [Strains]

Bolted column base plate [C. El Boustani]



Reinforced concrete bridge pier cap [H. Vincent]



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Topology optimization : elastic setting

Find $\Omega \subseteq \mathcal{D}$ minimizing the elastic compliance at fixed volume [Allaire, 2002]:



[TopOpt in Python, DTU]

$$\begin{array}{ll} \min_{\Omega, \boldsymbol{u}} & \int_{\partial \Omega} \boldsymbol{T} \cdot \boldsymbol{u} \, \mathrm{dS} \\ \mathrm{s.t.} & \boldsymbol{\sigma} = \mathbb{C} : \nabla \boldsymbol{u} \, \mathrm{in} \, \Omega \\ & \operatorname{div} \boldsymbol{\sigma} = \boldsymbol{0} \quad \mathrm{in} \, \Omega \\ \boldsymbol{\sigma} \boldsymbol{n} = \boldsymbol{T} \quad \mathrm{on} \, \partial \Omega_N \\ & |\Omega| \leq \eta |\mathcal{D}| \end{array}$$

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Find $\Omega \subseteq \mathcal{D}$ minimizing the elastic compliance at fixed volume [Allaire, 2002]:



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Density-based formulation

$$\min_{\substack{\rho, \boldsymbol{u}} \\ \text{s.t.}} \quad \int_{\partial \mathcal{D}} \boldsymbol{T} \cdot \boldsymbol{u} \, \mathrm{dS} \\ \text{s.t.} \quad \boldsymbol{\sigma} = \mathbb{C}(\rho) : \nabla \boldsymbol{u} \text{ in } \mathcal{D} \\ \text{div } \boldsymbol{\sigma} = 0 \quad \text{in } \mathcal{D} \\ \boldsymbol{\sigma} \boldsymbol{n} = \boldsymbol{T} \quad \text{on } \partial \mathcal{D}_{N} \\ \int_{\mathcal{D}} \rho \, \mathrm{d\Omega} \leq \eta |\mathcal{D}| \\ 0 \leq \rho(\boldsymbol{x}) \leq 1$$

 \Rightarrow **non-convex** problem, iterative procedure

e.g. SIMP method [Bendsoe and Kikuchi, 1988] : $\mathbb{C}(
ho)=
ho^{p}\mathbb{C}_{0}$ with ho>1

Objective : Find $\Omega \subseteq \mathcal{D}$ with **maximum limit load** for a given volume level η :

Proposed formulation:

$$\begin{array}{ll} \lambda^{+}(\eta) = \max_{\lambda,\sigma,\Omega} & \lambda \\ \text{s.t.} & \operatorname{div} \boldsymbol{\sigma} = 0 & \operatorname{in} \Omega \\ \boldsymbol{\sigma} \boldsymbol{n} = \lambda \boldsymbol{T} & \operatorname{in} \partial \Omega_{\boldsymbol{N}} \\ \boldsymbol{\sigma} \in \boldsymbol{G} & \operatorname{in} \Omega \\ |\Omega| \leq \eta |\mathcal{D}| \end{array}$$

Objective : Find $\Omega \subseteq \mathcal{D}$ with **maximum limit load** for a given volume level η :

extension by ${m \sigma}=0$ outside Ω

$$\begin{array}{ll} \lambda^{+}(\eta) = \max_{\lambda,\sigma,\rho} & \lambda \\ \text{s.t.} & \operatorname{div} \boldsymbol{\sigma} = 0 & \operatorname{in} \mathcal{D} \\ \boldsymbol{\sigma} \boldsymbol{n} = \lambda \boldsymbol{T} & \operatorname{in} \partial \mathcal{D}_{N} \\ \boldsymbol{\sigma} \in \rho \boldsymbol{G} & \operatorname{in} \mathcal{D} \\ \int_{\mathcal{D}} \rho \, \mathrm{d} \Omega \leq \eta |\mathcal{D}| \\ \rho \in \{0; 1\} \end{array}$$

ho being the characteristic function of Ω

Objective : Find $\Omega \subseteq \mathcal{D}$ with **maximum limit load** for a given volume level η :

problem convexification (LOAD-MAX)

$$\lambda^{+}(\eta) = \max_{\lambda, \sigma, \rho} \quad \lambda$$

s.t. div $\sigma = 0$ in \mathcal{D}
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ullet convex problem, akin to a limit analysis problem with an additional scalar variable ho

