

TOP Webinar

Topology Optimization Webinar

Data-driven Approaches in Topology Optimization (DATO), January 26, 2021



A new data-driven topology optimization framework for structural optimization

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Content

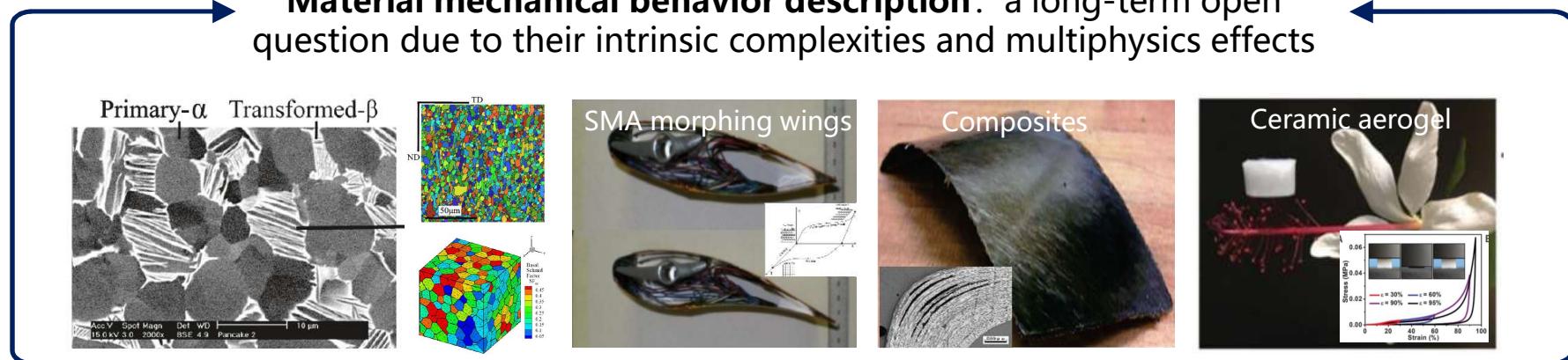
- 1. Research background**
- 2. Design methodology**
- 3. Numerical validation**
- 4. Conclusions & perspectives**

1. Research background

Topology optimization: lightweight and high-performance structures

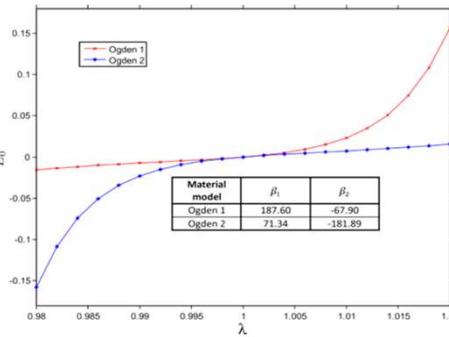
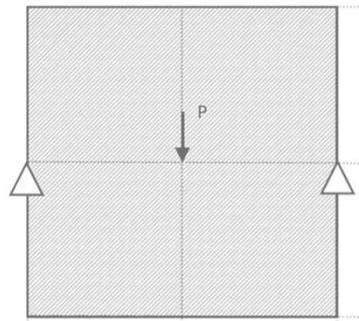


Material mechanical behavior description: a long-term open question due to their intrinsic complexities and multiphysics effects

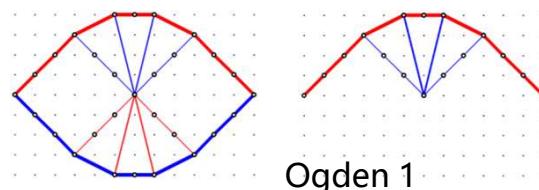


1. Research background

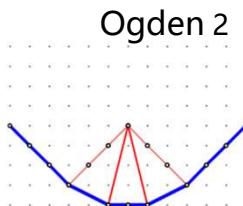
Material nonlinearity: One of the main concerns in nonlinear topology optimization



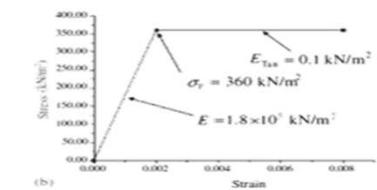
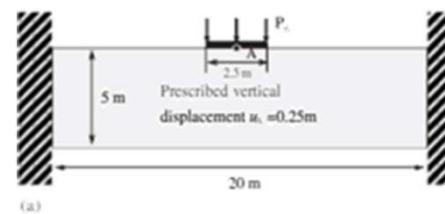
Linear elasticity



