MODEL-REDUCTION IN MICRO MECHANICS OF MATERIALS

(preserving the variational structure of constitutive relations)

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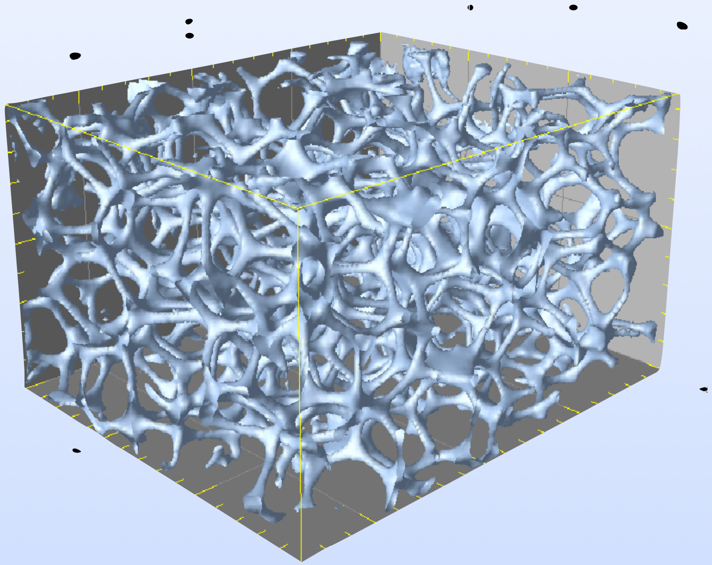
1. **Motivations and objectives**
2. **Reduced Order Modelling**
3. **Reduced variables**
4. **Reduced « dynamics » and variational structures**
5. **Examples**

1. Motivations and objectives

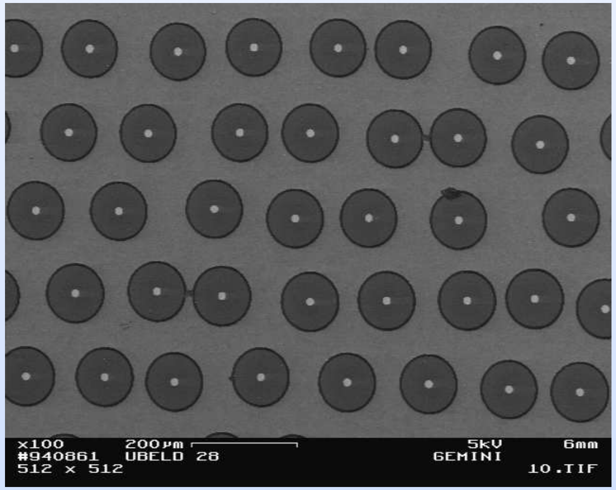
Micromechanics? Every material is heterogeneous at a small enough scale !

Natural materials

Bone:
2-phase
« composite »
solid+porous

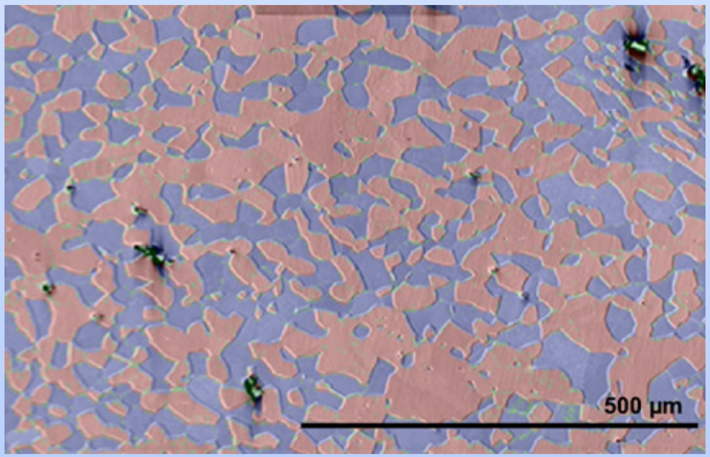


Man-made



Composite
(Ti/SiC)

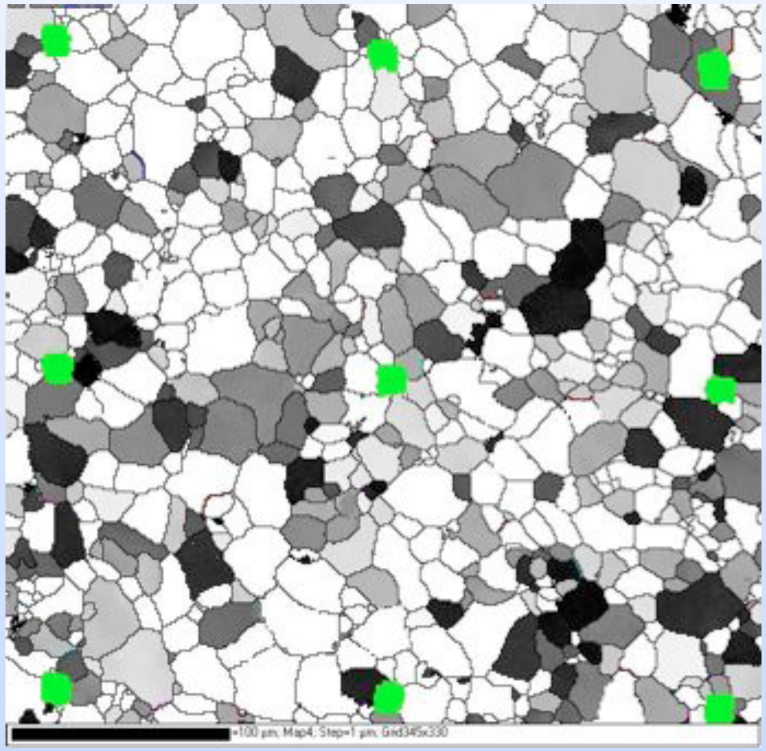
Polycrystalline
Ice



Duplex
steel

Different steps in a micromechanical analysis

Mechanics of solid materials at small scale.



1. **Microstructure description:**

   Representative volume element(s).

   Representativity? Statistical information?

2. **Mechanical properties of constituents**

   Constitutive relations known or identified *in situ.*

3. **Determination of local fields**

   Experimentally, numerically or theoretically.

4. **Homogenization**

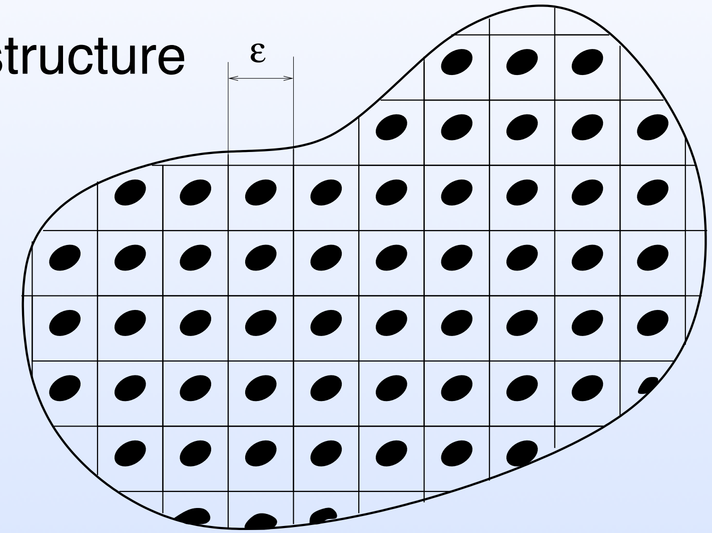
   (also called: coarse graining, upscaling ….).

   Averaging of certain quantities.

   Mathematically: weak limit of the fields when the size of the heterogeneities goes to 0.

Link with (periodic) mathematical homogenization

1. $\Omega = \Omega_\varepsilon^{(1)} \cup \Omega_\varepsilon^{(2)}$ domain with a fine microstructure



2. $$w^\varepsilon(\boldsymbol{\nabla} u) = \begin{cases} w^{(1)}(\boldsymbol{\nabla} u) \text{ in phase } 1, \\ w^{(2)}(\boldsymbol{\nabla} u) \text{ in phase } 2. \end{cases}$$

3. Assuming $w^{(i)}$ convex, then: $w^\varepsilon \xrightarrow{\Gamma} \widetilde{w}$

$$\widetilde{w}(\boldsymbol{\lambda}) = \inf_{u \text{ periodic}} \frac{1}{|V|} \int_V w(x, \boldsymbol{\lambda} + \boldsymbol{\nabla} u) \, d\boldsymbol{x}$$

V : unit-cell

4. $$u^\varepsilon = \underset{u}{\text{Argmin}} \int_\Omega w^\varepsilon(\boldsymbol{\nabla} u) \, d\boldsymbol{x} \quad \underset{\varepsilon \to 0}{\rightharpoonup} \quad u^0 = \underset{u}{\text{Argmin}} \int_\Omega \widetilde{w}(\boldsymbol{\nabla} u) \, d\boldsymbol{x}$$

Effective energy = minimum of the average energy

Here, more realistic constitutive relations

Individual constituents **Nonlinear dissipative constituents**

State of the system (state variables) : $\boldsymbol{\varepsilon}, \boldsymbol{\alpha}$ ex : $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}^{\mathrm{p}}, \ \gamma^{(s)}, ...$

Energy available in the system : $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha})$,

$\Rightarrow$ Driving forces : $\boldsymbol{\sigma} = \dfrac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \boldsymbol{\mathcal{A}} = -\dfrac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}),$

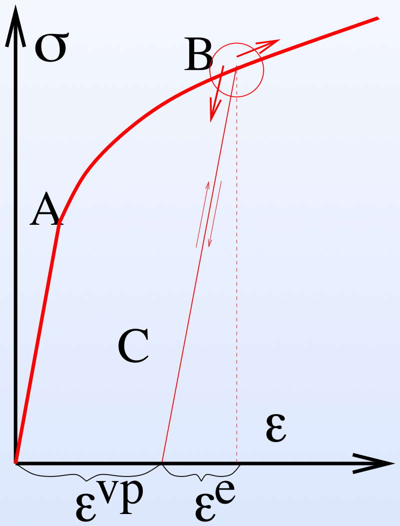
Evolution of the internal variables : $\dot{\boldsymbol{\alpha}} = \boldsymbol{\mathcal{F}}(\boldsymbol{\mathcal{A}}) \quad \Leftrightarrow \quad \boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{G}}(\dot{\boldsymbol{\alpha}}).$

When Onsager's symmetry relations are satisfied: Generalized Standard Materials (GSM) (Halphen & Nguyen, 1975):

$$\boldsymbol{\mathcal{F}}(\boldsymbol{\mathcal{A}}) = \frac{\partial \psi}{\partial \boldsymbol{\mathcal{A}}}(\boldsymbol{\mathcal{A}}) \quad \Leftrightarrow \quad \boldsymbol{\mathcal{G}}(\dot{\boldsymbol{\alpha}}) = \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}), \quad \psi = \varphi^*.$$

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) = 0, \quad w \text{ and } \varphi \text{ convex.}$$

Typical constitutive relations: (elasto-visco-plasticity)



$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\text{e}} + \boldsymbol{\varepsilon}^{\text{vp}},$$

$$\boldsymbol{\sigma} = \boldsymbol{L} : \boldsymbol{\varepsilon}^{\text{e}} = \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{vp}})$$

$$\dot{\boldsymbol{\varepsilon}}^{\text{vp}} = \frac{3}{2}\dot{\varepsilon}_0 \left(\frac{\sigma_{\text{eq}}}{\sigma_0}\right)^n \frac{\boldsymbol{s}}{\sigma_{\text{eq}}},$$

$$\sigma_{\text{eq}} = \left(\frac{3}{2}\boldsymbol{\sigma}^d : \boldsymbol{\sigma}^d\right)^{1/2}$$

Internal variable : $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}^{\text{vp}},$

Energy available in the system : $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\alpha}) : \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha}),$

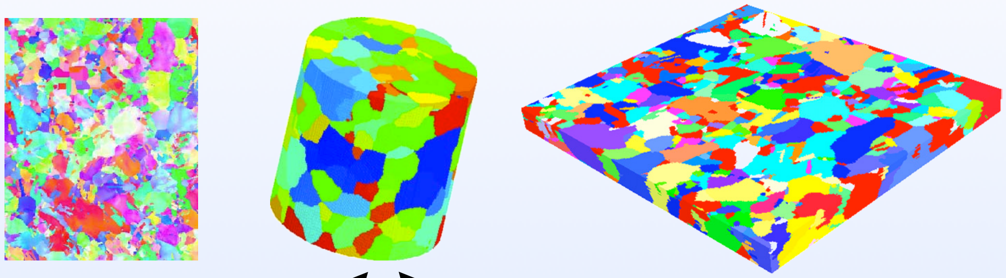
$\Rightarrow$ **Driving forces** : $\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha}), \quad \boldsymbol{\mathcal{A}} = -\frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \boldsymbol{\sigma},$

Dissipation potential : $\varphi(\dot{\boldsymbol{\alpha}}) = \frac{\sigma_0 \dot{\varepsilon}_0}{m+1}\left(\frac{\dot{\alpha}_{\text{eq}}}{\dot{\varepsilon}_0}\right)^{m+1}, \quad m = 1/n$

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) = 0.$$

Recent progress in Micromechanics…

New experimental techniques
(CT, EBSD, 3D XRD, 3D DIC…)



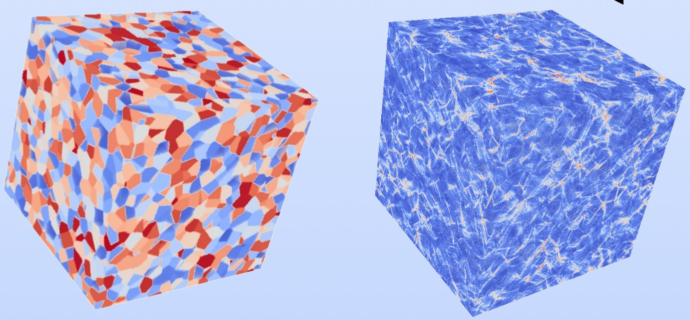
New homogenization approaches

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}),$$

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}) = \operatorname*{Inf}_{\boldsymbol{\varepsilon} \in \mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \langle w(\boldsymbol{\varepsilon}) \rangle \,,$$

Full-Field simulations
High resolution

Reduced order models



FEM: A. Needleman,… you!
Spectral methods: Khatchaturyan, PS & H. Moulinec, G. Milton, W. Muller, R. Lebensohn…

BUT:

- **Bounds and estimates through Linear Comparison Composite** (Willis, 1989, Ponte Castañeda 1991, PS, 1993).

- **1st moment AND fluctuations** of the fields (PPC, 1996, 2002).

Recent progress in Micromechanics…

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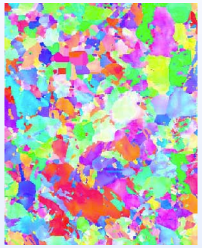
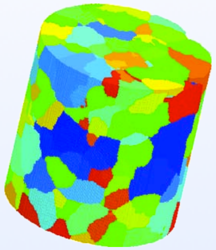
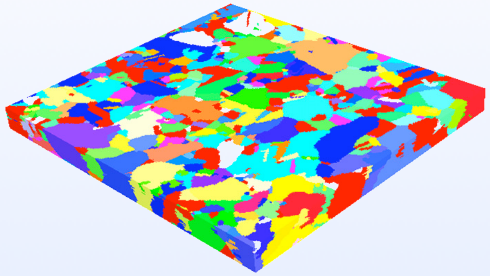
(CT, EBSD, 3D XRD, 3D DIC…)







New homogenization approaches

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}),$$

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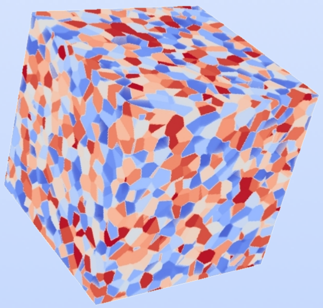
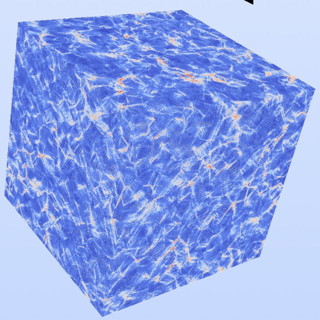
Full-Field simulations
High resolution

Reduced order models





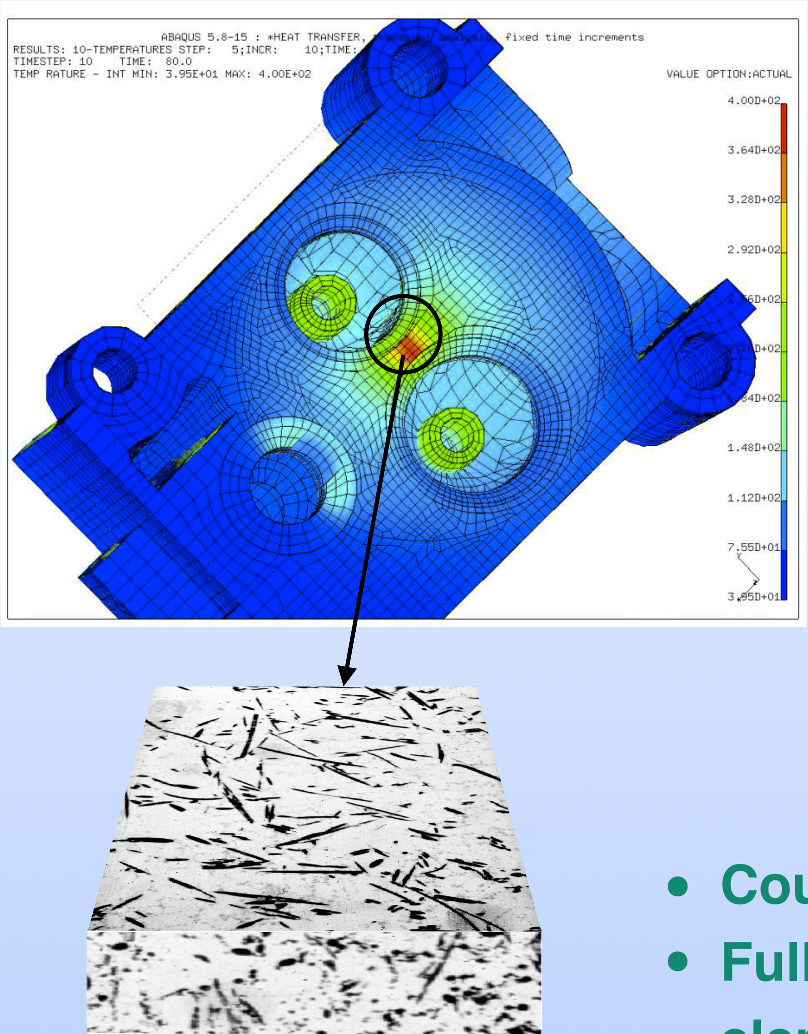
BUT:

- High cost
- no macroscopic constitutive relations

Limited: simple constitutive relations, microstructure, local fields

Objectives: 1) derive « reduced » constitutive relations

Fatigue a MMC insert subject to cyclic loading



- Al matrix (**viscous at 300°C**)
- Al2O3 fibers (elastic)
- Fibers parallel to the (x,y) plane with **random orientation**
- Aspect ratio ≃15; Vol. frac. = 10%
- Matrix with **nonlinear** kinematic hardening.