- related to a volume minimization problem [Kammoun, 2014; Herfelt et al., 2019]
- penalization procedure $\rho^{p} \approx \rho_{n}^{p_{n}} + p_{n}\rho_{n}^{p_{n}-1}\rho \implies black-and-white design$
- ullet slope limitation [Petersson & Sigmund, 1998] $\|
 abla
 ho\|\leq 1/\ell_0$ for mesh independency

Material with asymmetric strengths



(a) $f_c/f_t = 10$ (b) $f_c/f_t = 0.1$

Principal stresses (compression/traction)

Material without tensile strength



Material without tensile strength





(a) The Passion Façade



(b) After penalization

Extension to two materials

we want to optimize independently two phases (+ void) e.g. **steel** and **concrete**, **tension** and **compression**

Strength condition

$$\left\{egin{array}{l} oldsymbol{\sigma} = oldsymbol{\sigma}^1 + oldsymbol{\sigma}^2 \ oldsymbol{\sigma}^1 \in
ho_1 oldsymbol{G}^1 \ oldsymbol{\sigma}^2 \in
ho_2 oldsymbol{G}^2 \end{array}
ight.$$

G¹ possibly **anisotropic**

with
$$\rho_1 + \rho_2 \leq 1$$

12 m



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Objectives

Material constitutive law: $\sigma = F(\varepsilon)$

uncertain material properties \Rightarrow need for an effective behavior [Bleyer, JMPS, 2024]



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must account for history-dependent behaviors and thermodynamic consistency

Evolution equations of a standard material

Incremental potential

After time discretization, evolution equations of **Generalized Standard Materials** are obtained from the **incremental potential** [Ortiz & Stainier, Mielke, etc.]

$$\psi(\varepsilon, \alpha) + \Delta t \phi\left(\frac{\varepsilon - \varepsilon_n}{\Delta t}, \frac{\alpha - \alpha_n}{\Delta t}\right)$$

Simplifying assumptions: arepsilon is non-dissipative, ϕ is 1-homogeneous, single-step $oldsymbol{lpha}_n=0$

$$egin{aligned} &j(m{arepsilon}) := \inf_{lpha} \psi(m{arepsilon}, m{lpha}) + \phi(m{lpha}) \ &\Rightarrow m{\sigma} \in \partial_{m{arepsilon}} j \end{aligned}$$

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$$j(\varepsilon) := \inf_{\alpha} \psi(\varepsilon, \alpha) + \phi(\alpha)$$

 $\Rightarrow \sigma \in \partial_{\varepsilon} j$

Example: 1D linear elasticity + isotropic power-law hardening

$$\psi(\varepsilon, \alpha) = \psi_{\mathsf{el}}(\varepsilon - \alpha) + \psi_{\mathsf{h}}(\alpha)$$
$$= \frac{1}{2}E(\varepsilon - \alpha)^{2} + \frac{1}{m}H\alpha^{m}$$
$$\phi(\dot{\alpha}) = \sigma_{0}|\dot{\alpha}|$$



Uncertain elastoplastic case

Now j depends upon stochastic parameters ζ with known probability distribution **Goal**: formulate an **effective potential** to describe the effective behavior

 $j^{ ext{eff}}(arepsilon) = \mathcal{R}\left[j(arepsilon;oldsymbol{\zeta})
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$$\psi(\varepsilon,\alpha) = \frac{1}{2} E_{\zeta}(\varepsilon - \alpha)^2 + \frac{1}{m} H_{\zeta} \alpha^m \quad ; \quad \phi(\dot{\alpha}) = \sigma_{0\zeta} |\dot{\alpha}|$$



