Data Driven (Model Free) Mechanics

A new paradigm for multiscale mechanics of materials

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with A. Platzer, F. Figueredo Rocha, A. Leygue, . . .

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MecaMat Aussois, January 30, 2025

General context

The challenge of constitutive modeling:

- *physical principles*: well established, no intrinsic uncertainty
- *constitutive models*: approximation, interpretation, heuristics, uncertainty
  - models rely on postulates
  - relevant model can be strongly application-dependent
  - models are based on constitutive parameters, to be identified against experimental data
  - attempts to construct constitutive models from *ab initio* are confronted to complexity and difficulty of scale transitions

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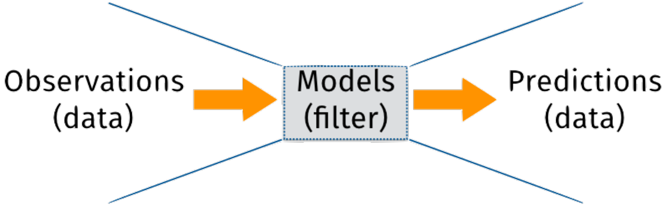

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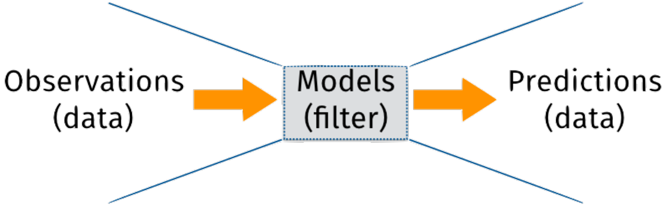


Approximation level of models difficult to control (convergence, UQ?)

Numerical materials

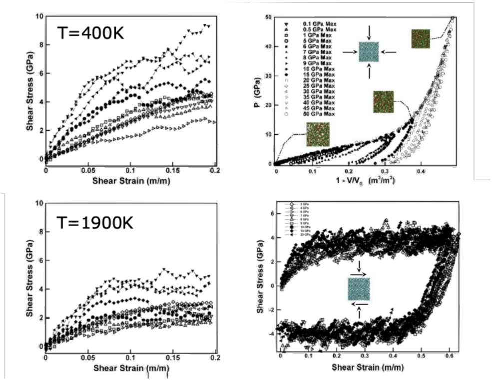
Complexity of (macroscopic) material behavior originates from interactions between unit mechanisms acting at fine (microscopic) scales:

- ▷ requires good understanding of unit mechanisms and mastered microscopic models
- ▷ effective (macroscopic) material response obtained by numerical modeling of representative samples (RVEs)

Examples:

SiO_2 amorphous glass

- ▷ molecular dynamics simulations (LAMMPS)
- ▷ pressure-shear loading at various temperatures and strain-rates



[W. Schill et al., JMPS 113 (2018) & 140 (2020)]

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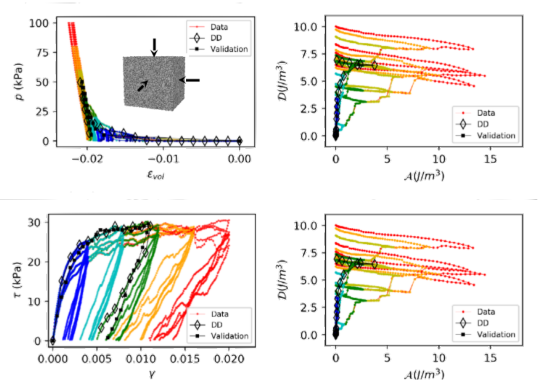
Examples:

Granular material (sand)

- ▷ 3D irregular rigid grains (LS-DEM)
- ▷ triaxial loading experiments
- ▷ frictional contact
- ▷ stored energy and dissipation

[K. Karapiperis et al., JMPS 144 (2020) & 147 (2021)]



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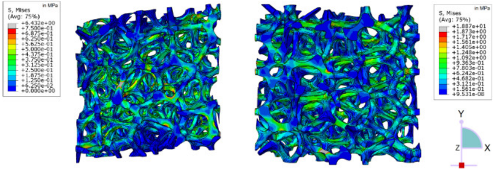
Examples:

Polyurethane foam

- ▷ continuum microstructured RVEs
- ▷ (an)isotropic (hyper)elasticity
- ▷ stochastic microstructures



[T.F. Korzeniowski and K. Weinberg, CMAME 400 (2022)]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QU'EST-CE QU'ON FAIT MAINTENANT ?

Multiscale mechanics

Objective: computations at structural (macroscopic) scale

- significant **cost** of systematic use of numerical material (RVE computations → e.g. FE^2)
- **difficulty** to construct explicit macroscopic model, reproducing results of numerical material model !

Solutions:

- linear material response → homogenization OK
- non-linear material response ?
  - mean field (MF) approaches
  - model reduction / modal approaches (NTFA, POD, PGD, ...)
  - *ad hoc* model parameters identification
  - surrogate models: neural networks (NN), machine learning (ML), ...
  - data-driven computing

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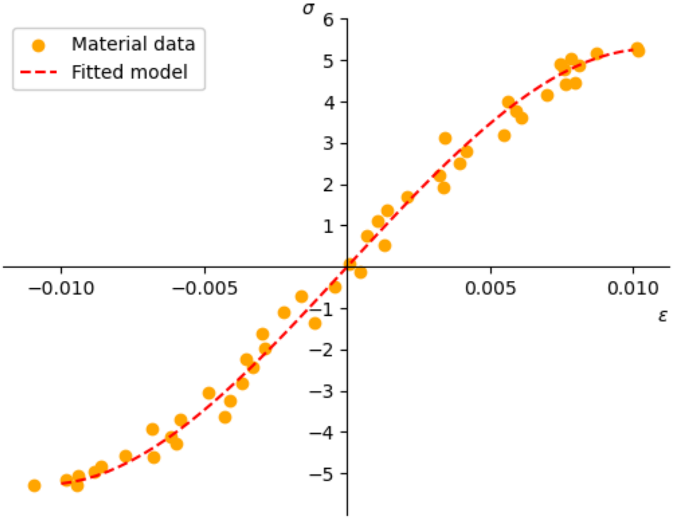
  - ◦ **data-driven computing**
- ▷ DD multiscale $\Longleftrightarrow$ **Active Learning (AL)** strategy