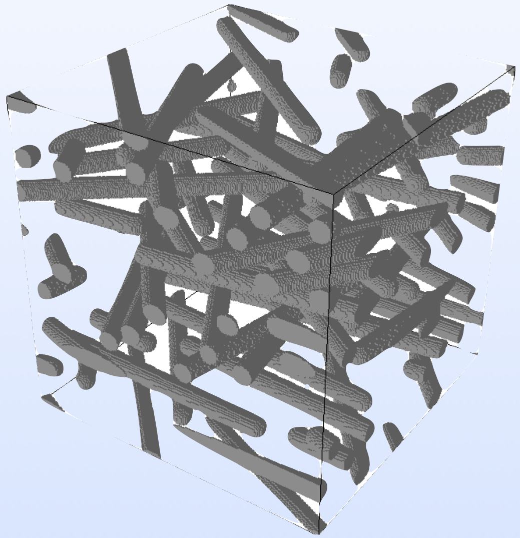
$$\dot{\boldsymbol{\sigma}} = \boldsymbol{L} : (\dot{\varepsilon} - \dot{\varepsilon}^{\text{vp}}), \quad \dot{\varepsilon}^{\text{vp}} = \frac{3}{2}\dot{p}\frac{\boldsymbol{s} - \boldsymbol{X}}{(\sigma - X)_{\text{eq}}},$$

$$\dot{p} = \left(\frac{((\sigma - X)_{\text{eq}} - \sigma_y)^+}{\eta}\right)^n, \quad \dot{\boldsymbol{X}} = \frac{2}{3}H\dot{\varepsilon}^{\text{vp}} - \eta\boldsymbol{X}\dot{p}.$$

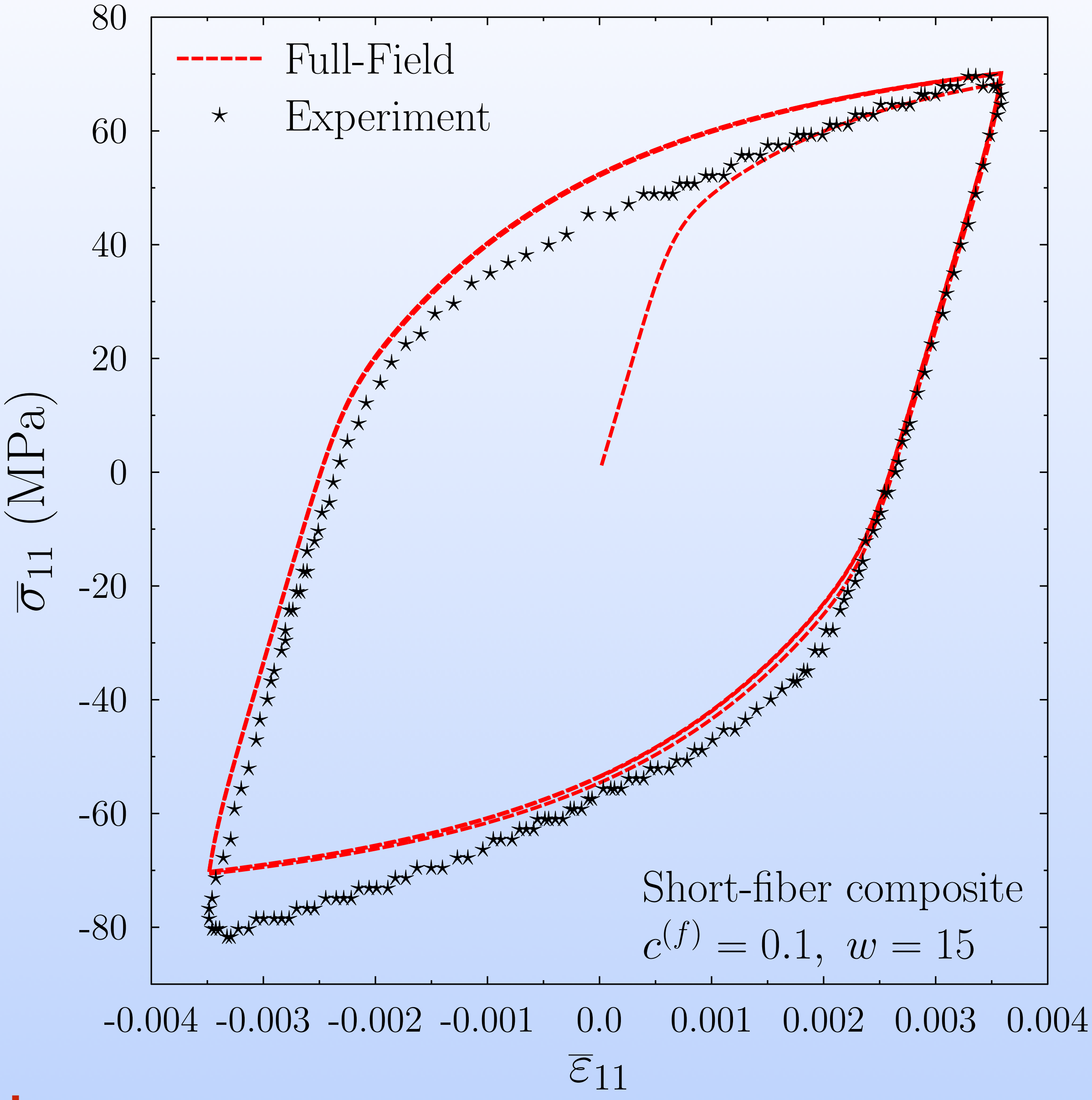
- **Coupled FEM2 still too expensive**
- **Full-field simulations on a Representative volume element**

Full-field simulations (FFT)

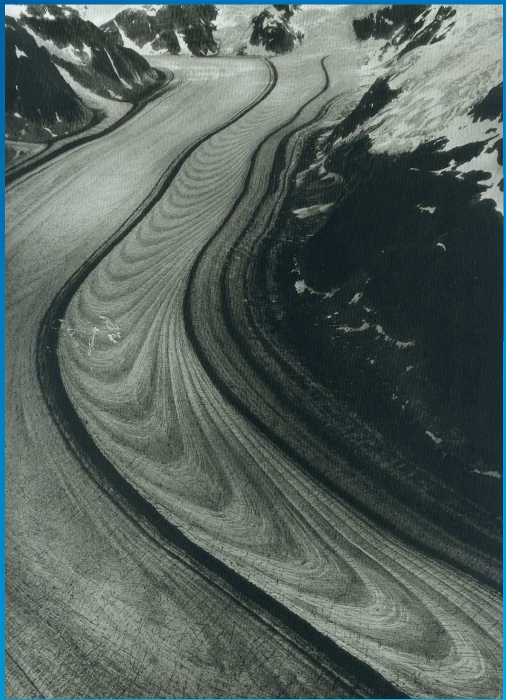
RVE (fibers alone)

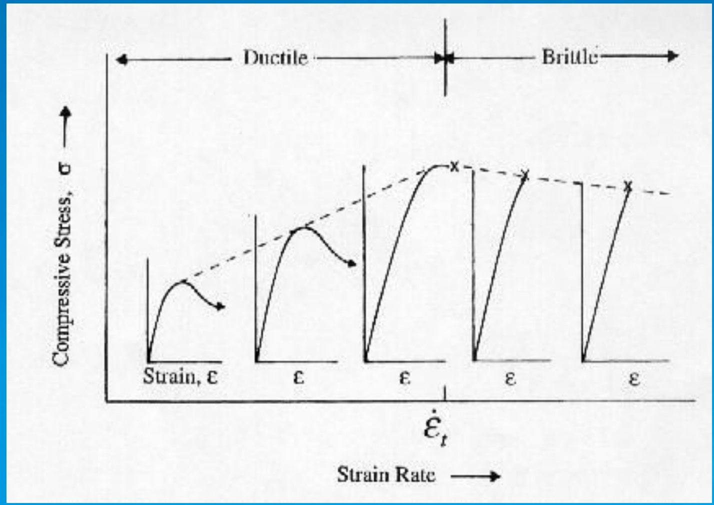


- **Full-field simulations do no provide effective constitutive relations.**
- **Can be used to calibrate a macroscopic model chosen *a priori.***
- **Huge quantity of information** (local fields) is generated but **lost.**

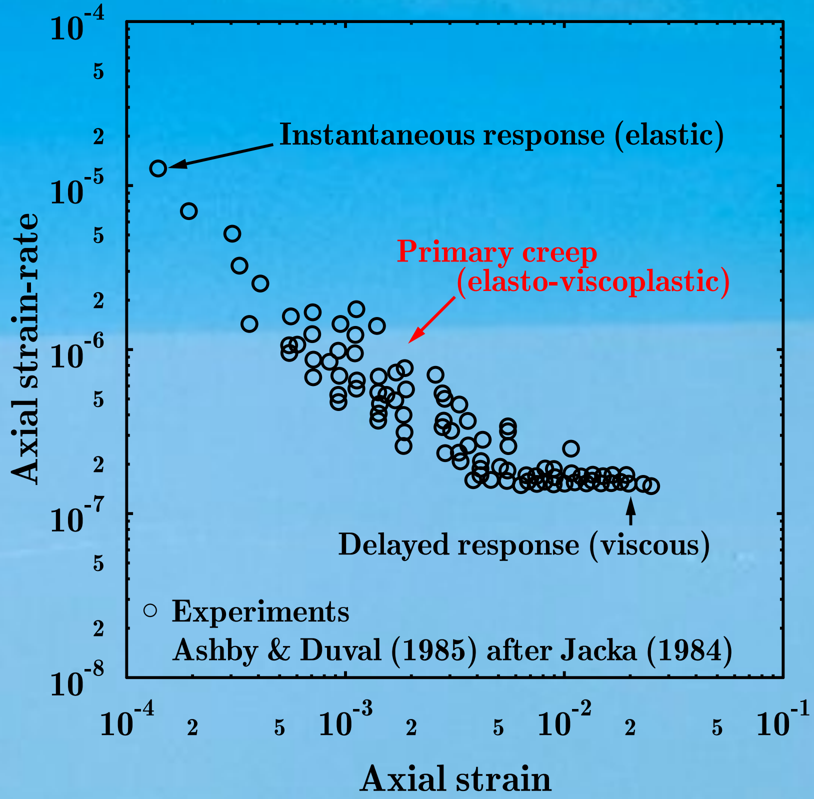


Objective 2: Cost reduction (for parameter calibration)





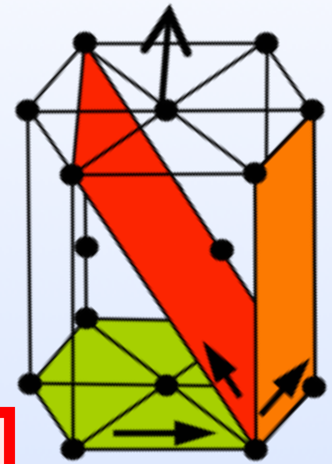
(Polycrystalline Ice)



Crystal plasticity model for Ice

SINGLE CRYSTALS deform by slip along 12 slip systems:

$$\dot{\varepsilon}^{vp} = \sum_{k=1}^{12} \dot{\gamma}^{(k)} \boldsymbol{m}^{(k)}$$



3 basal systems, 3 prismatic, 6 pyramidal

$$\dot{\varepsilon} = \dot{\varepsilon}^{\mathsf{e}} + \dot{\varepsilon}^{\mathsf{vp}}, \quad \dot{\varepsilon}^{\mathsf{e}} = \boldsymbol{M} : \dot{\boldsymbol{\sigma}},$$

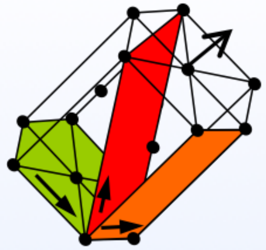
$$\dot{\gamma}^{(k)} = \dot{\gamma}_0^{(k)} \left(\frac{\left|\tau^{(k)} - X^{(k)}\right|}{\tau_0^{(k)}} \right)^{n^{(k)}} \operatorname{sign}\left(\tau^{(k)} - X^{(k)}\right), \quad \tau^{(k)} = \boldsymbol{\sigma} : \boldsymbol{m}^{(k)},$$

$$\dot{\tau}_0^{(k)} = \left(\tau_{sta}^{(k)} - \tau_0^{(k)}\right) \dot{p}^{(k)}, \quad \dot{p}^{(k)} = \sum_{\ell=1}^{12} h^{(k,\ell)} \left|\dot{\gamma}^{(\ell)}\right|,$$

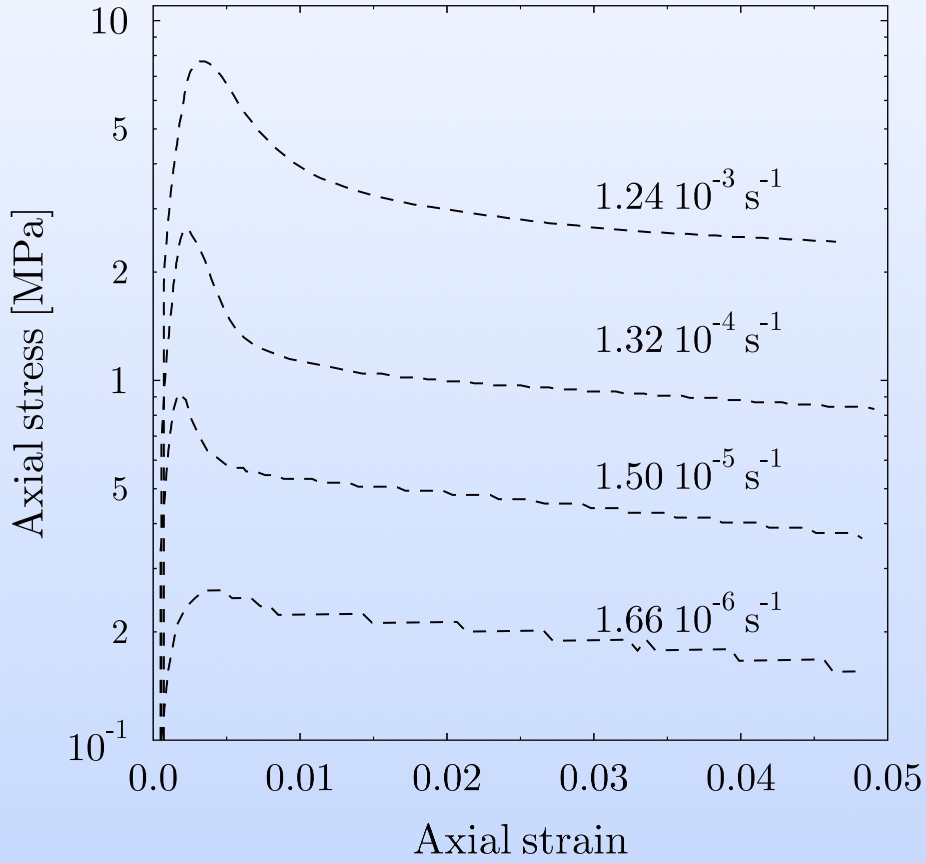
$$\dot{X}^{(k)} = c^{(k)} \dot{\gamma}^{(k)} - d^{(k)} X^{(k)} \left|\dot{\gamma}^{(k)}\right| - e^{(k)} \left|X^{(k)}\right|^m \operatorname{sign}\left(X^{(k)}\right).$$

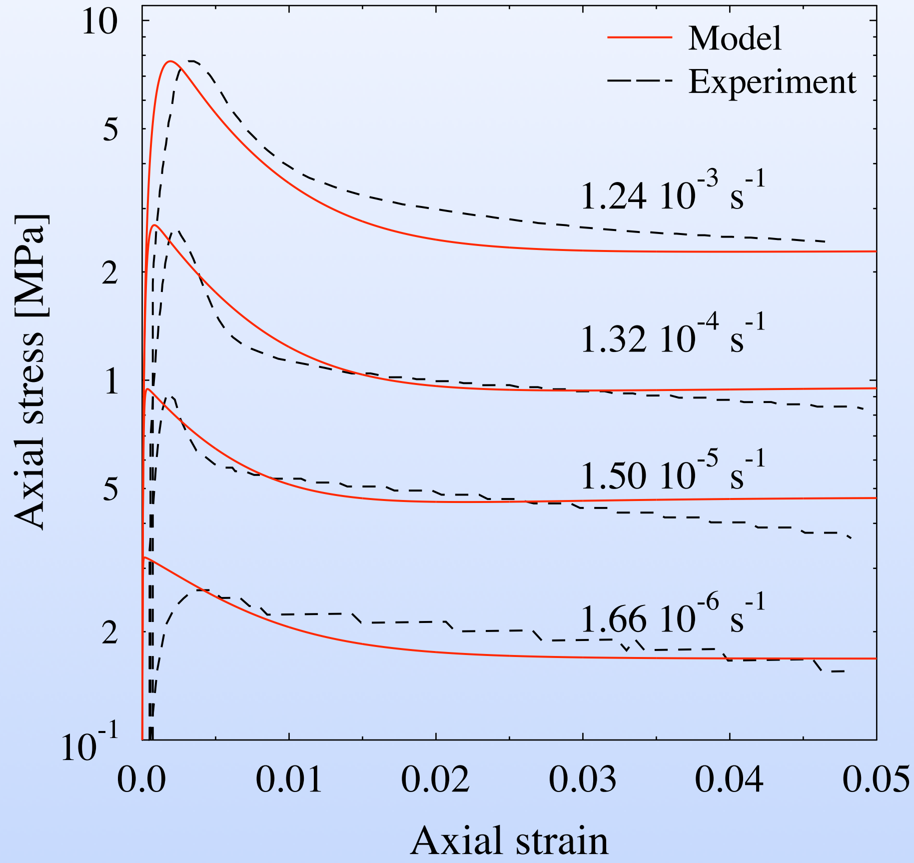
Involves many material parameters (and a few nontrivial)! CALIBRATION?