Risk-averse measures

Risk-measure \mathcal{R} : assume X be a random cost: $\mathbb{E}[X] = OK$ whereas $\mathcal{R}[X] = BAD$ e.g.:

- the safety margin $\mathcal{R}[X] = \mathbb{E}[X] + k \operatorname{std}[X]$, for k > 0
- the worst-case value: $\mathcal{R}[X] = \sup X$
- the Value-at-Risk (VaR) for a level $\beta \in [0; 1]$ (or the β -quantile):

$$\mathcal{R}[X] = \mathsf{VaR}_{\beta}(X) = \inf\{Z \text{ s.t. } \mathbb{P}[Z \ge X] \ge \beta\}$$

• and many more...

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- safety margin and VaR are not coherent
- worst-case value is coherent but too conservative
- expected value is coherent but risk-neutral

Conditional Value-at-Risk (CVaR)

The Conditional Value-at-Risk (CVaR) is a coherent risk measure [Rockafellar, 2000]

 $\operatorname{CVaR}_{\beta}(X) = \mathbb{E}\left[X \text{ s.t. } X \geq \operatorname{VaR}_{\beta}(X)\right]$



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Key result: convex optimization characterization

$$\mathsf{CVaR}_{\beta}(X) = \inf_{\lambda} \lambda + \frac{1}{1-\beta} \mathbb{E}\left[\langle X - \lambda \rangle_{+}\right]$$

Extends to random convex functions:

$$\mathsf{CVaR}_{\beta}(f)(\mathbf{x}) = \inf_{\lambda} \lambda + \frac{1}{1-\beta} \mathbb{E}\left[\langle f(\mathbf{x}; \boldsymbol{\zeta}) - \lambda \rangle_{+}\right]$$
 is convex

Examples

1D elasticity:
$$j(\varepsilon_{\zeta}; \zeta) = \frac{1}{2} E_{\zeta} \varepsilon_{\zeta}^{2}$$

 $j^{\text{eff}}(\varepsilon) = \text{CVaR}_{\beta}(\psi)(\varepsilon) = \frac{1}{2} \text{CVaR}_{\beta}(E) \varepsilon^{2}$

replaces uncertain Young modulus E_{ζ} with an **optimistic estimate** $\text{CVaR}_{\beta}(E)$

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General case

take CVaR on free-energy and dissipation potential + ε first-stage

$$j^{\mathsf{eff}}(\varepsilon) = \inf_{\boldsymbol{\alpha}_{\boldsymbol{\zeta}}} \mathsf{CVaR}_{\beta}\left(\psi(\varepsilon, \boldsymbol{\alpha}_{\boldsymbol{\zeta}}; \boldsymbol{\zeta})\right) + \mathsf{CVaR}_{\beta}\left(\phi(\boldsymbol{\alpha}_{\boldsymbol{\zeta}}; \boldsymbol{\zeta})\right)$$

• if $\beta = 0$, $CVaR = \mathbb{E}$ and we recover average formulation

• results in optimistic stiffness, strength and hardening

Examples

1D elasticity:
$$j(\varepsilon_{\zeta}; \zeta) = \frac{1}{2} E_{\zeta} \varepsilon_{\zeta}^{2}$$

 $j^{\text{eff}}(\varepsilon) = \text{CVaR}_{\beta}(\psi)(\varepsilon) = \frac{1}{2} \text{CVaR}_{\beta}(E) \varepsilon^{2}$

replaces uncertain Young modulus E_{ζ} with an optimistic estimate $\text{CVaR}_{\beta}(E)$