Material nonlinearity



A. Ramos, G. Paulino. SMO (2015) 51, 287-304



Linear elasticity



Material nonlinearity

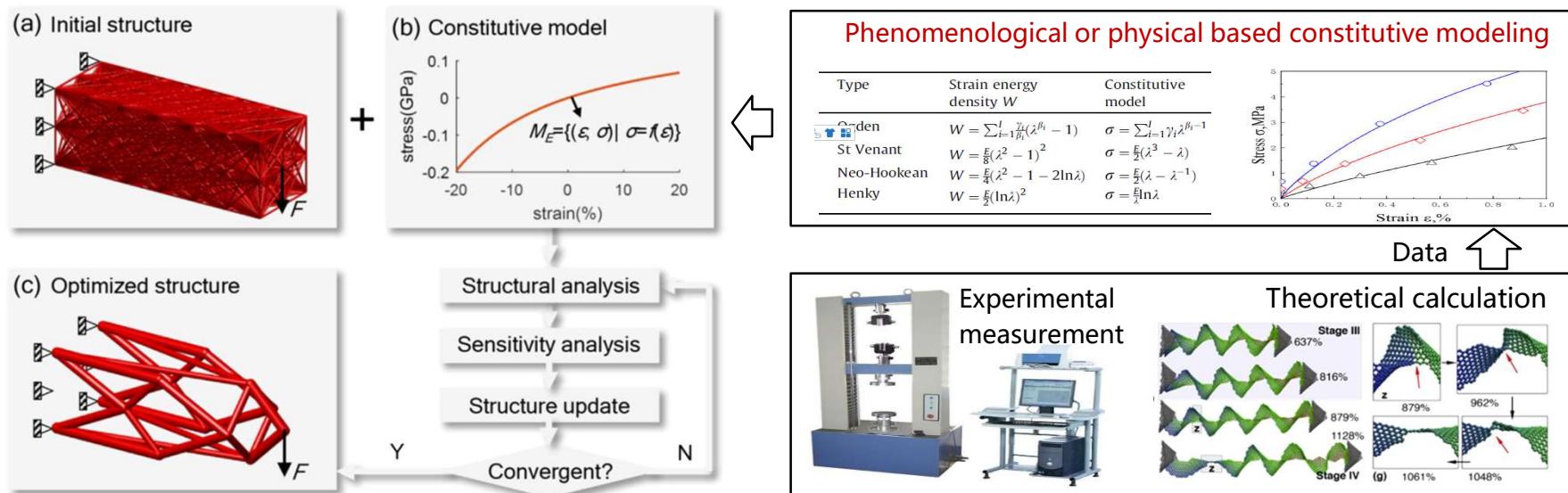


G.H. Yoon, Y.Y. Kim, IJNME (2007) 69, 2196-2218

1. Research background

Traditional topology optimization framework

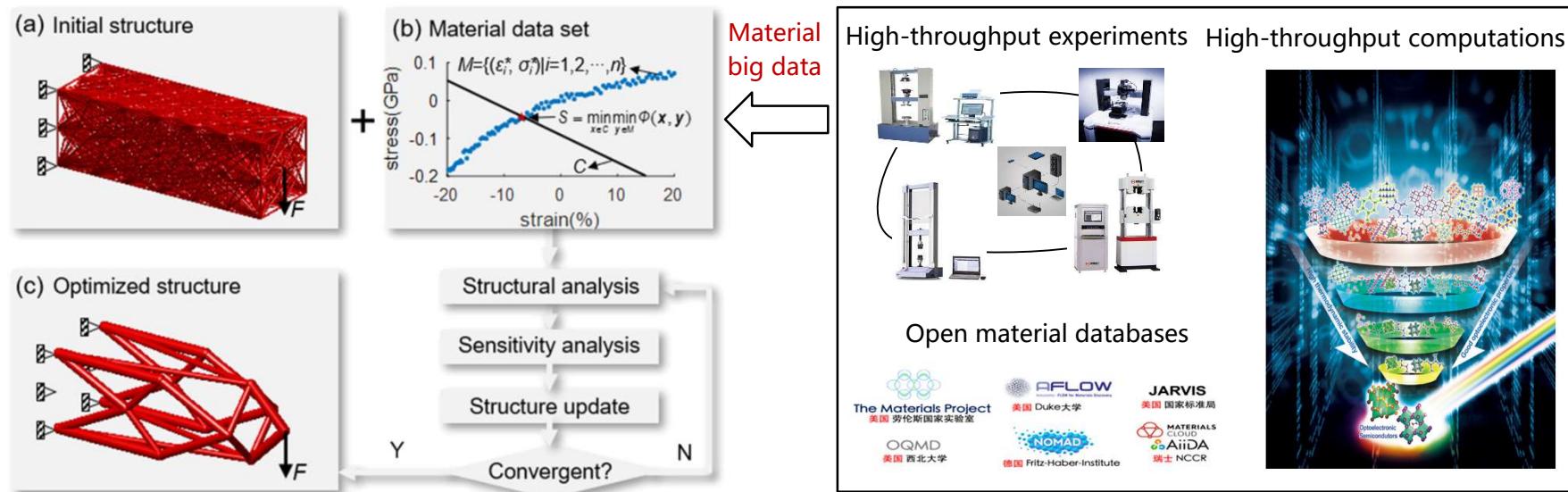
- Material nonlinearity: Described with **phenomenological or physical-based constitutive models** calibrated from experimental and computational data



1. Research background

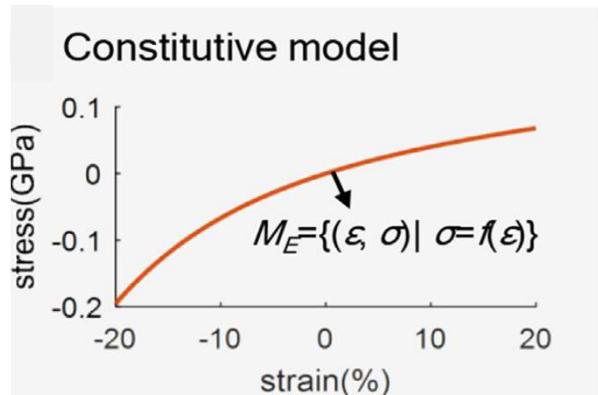
Data-driven topology optimization framework

