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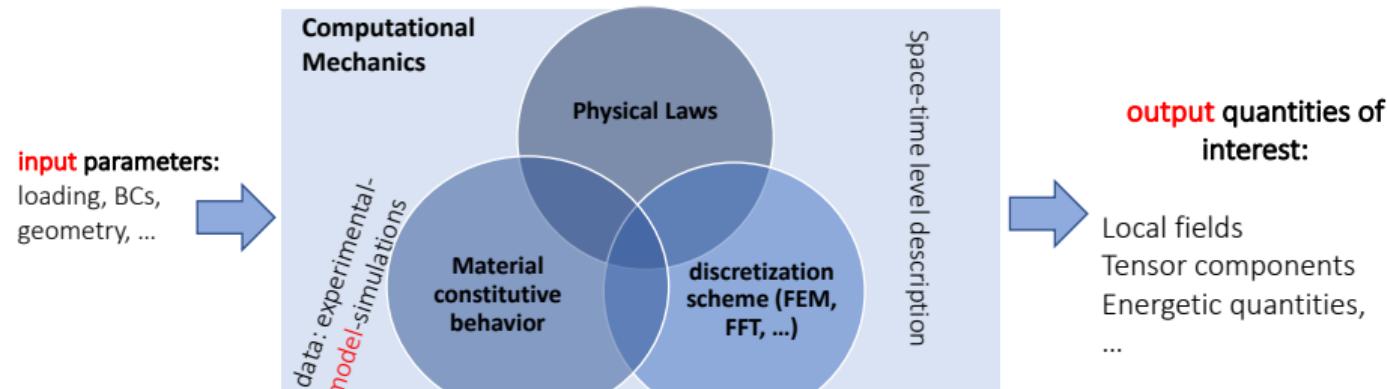
On thermodynamically admissible data driven computational mechanics

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Merging Computational Mechanics (CM) and Data Driven (DD) approaches

Data are ubiquitous in computational mechanics



Multi-dimensionality curse (in/out)
Material Model ignorance

- ✓ ROM based surrogate models: bypass expansive computational process
- ✓ Model Free solvers: bypass the modeling step (data-simulations paradigm)
- ✓ **Data are agnostic → Physically based approaches**



ROM based surrogate model

Real time 10D welding simulations

1

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- 1 Model free CM
- 2 Variational ROM
- 3 Φ HOPGD: real time simulations



Model free computational mechanics

Explicit model computational mechanics

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} & \mathbf{x} \in \Omega \\ \boldsymbol{\varepsilon} = \nabla^s \mathbf{u} & \mathbf{x} \in \Omega \\ \mathbf{u} = \mathbf{u}_0 & \mathbf{x} \in \Gamma^D; \quad \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}_0 \quad \mathbf{x} \in \Gamma^N \\ \boldsymbol{\sigma} = \partial_{\boldsymbol{\varepsilon}} \Psi \quad \text{and} \quad \dot{\boldsymbol{\alpha}} \in \partial_{\mathcal{A}} \varphi \end{cases}$$

Model free computational mechanics

$$\begin{cases} \operatorname{div} \boldsymbol{\sigma} + \mathbf{f} = \mathbf{0} & \mathbf{x} \in \Omega \\ \boldsymbol{\varepsilon} = \nabla^s \mathbf{u} & \mathbf{x} \in \Omega \\ \mathbf{u} = \mathbf{u}_0 & \mathbf{x} \in \Gamma^D; \quad \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}_0 \quad \mathbf{x} \in \Gamma^N \\ \mathcal{M} = \{z^* \mid z^* = (\boldsymbol{\varepsilon}^*, \boldsymbol{\sigma}^*)\} \end{cases}$$

Double distance problem: the DDCM solution is given by [T.Kirchdoerfer and M.Ortiz, 2016]

$$z^{\text{sol}} = \min_{z^* \in \mathcal{M}} \min_{z \in \mathcal{P}} \|z - z^*\|_*^2 \quad \text{with} \quad \mathcal{P} = \mathcal{C}^{\text{adm}} \cap \mathcal{S}^{\text{adm}}$$