Compression tests on single crystals at 45°/c axis



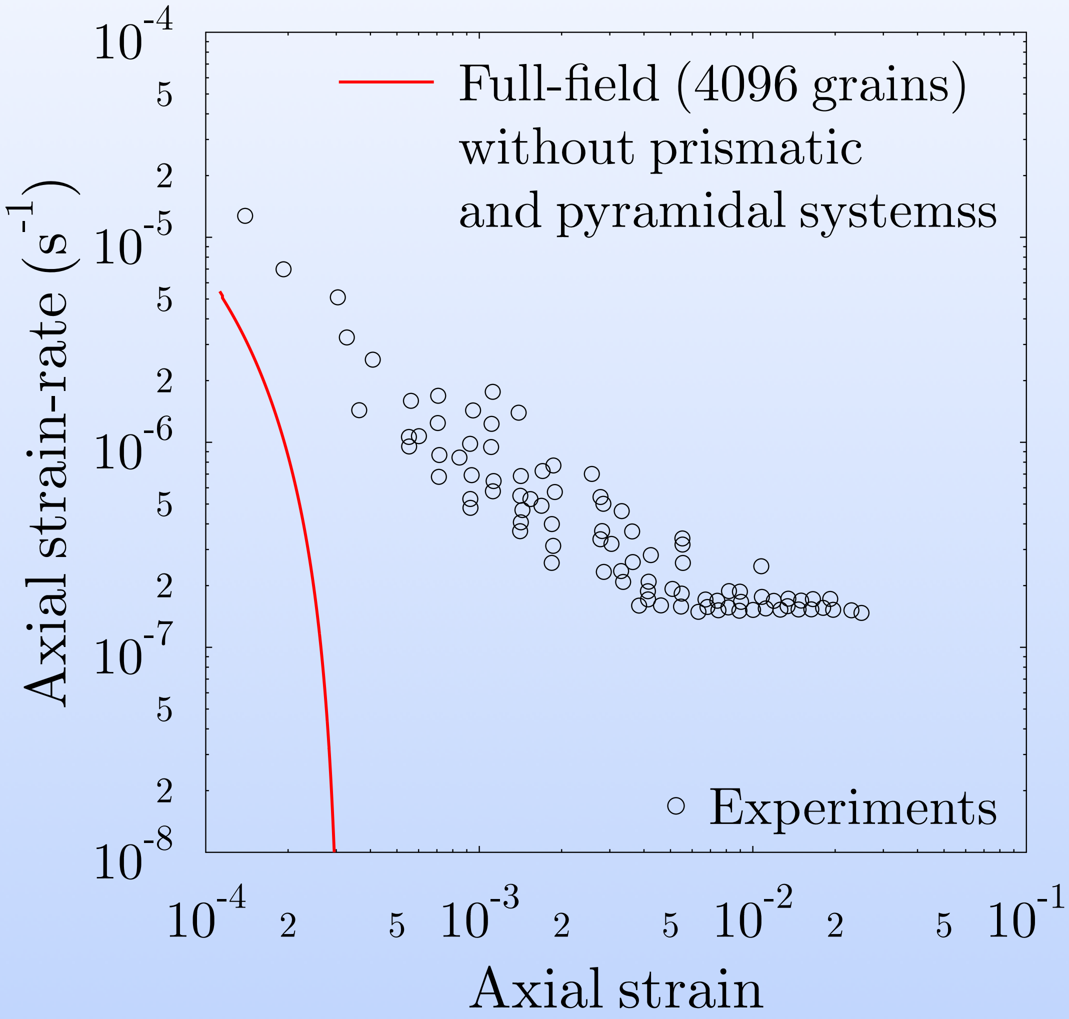
show significant **softening (and rate-dependence):**





Material parameters for basal systems can be identified from single crystal experiments. **But not for the prismatic and pyramidal systems.**

Prismatic and pyramidal systems?



- Prismatic and pyramidal systems **cannot be neglected**
- Their material parameters and latent hardening parameters **cannot be determined experimentally** (basal too soft)

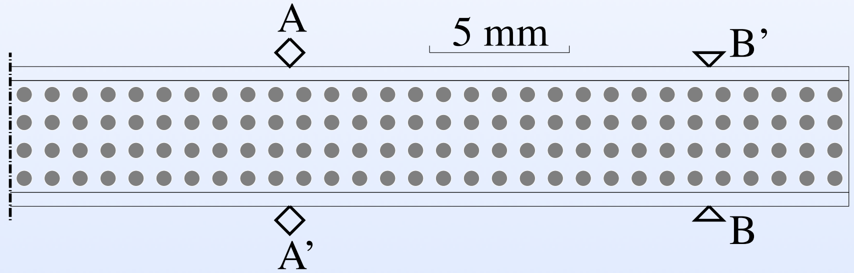
$\Rightarrow$ **Full-field simulations**

One full-field simulation on a 500 grain aggregate: 3 days.

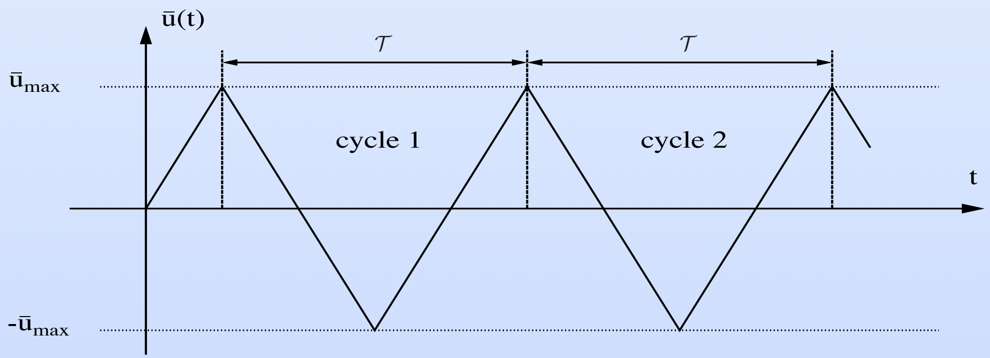
Identification of the major material parameters took us 6 months!

Objective 3: local fields reconstruction problem

Fatigue of a composite beam subject to 4-point bending



Half-beam (120 fibers)



Loading: prescribed vertical displacement at points A and A', frequency 0.1 Hz, 3 different amplitudes

$$\overline{u}_{max} = 0.15,\ 0.25,\ 0.5 \text{ mm}$$

Elastic fibers

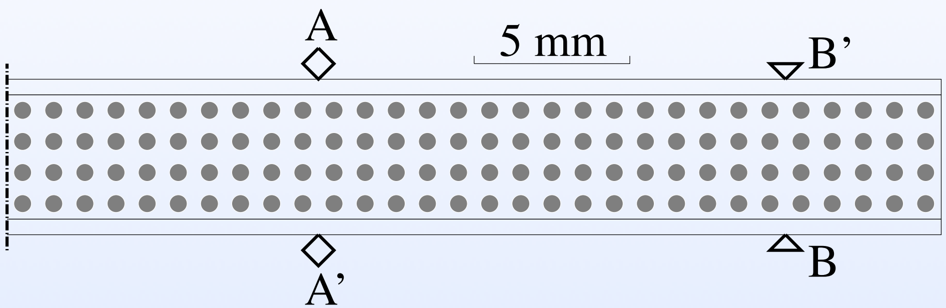
Elasto-viscoplastic matrix with isotropic and kinematic hardening (Armstrong Frederick law)

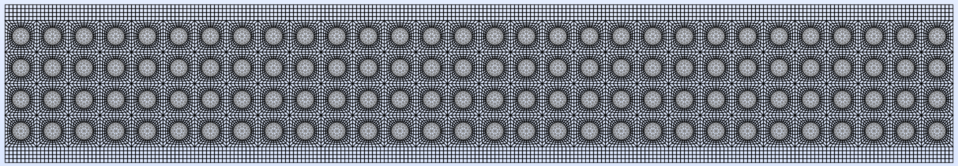
Local fatigue criterion (at point $\boldsymbol{x}$) based on the **energy dissipated** along the stabilized cycle

$$N_{cycle} = C\ w^{\beta}_{dissip},$$

$$w_{dissip}(\boldsymbol{x}) = \int_{cycle} \boldsymbol{\sigma}(\boldsymbol{x}, s) : \dot{\boldsymbol{\varepsilon}}^{\mathsf{vp}}(\boldsymbol{x}, s)\ ds$$

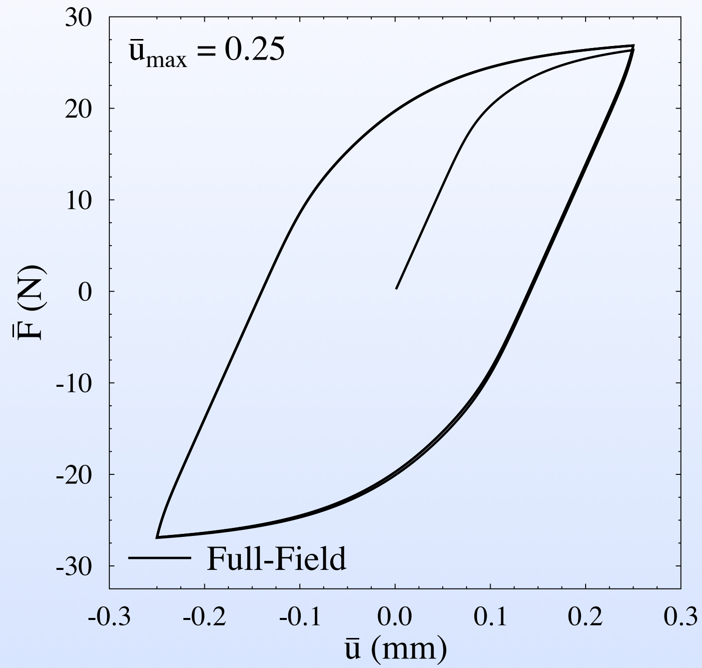
Full-field simulation of the composite structure

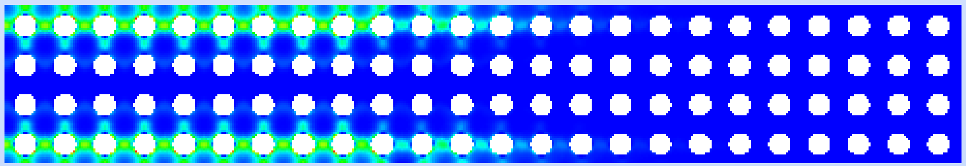




Fine mesh: 26880 elements (6 or 8 nodes)

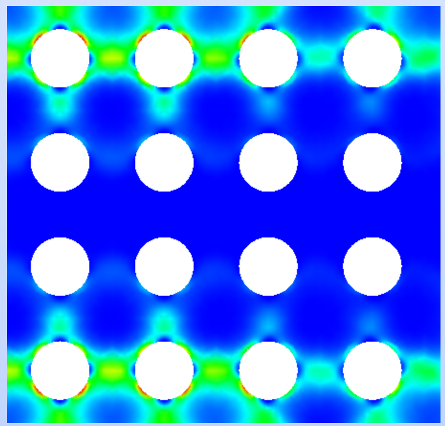
Structural response





Snapshot of the energy dissipated along the stabilized cycle

Local response: hot spots →



Can the global and local responses of the structure be predicted by a homogenization / localization approach? Location of « hot spots » ?

Objectives in brief

(a bit different from more general Reduced-Order-Modelling):

1) reduce COMPUTATIONAL COST (common to all ROM's),

2) Extract CONSTITUTIVE RELATIONS from « big data » (specific to micro mechanics)

3) Generate local fields where and when necessary,

- Define the local fields in the RVE **with only a few variables** describing physical mechanisms: **REDUCED VARIABLES (serve as macroscopic internal variables).**
- Derive **macroscopic constitutive relations for these variables = REDUCED « DYNAMICS » :**
  - preserving **variational structures** whenever possible,
  - accounting for **field statistics** (first and second moments).

⇒ **Two model reductions at the same time:**

- **computational model,**
- **mechanical model.**

2. Model reduction: what is this?

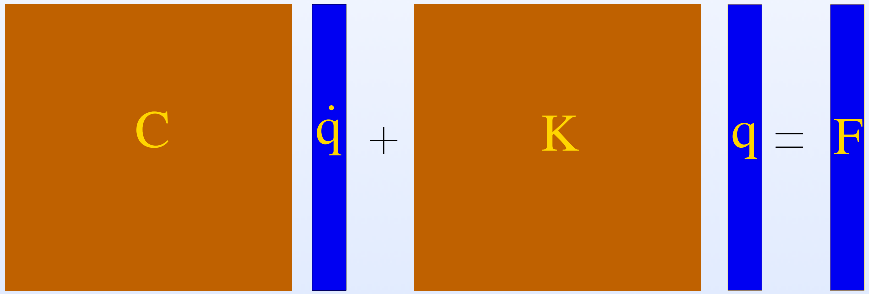
Linear systems

- Given a **large system of ordinary differential equations** (ODEs), typically

$$C(\dot{q}) + K(q) = F,$$

find a low-dimensional approximation.

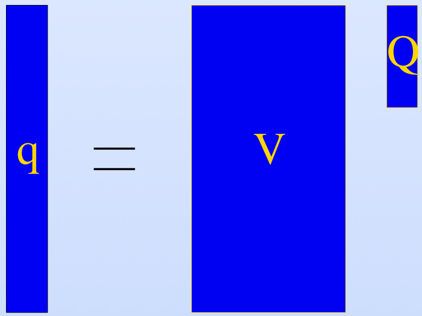
$$C.\dot{q} + K.q = F$$



- Main idea: the high-dimensional state vector *q* actually belongs to a **low-dimensional** subspace

***q* : fine variable, *Q* : coarse variable.**

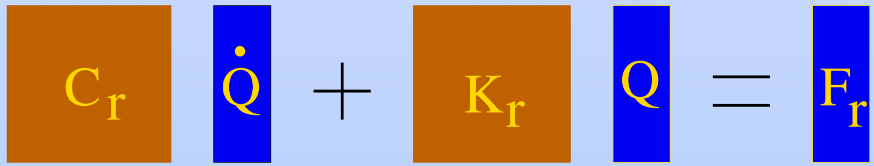
Projection



- **2 questions:**
  - What are the *Q*'s ?
  - How to get the ODE's for *Q*?

$$V^T.C.V.\dot{Q} + V^T.K.V.Q = V^T.F$$

For linear systems, the **ODEs can be projected on the low-dimensional space.**



Non trivial for nonlinear systems

More examples on http ://modelreduction.com !