General case

take CVaR on free-energy and dissipation potential + ε first-stage

$$j^{\mathsf{eff}}(\varepsilon) = \inf_{\alpha_{\zeta}} \mathsf{CVaR}_{\beta}\left(\psi(\varepsilon, \alpha_{\zeta}; \zeta)\right) + \mathsf{CVaR}_{\beta}\left(\phi(\alpha_{\zeta}; \zeta)\right)$$

• if $\beta = 0$, $CVaR = \mathbb{E}$ and we recover average formulation

• results in optimistic stiffness, strength and hardening

Pessimistic estimates

need to define an original dual CVaR



risk-neutral case $\beta = 0$



moderate risk-aversion $\beta = 0.5$



strong risk-aversion $\beta = 0.95$



risk-neutral case $\beta = 0$



moderate risk-aversion $\beta = 0.5$



strong risk-aversion $\beta = 0.95$

Risk-averse stochastic programming formulation at the structure scale Work directly on the **global** free-energy and dissipation potentials:

Optimistic formulation:

$$\boldsymbol{u}_{n+1}, \alpha_{\boldsymbol{\zeta}, n+1} = \operatorname*{arg \, inf}_{\boldsymbol{u} \in \mathcal{U}_{\mathsf{ad}}, \boldsymbol{\alpha}_{\boldsymbol{\zeta}}} \mathsf{CVaR}_{\beta}\left(\Psi\right)\left(\varepsilon, \boldsymbol{\alpha}_{\boldsymbol{\zeta}}\right) + \mathsf{CVaR}_{\beta}\left(\Phi\right)\left(\boldsymbol{\alpha}_{\boldsymbol{\zeta}}\right) - \langle \boldsymbol{F}, \boldsymbol{u} \rangle$$

Pessimistic formulation:

$$\boldsymbol{u}_{n+1}, \alpha_{\boldsymbol{\zeta}, n+1} = \underset{\boldsymbol{u} \in \mathcal{U}_{ad}, \alpha_{\boldsymbol{\zeta}}}{\operatorname{arg inf}} \operatorname{dCVaR}_{\beta}\left(\boldsymbol{\Psi}\right)\left(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}_{\boldsymbol{\zeta}}\right) + \operatorname{dCVaR}_{\beta}\left(\boldsymbol{\Phi}\right)\left(\boldsymbol{\alpha}_{\boldsymbol{\zeta}}\right) - \langle \boldsymbol{F}, \boldsymbol{u} \rangle$$



Risk-averse case: uncertainty on Young modulus only



Risk-averse case: uncertainty on hardening modulus only



Risk-averse case: uncertainty on yield stress only



Risk-averse case: combined uncertainty



Cyclic loading



Outline

1 Context

- 2 Conic programming for non-smooth optimization
- 3 Applications to limit analysis in civil engineering
- 4 Structural optimization
- 6 Risk-averse formulation of material behavior
- **6** Conclusions & perspectives

General conclusions

Conic optimization has many things to offer:

- rich physics: non-smooth, yielding behaviors
- modeling expressiveness: viscoplastic fluids, minimal cracks, membranes and shells, image processing, optimal transport
- numerical robustness: efficiency wrt Newton-Raphson, variational integration

Nonlinear membranes	Minimal crack surface	Funicular form-finding	Ş
Challenges & opportunities			
 integration in industrial software 			
 hybrid methods (Newton or first-order), warm-start 			
preconditioning			
Jeremy Blever (Laboratoire Navier)	HDR	November, 22 ^{n d} 2024	28/30

Research perspectives

Optimization under uncertainty

- fertile links to be drawn with robust optimization and stochastic programming
- computational cost reduction for adjustable formulations
- inclusion with robust topology optimization

Regularization of softening behaviors

- alternate minimization or fixed-point iterations of convex sub-problems
- damage gradient/phase-field models for heterogeneous materials
- softening plasticity: dissipation-based regularization [Bacquaert et al., JMPS, 2024]



Towards a Machine Learning era in computational mechanics ?

Learning plastic yield surfaces using implicit layers



Towards a Machine Learning era in computational mechanics ?

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Thank you for your attention !