Alternate minimization problem: iterative alternate global-local optimization

Global step : $(z)^k = \arg \min_{z \in \mathcal{P}} \|z - (z^*)^k\|_*^2 = \frac{1}{2} \int_{\Omega} (\boldsymbol{\varepsilon} : \mathbb{A} : \boldsymbol{\varepsilon} + \boldsymbol{\sigma} : \mathbb{A}^{-1} : \boldsymbol{\sigma}) dV$

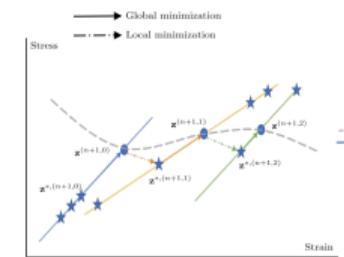
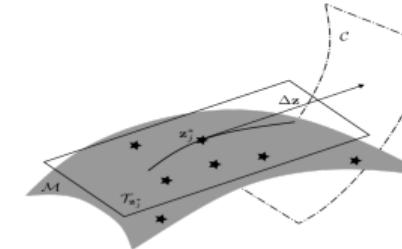
Local step : $(z^*)^{k+1} = \arg \min_{z^* \in \mathcal{M}} \|z^* - (z)^k\|_*^2 = \frac{1}{2} (\boldsymbol{\varepsilon} : \mathbb{A} : \boldsymbol{\varepsilon} + \boldsymbol{\sigma} : \mathbb{A}^{-1} : \boldsymbol{\sigma})$



Tangent distance DDCM for dissipative media¹

- Thermodynamically consistent model free framework
- Tangent distance minimization
- Observable state variables
- Material data basis: ε^* , σ^* , Ψ^* , \mathbb{C}_t
- Variational global problem at iteration $k + 1$ consists in:

$$\left\{ \begin{array}{l} \text{having the pair } z^* = (\varepsilon^*, \sigma^*) \text{, find the pair } z = (\varepsilon, \sigma) \text{ that minimizes the functional:} \\ \mathcal{L}(\mathbf{u}, \sigma, \Delta\varepsilon, \eta, \bar{\eta}, \lambda) = \| (\varepsilon - \varepsilon^* - \Delta\varepsilon, \sigma - \sigma^* - \mathbb{C}_t : \Delta\varepsilon) \|_{\mathbb{A}(\Omega)}^2 \\ + \int_{\Gamma_D} \lambda \cdot (\mathbf{u} - \mathbf{u}_0) dS + \int_{\Omega} \eta \cdot (\nabla \cdot \sigma + \mathbf{f}) dV + \int_{\Gamma_N} \bar{\eta} \cdot (\sigma \cdot \mathbf{n} - \mathbf{t}_0) dV \end{array} \right.$$



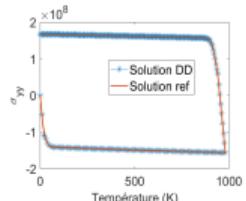
- Plasticity evolution: $(z, z^*) \rightarrow \Psi^*(\varepsilon^*) \rightarrow d = \sigma : \dot{\varepsilon} - \Psi^*(\varepsilon^*)$

¹ Pham, D., Blal, N., Gravouil, A., 2023. Tangent distance data driven computational mechanics for irreversible behaviors, (FEAD)

Tangent distance DDCM for dissipative media

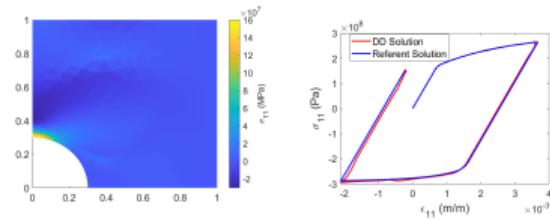
Applications

- Mixed Chaboche hardening
 - State laws: $\dot{\mathbf{X}} = \frac{2}{3} \mathbf{AC}\alpha, \mathbf{R} = \mathbf{bQq}$
 - Evolution laws: $\dot{\alpha} = \epsilon_p - \mathbf{C}\alpha\dot{\mathbf{p}}, \dot{\mathbf{R}} = (1 - \mathbf{b}\mathbf{q})\dot{\mathbf{p}}$
 - Yielding surface: $f(\sigma, \mathbf{X}, \mathbf{R}) = \sigma_{eq}(\sigma - \mathbf{X}) - \sigma_y - \mathbf{R}$