Data-Driven Computational Mechanics

Classical approach: fitting parametric representation of constitutive model to data



DDCM Illustration

Model-free data-driven computational mechanics on a 1D bar

[Kirchdoerfer & Ortiz, 2016]

DDCM Paradigm

Model-free data-driven computational mechanics [Kirchdoerfer-Ortiz, 2016]

- replace heuristic constitutive relation by **data**
- data set $\mathcal{D} = \{\hat{\boldsymbol{z}}_\alpha = (\hat{\boldsymbol{\varepsilon}}_\alpha, \hat{\boldsymbol{\sigma}}_\alpha), \alpha = 1, \ldots, N\}$
- manifold $\mathcal{E}$ of admissible states (compatible $\boldsymbol{\varepsilon}$ and balanced $\boldsymbol{\sigma}$)
- distance in phase space of mechanical states (with metric $\mathbb{C}$):

$$
\begin{aligned}
d(\boldsymbol{y}, \boldsymbol{z}) = \Big[& \frac{1}{2} (\boldsymbol{\varepsilon}_y - \boldsymbol{\varepsilon}_z) \cdot \mathbb{C} \cdot (\boldsymbol{\varepsilon}_y - \boldsymbol{\varepsilon}_z) \\
& + \frac{1}{2} (\boldsymbol{\sigma}_y - \boldsymbol{\sigma}_z) \cdot \mathbb{C}^{-1} \cdot (\boldsymbol{\sigma}_y - \boldsymbol{\sigma}_z) \Big]
\end{aligned}
$$

- best approximate solution = admissible state closest to data

$$
\inf_{\boldsymbol{z} \in \mathcal{E}} \inf_{\hat{\boldsymbol{z}} \in \mathcal{D}} d(\boldsymbol{z}, \hat{\boldsymbol{z}})
$$

Mixed-integer programming (MIP) problem

Constitutive distance

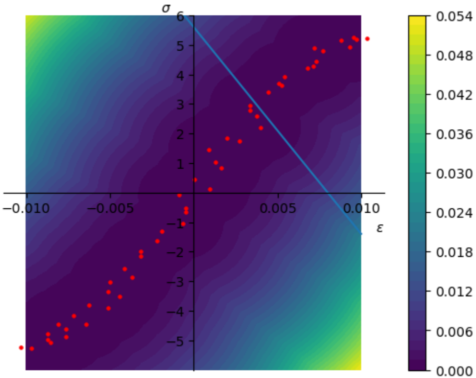
Constitutive response defined by data $\mathcal{D}$

$\implies$ constitutive distance $d_{\mathcal{D}}(\boldsymbol{z}) = \inf_{\boldsymbol{z}^* \in \mathcal{D}} d(\boldsymbol{z}, \boldsymbol{z}^*)$

Quadratic distance:

$$d(\boldsymbol{z}, \boldsymbol{z}^*) = \frac{1}{2} \|\boldsymbol{z} - \boldsymbol{z}^*\|^2_{\mathbb{C}} = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*) : \mathbb{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^*) + \frac{1}{2} (\boldsymbol{\sigma} - \boldsymbol{\sigma}^*) : \mathbb{C}^{-1} : (\boldsymbol{\sigma} - \boldsymbol{\sigma}^*)$$

based on metric $\mathbb{C}$



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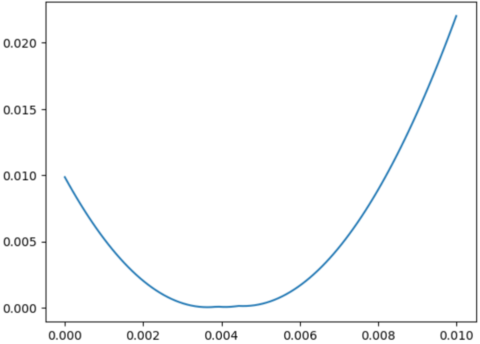

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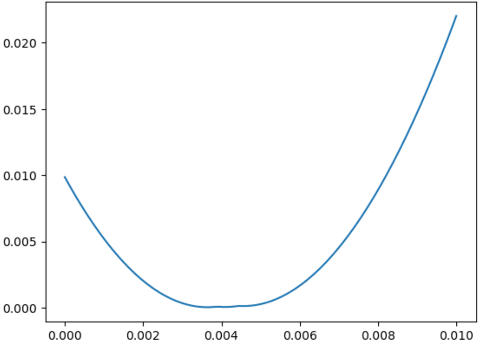


Regularisation (convexification) is possible [Kirchdoerfer & Ortiz, 2017]

DDCM Algorithm

Alternated minimization algorithm:

- ▷ projection on equilibrium manifold

$$\boldsymbol{z} = \arg \inf_{\boldsymbol{z}' \in \mathcal{E}} d(\boldsymbol{z}', \hat{\boldsymbol{z}}) = P_E(\hat{\boldsymbol{z}})$$

  minimization of a quadratic function with linear constraints

- ▷ *projection* on data set

$$\hat{\boldsymbol{z}} = \arg \inf_{\hat{\boldsymbol{z}}' \in \mathcal{D}} d(\boldsymbol{z}, \hat{\boldsymbol{z}}') = P_D(\boldsymbol{z})$$

  discrete nearest-neighbour (NN) search

- ▷ fixed point algorithm

$$\boldsymbol{z} = P_E(P_D(\boldsymbol{z}))$$

Alternative MIP algorithms are possible [Kanno, 2018, 2019], but with high computational cost.