Familiar procedure: vibrations of linear structures

« Fine » variables (displacement field)

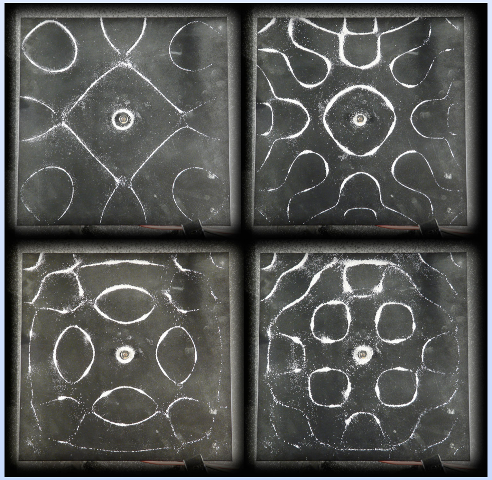
$$\boldsymbol{u}(\boldsymbol{x},t), \ \boldsymbol{x} \in \Omega$$

« Fine » dynamics

$$\boldsymbol{M}\ddot{\boldsymbol{u}}(t) + \boldsymbol{K}\boldsymbol{u}(t) = \boldsymbol{f}(t)$$

« Reduced » variables ξ :

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{k=1}^{M} \xi^{(k)}(t)\boldsymbol{\mu}^{(k)}(\boldsymbol{x})$$



1. Normal modes $\boldsymbol{\mu}^{(k)}$:

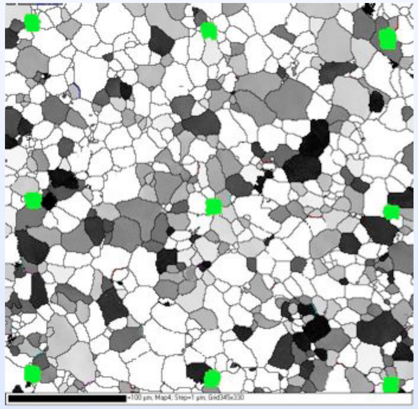
- Physical patterns (experimentally or through modal analysis of the whole structure),
- summation limited to $M \lll \infty$ modes, depending on f(t).

2. « Reduced » dynamics: $m^{(k)}(\ddot{\xi}^{(k)}(t) + \omega_k^2 \xi^{(k)}(t)) = F_k(t), \ k = 1, ..., M$

Finding the reduced dynamics is much more difficult for nonlinear systems!

Composites. Unit-cell problem

What are the « fine » variables and the ODE's?



Given: - the microstructure

- **the constitutive relations** of the phases ($\boldsymbol{\alpha}$ internal variables)
- the **history** $\overline{\varepsilon}(t)$ of macroscopic strain

Determine:

- the **local fields** $\boldsymbol{\sigma}(\boldsymbol{x},t), \boldsymbol{\varepsilon}(\boldsymbol{x},t), \boldsymbol{\alpha}(\boldsymbol{x},t)$
- the **effective response** $\overline{\boldsymbol{\sigma}}(t) = \widetilde{\boldsymbol{\mathcal{F}}}\left(\overline{\varepsilon}(s)|_{0\leq s\leq t}, \text{other variables ?}\right)$

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon},\boldsymbol{\alpha}), \quad \frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon},\boldsymbol{\alpha}) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) = 0, \quad \text{Constitutive relations}$$

$$\boldsymbol{\varepsilon} = \tfrac{1}{2}\left(\boldsymbol{\nabla u} + {}^{\mathsf{T}}\boldsymbol{\nabla u}\right) \quad \text{Compatibility}$$

$$\text{div}\,(\boldsymbol{\sigma}) = 0 \quad \text{Equilibrium}$$

$$\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}(t) \quad \text{Loading}$$

$$\boldsymbol{u}^* = \boldsymbol{u} - \overline{\varepsilon}.\boldsymbol{x} \text{ periodic, } \boldsymbol{\sigma}.\boldsymbol{n} \text{ anti-periodic} \quad \text{Boundary conditions}$$

Variational structure

It can be shown that the effective behavior derives RIGOUSLY from **2 effective potentials (PS 1982, 1985):**

$$\overline{\boldsymbol{\sigma}} = \frac{\partial \widetilde{w}}{\partial \overline{\boldsymbol{\varepsilon}}}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha}), \quad \frac{\partial \widetilde{w}}{\partial \boldsymbol{\alpha}}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha}) + \frac{\partial \widetilde{\varphi}}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) = 0,$$

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\alpha}) = \underset{\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}}{\text{Inf}} \langle w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) \rangle, \quad \widetilde{\varphi}(\dot{\boldsymbol{\alpha}}) = \langle \varphi(\dot{\boldsymbol{\alpha}}) \rangle .$$

Looks great:

- preserves the structure with 2 potentials,

- has a variational structure (similar to 1-potential nonlinear homogenization).

BUT IT IS NOT! $\boldsymbol{\alpha} = \left(\boldsymbol{\alpha}(\boldsymbol{x})|_{\boldsymbol{x} \in V}\right)$ is a **FIELD!**

In order to determine $\overline{\boldsymbol{\sigma}}$, one needs to determine the whole field of microscopic internal variables.

Can it be reduced to a finite number of variables ξ ?

What are the evolution equations for these variables? Preserve the structure with two potentials. (similar idea in Marsden & al, 2003)

« Fine » variables: 1. Fix the field $\boldsymbol{\alpha}(\boldsymbol{x})$ and solve for $\boldsymbol{\varepsilon}(\boldsymbol{x})$

$$\boldsymbol{\sigma} = \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\alpha}),\ \boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla \boldsymbol{u} + {}^{\mathsf{T}}\nabla \boldsymbol{u}\right),\ \operatorname{div}(\boldsymbol{\sigma}) = 0,\ \langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}} + \text{Boundary conditions}$$

$$\left(\operatorname{div}(\boldsymbol{L} : \nabla \boldsymbol{u}) = \operatorname{div}(\boldsymbol{L} : \boldsymbol{\alpha}),\ \langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}} + \text{Boundary conditions} \right)$$

$$\boldsymbol{\varepsilon}(\boldsymbol{x}, t) = \boldsymbol{A}(\boldsymbol{x}) : \overline{\boldsymbol{\varepsilon}}(t) + (\boldsymbol{D} * \boldsymbol{\alpha})(\boldsymbol{x}),\ \boldsymbol{D} \text{ nonlocal Green operator}$$

2. Solve the systems of differential equations

$$\frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{x}), \boldsymbol{\alpha}(\boldsymbol{x})) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}(\boldsymbol{x})) = 0, \quad \forall \boldsymbol{x} \in V.$$

ODE's to be reduced!

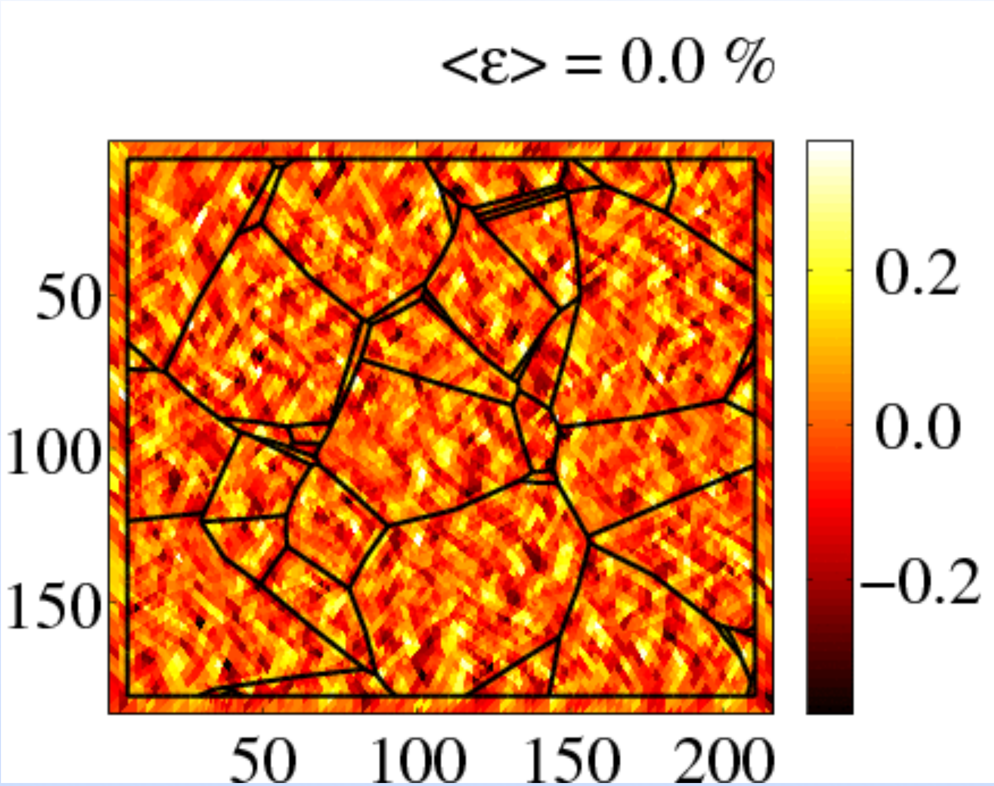
Fine variables: $\boldsymbol{\alpha}(\boldsymbol{x}),\ \boldsymbol{x} \in V.$

Note that the loading depends only on the 6 independent components of $\overline{\boldsymbol{\varepsilon}}$

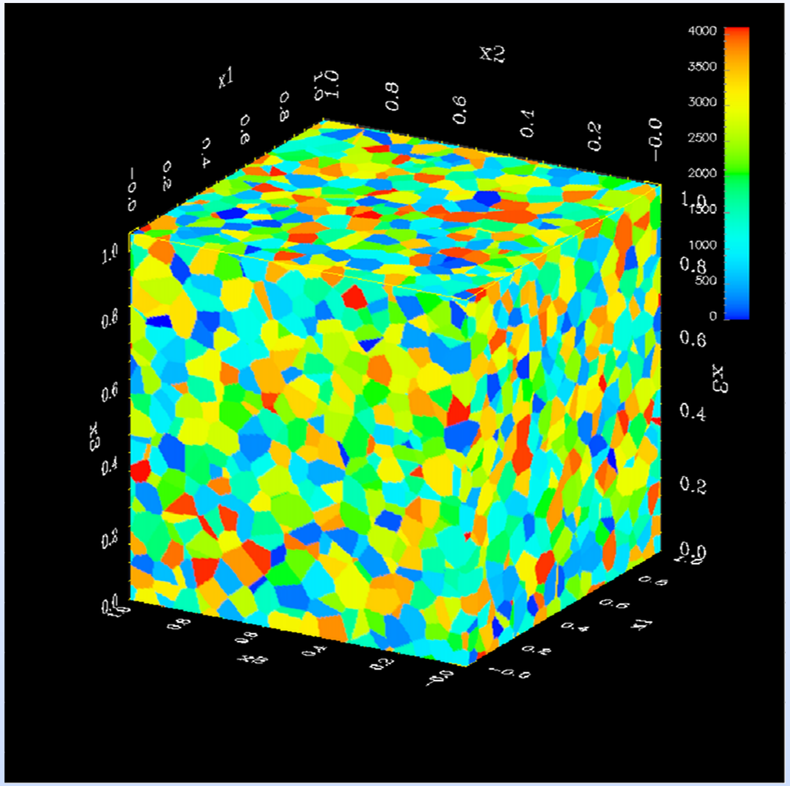
One can expect the fine variables to live in a finite-dimensional space!

3. Reduced variables (reduced basis)

Experiments © A. Guéry (LMT&EdF)



Full-field simulations by FFT (LMA)



- Limited number of features of the deformation field appearing gradually,
- The patterns remain stable with an increasing amplitude

$$\boldsymbol{\alpha}(\boldsymbol{x},t) = \sum_{k=1}^{M} \xi^{(k)}(t)\ \boldsymbol{\mu}^{(k)}(\boldsymbol{x}).$$

Reduced variables

1st approximation: finite number of internal variables: achieved by a decomposition on a finite set of « shape » functions

$$\boldsymbol{\alpha}(\boldsymbol{x},t) = \sum_{k=1}^{M} \xi^{(k)}(t)\ \boldsymbol{\mu}^{(k)}(\boldsymbol{x}).$$

- $\boldsymbol{\xi} = (\xi^{(k)})|_{k=1}^{M}$: **reduced variables (macroscopic internal variables).**
- The $\boldsymbol{\mu}^{(k)}$'s are the **plastic modes.**

- **Transformation Field Analysis (TFA)**: the $\boldsymbol{\mu}^{(k)}$ are uniform within each phase or subdomain (very stiff…) Dvorak 1992.

- **Nonuniform TFA (NTFA)**: the $\boldsymbol{\mu}^{(k)}$ are NON-uniform within each phase. Galvanetto, Michel &PS (2000), Michel &PS, 2003, 2004, Fritzen & Böhlke (2010)

- Unlike the usual decomposition in ROM (reduced order modelling), **decomposition of the field of internal variables**, not of the displacement field.

- A systematic procedure to determine the modes is the P.O.D. (proper orthogonal decomposition, although known as Karhunen-Loève decomposition, PCA….)

Mode selection by snapshot POD (or any other mean)

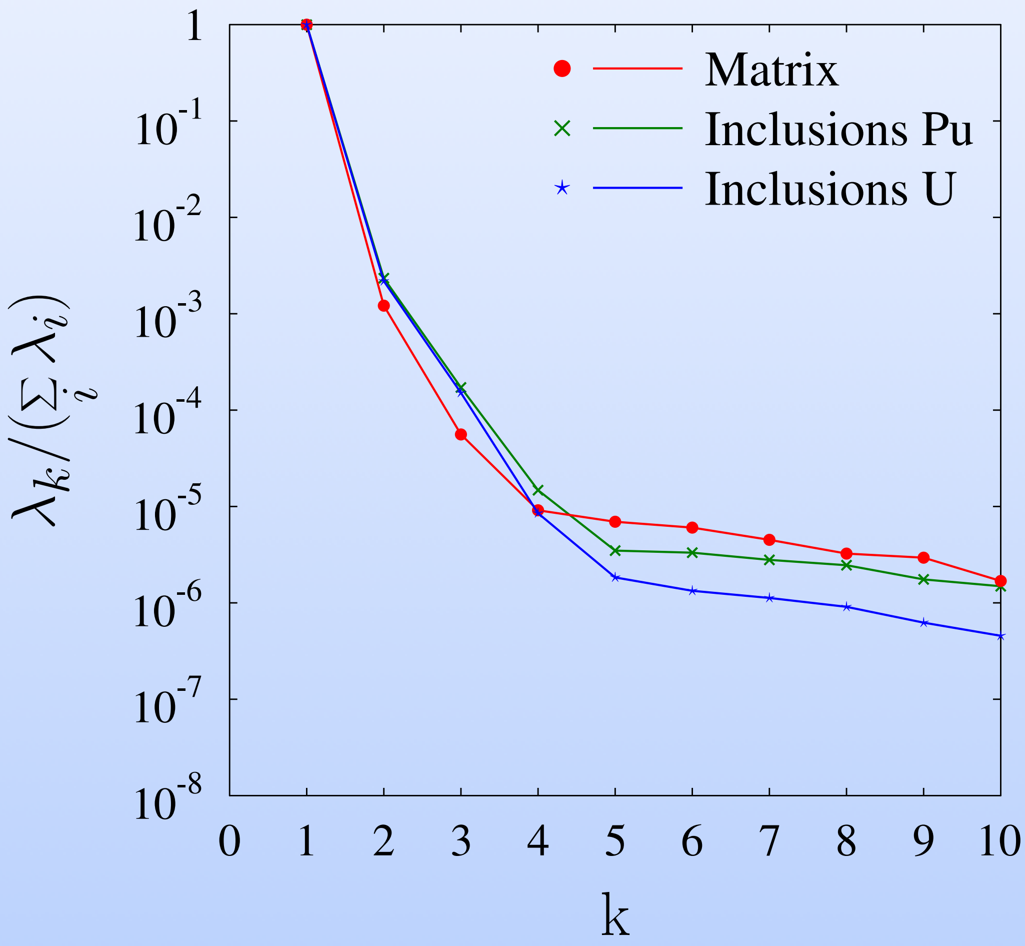
1. **Using full-field simulations**, generate snapshots $\boldsymbol{\theta}^{(i)}$ of the fields of internal variables along appropriately chosen **training** paths.
2. **Form and diagonalize the correlation matrix:**

$$g_{ij} = \left\langle \boldsymbol{\theta}^{(i)} : \boldsymbol{\theta}^{(j)} \right\rangle,$$

$$\sum_{j=1}^{M} g_{ij} v_j^{(k)} = \lambda_k v_i^{(k)}$$

The higher λ_k, the better the correlation of $\boldsymbol{v}^{(k)}$ with the snapshots

3. $$\boldsymbol{\mu}^{(k)}(\boldsymbol{x}) = \sum_{k=1}^{M_T} v_\ell^{(k)} \boldsymbol{\theta}^{(\ell)}(\boldsymbol{x}).$$

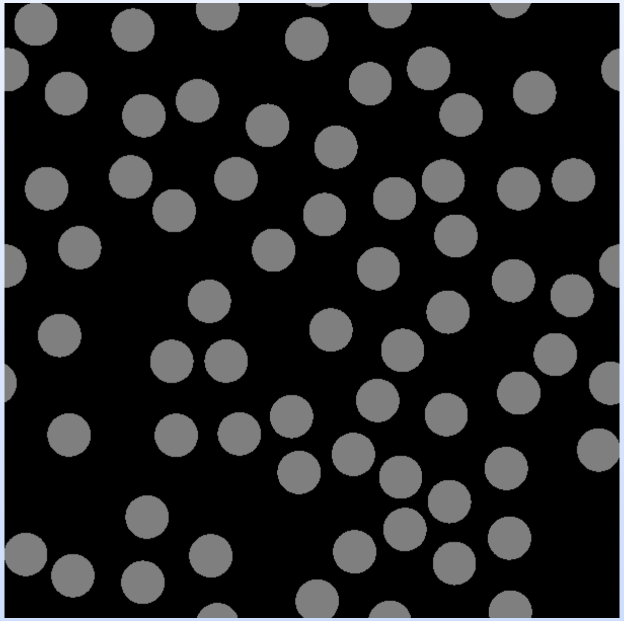


Number of modes $\Leftrightarrow$ information contained in the modes

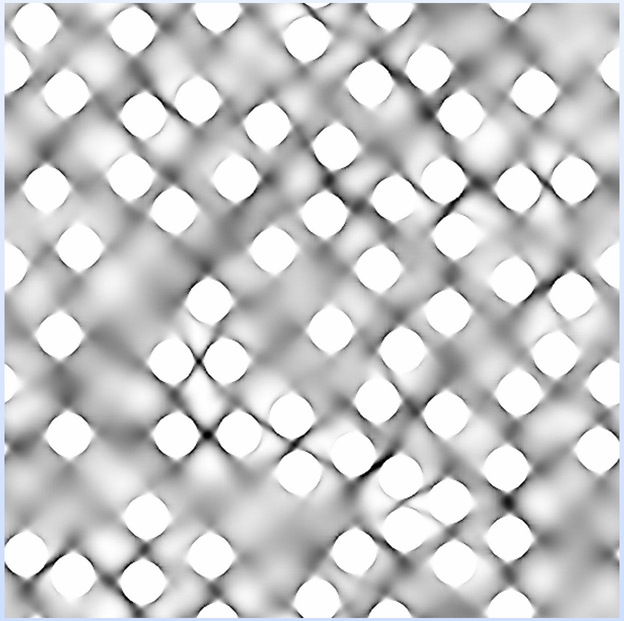
What do these modes look like?