- Non-linear isotropic hardening

$$R(p) = \sigma_\infty + (\sigma_y - \sigma_\infty) \exp(-bp)$$



Concluding remarks

- Good agreement compared to standard FEM
- Data greedy strategy
- Difficulty to experimentally obtain all the needed data
- An hybrid approach: $\|z^* - z^{BK} + \delta z\|$



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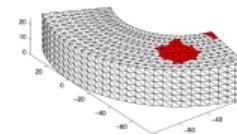
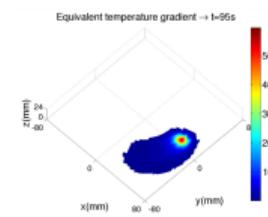
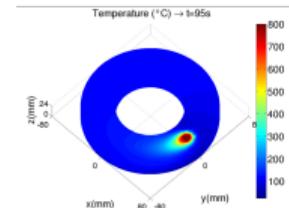


Reduced Order Models

- Reducing the system dimension complexity
- Linear(ized) system size significantly reduced
- Need to reduce the dissipation flow equations → Hyper-reduction
- Multi-parametric simulations: rapid simulations and **real time** simulations

Variational Reduced Order Modeling (VROM)

Propose reduced order models devoted to dissipative continua within a variational framework that preserves the constitutive laws structure



(a) Selected element in control volume

D.Ryckelynck. A priori hyperreduction model : an adaptive approach. International Journal of Computational Physics, 202 :346–366. 2005
Zhang and al. Efficient hyper reduced-order model (HROM) for parametric studies of the 3D thermo-elasto-plastic calculation. FEAD, 2014



Thermodynamically admissible Full Order Model

► Generalized Standard Materials (GSM) framework

- State variables: ε strain field, θ the temperature and α internal variables
- Convex positive semi-continuous potentials: Ψ and φ (or equivalently φ^*)

$$\left\{ \begin{array}{l} s = \frac{\partial \Psi}{\partial \theta}, \quad \sigma^{\text{rev}} = \frac{\partial \Psi}{\partial \varepsilon}, \quad X_\alpha = \frac{\partial \Psi}{\partial \alpha} \\ \frac{\nabla \theta}{\theta} \in \frac{\partial \varphi}{\partial q}, \quad \sigma^{\text{irr}} \in \frac{\partial \varphi}{\partial \dot{\varepsilon}}, \quad A \in \frac{\partial \varphi}{\partial \dot{\alpha}} \Leftrightarrow q \in \frac{\partial \varphi^*}{\partial \nabla \theta / \theta}, \quad \dot{\varepsilon} \in \frac{\partial \varphi^*}{\partial \sigma^{\text{irr}}}, \quad \dot{\alpha} \in \frac{\partial \varphi^*}{\partial A} \end{array} \right. ; \quad \sigma = \sigma^{\text{rev}} + \sigma^{\text{irr}}$$

► Extended Lagrangian functional for dissipative media

$$\mathcal{A} = \int_I \int_{\Omega} \underbrace{\rho \|\dot{\mathbf{u}}\|^2}_{2\mathcal{K}} dV dt \Rightarrow \boxed{\mathcal{L}(\mathbf{u}, \theta, \alpha) = \int_I \left(\mathcal{K} - \mathcal{E}_p - \int_{\Omega} \int \left(\rho \dot{\theta} s - \mathbf{q} \cdot \frac{\nabla \theta}{\theta} \right) d\tau dV - \int_{\Omega} \int \mathcal{D} d\tau dV \right) dt}$$

with : $\mathcal{D} = \rho \theta s^{\text{irr}} = \sigma^{\text{irr}} : \dot{\varepsilon} - \frac{\partial \Psi}{\partial \alpha} \cdot \dot{\alpha}$ the irreversible entropy production