DDCM in practice (1)

- discrete balance and compatibility equations

$$\sum_{e=1}^{M} w_e \mathbf{B}_e^T \boldsymbol{\sigma}_e = \mathbf{f} \quad \text{and} \quad \boldsymbol{\varepsilon}_e = \mathbf{B}_e \mathbf{u} \; (e = 1, \ldots, M)$$

- global distance to minimize

$$d(\mathbf{z}, \hat{\mathbf{z}}) = \Big[\sum_{e=1}^{M} w_e \Big(\frac{1}{2} (\boldsymbol{\varepsilon}_e - \hat{\boldsymbol{\varepsilon}}_{\alpha_e}) \cdot \mathbb{C} \cdot (\boldsymbol{\varepsilon}_e - \hat{\boldsymbol{\varepsilon}}_{\alpha_e}) + \frac{1}{2} (\boldsymbol{\sigma}_e - \hat{\boldsymbol{\sigma}}_{\alpha_e}) \cdot \mathbb{C}^{-1} \cdot (\boldsymbol{\sigma}_e - \hat{\boldsymbol{\sigma}}_{\alpha_e})\Big)\Big]$$

- constrained minimization $\Longrightarrow$ Lagrange multipliers $\boldsymbol{\lambda}$

$$\sup_{\boldsymbol{\lambda}} \inf_{\mathbf{u},\boldsymbol{\sigma}} \left[d\left((\mathbf{B}\mathbf{u}, \boldsymbol{\sigma}), \hat{\mathbf{z}}\right) - \boldsymbol{\lambda}^T \left(\sum_{e=1}^{M} w_e \mathbf{B}_e^T \boldsymbol{\sigma}_e - \mathbf{f} \right) \right]$$

DDCM in practice (2)

Constrained minimization leads to two (uncoupled) linear algebraic systems

$$\sum_{e=1}^{M} w_e \mathbf{B}_e^T \mathbb{C} \mathbf{B}_e \mathbf{u} = \sum_{e=1}^{M} w_e \mathbf{B}_e^T \mathbb{C} \hat{\boldsymbol{\varepsilon}}_{\alpha_e}$$

$$\sum_{e=1}^{M} w_e \mathbf{B}_e^T \mathbb{C} \mathbf{B}_e \boldsymbol{\lambda} = \mathbf{f} - \sum_{e=1}^{M} w_e \mathbf{B}_e^T \hat{\boldsymbol{\sigma}}_{\alpha_e}$$

with $\boldsymbol{\varepsilon}_e = \mathbf{B}_e \mathbf{u}$ and $\boldsymbol{\sigma}_e = \hat{\boldsymbol{\sigma}}_{\alpha_e} + \mathbb{C} \mathbf{B}_e \boldsymbol{\lambda}$.

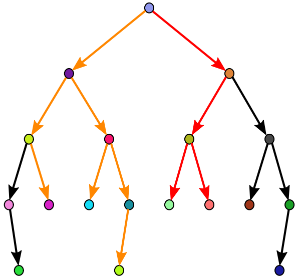
Projection $P_E(\hat{\mathbf{z}})$ amounts to solving above systems:

- ▷ structure of linear elasticity stiffness matrices
- ▷ can be factorized once for all load cases
- ▷ can use off-the-shelf FE solvers (for example)

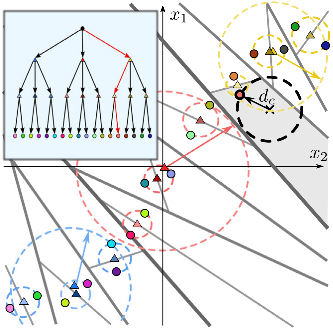
$\Longrightarrow$ main computational cost in NN searches $(P_D(\mathbf{z}))$!

Computational Cost

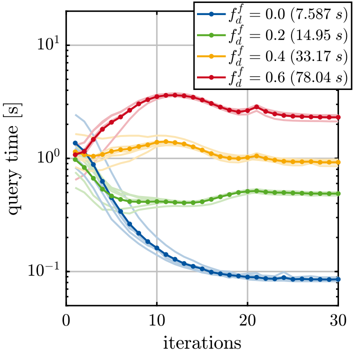
Optimized NN search algorithms ([Eggersmann et al., CMAME 382, 2021])



approximate kd-tree search



kmeans-tree search

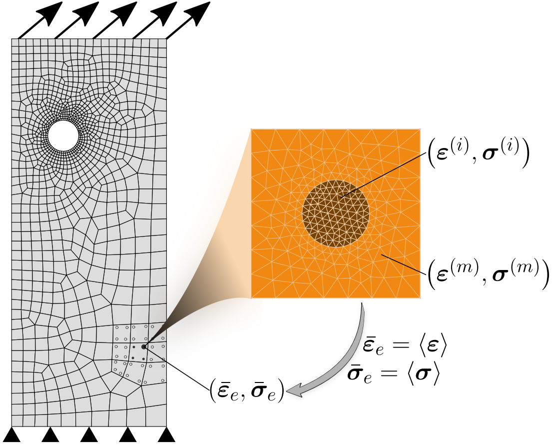


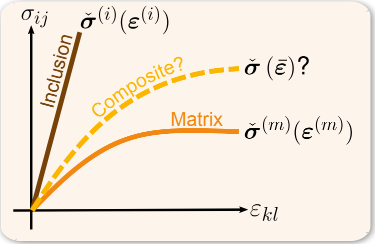
10^9 *points query time* $\sim$ *1s*

Additional benefits:

- ▷ no tangent operator for non-linear problems
- ▷ no need for incremental loading (history-independent materials)

Multiscale computational mechanics





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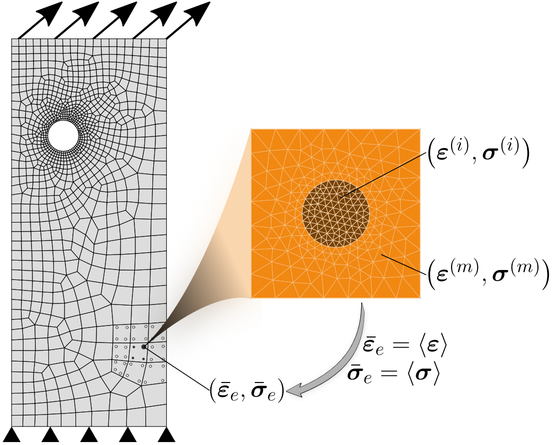

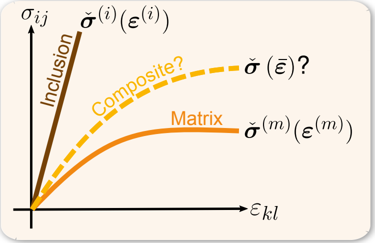

Available solutions

- concurrent multiscale methods (FE^2) [Feyel, 1999]
- offline database from micro computation
  - macroscopic models (fitted, incl. NN)
  - DDCM [Xu et al., 2020]