Elastic fibers. Elasto-plastic matrix with isotropic hardening.

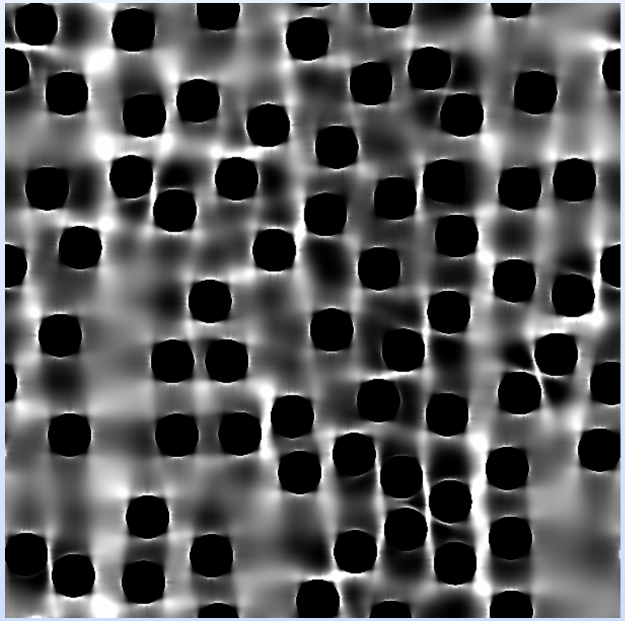
Fiber volume fraction : 0.25.



VER (64 fibers)



$\mu_{22}^{(1)}$



$\mu_{12}^{(2)}$

NTFA : 2 modes $\boldsymbol{\mu}^{(k)}$ generated from the plastic strain field along two loading paths

$$\overline{\boldsymbol{\sigma}} = \overline{\sigma}(t)\boldsymbol{\Sigma}^{(k)}, \quad \boldsymbol{\Sigma}^{(1)} = \text{simple tension}, \quad \boldsymbol{\Sigma}^{(2)} = \text{pure shear}, \quad \overline{\varepsilon}_t : \boldsymbol{\Sigma}^{(k)} = 5\%.$$

4. Reduced « Dynamics » (structure-preserving…)

Initial version in Michel & PS (IJSS 2003)

- improved in the hybrid model of Fritzen & Leuschner (IJSS 2013) using variational techniques.
- improved by Michel & PS (JMPS 2016, Comput. Mech 2016) using nonlinear homogenization techniques.

For simplicity: **elasto-(visco)plastic constituents** $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}^{\mathrm{p}}$

w **is quadratic**

$$w^{(r)}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{p}}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}) : \boldsymbol{L}^{(r)} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\mathrm{p}}) \quad \text{in phase } r,$$

Effective constitutive relations derived from 2 effective potentials:

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\varepsilon}^{\mathrm{vp}}|_{\boldsymbol{x}\in V}) = \operatorname*{Inf}_{\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}} \langle w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{vp}}) \rangle, \quad \widetilde{\varphi}(\dot{\boldsymbol{\varepsilon}}^{\mathrm{vp}}|_{\boldsymbol{x}\in V}) = \left\langle \varphi(\dot{\boldsymbol{\varepsilon}}^{\mathrm{vp}}) \right\rangle$$

Using the NTFA decomposition

$$\boldsymbol{\varepsilon}^{\mathrm{p}}(\boldsymbol{x}, t) = \sum_{k=1}^{M} \xi^{(k)}(t) \boldsymbol{\mu}^{(k)}(\boldsymbol{x}),$$

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\xi}) = \operatorname*{Inf}_{\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}} \langle w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{p}}) \rangle, \quad \widetilde{\varphi}(\dot{\boldsymbol{\xi}}) = \left\langle \varphi(\dot{\boldsymbol{\varepsilon}}^{\mathrm{p}}) \right\rangle.$$

$(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\xi})$ **macroscopic state variables**

1st potential is easy

$$\widetilde{w}(\overline{\varepsilon}, \boldsymbol{\xi}) = \underset{\langle \varepsilon \rangle = \overline{\varepsilon}}{\text{Inf}} \langle w(\varepsilon, \varepsilon^{\text{p}}) \rangle, \quad \varepsilon^{\text{p}}(\boldsymbol{x}, t) = \sum_{k=1}^{M} \xi^{(k)}(t)\, \boldsymbol{\mu}^{(k)}(\boldsymbol{x}).$$

$\boldsymbol{\sigma} = \boldsymbol{L} : (\varepsilon - \varepsilon^{\text{p}}), \quad \text{div}\,(\boldsymbol{\sigma}) = 0,$ Boundary conditions,

$$\varepsilon(\boldsymbol{x}, t) = \boldsymbol{A}(\boldsymbol{x}) : \overline{\varepsilon}(t) + \sum_{k=1}^{M} \xi^{(k)}(t) \boldsymbol{D} * \boldsymbol{\mu}^{(k)}(\boldsymbol{x})$$

$$\boldsymbol{\sigma}(\boldsymbol{x}, t) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{A}(\boldsymbol{x}) : \overline{\varepsilon}(t) + \sum_{k=1} \xi^{(k)}(t) \boldsymbol{\rho}^{(k)}(\boldsymbol{x}),$$

$$\widetilde{w}(\overline{\varepsilon}, \boldsymbol{\xi}) = \frac{1}{2} \overline{\varepsilon} : \widetilde{\boldsymbol{L}} : \overline{\varepsilon} - \overline{\varepsilon} : \sum_{k=1}^{M} \boldsymbol{a}^{(k)} \xi^{(k)} + \frac{1}{2} \sum_{k,\ell=1}^{M} \mathcal{L}^{(k\ell)} \xi^{(k)} \xi^{(\ell)},$$

↓ **Pre-computed by solving elastic problems**

- $\boldsymbol{A}(\boldsymbol{x})$ **elastic strain localization tensor,** $\boldsymbol{D}$ **Green operator,**
- $\boldsymbol{D} * \boldsymbol{\mu}^{(k)}(\boldsymbol{x})$ **strain field induced elastically by** $\boldsymbol{\mu}^{(k)}$

Derivation $\Rightarrow$

$$\overline{\boldsymbol{\sigma}}(t) = \frac{\partial \widetilde{w}}{\partial \overline{\varepsilon}}(\overline{\varepsilon}, \boldsymbol{\xi}) = \widetilde{\boldsymbol{L}} : \overline{\varepsilon}(t) - \sum_{k=1}^{M} \boldsymbol{a}^{(k)} \xi^{(k)}(t).$$

2nd potential is difficult

1. **Computing** $\widetilde{\varphi}(\dot{\boldsymbol{\xi}}) = \left\langle \varphi\left(\sum_{k=1}^{M} \dot{\xi}^{(k)}(t)\boldsymbol{\mu}^{(k)}(\boldsymbol{x})\right)\right\rangle$ **is expensive:**

- store the modes (memory)
- **compute the local plastic strain-rate at each local point** $\boldsymbol{x}$
- average.

2. **Doubly nonlinear differential equation**

$$\frac{\partial \widetilde{w}}{\partial \boldsymbol{\xi}}(\overline{\varepsilon}, \boldsymbol{\xi}) + \frac{\partial \widetilde{\varphi}}{\partial \dot{\boldsymbol{\xi}}}(\dot{\boldsymbol{\xi}}) = 0.$$

alternatively

$$\mathfrak{a} = -\frac{\partial \widetilde{w}}{\partial \boldsymbol{\xi}}(\overline{\varepsilon}, \boldsymbol{\xi}), \quad \dot{\boldsymbol{\xi}} = \frac{\partial \widetilde{\varphi}^*}{\partial \mathfrak{a}}(\mathfrak{a}).$$

Hybrid model of Fritzen & Leuschner (2013): approximate the dual potential $\widetilde{\varphi}^*(\mathfrak{a})$:

$$\widetilde{\varphi}^*(\mathfrak{a}) \simeq \langle \varphi^*(\boldsymbol{\sigma}(\overline{\varepsilon}, \boldsymbol{\xi}))\rangle, \text{ where } \quad \boldsymbol{\sigma}(\boldsymbol{x}, \overline{\varepsilon}, \boldsymbol{\xi}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{A}(\boldsymbol{x}) : \overline{\varepsilon}(t) + \sum_{k=1} \xi^{(k)}(t)\boldsymbol{\rho}^{(k)}(\boldsymbol{x}),$$

Nice feature: the approximation is reasonably accurate. **But**

1) still the cost of computing $\langle \varphi^*(\boldsymbol{\sigma}(\overline{\varepsilon}, \boldsymbol{\xi}))\rangle$, **remains very high.**

2) Does not provide an explicit macroscopic constitutive relation.

Dramatic acceleration: NL homogenization

Choose your favorite homogenization scheme

Option 1

closely related to the Tangent Second-Order Method (Ponte Castañeda, JMPS, 1996, 2002).

$$\langle \psi(\boldsymbol{\sigma}(\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\xi})) \rangle \simeq \sum_{r=1}^{P} c^{(r)} \left(\psi^{(r)}(\overline{\boldsymbol{\sigma}}^{(r)}) + \frac{1}{2} \frac{\partial^2 \psi^{(r)}}{\partial \boldsymbol{\sigma}^2}(\overline{\boldsymbol{\sigma}}^{(r)}) : \boldsymbol{C}^{(r)}(\boldsymbol{\sigma}) \right), \quad (\psi = \varphi^*)$$

where $\overline{\boldsymbol{\sigma}}^{(r)}, \ \boldsymbol{C}^{(r)}(\boldsymbol{\sigma})$ can be expressed in terms of $\overline{\boldsymbol{\varepsilon}}, \boldsymbol{\xi}$ and **pre-computed quantities** $\overline{\boldsymbol{\rho}}^{(k,r)}, \ \boldsymbol{C}^{(r)}(\boldsymbol{\rho}^{(k)})$.

Advantage: Really fast, Exact to second-order

BUT: limitations of the TSO (very poor for porous materials), requires a tangent operator

Option 2 (for polycrystals only)

$$\psi(\boldsymbol{x}, \boldsymbol{\sigma}) = \sum_{r=1}^{P} \chi^{(r)}(\boldsymbol{x}) \sum_{s=1}^{S} \psi_s^{(r)}(\tau_s^{(r)}), \quad \tau_s^{(r)} = \boldsymbol{\sigma} : \boldsymbol{m}_s^{(r)}$$

closely related to the Fully Optimized Method, Ponte Castañeda, PRS 2015,

$$\langle \psi(\boldsymbol{\sigma}(\overline{\varepsilon}, \boldsymbol{\xi})) \rangle \simeq \sum_{r=1}^{P} c^{(r)} \sum_{s=1}^{S} \frac{1}{2} \left(\psi_s^{(r)}(\hat{\tau}_s^{(r)}) + \psi_s^{(r)}(\check{\tau}_s^{(r)}) \right),$$

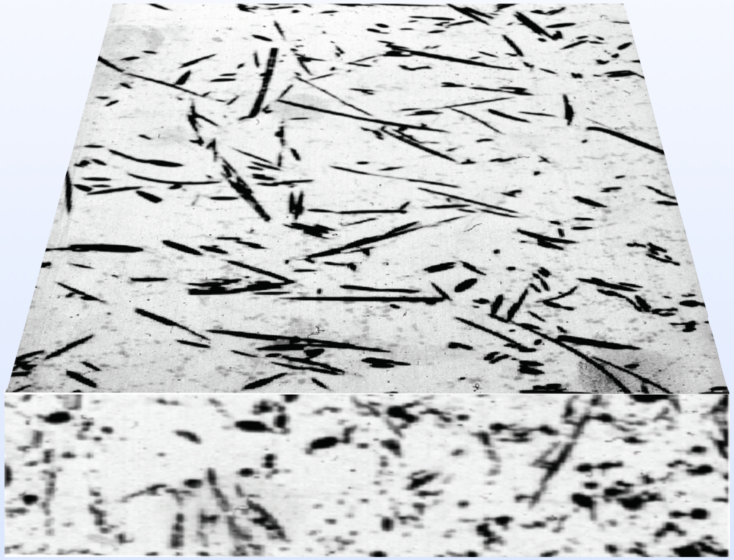
$$\hat{\tau}_s^{(r)} = \overline{\tau}_s^{(r)} + \sqrt{C^{(r)}(\tau_s^{(r)})}, \quad \check{\tau}_s^{(r)} = \overline{\tau}_s^{(r)} - \sqrt{C^{(r)}(\tau_s^{(r)})},$$

$$\overline{\tau}_s^{(r)} = \langle \tau_s \rangle^{(r)}, \quad C^{(r)}(\tau_s^{(r)}) = \left\langle (\tau_s - \overline{\tau}_s^{(r)})^2 \right\rangle^{(r)}$$

where $\overline{\tau}_s^{(r)}$, $C^{(r)}(\tau_s^{(r)})$ can be expressed in terms of $\overline{\varepsilon}, \boldsymbol{\xi}$ and **pre-computed quantities** $\overline{\boldsymbol{\rho}}^{(k,r)}$, $\boldsymbol{C}^{(r)}(\boldsymbol{\rho}^{(k)})$.

Advantage: Really fast, does not require a tangent operator, works for porous materials

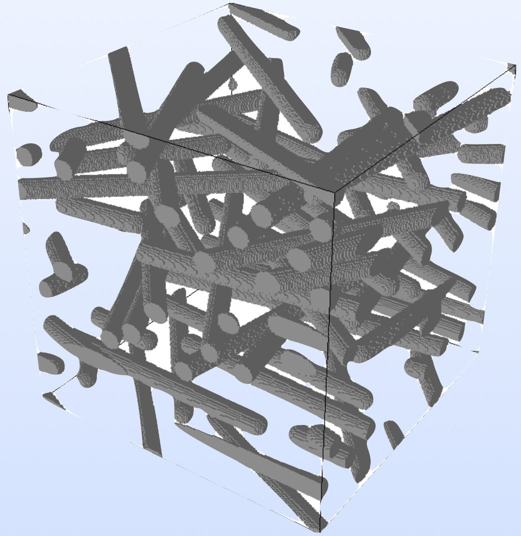
Examples. 1. Metal-matrix composites (short-fiber)



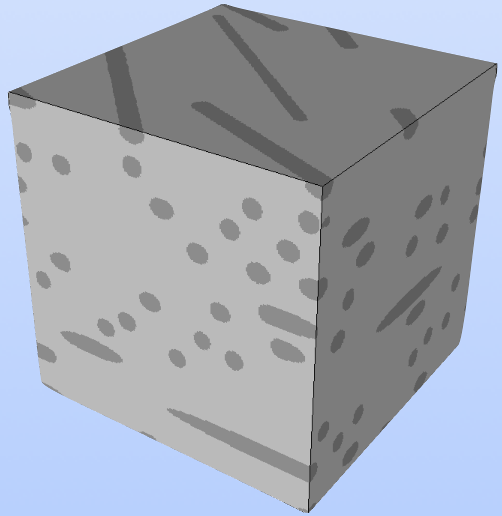
- Al matrix (**viscous at 300°C**)
- Al2O3 fibers (elastic)
- Fibers parallel to the (x,y) plane with **random orientation**
- Aspect ratio$\simeq$15; Vol. frac. = 10%
- Matrix identification with **nonlinear** kinematic hardening.
- no residual stress accounted for (hence the error in compression)

Full-field simulations (FFT)