- Instead of using empirical constitutive models, **material data sets** are directly used to describe the nonlinear constitutive relationship



2. Design methodology

Structural analysis with empirical constitutive model



- ❖ Conservation laws
- Equilibrium + Neumann
 $\operatorname{div} \sigma + f = \mathbf{0}$ in Ω
- $\sigma \cdot n = t$ on Γ_N
- Kinematics + Dirichlet
 $\epsilon(\mathbf{u}) = 1/2(\nabla \mathbf{u} + \nabla^T \mathbf{u})$
- $\mathbf{u} = \bar{\mathbf{u}}$ on Γ_D

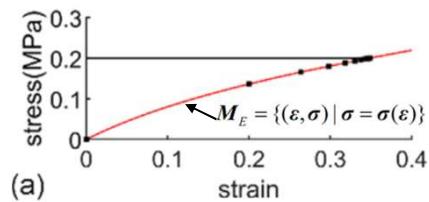
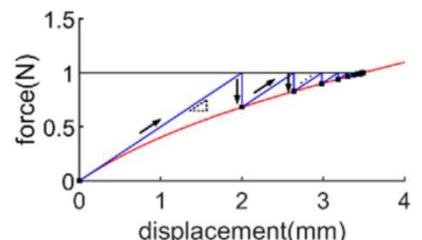
Newton-Raphson solver

Principal of minimum potential energy $\epsilon = \mathbf{B}\mathbf{U}$ $\mathbf{u} = \mathbf{N}\mathbf{U}$

$$\min \Pi = \Pi^{\text{int}} - \Pi^{\text{ext}} = \frac{1}{2} \int_{\Omega} \sigma^T \epsilon d\Omega - \int_{\Omega} \mathbf{f}^T \mathbf{u} d\Omega - \int_{\Gamma_N} \mathbf{t}^T \mathbf{u} d\Gamma$$

$$\text{Variational theory } \delta \Pi(\mathbf{U}) = 0 \Rightarrow \int_{\Omega} \mathbf{B}^T \sigma d\Omega = \int_{\Omega} \mathbf{N}^T \mathbf{f} d\Omega - \int_{\Gamma_N} \mathbf{N}^T \mathbf{t} d\Gamma \Rightarrow \mathbf{F}_{\text{int}}(\mathbf{U}) = \mathbf{F}_{\text{ext}}$$

$$\text{Linearization } \mathbf{F}_{\text{int}}(\mathbf{U}^{k+1}) \approx \mathbf{F}_{\text{int}}(\mathbf{U}^k) + \mathbf{K}_{\tan}^k(\mathbf{U}^k) \Delta \mathbf{U}^k = \mathbf{F}_{\text{ext}}$$



Global space

Local constitutive model

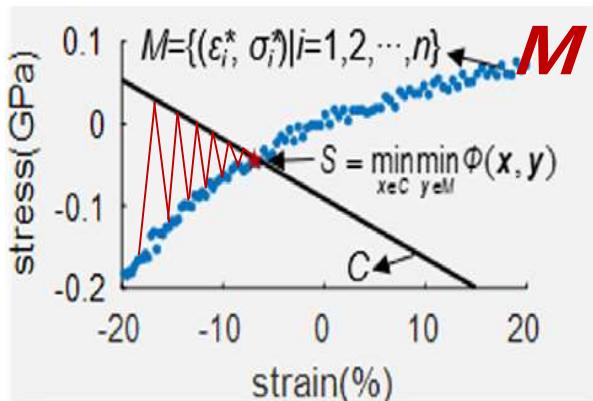
$$\begin{aligned} \text{Residual } \mathbf{R} \\ \Leftrightarrow \begin{cases} \mathbf{K}^{\tan} \Delta \mathbf{U}^k = \mathbf{F}_{\text{ext}} - \mathbf{F}_{\text{int}} \\ \mathbf{U}^{k+1} = \mathbf{U}^k + \Delta \mathbf{U}^k \end{cases} \end{aligned}$$

$$\begin{aligned} \Leftrightarrow \begin{cases} \epsilon = \mathbf{B}\mathbf{U} \\ \sigma = \sigma(\epsilon) \end{cases} \end{aligned}$$

Convergence criteria $\|\mathbf{R}\| \leq 10^{-\gamma}$ or $\|\Delta \mathbf{U}\| \leq 10^{-\gamma}$

2. Design methodology

Structural analysis with discrete material dataset



- ❖ Conservation laws
- Equilibrium + Neumann
 $\operatorname{div}\sigma + f = 0 \text{ in } \Omega$
 $\sigma \cdot n = t \text{ on } \Gamma_N$
- Kinematics + Dirichlet
 $\varepsilon(u) = 1/2(\nabla u + \nabla^T u)$
 $u = \bar{u} \text{ on } \Gamma_D$

■ Data-driven solver

Local strain and stress pair $z = (\varepsilon, \sigma) \in C$ and $z^* = (\varepsilon^*, \sigma^*) \in M$

$$\text{Distance metric } d(z, z^*) = \sqrt{\Psi(\varepsilon - \varepsilon^*) + \Psi'(\sigma - \sigma^*)}$$

$$\text{where } \Psi(\varepsilon) = \frac{1}{2} \varepsilon^T D \varepsilon \text{ strain energy density}$$

$$\Psi'(\sigma) = \frac{1}{2} \sigma^T D^{-1} \sigma \text{ complementary energy density}$$