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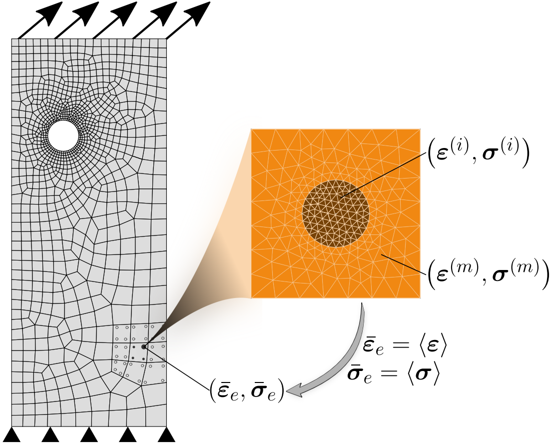

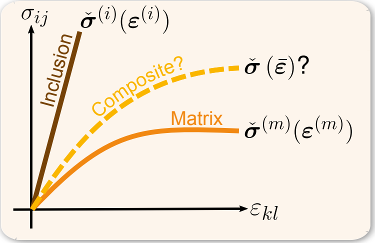

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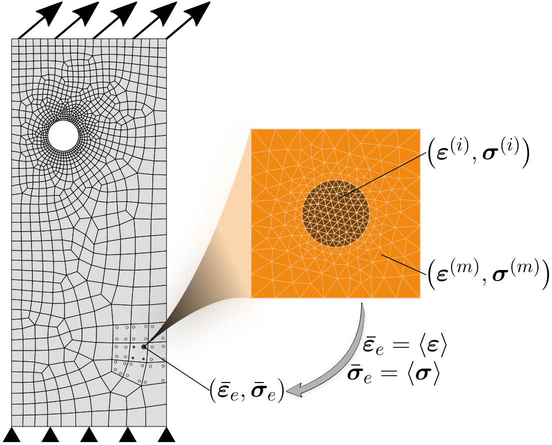

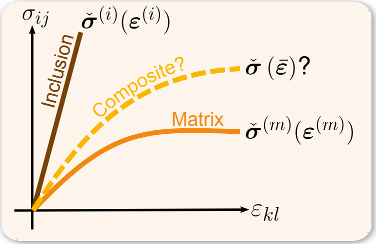

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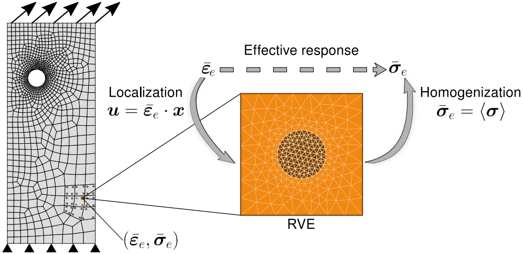
Accelerating FE^2



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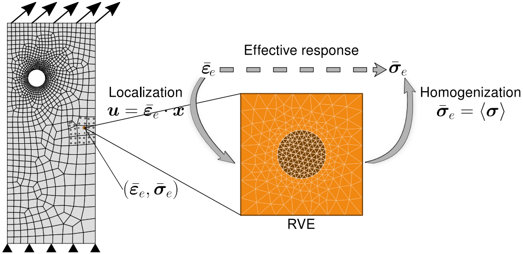

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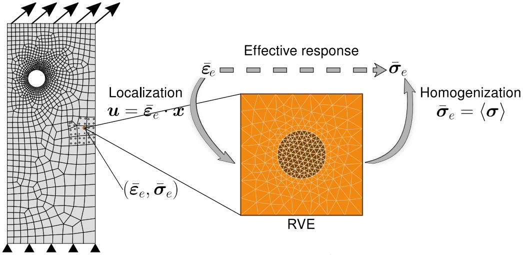

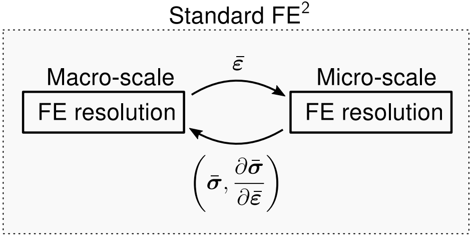

High computational cost

- **systematic** and **redundant** evaluations
- tangent operator

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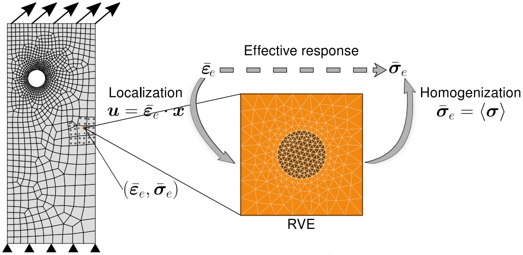

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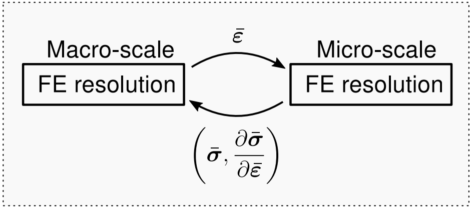
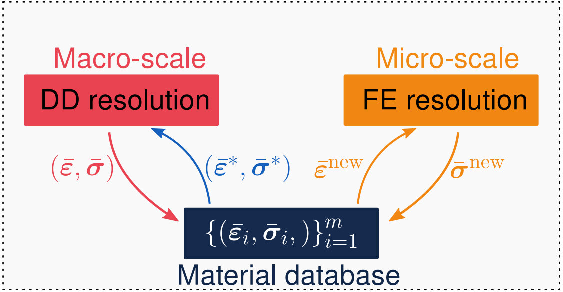
Standard FE^2



Data-driven FE^2



Dynamic database construction (A. Platzer's Ph.D. thesis)

Example: multiscale data generation

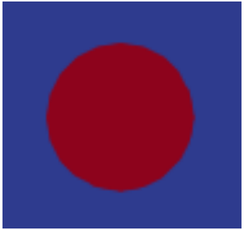
- ▷ Nonlinear strain energy:

$$\Psi(\boldsymbol{\varepsilon}) = \frac{\lambda}{2}\left(\mathrm{tr}\boldsymbol{\varepsilon}^2 + \frac{\alpha}{2}\mathrm{tr}\boldsymbol{\varepsilon}^4\right) + \mu\left(|\boldsymbol{\varepsilon}|^2 + \frac{\alpha}{2}|\boldsymbol{\varepsilon}|^4\right)$$