Fibers alone



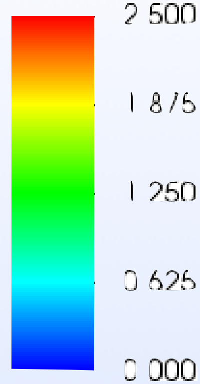
Matrix + Fibers

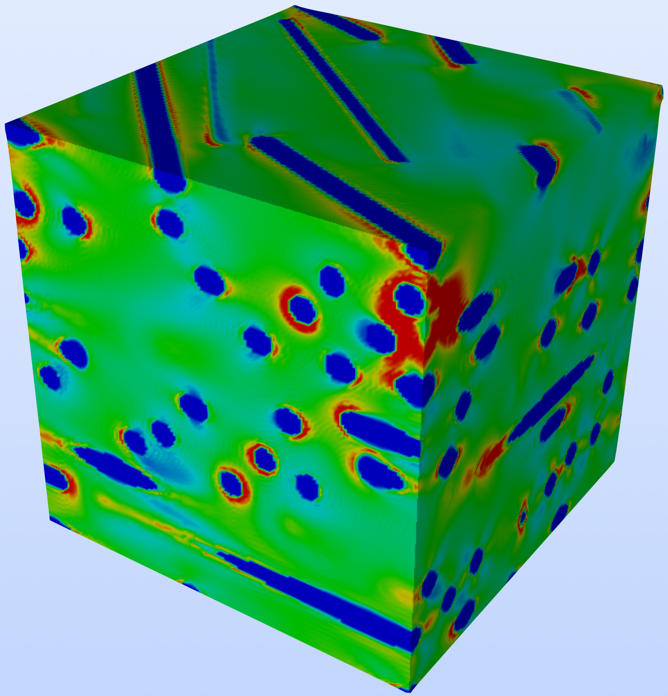


NTFA Modes

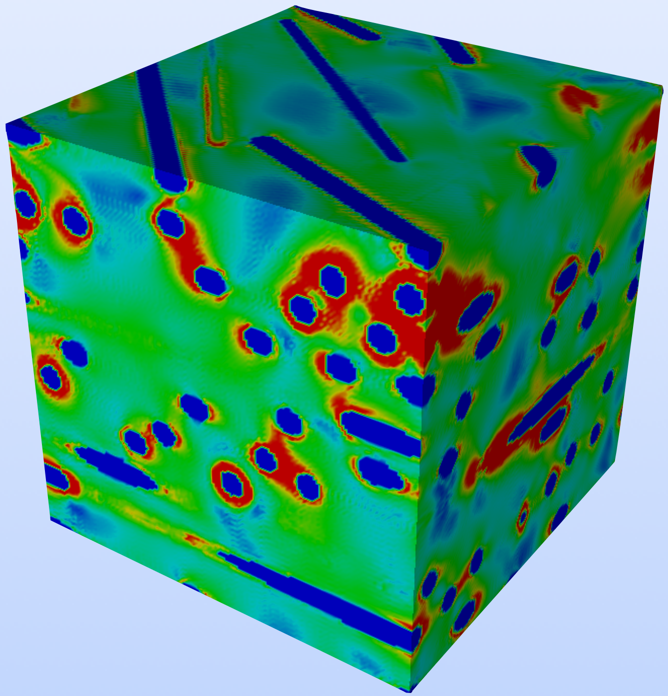
- 100 snapshots generated from the FF simulations
- POD : modes with 99.99% « information »
- $\longrightarrow$ 5 modes for NLKH

μ_{eq}

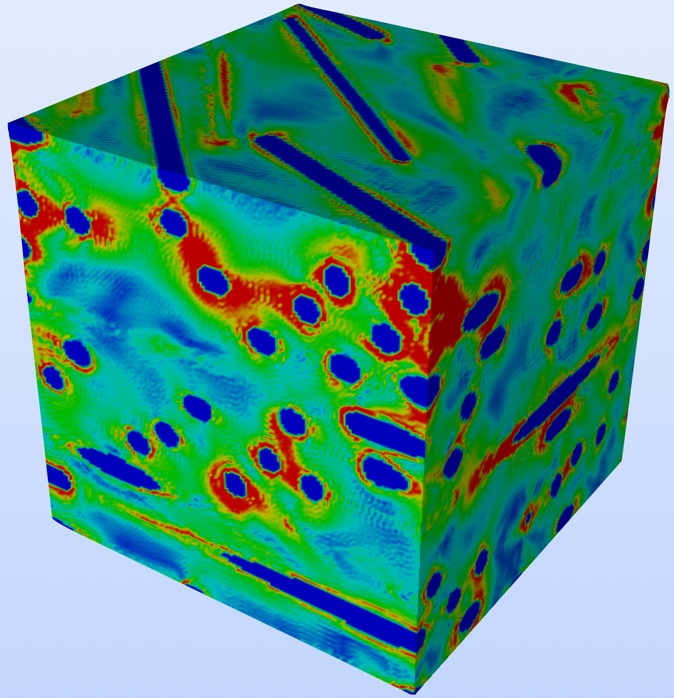




Mode 1 (NL)



Mode 2 (NL)

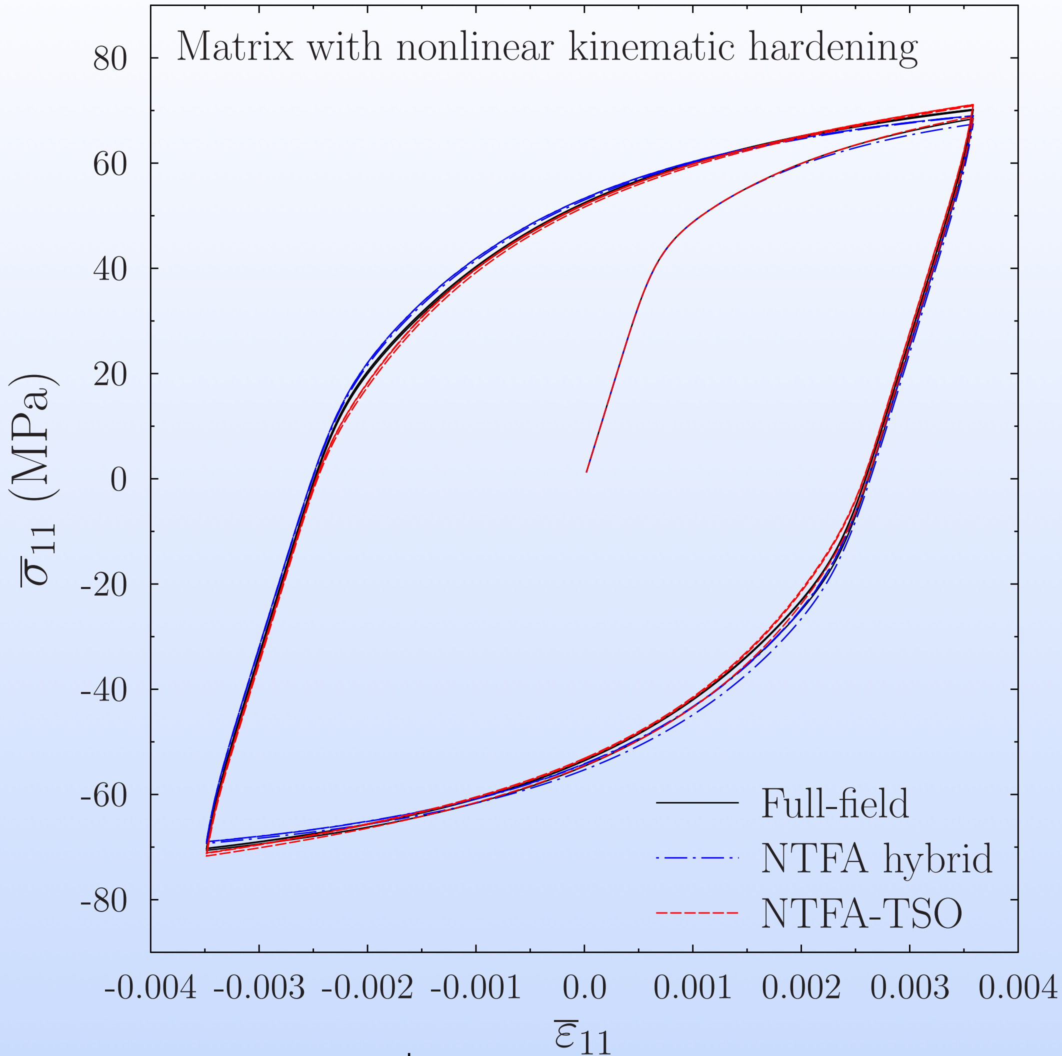


Mode 3 (NL)

Overall response:

Full-Field versus NTFA.

NTFA: Integration of the effective constitutive relations at a **single material point**

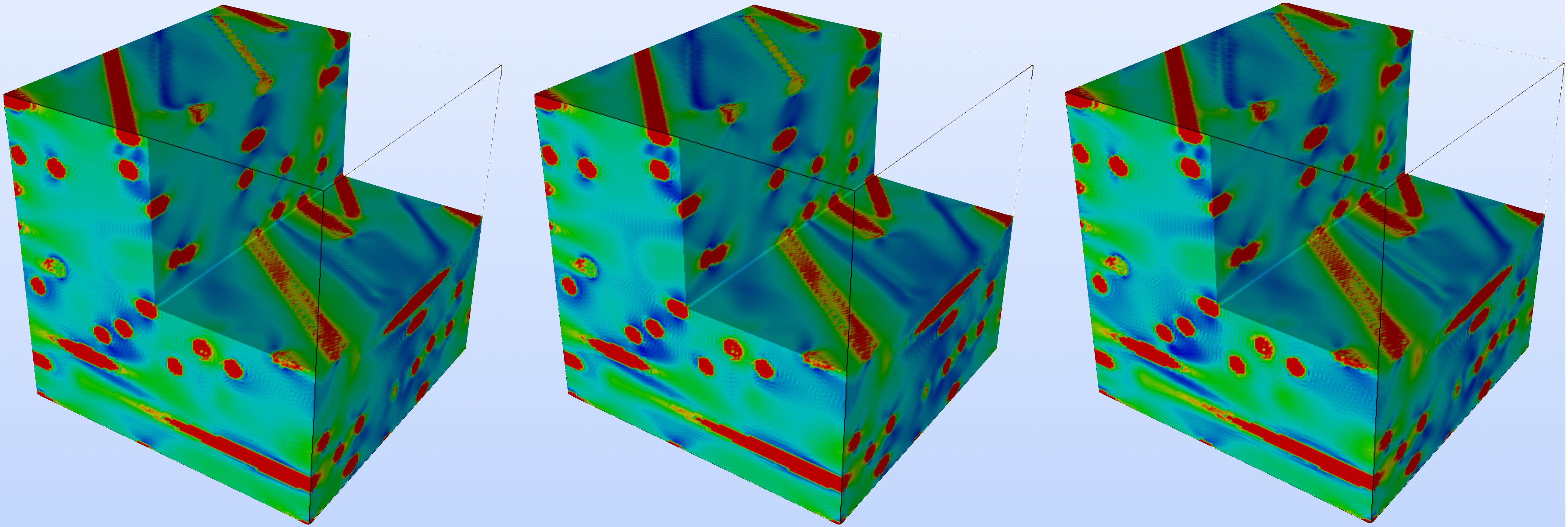


Full-field (FFT) Reference	NTFA hybrid (CPU ratio= FFT/ hybrid)	NTFA-TSO (CPU ratio= FFT/TSO)
189 800 s.	72 159 s.	15.96 s.
$\geq$ 2 days	**(CPU ratio = 2.63)**	**(CPU ratio = 11 892)**

Spectacular speed-up due to the NL homogenization approximation!

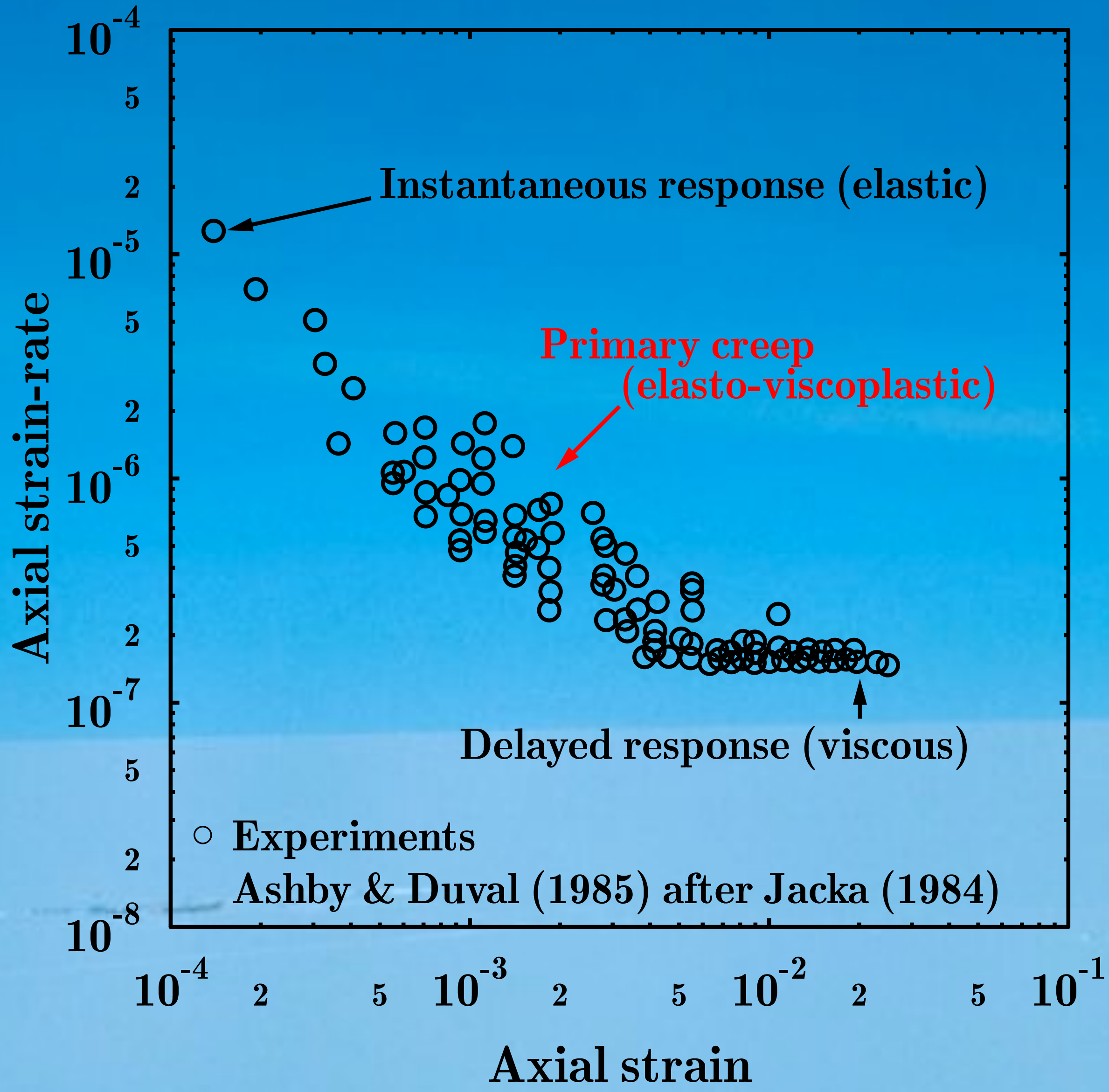
Reconstruction of the local (stress) field

$$(\overline{\varepsilon}(t), \boldsymbol{\xi}(t)) \text{ known } \Rightarrow \boldsymbol{\sigma}(\boldsymbol{x}, t) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{A}(\boldsymbol{x}) : \overline{\varepsilon}(t) + \sum_{k=1}^{M} \xi^{(k)}(t) \boldsymbol{\rho}^{(k)}(\boldsymbol{x}).$$

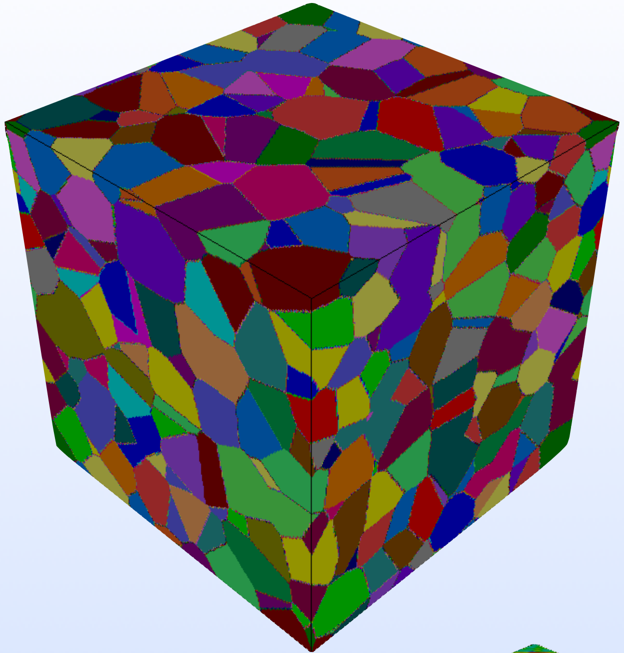


Full-field (reference) NTFA-hybrid NTFA-TSO

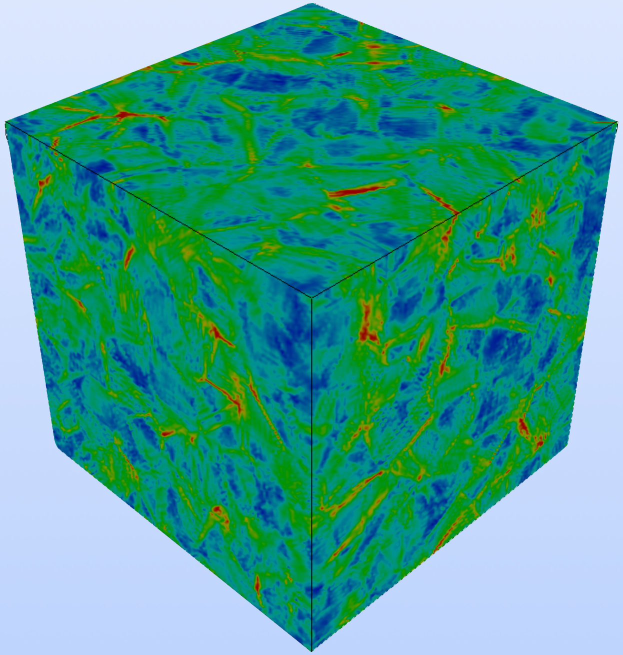
2. Creep of polycrystalline ice



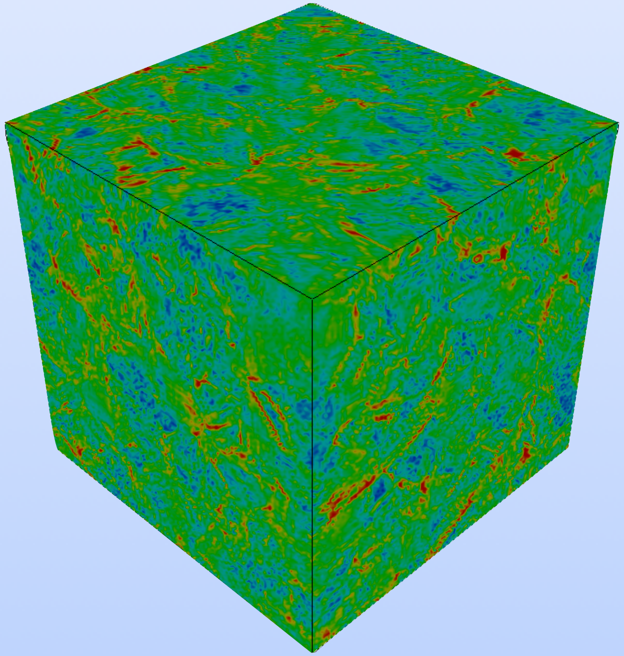
1) Run full-field simulations with 1st guess of parameters.
2) Extract modes by P.O.D.
3) Use the ROM to calibrate material parameters.
4) Fine tune with Full-field sim.