Minimize an energy-based distance between C and M

Nested optimization problem

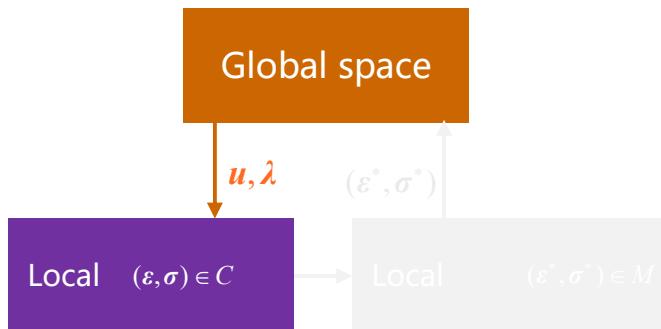
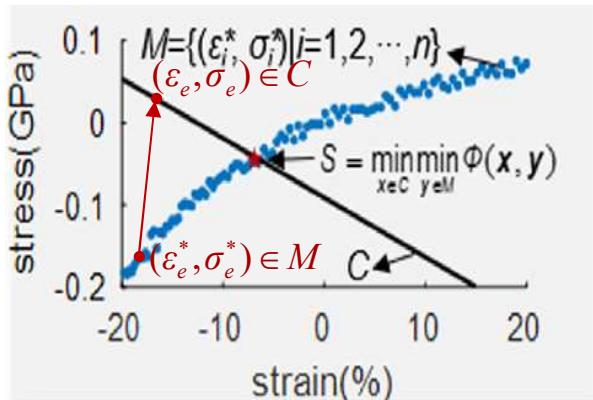
$$\min_{z^* \in M} \min_{z \in C} \Phi = \int_{\Omega} d(z, z^*)^2 d\Omega = \int_{\Omega} \Psi(\varepsilon - \varepsilon^*) + \Psi'(\sigma - \sigma^*) d\Omega$$

Inner subproblem

Outer subproblem

2. Design methodology

Structural analysis with discrete material dataset



■ Data-driven solver (Inner subproblem)

given $(\varepsilon_e^*, \sigma_e^*) \in M \quad e = 1, 2, \dots, m$

Lagrange multiplier method

$$\min_{(\varepsilon_e, \sigma_e)} \Phi = \sum_{e=1}^m \int_{A_e} \int_{L_e} \Psi(\varepsilon_e - \varepsilon_e^*) + \Psi'(\sigma_e - \sigma_e^*) dAdL + \lambda \left(\sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e dAdL - \mathbf{F}_{\text{ext}} \right) = \tilde{\Phi}$$

s.t. $\sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e dAdL = \mathbf{F}_{\text{ext}}$ (equilibrium)

$\varepsilon_e = \mathbf{B}_e \mathbf{u} \quad e = 1, 2, \dots, m$ (compatibility)

$$\begin{cases} \mathbf{K}\mathbf{u} = \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T D_e \varepsilon_e^* dAdL \\ \mathbf{K}\lambda = \mathbf{F}_{\text{ext}} - \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e^* dAdL \\ \mathbf{F}_{\text{int}} \text{ correspond to guess } \sigma_e^* \end{cases}$$

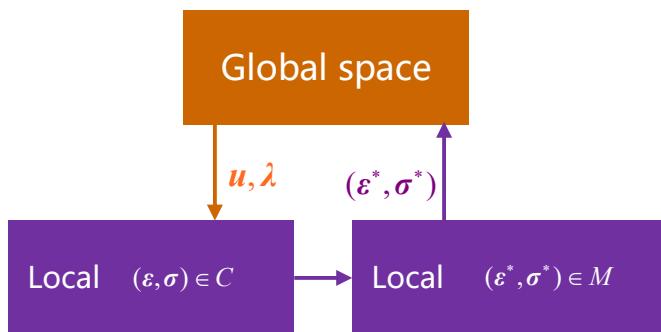
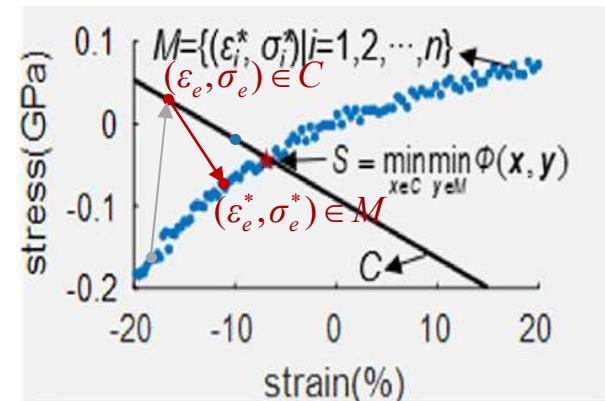
Taking all variations $\delta \tilde{\Phi}(\mathbf{u}, \lambda, \sigma_e) = 0$

$$\begin{cases} \delta \mathbf{u} = 0 \Rightarrow \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T D_e (\mathbf{B}_e \mathbf{u} - \varepsilon_e^*) dAdL = 0 \\ \delta \lambda = 0 \Rightarrow \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e dAdL = \mathbf{F}_{\text{ext}} \\ \delta \sigma_e = 0 \Rightarrow \sigma_e = D_e \mathbf{B}_e \lambda + \sigma_e^* \quad e = 1, 2, \dots, m \end{cases}$$

$$\mathbf{K} = \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T D_e \mathbf{B}_e dAdL$$