- ▷ Heterogeneities:

$$\Psi(\boldsymbol{\varepsilon}(\boldsymbol{y})) = \begin{cases} \Psi^M(\boldsymbol{\varepsilon}(\boldsymbol{y})) & \text{for } \boldsymbol{y} \text{ in the matrix} \\ \gamma\Psi^M(\boldsymbol{\varepsilon}(\boldsymbol{y})) & \text{for } \boldsymbol{y} \in \text{ in the inclusions} \end{cases},$$

with $\gamma = 10^3$, $\alpha = 0$ or 10^4, $E^M = 24[F/L^2]$, $\nu = 0.3$



- ▷ Periodic boundary conditions.
- ▷ $(\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{12}) = (\theta_0\theta_1, \theta_0(1-\theta_1), \theta_2)$
- ▷ θ_is are sampled by the Latin Hyper Cube.
- ▷ Database size: $N_d = 10K$

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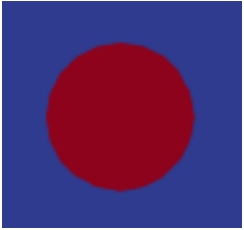
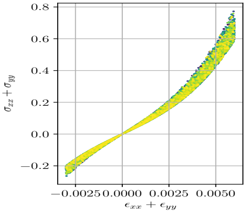
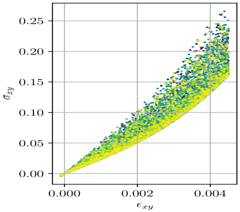


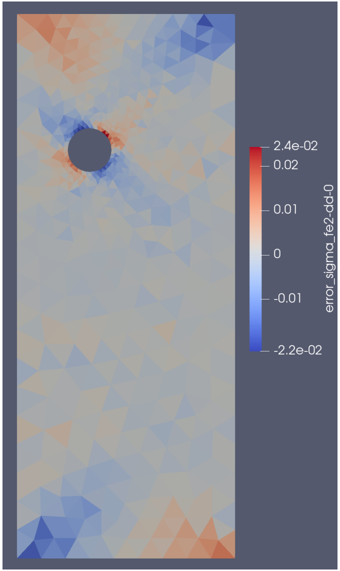




Example: DDCM perforated plate

- $\Omega : \begin{cases} \text{height} = 50, \text{width} = 20 \\ \text{hole radius} = 2 \end{cases} \quad [L]$
- Dirichlet BCs: $\begin{cases} \boldsymbol{u}_{bot} = (0,0)[L] \\ \boldsymbol{u}_{top} = (0.3, 0.05)[L] \end{cases}$
- Meshes P1 ($N_{el} = 905$)
- DDCM via **ddfenics**[1] .
- Reference FE^2 via **micmacsFenics**[2] .
- Static DB of $10K$ samples.
- Estimation[3] of $\mathbb{C} := \mathrm{sym}(\boldsymbol{A}_\sigma \boldsymbol{A}_\varepsilon^{-1})$, s.t.

  $$[\boldsymbol{DB}] = \boldsymbol{U}\boldsymbol{\Sigma} \begin{bmatrix} \boldsymbol{A}_\varepsilon & \dots \\ \boldsymbol{A}_\sigma & \dots \end{bmatrix}$$



[1] github.com/felipefr/ddfenics

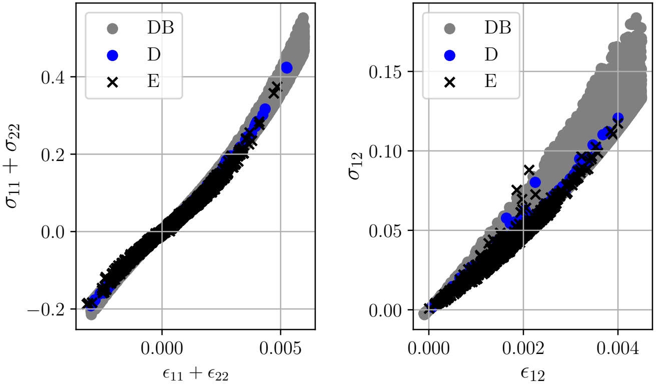
[2] github.com/felipefr/micmacsFenics

[3] [Eggersmann et al, 2019]

Example: DDCM with Static DB vs FE^2

Method	NR it	DD it	N_{eval}^{σ}	N_{eval}^{tan}	$t_{DBgen}(s)$	$t_{total}(s)$	speedup	$e_{L^2}^{rel}(u, u_{ref})$
FE^2	5	-	10020	10020	-	180.8	1	-
DDCM	-	8	10000	-	78.07	80.95	**2.233**	6.12e-03

Phase Space DD : Perf. Plate



Prototype adaptive solver (small strain)

0 Initial database

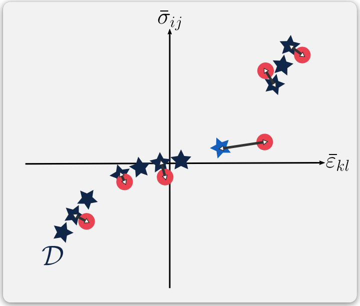
$\mathcal{D}^{(0)}$

DDCM simulation

1 Mechanical response

$\{(\bar{\boldsymbol{\varepsilon}}_e, \bar{\boldsymbol{\sigma}}_e)\}_{e=1}^{M}$

Macro strain-stress space



(from A. Platzer's PhD thesis)

Prototype adaptive solver (small strain)

