An homogenization example of a material with non-conventional microstructure: thermal memory effect and uncertainties

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Motivations

- Materials with microstructure
  - Composites, on-demand tunable material (3D printed)…
- Mechanical engineering
  - Thermo-mechanical behaviors
  - Continuum mechanics models at both scales
  - Microscale length ~ 0.01 mm – 1 cm
- Scale change: homogenization & relocalization

Outlines

- Kind of the scale transition approaches we use
- A specific example

  (not new: [Auriault 1983])

  Transient thermal behavior / high contrast phase

  A macroscopic memory effect
- Numerization of the homogenization

  (more recent: [DD et al 2015])

  Cell model, microscopic problem, macroscopic quantities
- Uncertainties in the micro-structure

  (on the way)

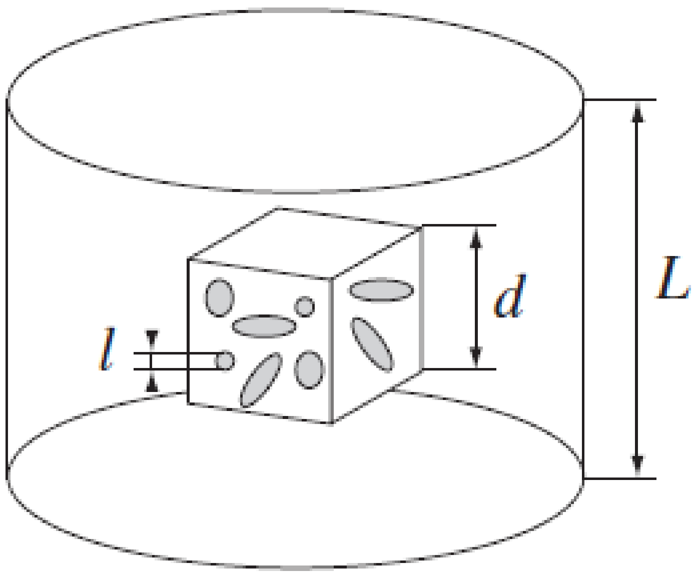
  Geometric parameters, non-intrusive approach

Our typical approach

- Spatial scales?
  - Microstructure component: *l*
  - Elementary representative volume: *d*
  - Studied structure: *L*

  Separation ? $l < d << L$

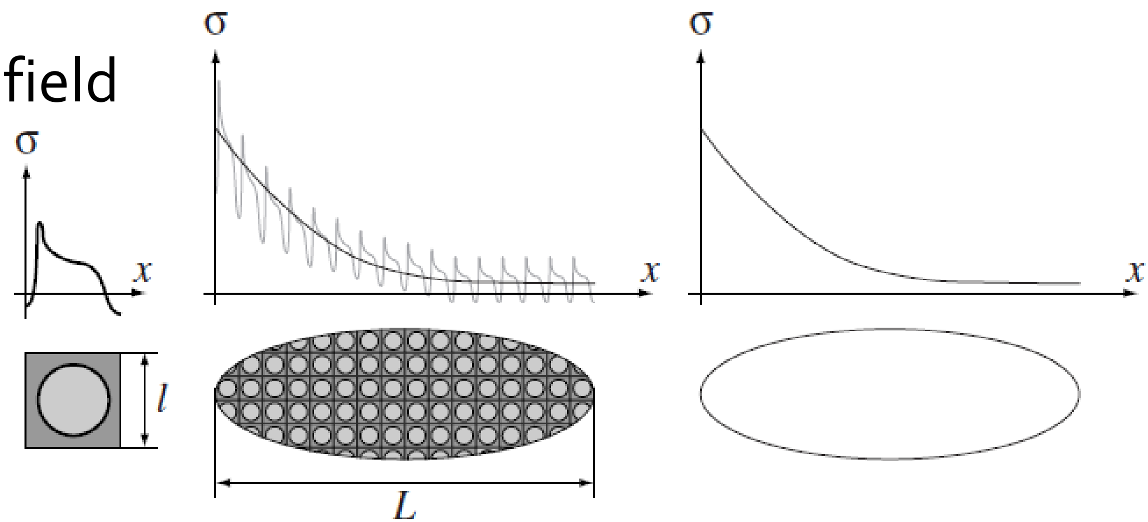
  $\varepsilon = d / L$ small



[a synthesis in: DD 2000]