► Going variational

$$\left\{ \begin{array}{l} \int_{\Omega} \rho \ddot{\mathbf{u}} \cdot \delta \mathbf{u} dV - \int_{\Omega} (\nabla \cdot \Psi_{,\epsilon} + \mathbf{f}) \cdot \delta \mathbf{u} dV = 0 \quad ; \int_{\partial\Omega} (\boldsymbol{\sigma} \cdot \mathbf{n} - \mathbf{t}) \cdot \delta \mathbf{u} dV = 0 \quad \forall \delta \mathbf{u} \in \mathcal{V}_u \\ \int_I \int_{\Omega} \left(\frac{\partial \Psi}{\partial \alpha} + \frac{\partial \varphi}{\partial \dot{\alpha}} \right) \cdot \delta \alpha dt = 0 \quad \forall \delta \alpha \in \mathcal{V}_{\alpha} \\ \int_I \int_{\Omega} \left(\rho c_p \dot{\theta} + \operatorname{div} \mathbf{q} - \rho \theta \frac{\partial}{\partial \theta} (\boldsymbol{\sigma}^{\text{rev}} : \dot{\epsilon} - \mathcal{A} : \dot{\alpha}) - (\boldsymbol{\sigma}^{\text{irr}} : \dot{\epsilon} + \mathcal{A} \cdot \dot{\alpha}) - r \right) \delta \theta \textcolor{red}{d\tau} dV dt = 0 \end{array} \right.$$

► FOM thermo-mechanical local field equations

$$\Rightarrow \left\{ \begin{array}{l} \rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \quad \forall \mathbf{x} \in \Omega \quad \text{and} \quad \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t} \quad \forall \mathbf{x} \in \partial\Omega \\ \frac{\partial \Psi}{\partial \alpha} + \frac{\partial \varphi}{\partial \dot{\alpha}} = 0 \quad \forall \mathbf{x} \in \Omega \\ \rho c_p \dot{\theta} + \operatorname{div} \mathbf{q} = \rho \theta \frac{\partial}{\partial \theta} (\boldsymbol{\sigma}^{\text{rev}} : \dot{\epsilon} - \mathcal{A} : \dot{\alpha}) + (\boldsymbol{\sigma}^{\text{irr}} : \dot{\epsilon} + \mathcal{A} \cdot \dot{\alpha}) + r \quad \forall \mathbf{x} \in \Omega \end{array} \right.$$



Revisiting dissipative ROM within a variational thermodynamically admissible framework

- Reduced state variables bases

$$(\mathbf{u}, \theta, \boldsymbol{\alpha}) \in \text{Span} \{ \boldsymbol{\Upsilon}_i \}_{i=1..N_u} \times \text{Span} \{ \Theta_i \}_{i=1..N_\theta} \times \text{Span} \{ \boldsymbol{\Phi}_i \}_{i=1..N_a}$$

- Variational Reduced Model (VROM) ansatz

$$\mathbf{u}(\mathbf{x}, t; \boldsymbol{\mu}) = \sum_{i=1}^{N_u} \boldsymbol{\Upsilon}_i(\mathbf{x}, \boldsymbol{\mu}) \xi_i(t) \quad \boldsymbol{\alpha}(\mathbf{x}, t, \boldsymbol{\mu}) = \sum_{i=1}^{N_a} \boldsymbol{\Phi}_i(\mathbf{x}, \boldsymbol{\mu}) \alpha_i(t) \quad \theta(\mathbf{x}, t; \boldsymbol{\mu}) = \sum_{i=1}^{N_a} \Theta_i(\mathbf{x}, \boldsymbol{\mu})_i \theta_i(t)$$

- VROM framework: find the reduced variables solution of the stationary problem

$$\mathcal{L}^{\text{ROM}} \rightarrow \underset{\{\alpha_i\}, \{\xi_i\}, \{\theta_i\}}{\text{Stat}}$$

keeping a GSM framework:

$$\Psi^{\text{ROM}}(\bar{\boldsymbol{\xi}}, \bar{\boldsymbol{\alpha}}) \quad \text{and} \quad \varphi^{\text{ROM}}(\dot{\bar{\boldsymbol{\alpha}}}) \quad \text{s.t.} \quad \left\{ \begin{array}{l} \tau = \partial_{\bar{\boldsymbol{\xi}}} \Psi^{\text{ROM}} \quad \bar{X}_a = \partial_{\bar{\boldsymbol{\alpha}}} \Psi^{\text{ROM}} \\ \bar{\mathbf{a}} \in \partial_{\dot{\bar{\boldsymbol{\alpha}}}} \varphi^{\text{ROM}} \Leftrightarrow \dot{\bar{\boldsymbol{\alpha}}} \in \partial_{\bar{\mathbf{a}}} (\varphi^{\text{ROM}})^* \end{array} \right.$$