2. Design methodology

Structural analysis with discrete material dataset



■ Data-driven solver (Outer subproblem)

$$\text{given } (\varepsilon_e, \sigma_e) \in C \quad e = 1, 2, \dots, m \quad \min_{(\varepsilon_e^*, \sigma_e^*) \in M} \varphi_e = d(z_e, z_e^*)^2 = \Psi(\varepsilon_e - \varepsilon_e^*) + \Psi'(\sigma_e - \sigma_e^*) \quad e = 1, 2, \dots, m$$

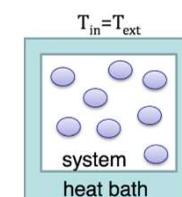
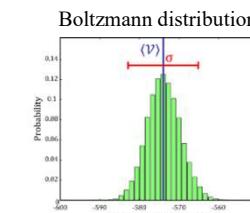
$$\min_{(\varepsilon_e^*, \sigma_e^*) \in M} \Phi = \sum_{e=1}^m \int_{A_e} \int_{L_e} \frac{\Psi(\varepsilon_e - \varepsilon_e^*) + \Psi'(\sigma_e - \sigma_e^*)}{\text{Non-negativity}} dAdL$$

Nearest-neighbour-search (NNS)
- overwhelm the influence of the nearest data point
- sensitive to noises and outliers

Probabilistic data cluster

$$p_i(z_e^k, \beta^k) = \frac{1}{Z(z_e^k, \beta^k)} e^{-\beta^k d^2(z_e^k, z_i^*)} \quad i = 1, 2, \dots, n$$

$$\text{where } Z(z_e^k, \beta^k) = \sum_{i=1}^n e^{-\beta^k d^2(z_e^k, z_i^*)}$$



Minimize the free energy

$$F(z_e^k, \beta^k) = -\frac{1}{\beta^k} \log Z(z_e^k, \beta^k)$$

$$\begin{cases} \varepsilon_e^{*k+1} = \sum_{i=1}^n p_i(z_e^k, \beta^k) \varepsilon_i^* \\ \sigma_e^{*k+1} = \sum_{i=1}^n p_i(z_e^k, \beta^k) \sigma_i^* \end{cases}$$

Simulate annealing to adjust β

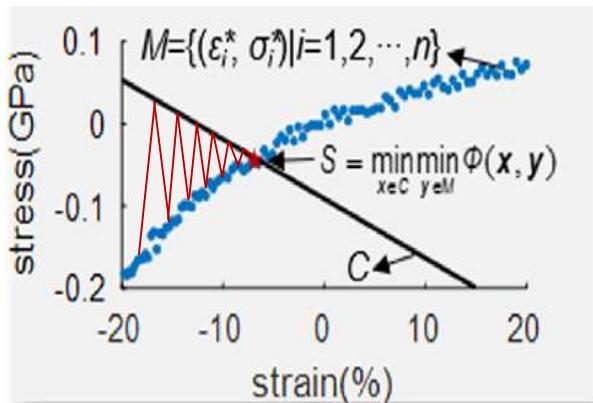
- Initially set β sufficient small that $F(z, \beta)$ is convex (sufficient high temperature T that a large data cluster accounts)
- Increase β to guide the solver towards minimum (decrease temperature T that a small data cluster accounts and the effect of outlier that is close to C than the data cluster is neglected)

$$\frac{1}{\beta} \propto T$$

T. Kirchdoerfer, M. Ortiz. CMAME (2017) 326, 622-641

2. Design methodology

Structural analysis with discrete material dataset



■ Data-driven solver (Convergence criteria)

It is difficult to determine the threshold $10^{-\gamma}$

$$\|\mathbf{R}^*\| \leq 10^{-\gamma} \text{ or } \|\boldsymbol{\lambda}\| \leq 10^{-\gamma}$$

The data-driven solver terminates when

$$(\varepsilon_e^{(K+1)}, \sigma_e^{(K+1)}) = (\underline{\varepsilon_e^{(K)}, \sigma_e^{(K)}}) \quad \text{for all } e = 1, 2, \dots, m$$

Solution

$$\begin{cases} \mathbf{Ku} = \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T D_e \varepsilon_e^* dAdL & \text{①} \\ \mathbf{K\lambda} = \mathbf{F}_{\text{ext}} - \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e^* dAdL & \text{②} \end{cases}$$

$$\begin{cases} \varepsilon_e = \mathbf{B}_e \mathbf{u} & \text{③} \\ \sigma_e = D_e \mathbf{B}_e \boldsymbol{\lambda} + \sigma_e^* & \text{④} \end{cases}$$

Structural equilibrium

$$\mathbf{F}_{\text{int}} = \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \underline{\sigma_e^k} dAdL \quad \text{④}$$

$$\mathbf{F}_{\text{int}} = \left(\sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T D_e \mathbf{B}_e dAdL \right) \boldsymbol{\lambda}^k + \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e^{*k} dAdL \quad \text{②}$$

$$\mathbf{R} = \mathbf{F}_{\text{int}} - \mathbf{F}_{\text{ext}} = \mathbf{0}$$

Structural end-compliance

$$\begin{aligned} J(\mathbf{A}, \mathbf{u}) &= \sum_{e=1}^m \int_{A_e} \int_{L_e} (\underline{\sigma_e^K})^T \underline{\varepsilon_e^K} dAdL \\ &= \sum_{e=1}^m \int_{A_e} \int_{L_e} (D \mathbf{B}_e \boldsymbol{\lambda}^K + \sigma_e^{*K})^T (\mathbf{B}_e \mathbf{u}^K) dAdL \\ &= (\mathbf{K\lambda}^K + \sum_{e=1}^m \int_{A_e} \int_{L_e} \mathbf{B}_e^T \sigma_e^* dAdL)^T \mathbf{u}^K \\ &= \underline{\mathbf{F}_{\text{ext}}^T \mathbf{u}^K} \quad \text{②} \end{aligned}$$

