« Data-driven » en Mécanique des Matériaux et des Structures

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Data-driven Computational Mechanics

new philosophy based on the intensive use of data

: a future revolution

in computational engineering

Data-driven Computational Solid Mechanics

Data :geometry, loading, material

Data-driven Computational Mechanics

- **Pioneer works : Data used without Material Science**
  Ortiz et al 2016,2017…; Chinesta et al 2016,2017…

Data-driven Computational Mechanics

- **Today works**
  - numerous
  - many of them: hybrid
  - interesting solutions **but** for particular situations

Challenge: history-dependent materials in 2D and 3D

OUTLINE

Data-driven computation(material)

1. Today approach in computational solid mechanics

2. Data-driven computational approaches (complex nonlinear materials)

3. A DD approach for complex materials with memory: basic features and numerical tools

4. A DD approach for complex materials with :illustrations

5. Conclusion

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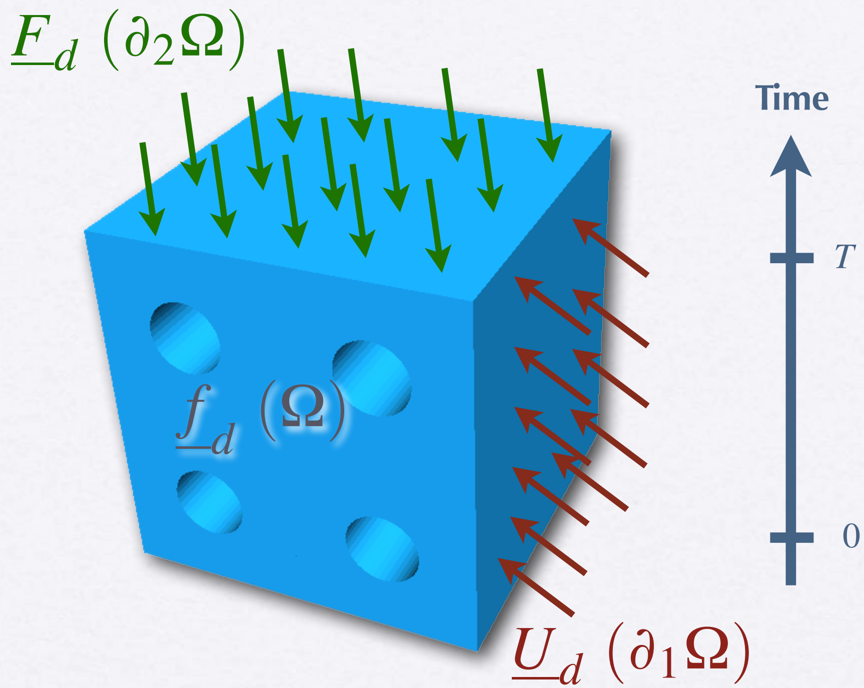
Today computational approach over $[0, T] \times \Omega$

Find $s = (\dot{\boldsymbol{\varepsilon}}^p, \boldsymbol{\sigma}) \in \boldsymbol{S}^{[0,T]}$

such that



Kinematic admissibility

$$\varepsilon^p = \varepsilon - \varepsilon^e \qquad \varepsilon^e = K^{-1}\sigma$$

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\underline{U}) \qquad \underline{U}_{|\partial_1\Omega} = \underline{U}_d$$

Static admissibility

$$\forall \underline{U}^\star \in \boldsymbol{\mathcal{U}}_0^{[0,T]},$$

$$-\int_{[0,T]} \mathrm{Tr}[\boldsymbol{\sigma}\boldsymbol{\varepsilon}^\star] d\Omega dt + \int_{[0,T]\times\Omega} \underline{f}_d \cdot \underline{U}^\star d\Omega dt + \int_{[0,T]\times\partial_2\Omega} \underline{F}_d \cdot \underline{U}^\star dS dt = 0$$

Constitutive relations

Today computational approach over $[0, T] \times \Omega$

Find s defined over $[0,T] \times \Omega$ such that:

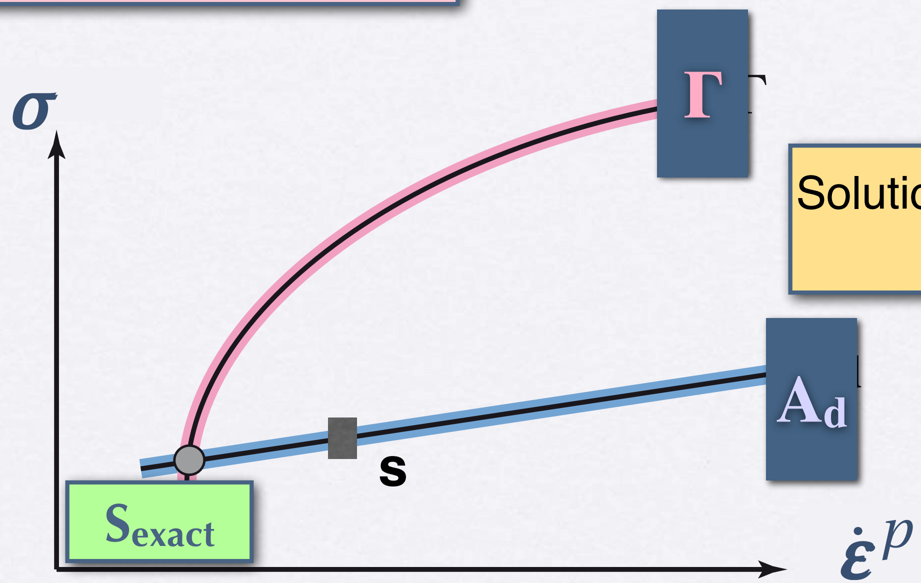
- admissibility(exact)
- constitutive relations (from experimental data)

Geometric representation

Find $s = (\dot{\boldsymbol{\varepsilon}}^p, \boldsymbol{\sigma}) \in \boldsymbol{S}^{[0,T]}$ such that:

A_d • admissibility(exact) — linear, possibly global

Γ • constitutive relations — local, possibly nonlinear



Solution: distance(s ,(Γ)) = 0
or minimun

Material Science

Today computational approach- The Material Science approaches

- **Functional approach**: identification needs a lot of experimental histories

- **Internal variable approach** : identification needs much less data

Classical Computational approach- Internal (hidden) variable approach

State $\mathbf{s} = (\dot{\boldsymbol{\varepsilon}}^p, \dot{\mathbf{X}}, \boldsymbol{\sigma}, \mathbf{Y}) \in S^{[0,T]}$

X ,Y : additional internal hidden variables

State equations

$$\mathbf{Y} = \boldsymbol{\Lambda}\mathbf{X}$$

State evolution laws

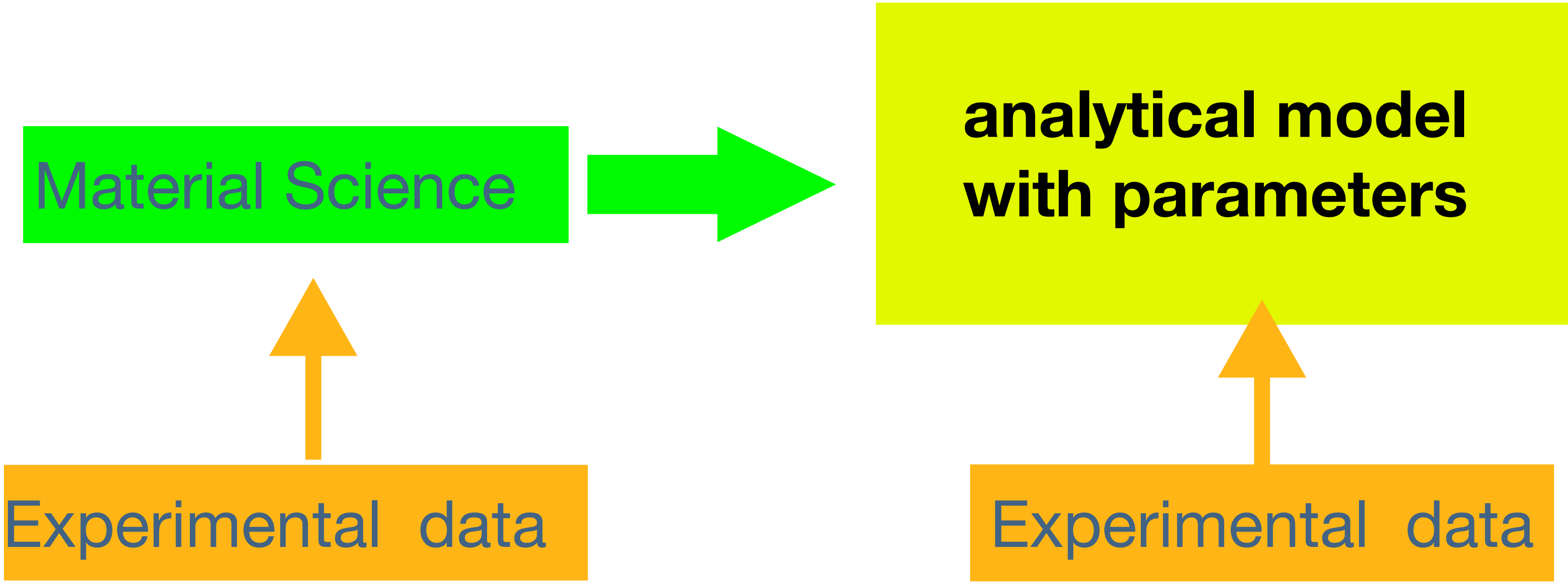
$$\begin{bmatrix} \dot{\boldsymbol{\varepsilon}}_p \\ -\dot{\mathbf{X}} \end{bmatrix} = \mathbf{B}\left(\begin{bmatrix} \boldsymbol{\sigma} \\ \mathbf{Y} \end{bmatrix}\right)$$