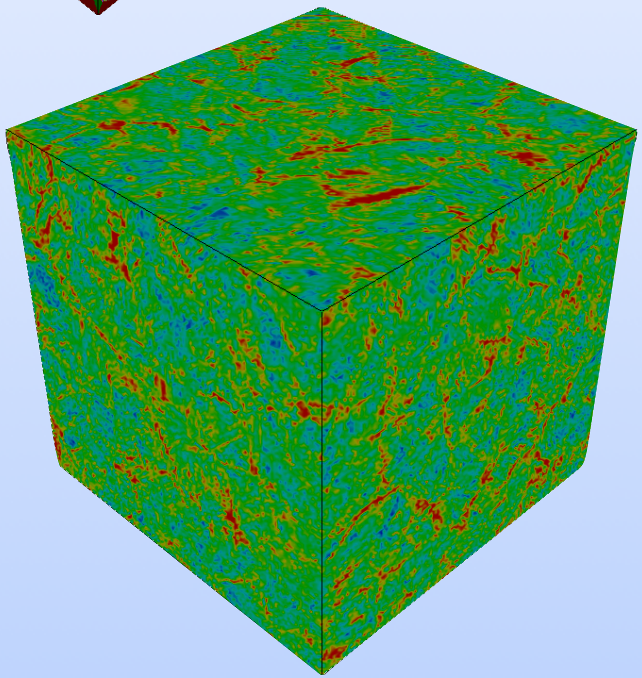
500 grains



Mode 1

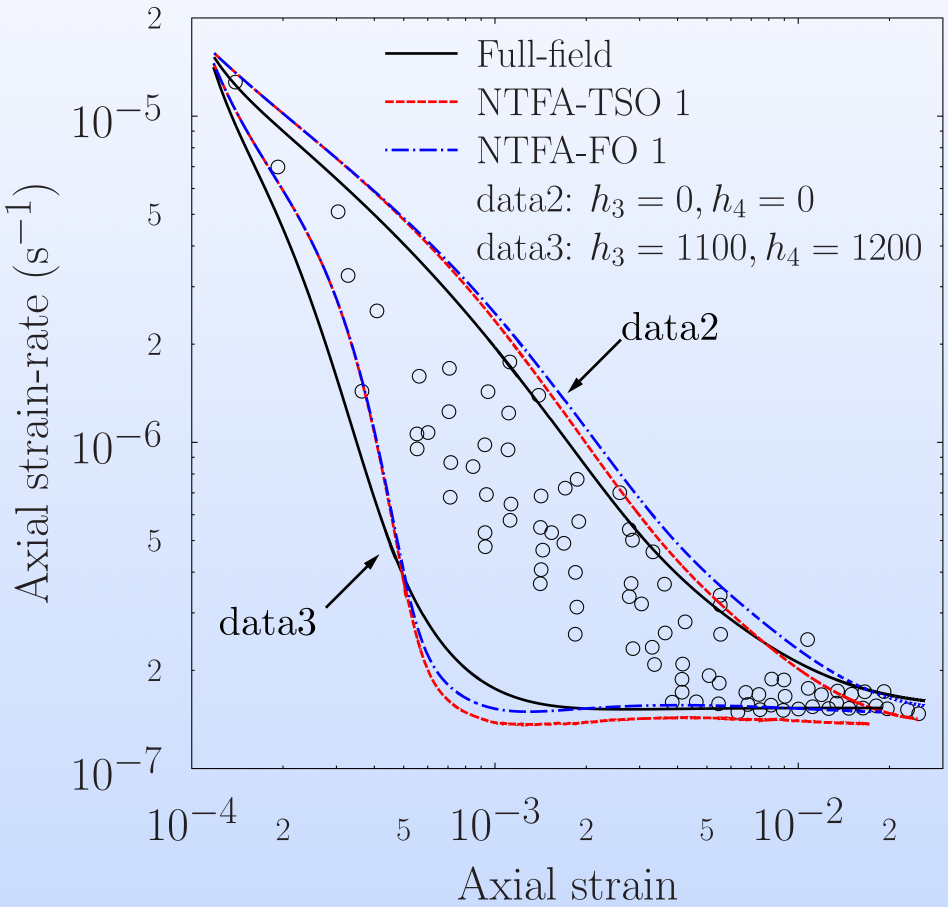


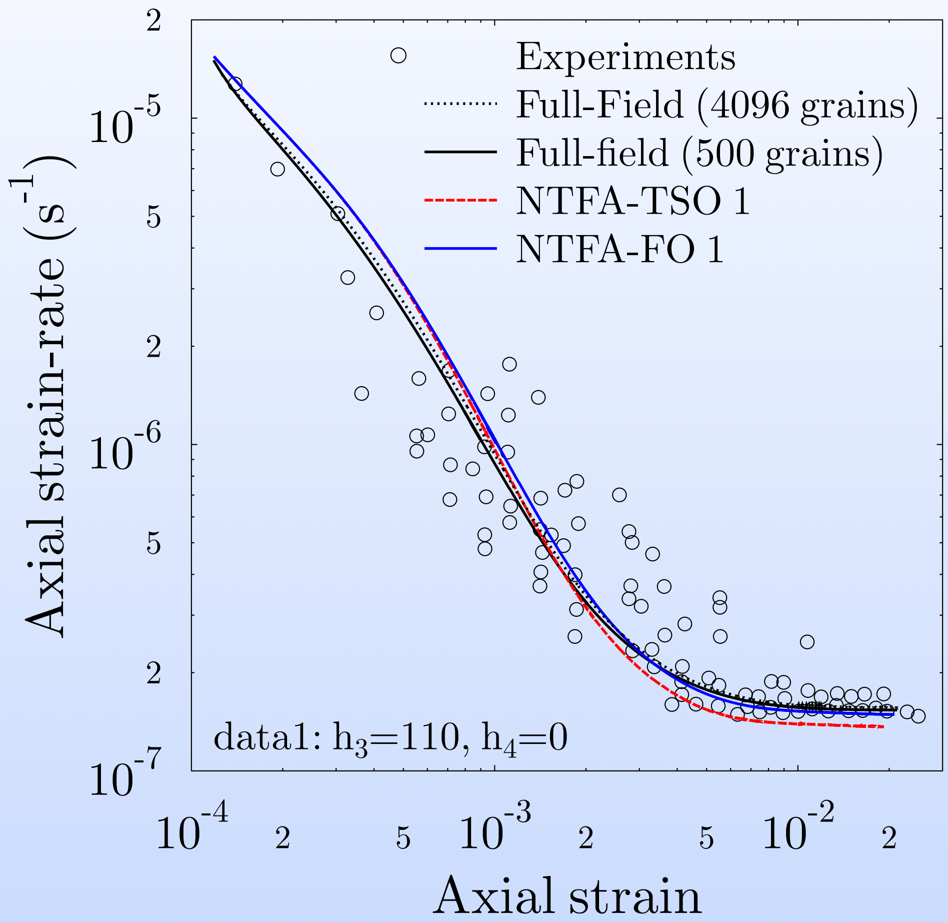
Mode 2



Mode 3

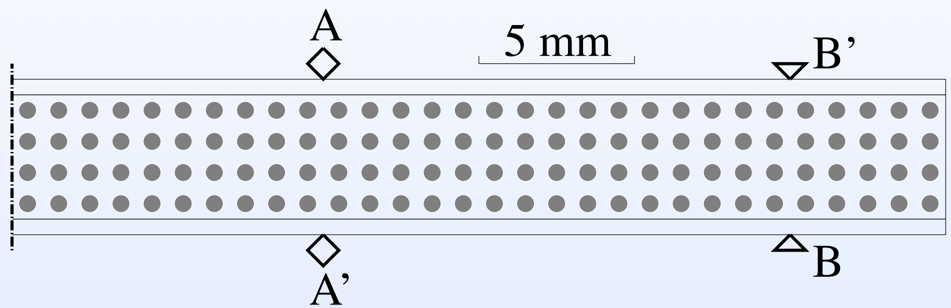
Calibration: latent hardening prismatic/pyramidal

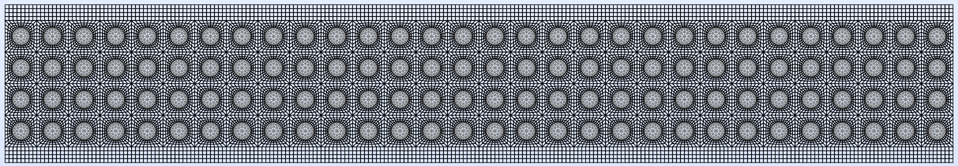




	Full-field (FFT)	NTFA-TSO	NTFA-FO
CPU Intel Xeon X5687 @ 3.6 GHz	261 499 s. **3 days**	614 s. **10 min** **Acceleration $\simeq$ 400**	540 s. **less than 10 min** **Acceleration $\simeq$ 500**

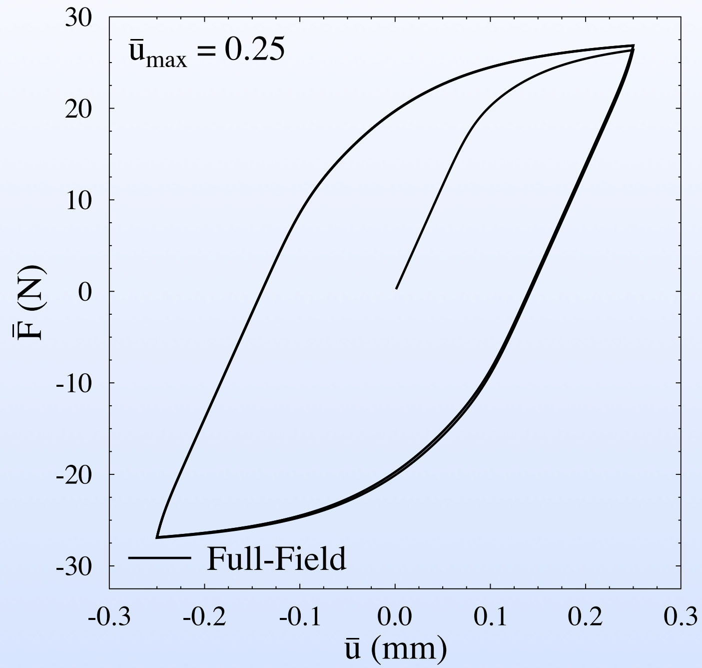
EX3: Structural problem, composite structure

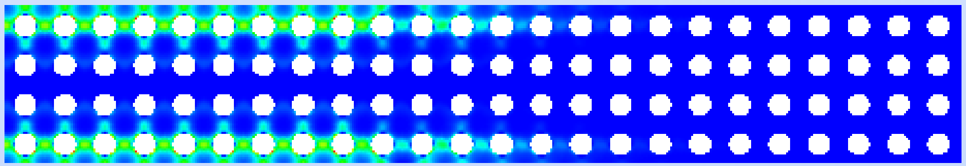




Fine mesh: 26880 elements (6 or 8 nodes)

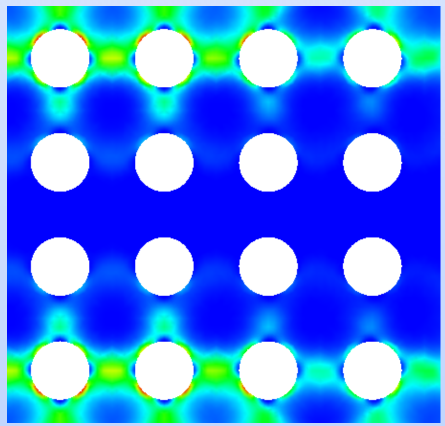
Structural response



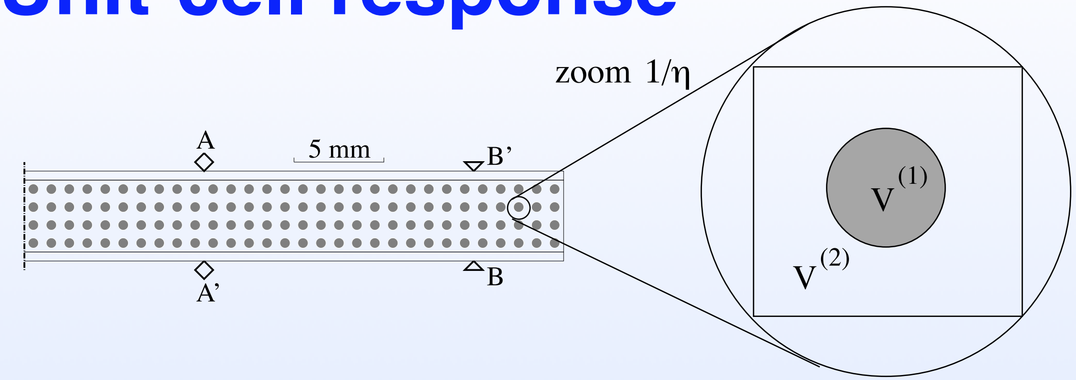


Snapshot of the energy dissipated along the stabilized cycle

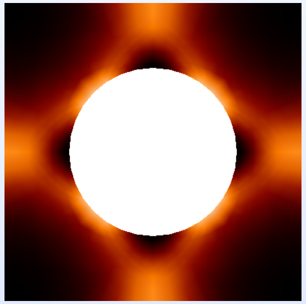
Local response: hot spots →

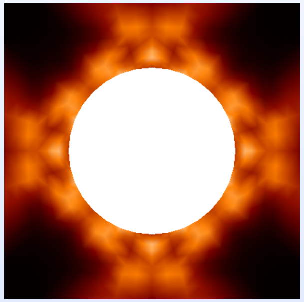


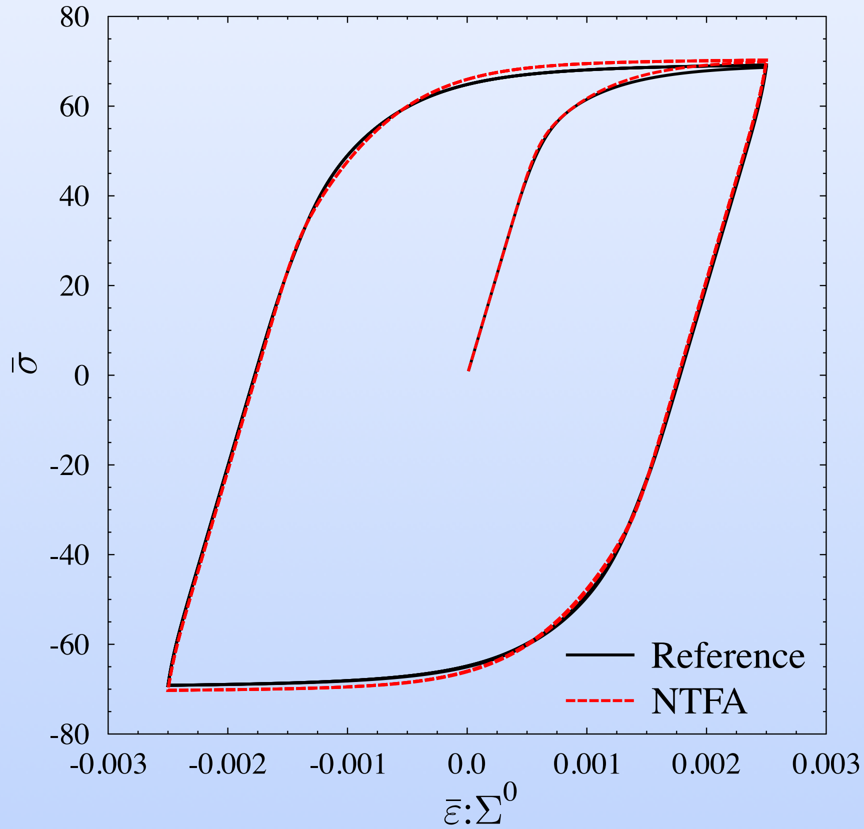
Unit-cell response

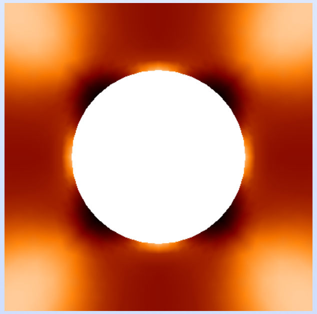


Determination of modes with 99.99% of the information:



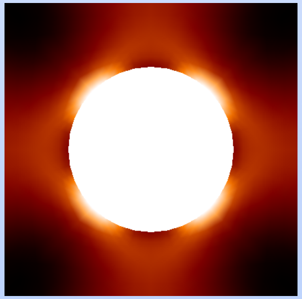


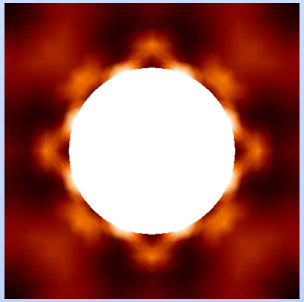




5 modes generated from tensile and shear « tests ».