Our typical approach

- Flavor of the solution field



a) cellule b) structure c) structure homogène équivalente

Reference problem: resolve the micro scale on the whole structure

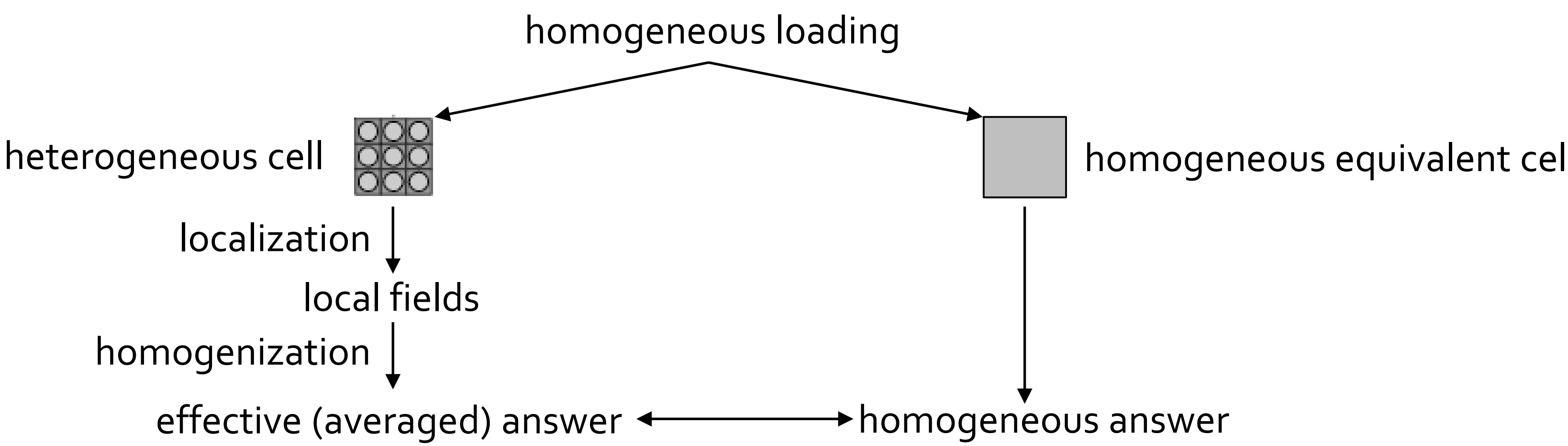
Often unaffordable…

⇒ “Decouple” the local resolution (at a micro/cell scale) from the global resolution (at the structure/macro/homogenized scale)

e.g. precompute on a single cell

Our typical approach

- Equivalence for the homogenized model



Which boundary conditions on the micro cell?

Dirichlet, Neumann, self-consistent, periodic superposition…

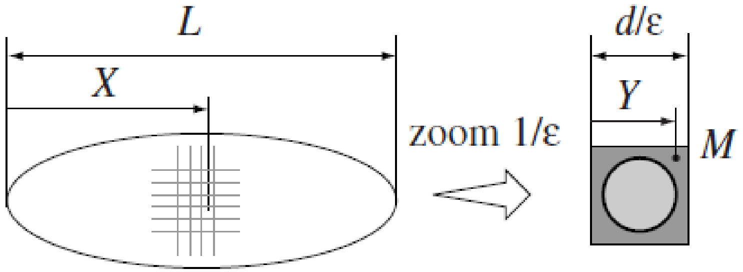
Different approaches, different results (bounds?)

Our typical approach

- (quasi-)Periodic homogenization

The elementary representative volume is an elementary (small) cell

1. A description with two spatial coordinates



Note that the spatial derivative is now

$$\frac{\partial}{\partial M} = \frac{\partial}{\partial x} + \frac{1}{\epsilon}\frac{\partial}{\partial y}$$

2. Each field in your solution is asymptotically developed as:

$U(x,y) = U_0(x,y) + \varepsilon U_1(x,y) + \varepsilon^2 U_2(x,y) + \ldots$

each being Y-periodical

[Sanchez-Palencia 1980]