B : positive

+ initial cond

Modelling of materials

Today



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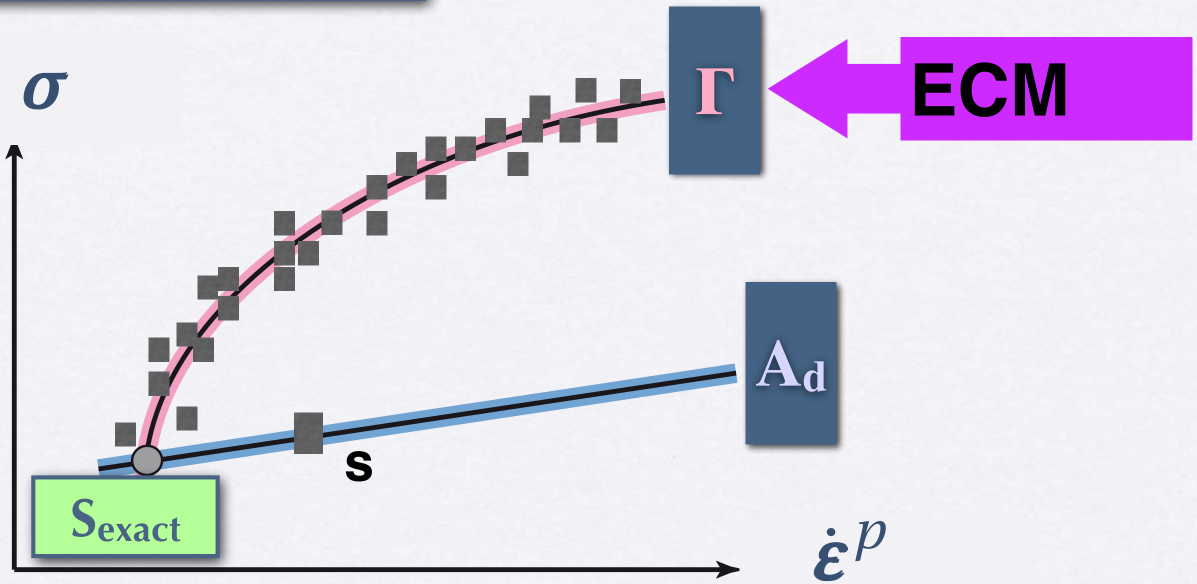
Data-driven computation
Ideal situation

Find $s = (\dot{\boldsymbol{\varepsilon}}^p, \boldsymbol{\sigma}) \in \mathcal{S}^{[0,T]}$ such that:

$\mathcal{A}_d$ • admissibility (exact) — linear, possibly global

Γ • constitutive relations — local, possibly nonlinear



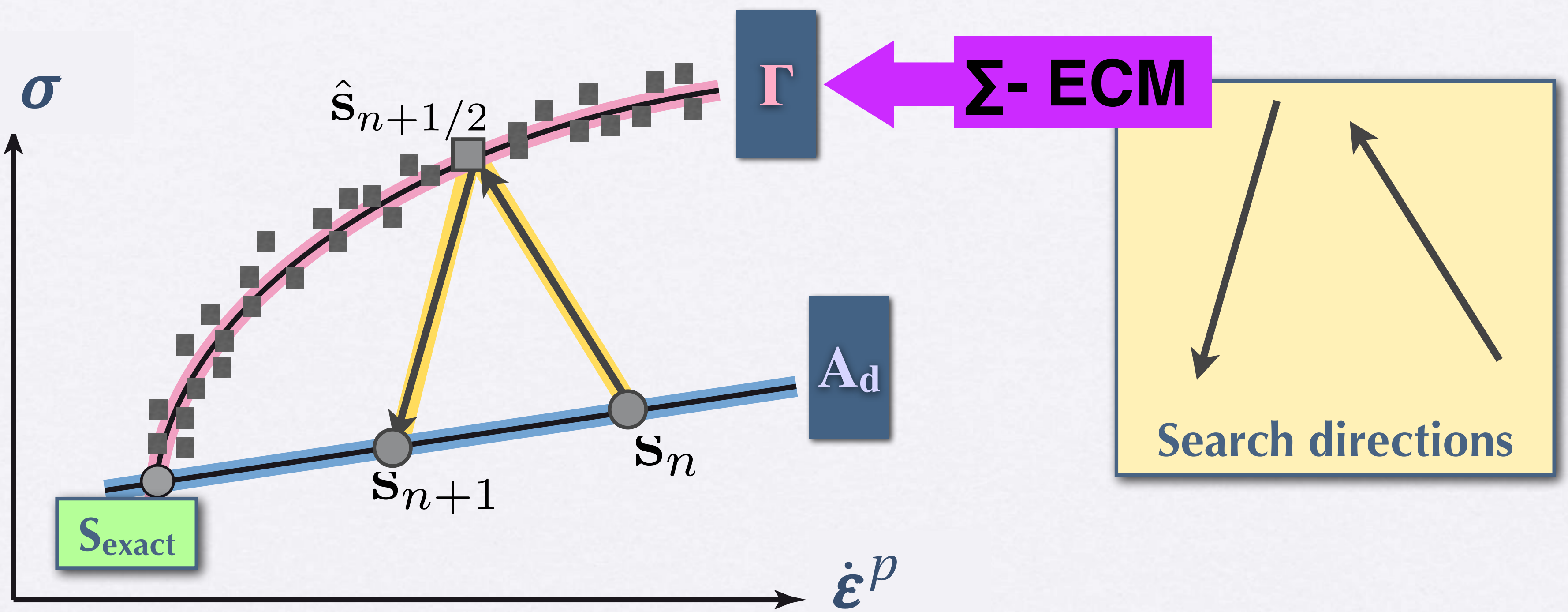
Data-driven computation-the solver LATIN