Rate dependent materials

- FOM dissipation potential and non-conservative thermodynamical forces

$$\varphi(\dot{\alpha}) = \frac{1}{2}\eta\|\dot{\alpha}\|^2 \quad \text{where} \quad \mathcal{A} = \frac{\partial\varphi}{\partial\dot{\alpha}} = \eta\dot{\alpha}$$

- VROM associated dissipation potential and non-conservative reduced thermodynamical forces

$$\Psi^{\text{ROM}}(\bar{\xi}, \bar{\alpha}, \bar{\theta}) = \oint_{\Omega} \Psi dV \quad \text{and} \quad \varphi^{\text{ROM}}(\dot{\bar{\alpha}}) = \oint_{\Omega} \varphi dV$$

Rate dependent materials: e.g. visco-elasticity

► FOM

$$\begin{cases} \mathcal{L}^{\text{vis}}(\mathbf{u}, \boldsymbol{\varepsilon}, \lambda) = \int_I \left(\mathcal{K} - \mathcal{E}_p - \int_{\Omega} \mathcal{A} : \boldsymbol{\varepsilon}^{\text{vis}} dV \right) dt + \int_I \int_{\Omega} \lambda \operatorname{tr}(\dot{\boldsymbol{\varepsilon}}^{\text{vis}}) dV dt \\ \Psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\text{vis}}) = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{vis}}) : \mathbb{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{vis}}) \quad \text{and} \quad \varphi(\dot{\boldsymbol{\varepsilon}}^{\text{vis}}) = \frac{1}{2} \eta \|\dot{\boldsymbol{\varepsilon}}^{\text{vis}}\|^2 \end{cases} \xrightarrow{\delta \mathcal{L}^{\text{vis}}} \begin{cases} \rho \ddot{\mathbf{u}} = \operatorname{div} \boldsymbol{\sigma} + \mathbf{f} \\ \eta \dot{\boldsymbol{\varepsilon}}^{\text{vis}} = \boldsymbol{\sigma} - \operatorname{tr} \boldsymbol{\sigma} \mathbf{I} \end{cases}$$

► VROM

$$\begin{cases} \Psi^{\text{ROM}}(\bar{\boldsymbol{\xi}}, \bar{\boldsymbol{\alpha}}) = \frac{1}{2} \bar{\boldsymbol{\xi}} \cdot \mathbf{K} \cdot \bar{\boldsymbol{\xi}} + \frac{1}{2} \bar{\boldsymbol{\alpha}} \cdot \mathbf{K}^{\text{vis}} \cdot \bar{\boldsymbol{\alpha}} - \bar{\boldsymbol{\xi}} \cdot \mathbf{K}^c \cdot \bar{\boldsymbol{\alpha}} \\ \varphi^{\text{ROM}}(\dot{\bar{\boldsymbol{\alpha}}}) = \eta \|\dot{\bar{\boldsymbol{\alpha}}}\|_2^2 \Rightarrow \bar{\mathbf{a}} = \frac{\partial \varphi^{\text{ROM}}}{\partial \bar{\boldsymbol{\alpha}}} = \eta \dot{\bar{\boldsymbol{\alpha}}} \\ \mathcal{L}_{\text{ROM}}^{\text{vis}}(\bar{\boldsymbol{\xi}}, \bar{\boldsymbol{\alpha}}) = \int_I \left(\mathcal{K}^{\text{ROM}} - \mathcal{E}_p^{\text{ROM}} - \bar{\boldsymbol{\alpha}} \cdot \bar{\mathbf{a}} \right) dt \end{cases} \quad \text{with} \quad \begin{cases} K_{ij} = \int_{\Omega} \nabla^s \boldsymbol{\Upsilon}_i : \mathbb{C} : \nabla^s \boldsymbol{\Upsilon}_j dV \\ K_{ij}^{\text{vis}} = \int_{\Omega} \boldsymbol{\Phi}_i : \mathbb{C} : \boldsymbol{\Phi}_j dV \\ K_{ij}^c = \int_{\Omega} \nabla^s \boldsymbol{\Upsilon}_i : \mathbb{C} : \boldsymbol{\Phi}_j dV \end{cases}$$