Our typical approach

- (quasi-)Periodic homogenization

3. Write the problem ODE,PDE… for any $\varepsilon \to 0$: identify the different powers of ε

One should obtain in the best case:

what the macro fields are

what the cell micro-problem is

what the homogenized macro problem is

and what the homogenized parameters are, how to relocalize the macro fields on the micro cell

Interesting features

- The approach embed the derivation of the homogenized model: used as a modeling tool
- Few parasitic boundary effects on the cell

[Sanchez-Palencia 1980]

A specific example [Auriault 1983]

- Transient thermal (but linear) bi-phasic material with a large contrast in conductivity

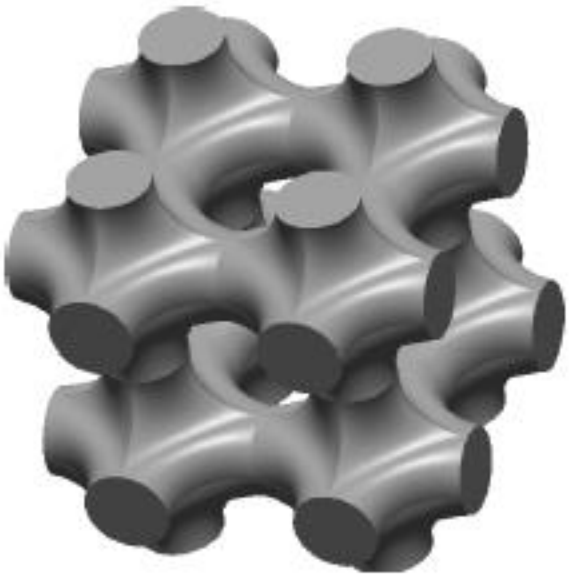
  Phases F and S

  $$\rho_F c_F \approx \rho_S c_S$$
  $$k_F = \varepsilon^2 k'_F \text{ with } k'_F \approx k_S$$

  Perfect interface between the phases

  Characteristic times

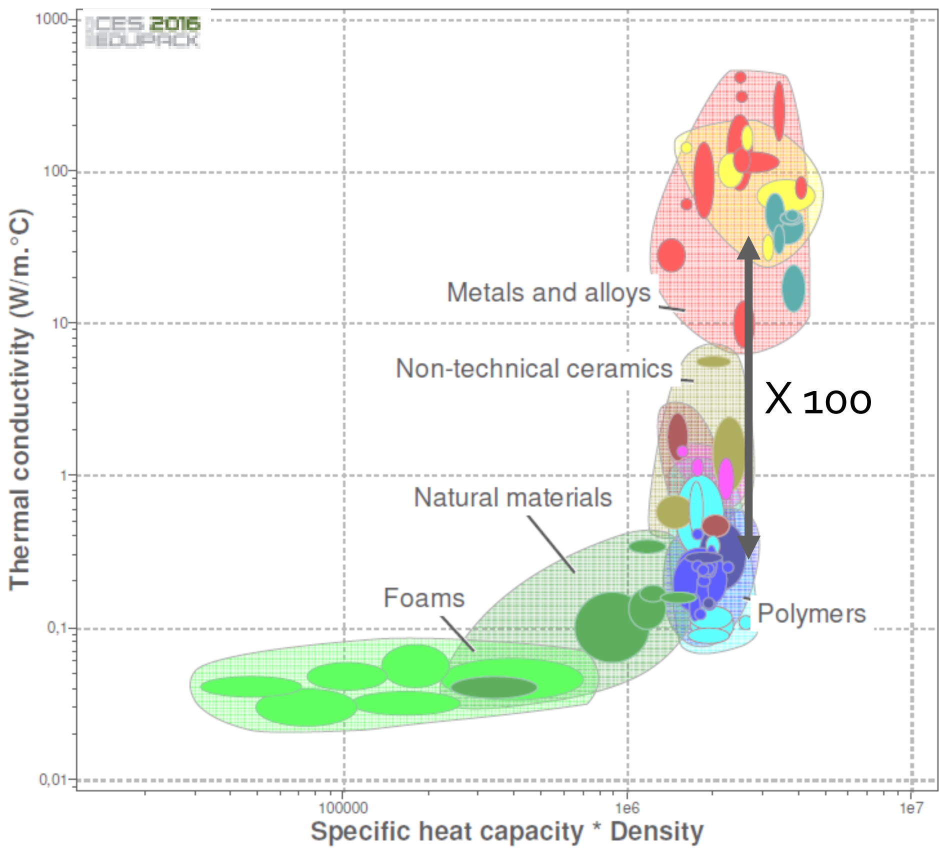
  $$\tau_S = (\rho_S c_S / k_S)(l_S/\pi)^2$$
  $$\tau_F = \frac{\rho_F c_F l_F^2}{k_F \pi^2} \approx \frac{\rho_F c_F L_F^2}{k'_F \pi^2} \approx \tau_S/\varepsilon^2 \approx \tau_M$$