Optimization problem

$$\min_{\mathbf{A}} \quad J(\mathbf{A}, \mathbf{u}) = \mathbf{F}_{\text{ext}}^T \mathbf{u}$$

$$\text{s.t.} \quad \mathbf{R}(\mathbf{A}, \mathbf{u}) = \mathbf{F}_{\text{ext}} - \mathbf{F}_{\text{int}} = \mathbf{0}$$

$$V(\mathbf{A}) = \sum_{e=1}^m A_e L_e \leq V_{\max}$$

$$A_e \geq 0, \quad e = 1, 2, \dots, m$$

2. Design methodology

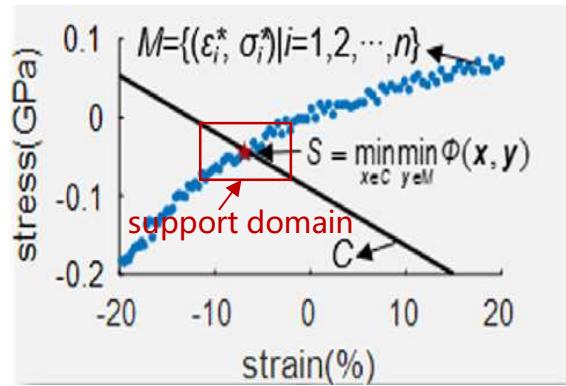
Sensitivity analysis with discrete material dataset

Adjoint method $R = \mathbf{0}$

$$\tilde{J} = \mathbf{F}_{\text{ext}}^T \mathbf{u} + \boldsymbol{\beta}^T \mathbf{R}$$

$$\frac{\partial \tilde{J}}{\partial A_e} = \mathbf{F}_{\text{ext}}^T \frac{\partial \mathbf{u}^K}{\partial A_e} + \boldsymbol{\beta}^T \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}^K} \frac{\partial \mathbf{u}^K}{\partial A_e} + \frac{\partial \mathbf{R}}{\partial A_e} \right) = \underbrace{\left(\mathbf{F}_{\text{ext}}^T - \boldsymbol{\beta}^T \frac{\partial \mathbf{F}_{\text{int}}}{\partial \mathbf{u}^K} \right)}_{?} \frac{\partial \mathbf{u}^K}{\partial A_e} - \boldsymbol{\beta}^T \frac{\partial \mathbf{F}_{\text{int}}}{\partial A_e}$$

$$\frac{\partial J}{\partial A_e} = -\boldsymbol{\beta}^T \frac{\partial \mathbf{F}_{\text{int}}}{\partial A_e}$$



Representation of $(\varepsilon_e^K, \sigma_e^K)$ with a data cluster in M

Data cluster $(\varepsilon_{i_e}^*, \sigma_{i_e}^*) \in M \quad i_e = 1, 2, \dots, N_e$ within a support domain of $(\varepsilon_e^K, \sigma_e^K)$

where $d(\varepsilon_{i_e}^*, \varepsilon_e^K) \leq d_I$ with d_I denoting the radius of the support domain

Define the relevance of each data $(\varepsilon_{i_e}^*, \sigma_{i_e}^*) \in M \quad i_e = 1, 2, \dots, N_e$ to $(\varepsilon_e^K, \sigma_e^K)$

$p_{i_e}(\varepsilon_e^K) \quad i_e = 1, 2, \dots, N_e$

Probabilistic representation $\sigma_e^K = \sum_{i_e=1}^{N_e} p_{i_e}(\varepsilon_e^K) \sigma_{i_e}^* \Rightarrow \frac{\partial \sigma_e^K}{\partial \varepsilon_e^K} = \sum_{i_e=1}^{N_e} \frac{\partial p_{i_e}(\varepsilon_e^K)}{\partial \varepsilon_e^K} \sigma_{i_e}^*$

2. Design methodology

Sensitivity analysis with discrete material dataset

Moving Least Square (MLS) $p(\varepsilon_e^K) = [p_1(\varepsilon_e^K), p_2(\varepsilon_e^K), \dots, p_{N_e}(\varepsilon_e^K)]^T$

$$p(\varepsilon_e^K) = \mathbf{N}^T(\varepsilon_e^K) \mathbf{A}^{-1}(\varepsilon_e^K) \mathbf{B}^{-1}(\varepsilon_e^K)$$

$$\mathbf{A}(\varepsilon_e^K) = \sum_{i_e=1}^{N_e} w(\varepsilon_e^K - \varepsilon_{i_e}^*) \mathbf{N}(\varepsilon_{i_e}^*) \mathbf{N}^T(\varepsilon_{i_e}^*)$$