► VROM Euler-Lagrange field equations

$$\begin{cases} \mathbf{M} \cdot \ddot{\bar{\boldsymbol{\xi}}} = \mathbf{K} \cdot \bar{\boldsymbol{\xi}} - \mathbf{K}^c \cdot \bar{\boldsymbol{\alpha}} - \mathbf{f} \quad (f_i = \langle \mathbf{f}, \boldsymbol{\Upsilon}_i \rangle_{L_2} \quad \text{reduced external force}) \\ \eta \dot{\bar{\boldsymbol{\alpha}}} = \mathbf{K} \cdot \bar{\boldsymbol{\xi}} - \mathbf{K}^c \cdot \bar{\boldsymbol{\alpha}} \end{cases}$$



Rate independent materials

- FOM dissipation potential and non-conservative thermodynamical forces

$$\varphi(\dot{\alpha}) = \sigma \|\dot{\alpha}\| \quad \text{where} \quad \mathcal{A} \in \frac{\partial \varphi}{\partial \dot{\alpha}} = \sigma \frac{\dot{\alpha}}{\|\dot{\alpha}\|}$$

- VROM associated dissipation potential and non-conservative thermodynamical reduced forces

$$\varphi^{\text{ROM}}(\dot{\bar{\alpha}}) = \int_{\Omega} \varphi(\dot{\alpha}) dV \rightarrow \tilde{\varphi}(\dot{\bar{\alpha}}) = \sigma \|\dot{\bar{\alpha}}\|_2 \Rightarrow \quad \bar{\mathbf{a}} \in \frac{\partial \tilde{\varphi}}{\partial \dot{\bar{\alpha}}} \Leftrightarrow \bar{\mathbf{a}} \in \sigma \frac{\dot{\bar{\alpha}}}{\|\dot{\bar{\alpha}}\|_2}$$

- Reduced evolution law: $\dot{\bar{\alpha}} = \lambda \frac{\partial \tilde{f}}{\partial \bar{\mathbf{a}}}$ with the yielding VROM surface $\tilde{f}(\mathbf{a}) = \|\bar{\mathbf{a}}\|_2 - \sigma \leq 0$

VROM for rate independent materials

Theorem

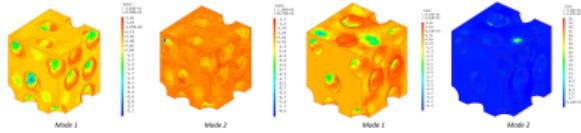
- The reduced dissipation potential $\tilde{\varphi} = \sigma \|\dot{\bar{\alpha}}\|_2$ defines a VROM upper bound: $\varphi^{\text{ROM}} \leq \tilde{\varphi}$

Proof

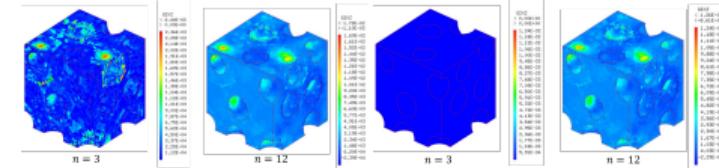
Consider the concave function $g : \bullet \longmapsto \sigma \sqrt{\bullet}$. The dissipation potential function $\tilde{\varphi}$ can be then written as $\varphi^{\text{ROM}}(\dot{\bar{\alpha}}) = g\left(\|\dot{\bar{\alpha}}\|_2^2\right)$. The concavity of g and the L2-orthogonality of the reduced modes Φ_i ensure