  $\Rightarrow$ A macro thermal load will lead to a micro answer visible at macro scale…

In practice…

- Finite value of $\varepsilon = l / L$



$\varepsilon = 1/10$: a big microstructure

Does a *given* microstructure lead to a macroscopic memory effect? Depends on the structure size!

A macro memory effect arises only with contrast $O(\varepsilon^2)$

A specific example [Auriault 1983]

Lets do it…

- Asymptotic development of temperature fields $$\theta = \sum_{\alpha=0}^{\infty} \varepsilon^{\alpha} \theta_{\alpha}(x, y, t)$$
- Develop the models (heat balance, bcs…)

We obtain successively :

- A macro S-temperature $\theta_{S0} = \theta_{S0}(x, t)$ $\underline{Z}_{S0}(x, t) = \underline{\mathrm{grad}}_x \theta_{S0}$
- The micro problem for θ_{S1}:

  a steady-state thermal problem, parametered with $\underline{Z}_{S0}$ as a load, on S-phase only

  leads to a relocalization operator for the micro-temperature gradient

$$\underline{Z}_{S1}(x, y, t) = -\boldsymbol{L}_S(y)\underline{Z}_{S0}(x, t)$$

  (note the linear dependency, $\boldsymbol{L}_S$ is computed once for all)

A specific example [Auriault 1983]

Lets do it…

We obtain successively:

- The problem giving θ_{F0}: a transient thermal problem on the F-phase only, loaded with a boundary condition on the interface with θ_{S10}
  but now $\theta_{F0}(x, y, t)$ is not a macro-field only!

- A macro problem with a 2-field unknown…

$$C_{MS}\dot{\theta}_{S0} = \mathrm{div}_x(k_{MS}\underline{Z}_{S0}) - \left\langle \rho_F c_F \dot{\theta}_{F0} \right\rangle_F$$

  with homogenized material parameters:
  capacity $C_{MS} = \langle \rho_S c_S \rangle_S$
  conductivity $k_{MS} = \langle k_S(1 - L_S) \rangle_S$

And we stop here the asymptotic development…

A specific example [Auriault 1983]

Lets do it…

Interpretation:

$$C_{MS}\dot{\theta}_{S0} = \mathrm{div}_x(k_{MS}\underline{Z}_{S0}) - \left\langle \rho_F c_F \dot{\theta}_{F0} \right\rangle_F$$

At this scale, θ_{F0} can be seen as a field of internal variables, serving as memorizing the past evolution of the material

But, defined at the micro scale, it is too huge to store at every time step

$\Rightarrow$ An equivalent (hereditary) model with a memory function

$$C_{MS}\dot{\theta}_{S0} = \mathrm{div}_x(k_{MS}\underline{Z}_{S0}) + \int_{\tau=-\infty}^{\tau=t} \ddot{\theta}_{S0}(\tau)\beta(t-\tau)d\tau$$

A specific example [Auriault 1983]

Lets do it…

Interpretation:

$$C_{MS}\dot{\theta}_{S0} = \mathrm{div}_x(k_{MS}\underline{Z}_{S0}) + \int_{\tau=-\infty}^{\tau=t} \ddot{\theta}_{S0}(\tau)\beta(t-\tau)d\tau$$

$\beta(t)$ is also a macroscopic material characteristic (back-in-time function)

- Semi-analytical solution (1D stratified composite):

$$\beta(t) \approx \rho_F c_F n \frac{8}{\pi^2} \exp[-t/\tau_F]$$

evanescent memory with a characteristic time τ_F

a.k.a. kernel, resolvent, Duhamel integral… see also Prony series…

Numerization

- For a 3D microstructure… rely on simulation
  - Pre-compute on a cell to provide

    Capacity C_M: simple average (analytical)