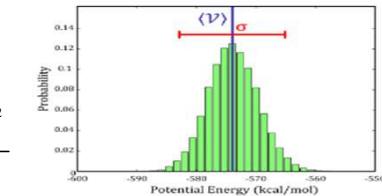
$$\mathbf{B}(\varepsilon_e^K) = [w(\varepsilon_e^K - \varepsilon_1^*) \mathbf{N}(\varepsilon_1^*) \cdots w(\varepsilon_e^K - \varepsilon_{N_e}^*) \mathbf{N}(\varepsilon_{N_e}^*)]$$

$\mathbf{N}^T(\varepsilon_e^K)$ - basis function (independent of the material dataset)

$w(\varepsilon_e^K - \varepsilon_{i_e}^*)$ - weight function

$$\text{Gauss function } w(\varepsilon_e^K - \varepsilon_{i_e}^*) = \frac{e^{-\eta^2 (\varepsilon_e^K - \varepsilon_{i_e}^*)^2 / d_i^2} - e^{-\eta^2}}{1 - e^{-\eta^2}}$$

$$\frac{\partial \sigma_e^K}{\partial \varepsilon_e^K} = \sum_{i_e=1}^{N_e} \frac{\partial p_{i_e}(\varepsilon_e^K)}{\partial \varepsilon_e^K} \sigma_{i_e}^*$$



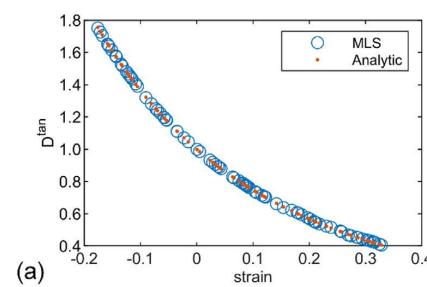
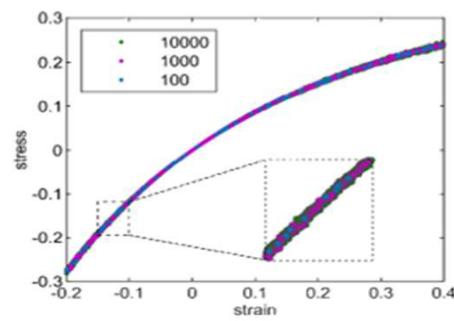
Henky model

$$\sigma = \frac{E}{1+\varepsilon} \ln(1+\varepsilon)$$

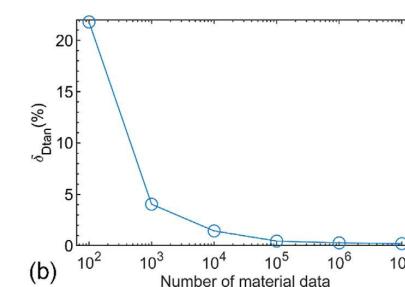
$$E = 1$$

Material dataset

$$M = \{(\varepsilon_i^*, \sigma_i^*) \mid i = 1, 2, \dots, n\}$$



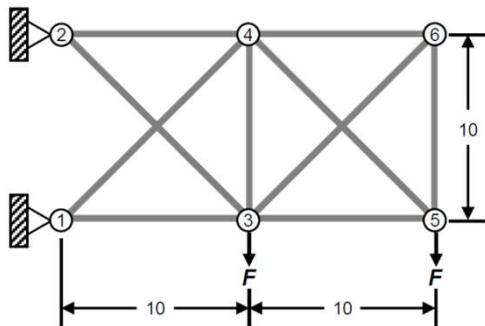
(a)



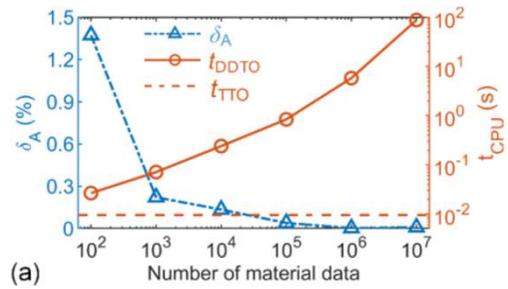
(b)

3. Numerical validation

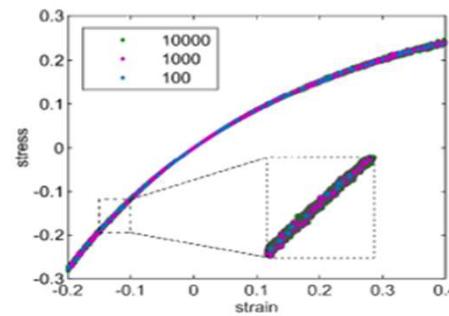
10-bar plane truss



Discrepancy vs. Computational cost



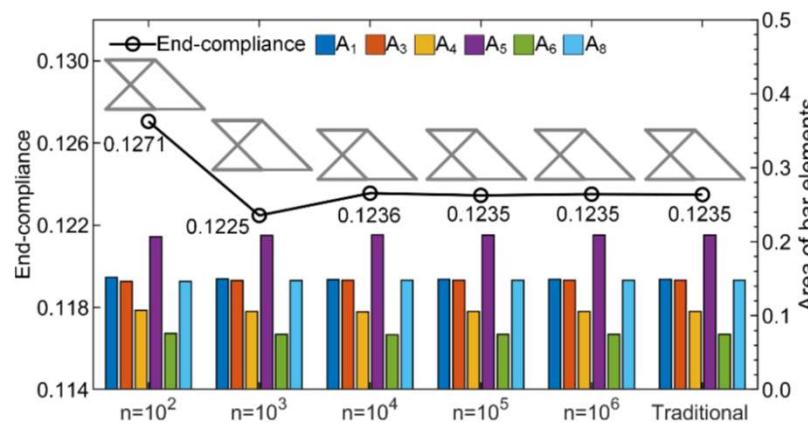
Material dataset I



Henky model

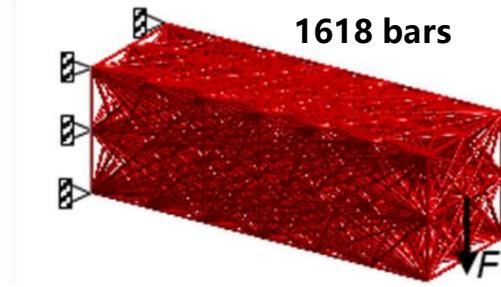
$$\sigma = \frac{E}{1+\varepsilon} \ln(1 + \varepsilon)$$