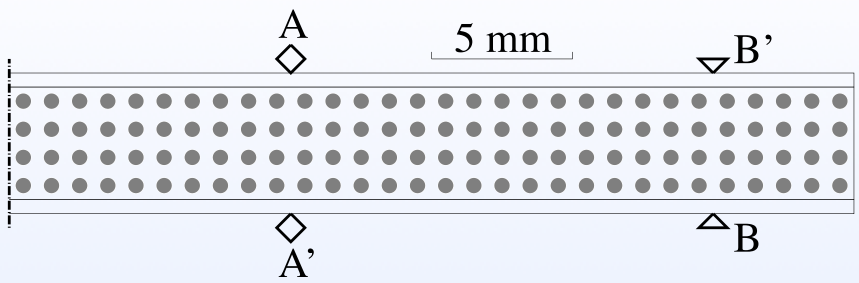
5 internal variables



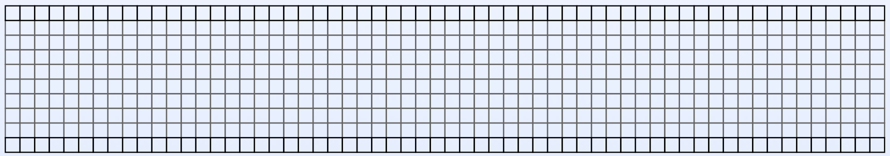


Unit-cell response to a uniaxial tensile test

Structural response

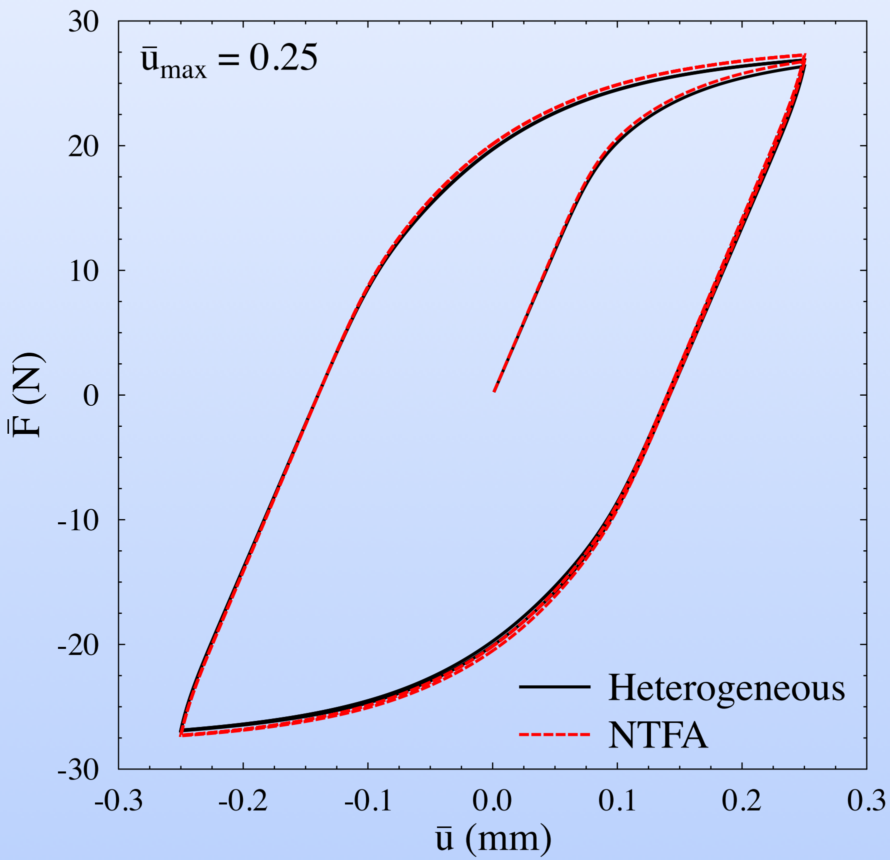


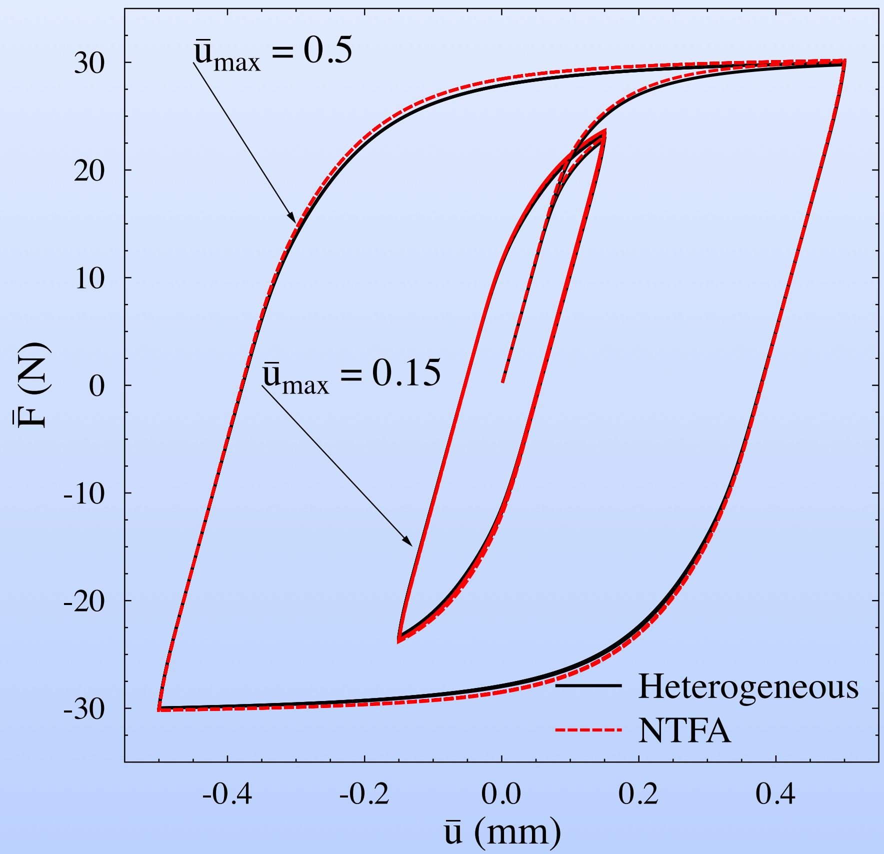
Coarse mesh



Structural response:

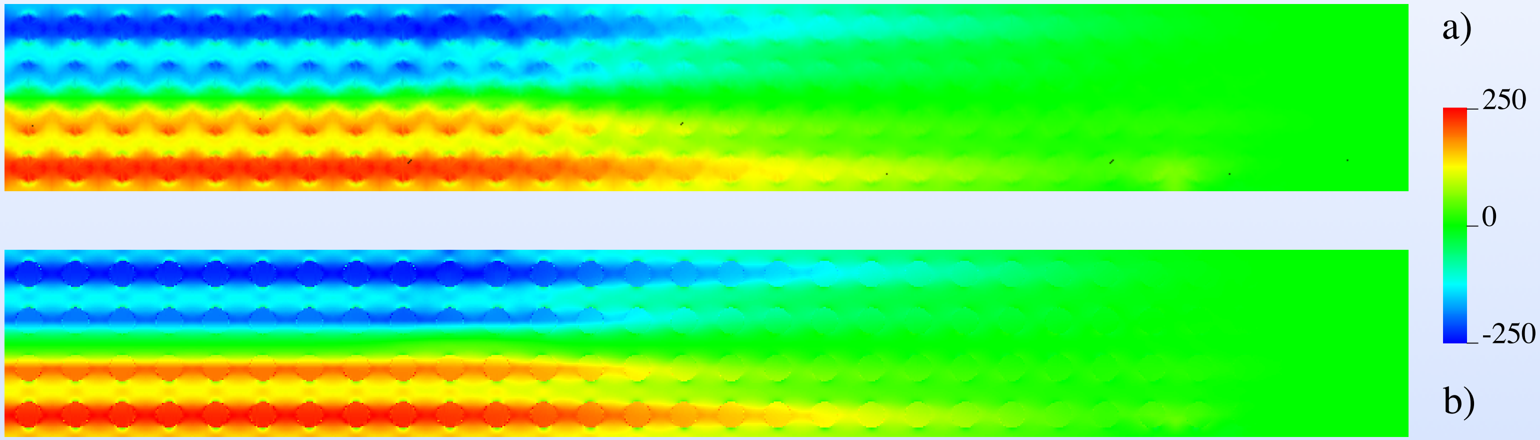
Force/displacement at point A





Local fields

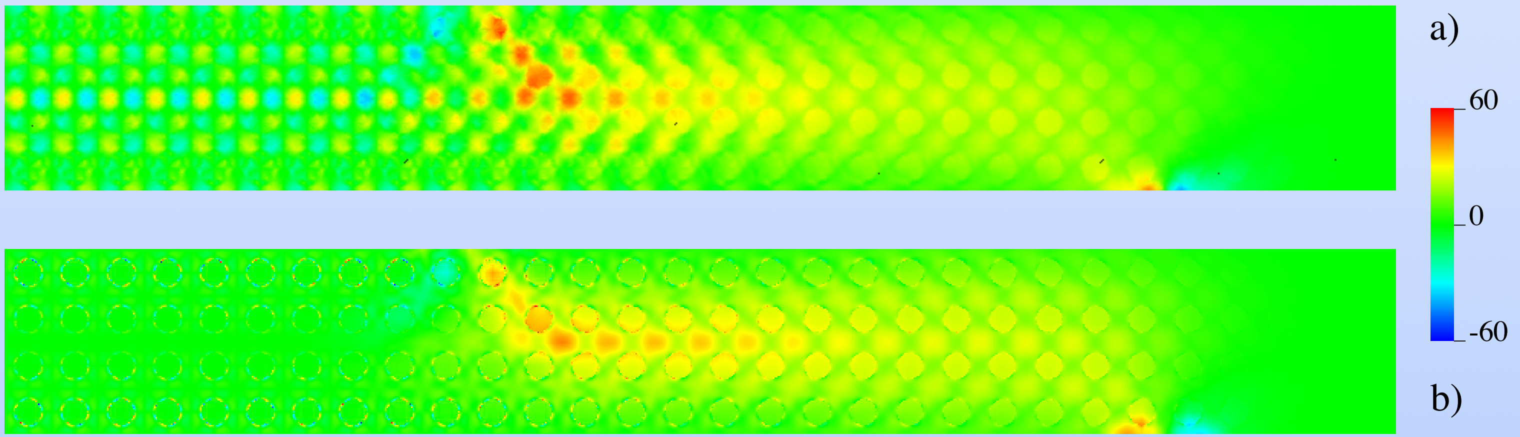
$$\boldsymbol{\sigma}(\boldsymbol{X},\boldsymbol{x},t) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{A}(\boldsymbol{x}) : \overline{\boldsymbol{\varepsilon}}(\boldsymbol{X},t) + \sum_{k=1} \xi^{(k)}(\boldsymbol{X},t)\boldsymbol{\rho}^{(k)}(\boldsymbol{x})$$



Full-field

σ_{11}

NTFA+ **localization**



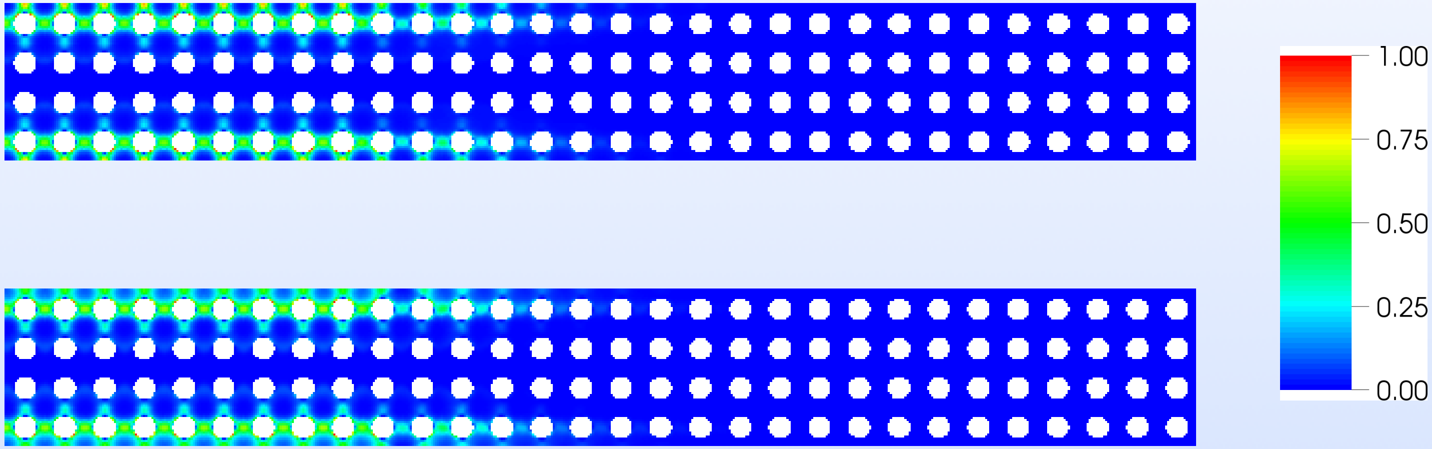
Full-field

σ_{12}

NTFA+ **localization**

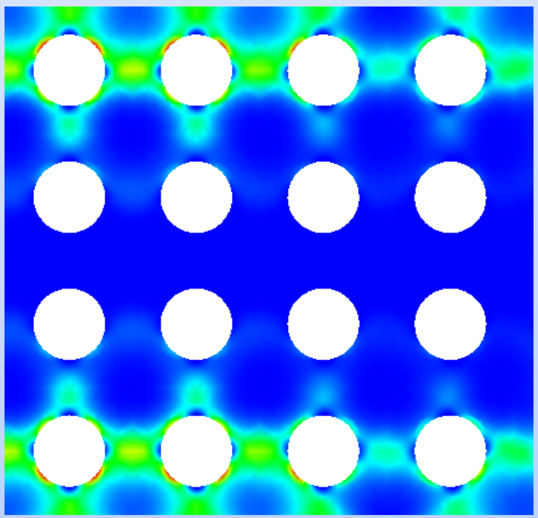
Localization by postprocessing the response of the homogenized model.

Energy dissipated along the stabilized cycle

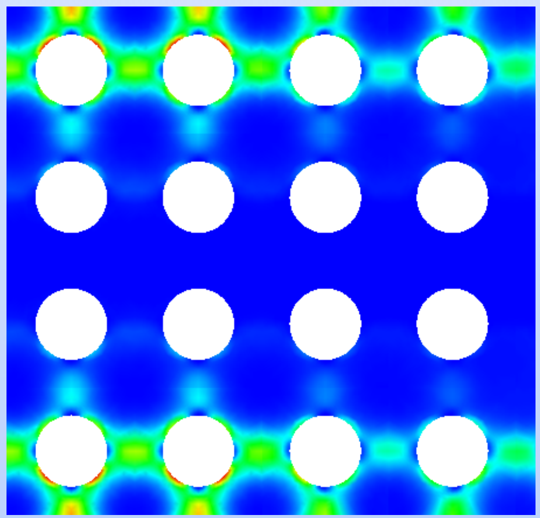


a) Full-field

b) NTFA+ **localization**



a) Full-field



b) NTFA+ **localization**

Take-home messages

- **Reduced-order modeling is useful** in order to:
  - arrive at **tractable macroscopic constitutive relations**,
  - expressed in terms of **quantities computed off-line** (entailing the morphological information).
  - benefit from progress recently made in **full-field simulations and theoretical homogenization**,
  - solve efficiently **inverse problems**.
- **The Nonuniform Transformation Field Analysis** (NTFA) is one possibility based on **observed plastic strain patterning**. Localization can be a linear operation, even for nonlinear constituents.
- **Reducing the « dynamics » is essential** and much more cost-effective than only reducing the variables (by orders of magnitude).

Open problems

- **Domain of validity (in loading space):**

  - The NTFA has a limited domain of validity.

  - Can this domain be predicted from the sole knowledge of the training paths?

- **Convergence/ error estimates:**

  - CV as the number of modes goes to infinity?
  - error estimate for a finite number of modes?

- **Mode determination:**

  - « on-the-fly »: PGD (Chinesta et al), else?
  - optimized for specific loadings?

- **Uncertainties.**

A few references

- **Nonuniform Field Analysis:**

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- **Variational version of NTFA.**

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A few general references (non-exhaustive)

- **Model reduction in general:**

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