    Conductivity $\boldsymbol{k}_M$: requires to solve few (3) steady-state thermal micro-problems, and provides also the relocalization operator $\boldsymbol{L}_S$ to rebuilt the micro-solution as post-treatment once the homogenized problem is solved

    Memory effect function $\beta(t)$: requires to solve a transient thermal micro-problem

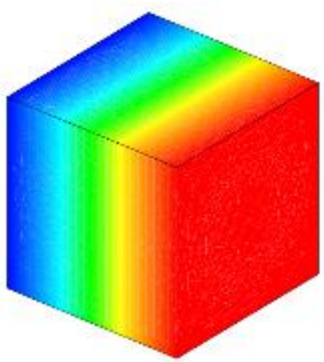
    (every micro-problem is linear here, hence easy to pre-compute once for all, with periodic boundary conditions and macro loading)

[DD et al 2015]

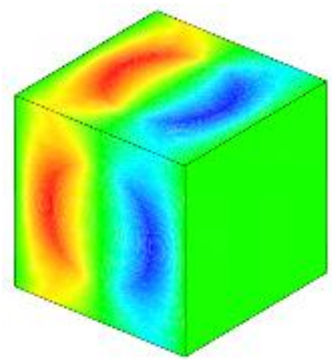
A specific example [Auriault 1983]

A 3D example

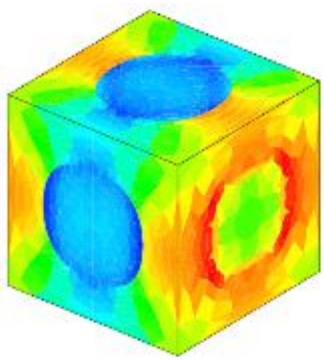
(a) Phase S (b) Phase F (c) Cellule élémentaire



Macro temperature field (load)



Micro temperature field (answer)

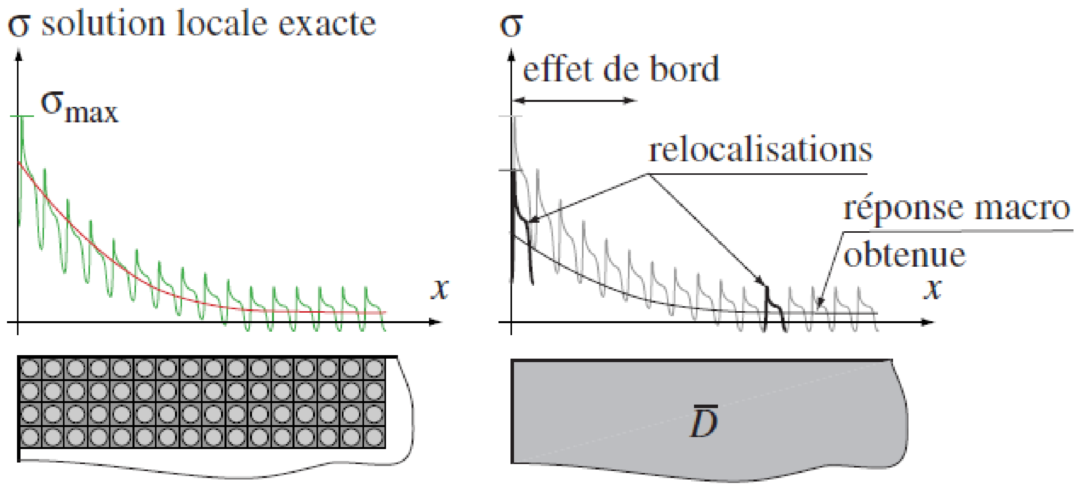


Micro temperature gradient (relocalization)

Limitations

- As for any approach: edge effects

  Close to structure boundary: periodicity assumption does not hold any more…



$\Rightarrow$ Higher order corrections or local reanalysis (DDM, MGM, zoom…)