$$E = 1$$



3. Numerical validation

Cantilevered space truss



Ogden model

$$\sigma = \sum_{i=1}^I \frac{\gamma_i}{\beta_i} ((1+\varepsilon)^{\beta_i} - 1)$$

$$I = 2, \gamma_i = -\gamma_i = E/(\beta_1 - \beta_2)$$

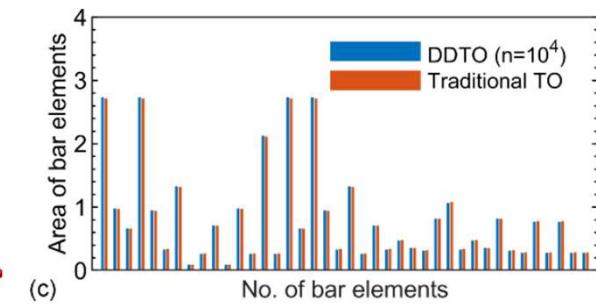
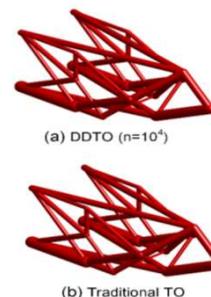
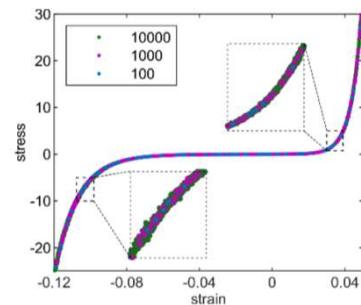
Material I

$$E = 1, \beta_1 = 187.6, \beta_2 = -67.9$$

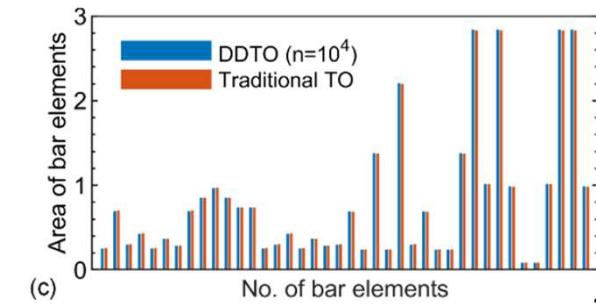
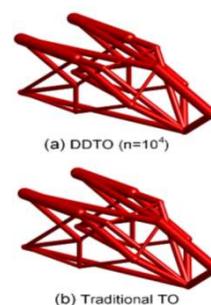
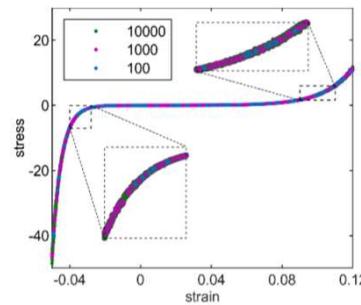
Material II

$$E = 1, \beta_1 = 71.34, \beta_2 = -181.89$$

Material I

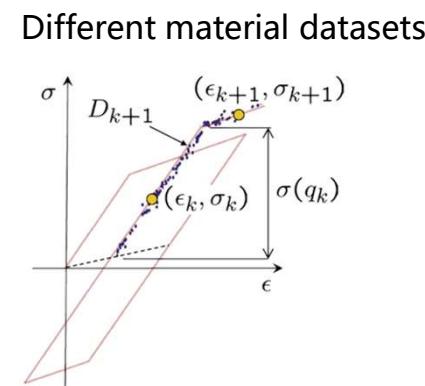
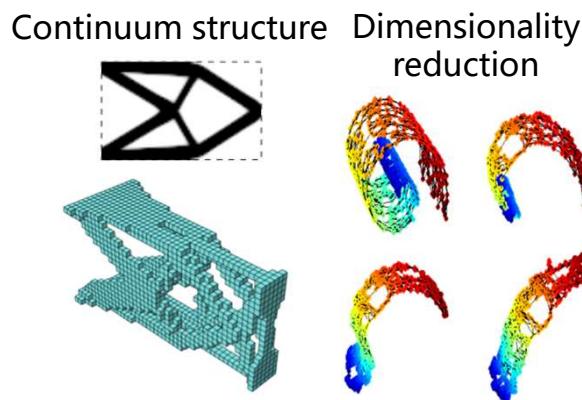


Material II



4. Conclusions & perspectives

- First and preliminary studies are made using datasets for the description of material behavior in truss topology optimization
- Data-driven structural analysis employed for structural response analysis and sensitivity analysis are developed based on MLS approach
- The proposed DDTO framework is appealing in engineering applications with emerging new materials



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