$$\begin{aligned} \int_{\Omega} g(\|\dot{\bar{\alpha}}\|_2^2) dV &\leq g\left(\int_{\Omega} \|\dot{\bar{\alpha}}\|_2^2 dV\right) \Rightarrow \int_{\Omega} \sigma \|\dot{\bar{\alpha}}\| \leq \sigma \sqrt{\left(\int_{\Omega} \|\dot{\bar{\alpha}}\|_2^2 dV\right)} \\ &\Rightarrow \varphi^{\text{ROM}} \leq \sigma \sqrt{\int_{\Omega} (\Phi_i \cdot \Phi_j dV) \dot{\alpha}_i \dot{\alpha}_j} = \sigma \sqrt{\dot{\alpha}_i^2} = \sigma \|\dot{\bar{\alpha}}\|_2 = \tilde{\varphi}(\dot{\bar{\alpha}}) \end{aligned}$$

► Example of the reduced basis modes for a heterogeneous matrix-inclusion medium within J2 von Mises plasticity (3 modes)



► Local plastic field obtained with the VROM





VROM: concluding remarks

- **Clustering** into N_c clusters $\Omega = \bigcup_{c=1}^{N_c} \Omega_c$ with the ROM ansatz

$$\boldsymbol{\alpha}(\mathbf{x}, t) = \sum_{i=1}^{\tilde{N}_c} \boldsymbol{\Phi}_i^{(c)}(\mathbf{x}) \alpha_i^{(c)}(t) \quad \forall \mathbf{x} \in \Omega_c$$

The flow evolution law fulfills the normality law $\dot{\overline{\boldsymbol{\alpha}^{(c)}}} = \lambda^{(c)} \frac{\overline{\dot{\mathbf{a}}^{(c)}}}{\|\overline{\mathbf{a}^{(c)}}\|_2}$ $\forall c = 1..N_c$ where the internal variables flow is orthogonal to the boundary of the reduced domain

$$\tilde{f}^{(c)}\left(\overline{\mathbf{a}^{(c)}}\right) = \|\overline{\mathbf{a}^{(c)}}\|_2 - k_c \sigma \quad k_c = |\Omega_c|/|\Omega|$$

- Weakly intrusive reduced order model
- Suquet NTFA approach for multi-scale simulations
- The proposed rate independent VROM is equivalent to a **Linear Comparison Reduced Order Model**²

² N. BLAL. Variational Reduced Order Models for dissipative problems within the formalism of standard generalized materials and the extended Lagrangian functional. Submitted.



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ΦHOPGD: Physically based High Order Proper Generalized Decomposition (ongoing)

- Variables separation representation of the QoI w.r.t the model extra-coordinates

$$\mathbf{u}^{\text{ROM}}(\mathbf{x}, t, \boldsymbol{\mu}) = \sum_{i=1}^N \boldsymbol{\Upsilon}_i(\mathbf{x}) \xi_i(t) \prod_{j=1}^d \zeta_i^j(\mu_j) \quad \text{s.t.} \quad \min \|\mathbf{u}^{\text{ROM}} - \mathbf{u}^*\|$$

- Offline-online approach → Adaptive solutions without any need to re-run FE simulations
- ROM builder complexity: data (primal and dual QoI)
- Respecting the material behavior with only primal data and a small number of ROM modes

$$\mathbf{u}^{\text{ROM}}(\mathbf{x}, t, \boldsymbol{\mu}) = \sum_{i=1}^N \boldsymbol{\Upsilon}_i(\mathbf{x}) \xi_i(t) \prod_{j=1}^d \zeta_i^j(\mu_j) \quad \text{s.t.} \quad \min \|\mathbf{u}^{\text{ROM}} - \mathbf{u}^*\| + \langle \Lambda, F(\mathbf{u}, \boldsymbol{\alpha}; \dot{\boldsymbol{\alpha}}) \rangle$$



Conclusions

Data driven approaches are efficient tools to deal with complex multiscale, multi-physics and multi-parametric computational mechanics

- High-dimensional spaces
- Real time simulations
- Uncertainty and variability issues
- Rapid design

Data sciences should not be purely used as data driven process in CM. They need a scientific approach keeping

- Experimental investigations and computational needs
- Physical foundations
- Mathematical considerations