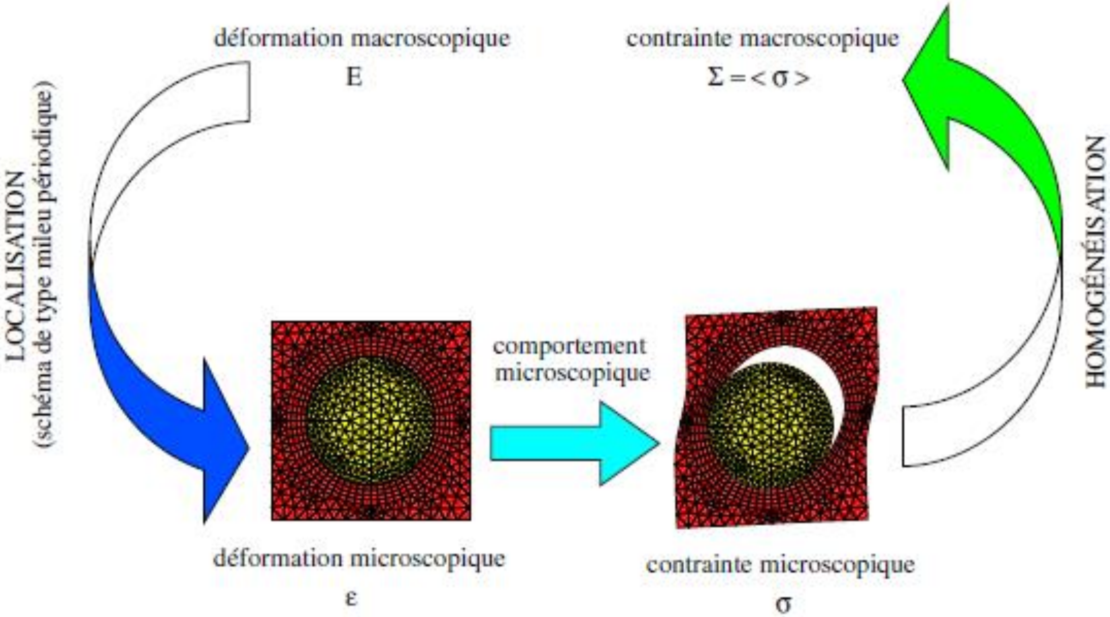
Limitations

- Non-linear behavior issue

  Linear ⇒ superposition, easy pre-computation

  Non-linear ⇒ less easy…

  A “no pre-computation” solution: FE2 approach [Feyel et al 2001]



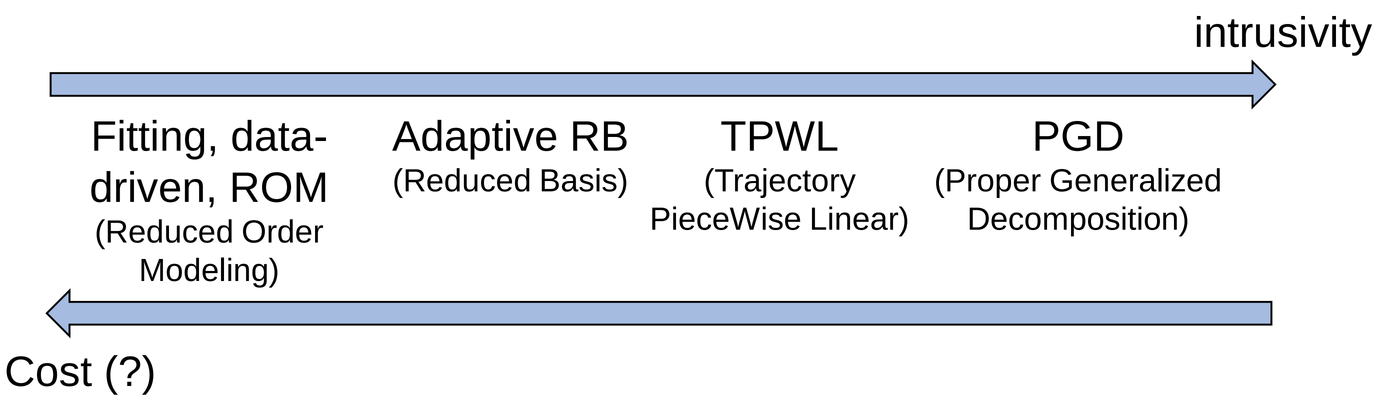
Limitations

- Non-linear behavior issue

  Linear $\Rightarrow$ superposition, easy pre-computation

  Non-linear $\Rightarrow$ less easy…

    Try to avoid identical or similar solves (and store computed knowledge)



Uncertainties

- Motivation

  On-demand material tuning:

  Goal-oriented design of the microstructure

  Target performance of the macroscopic behavior

  First step:

  manufacturing process uncertainties $\Rightarrow$ influence on the macroscopic behavior

- Issues
  - Multiple parameters
  - Multiple queries

Carnot Ingénierie@Lyon project: MURMUR (Multiscale robust design of material microstructures), LaMCoS project: MaDAMe_R^2 (Multiscale Design of Advanced Materials using Rapid and Robust approaches))

Uncertainties

- Issues
  - Multiple parameters
  - Multiple queries
  - What is needed (which quantity of interest?, full cdf, first moments, level of confidence, envelops…)

intrusivity →

Black-box MCS (Monte-Carlo Simulations)	QMS ROM Collocation-PCE (Quasi Monte-Carlo, Surrogate models)	Stochastic FE code / PCE (Polynomial chaos expansion)

← Cost (?) – depends on the number of parameters…

Uncertainties

- Non-intrusive collocation-based PCE

Input parameters values → Black-box model → Quantity of interest (QoI)

  - No matter if linear or non-linear (black-box)
  - Computational complexity ↑ with the number of parameters
  - If QoI = macro characteristics (C_M, $\boldsymbol{k}_M$, β),

$\Rightarrow$ How do uncertainties propagate through scales?

Uncertainties

- Non-intrusive collocation-based PCE

Input parameters values → Black-box model → Quantity of interest (QoI)

Representation of a random variable X :

from a basic r.v. set ξ

ψ_i = orthogonal polynomial basis

X_i = coefficient

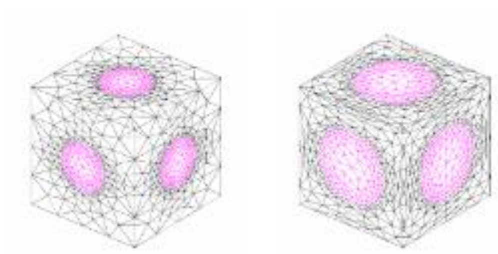
$$X(\boldsymbol{\xi}) = \sum_{i=0}^{p} X_i \psi_i(\boldsymbol{\xi})$$

Input: given a stochastic distribution $\Rightarrow$ particular polynomial basis

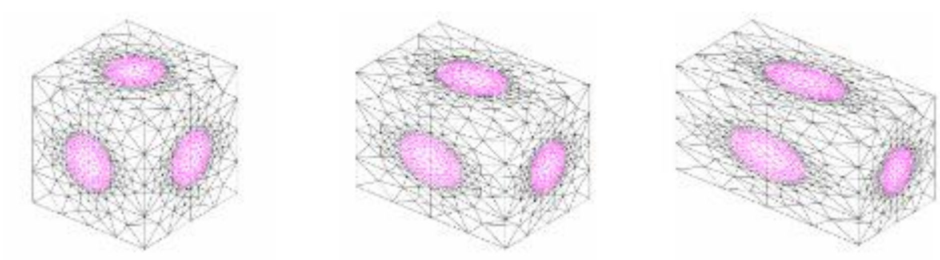
QoI: identify the coefficients by projection/least square on a set of runs (collocation points for inputs)

Uncertainties

- Uncertain input parameters:
  - Phase material characteristics
  - Geometry parametrization



distortion
(stochastic distribution: uniform)



(a) $\alpha = 0$ (b) $\alpha = 0,5$ (c) $\alpha = 1$

elongation
(stochastic distribution: uniform)

Uncertainties

- Uncertain QoI:
  example of macroscopic conductivity $\boldsymbol{k}_M$ eigenvalues coefficients of variation:

inputs			QoI	
micro conductivity k_F	distortion	elongation	$k_{MI} = k_{MII}$	k_{MIII}
0	0	1	0	0
0.3536	0		0.0845	0.0919
0	2.582		0.0907	0.0921
0.3536	2.582		0.1718	0.181

Outlooks and prospects

- Robust design of ad hoc microstructures
- Optimization (many query problem also)
  - Performance $\Rightarrow$ QoI = macro characteristics
  - Integrity $\Rightarrow$ QoI = relocalization operator/field

    (tensor representation/decomposition…)
- Topological optimization at both scales
- Increasing the number of parameters

  (curse of dimensionality)

Some references

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