0 Initial database

$\mathcal{D}^{(0)}$

↓ DDCM simulation

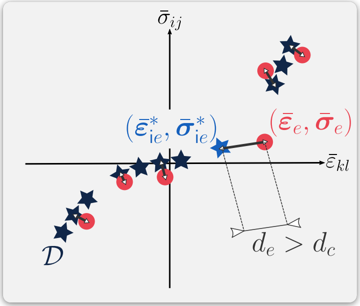
1 Mechanical response

$\{(\bar{\boldsymbol{\varepsilon}}_e, \bar{\boldsymbol{\sigma}}_e)\}_{e=1}^{M}$

↓ select isolated points

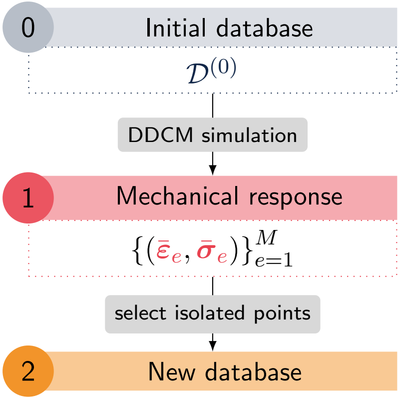
2 New database

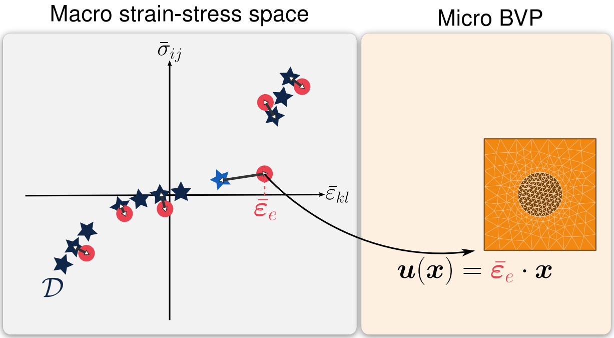
Macro strain-stress space



(from A. Platzer's PhD thesis)

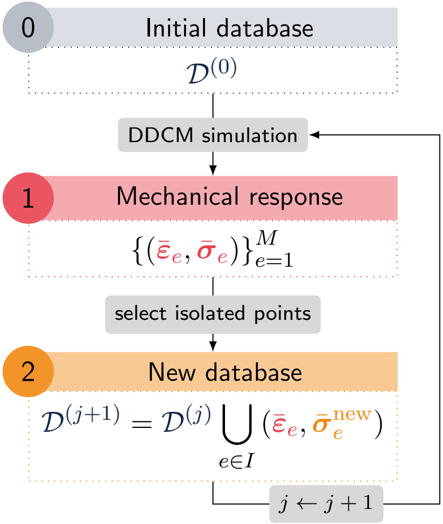
Prototype adaptive solver (small strain)

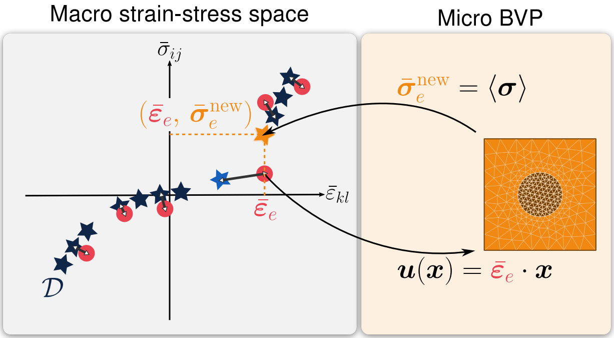




(from A. Platzer's PhD thesis)

Prototype adaptive solver (small strain)

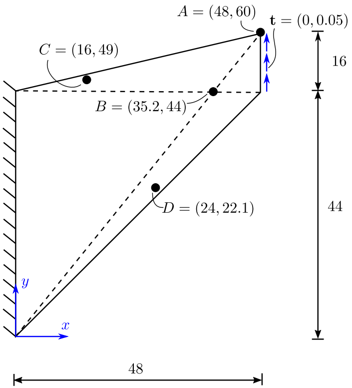


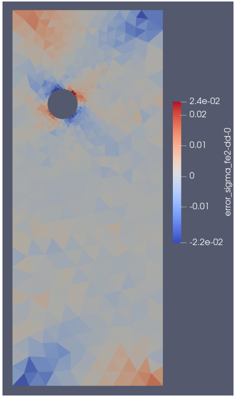


(from A. Platzer's PhD thesis)

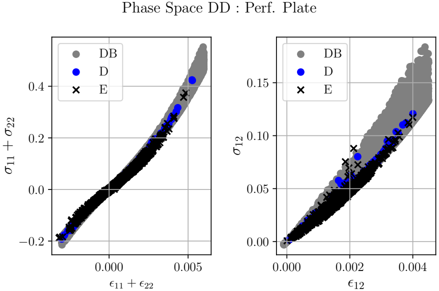
Numerical Examples

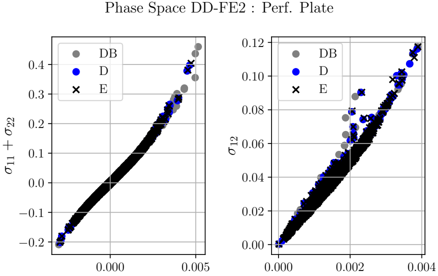
- ▷ 1) Cook Membrane, 2) Perforated plate
- ▷ Meshes P1 (N_{el}): 868 (Cook) , 905 (PP Coarse), 2004 (PP Fine)
- ▷ Parameters: $N_d = 10$, $\texttt{maxupdate} = 20$, $\mathbb{C}$ estimated/updated





Comparison Pure DDCM to DD-FE^2





Perforated plate

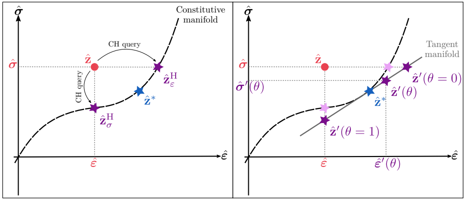
-	DDCM	DD-FE2
N_d^0	10000	10
dist_{rel}	6.81e-02	9.76e-4
$e_{L^2}^{rel}(u, u_{ref})$	6.12e-03	1.48e-04
$e_{L^2}^{rel}(\boldsymbol{\sigma}, \boldsymbol{\sigma}_{ref})$	4.39e-02	8.43e-03
$e_{L^2}^{rel}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_{ref})$	9.62e-02	7.41e-03
N_d	10000	931
$\mathtt{it}_{\mathtt{out}}$	-	46
$\mathtt{it}_{\mathtt{total}}$	8	69
$t_{\text{online}}(s)$	2.88	14.89
$t_{\text{offline}}(s)$	78.07	0.078
$t_{Total}(s)$	80.95	14.97
Speed-up	1	$\mathbf{5.41}$

$\longrightarrow$ speedup w.r.t. FE^2 $\approx 11\times$

Active learning

DD-AL method:

- ▷ enhanced DDCM strategy:
  - ◦ accelerated projection on equilibrium manifold
  - ◦ Sylvester mean metric estimation for $\mathbb{C}$
  - ◦ locally convex reconstruction
  - ◦ tangent reconstruction
- ▷ AL labellisation:
  - ◦ Greedy (G) score: $G_{(v)}^{(j)} = (\sqrt{w_j})d_{1j}$
  - ◦ Entropy (E) score: $E^{(j)} = \tilde{E}^{(j)} \times G^{(j)}$

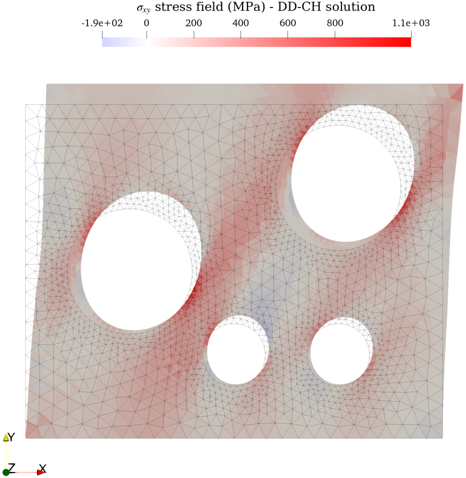


$$\tilde{E}^{(j)} = -\sum_{i=1}^{k} p_{ij}\log(p_{ij}) \ , \ p_{ij} = \frac{\exp(-\bar{d}_{ij})}{\sum_{l=1}^{k}\exp(-\bar{d}_{lj})} \ , \ \bar{d}_{ij} = \frac{d_{ij} - \max_{l\in[1,k]} d_{lj}}{\max_{l\in[1,k]} d_{lj}}$$

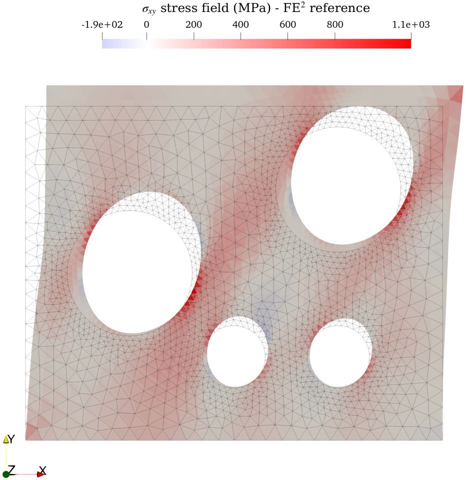
[Rocha *et al.*, *under review*]

DD-AL example

DD vs. FE^2 simulation of a holed plate (σ_{xy} stress component)



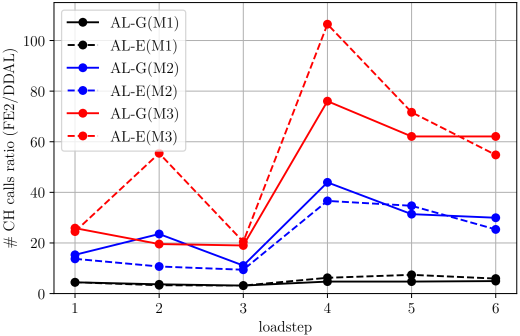
DD-CH



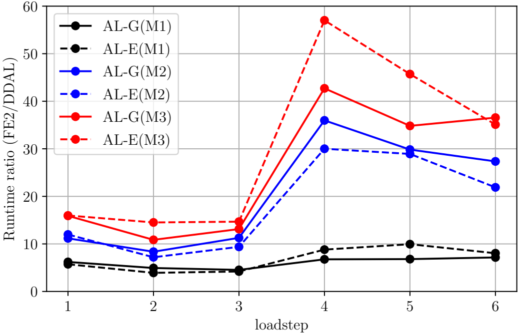
FE^2

DD-AL example

Improved efficiency of AL strategies: speedup w.r.t. FE^2



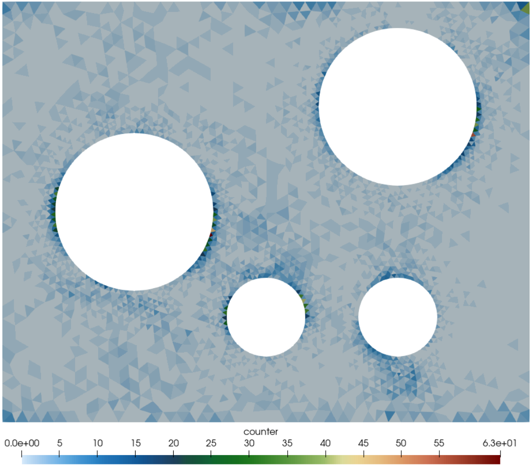
CH calls



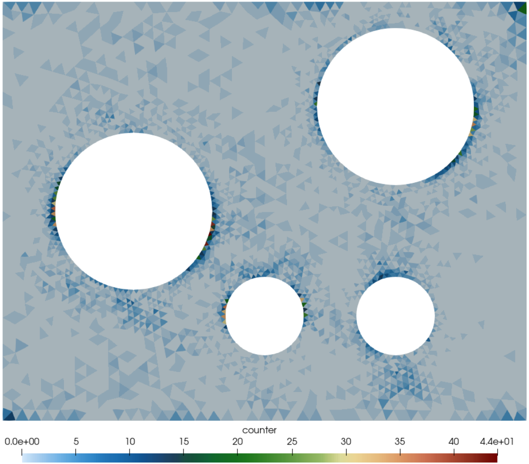
CPU

DD-AL example

Improved efficiency of AL strategies: # of call to CH



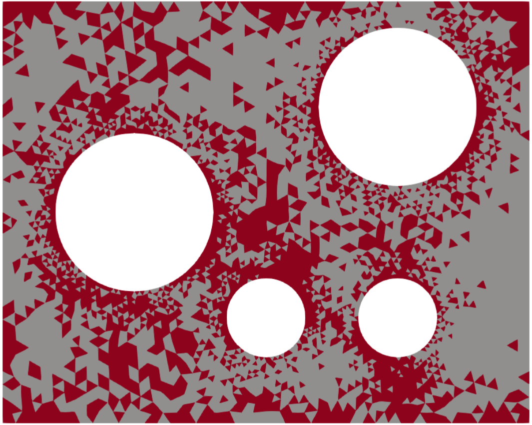
G-score



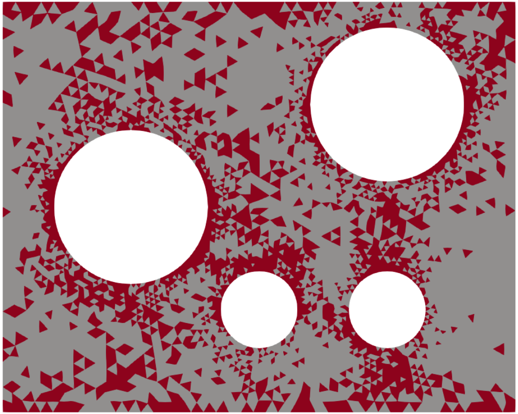
E-score

DD-AL example

Improved efficiency of AL strategies: # of call to CH (binary view)



G-score



E-score

DD Multiscale Nonlinear Elasticity

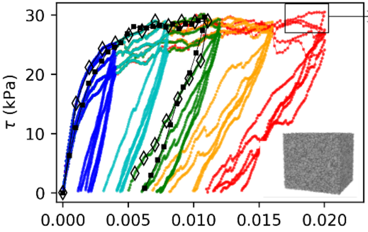
Main observations:

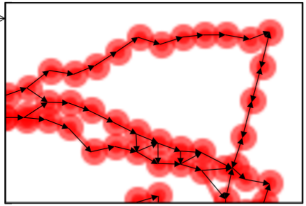
- On-the-fly databases can drastically speed-up pure FE^2 approaches.
- Larger speedups are obtained for larger problems
- Active Learning strategy with Entropy score offers further performance gains
- The recreation of BallTree, KDTree using sklearn have not shown to be a bottleneck in terms of computational costs.
- **ddfenics**[1] has been shown to be an efficient toolbox to test new formulations in DDCM : nonlinear problems, functional spaces, solvers, ...

[1] `github.com/felipefr/ddfenics`

Incremental data driven inelasticity

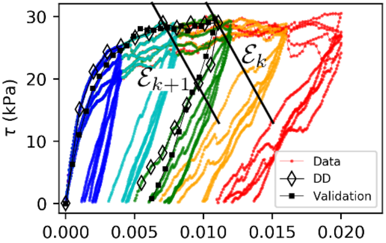
Construction of connected paths (observations + thermodynamics)





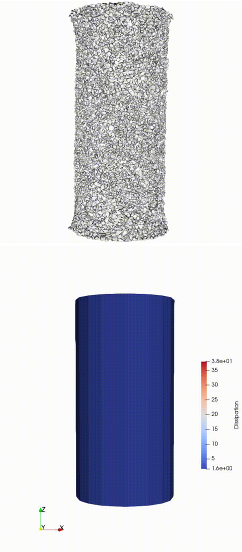
Data points and connections

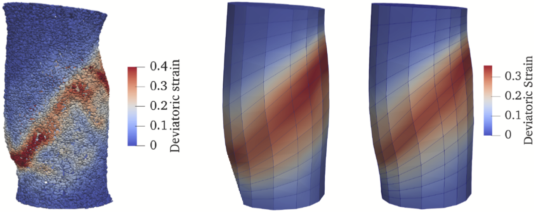
Incremental DDCM problem



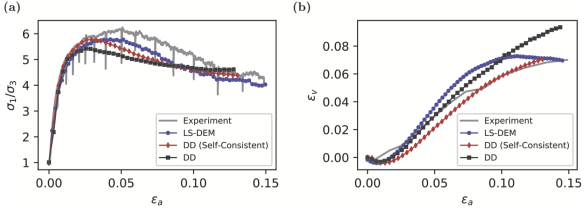
Application: shear-banding in sand

Formation of a shear band in sand (triaxial experiment)





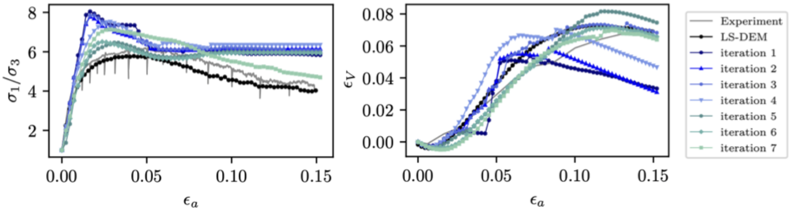
LS-DEM DD DD (self-consistent)



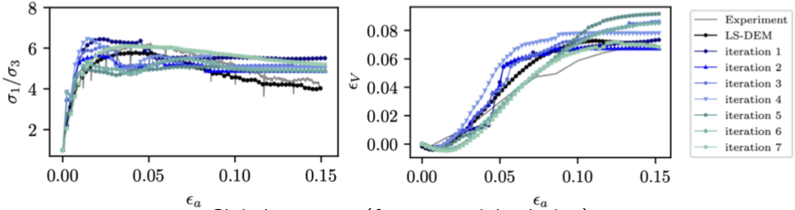
[Karapiperis et al., 2021]

Reinforcement learning

Iterative approach (identify relevant strain path to sample)



Global response (from mechanical solution)



Global response (from material solution)

[Gorgogianni et al., 2023]

Data-driven multiscale paradigm(s)

Overview:

- data generation by computations on RVEs (numerical material):
  FE, FFT, mean-field, ...
- *a priori* generation of a data base
  - **offline** computations (low marginal cost)
  - difficulty = sampling (range, density, distribution, ...)
- *dynamic* data generation
  - automatic **sampling** (distance criterion, or other $\sim$ adaptive learning)
  - difficulty = storage / history effects (*cf.* [Chaouch & Yvonnet, 2024])
  - higher initial cost, with asymptotic reduction ($<$ FE^2)
- *iterative* data generation
  - improvement / enrichment of database through repeated simulations [Prume *et al.*, 2025]
  - more significant computational cost
  - can be seen as **reinforcement learning**

Perspectives

Main conclusion:

- DDCM allows to generate multi-scale data only when and where needed
  - importance sampling
  - $\sim$ parcimony
- applicable to numerical and semi-analytical homogenization approaches

Perspectives:

- data reuse: pick data in existing set *vs.* generating new data
- data storage issue (full micro-fields) !
- potential combination with data-reduction techniques
- community effort ?