Iterative and alternative scheme

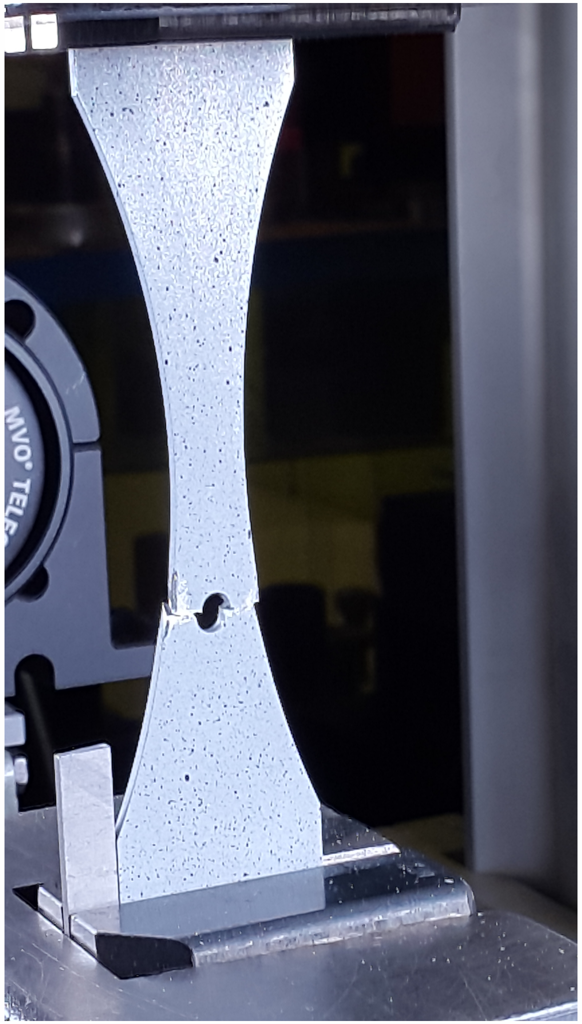
Local stage | Linear stage

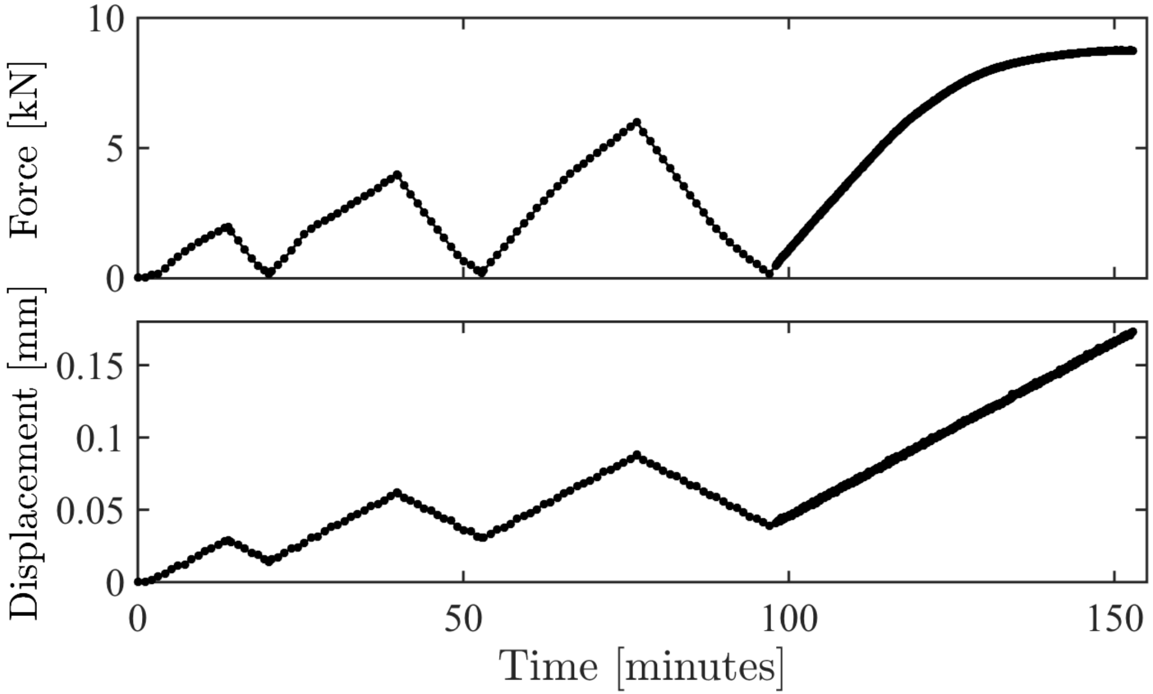
$$\cdots \longrightarrow \mathbf{s}_n \in \mathbf{A_d} \longrightarrow \underbrace{\hat{\mathbf{s}}_{n+1/2} \in \Gamma \longrightarrow \mathbf{s}_{n+1} \in \mathbf{A_d}}_{\text{Iteration } n+1} \longrightarrow \hat{\mathbf{s}}_{n+3/2} \longrightarrow \cdots$$

$$\mathbf{s}_{ex} = \mathbf{A_d} \cap \Gamma$$

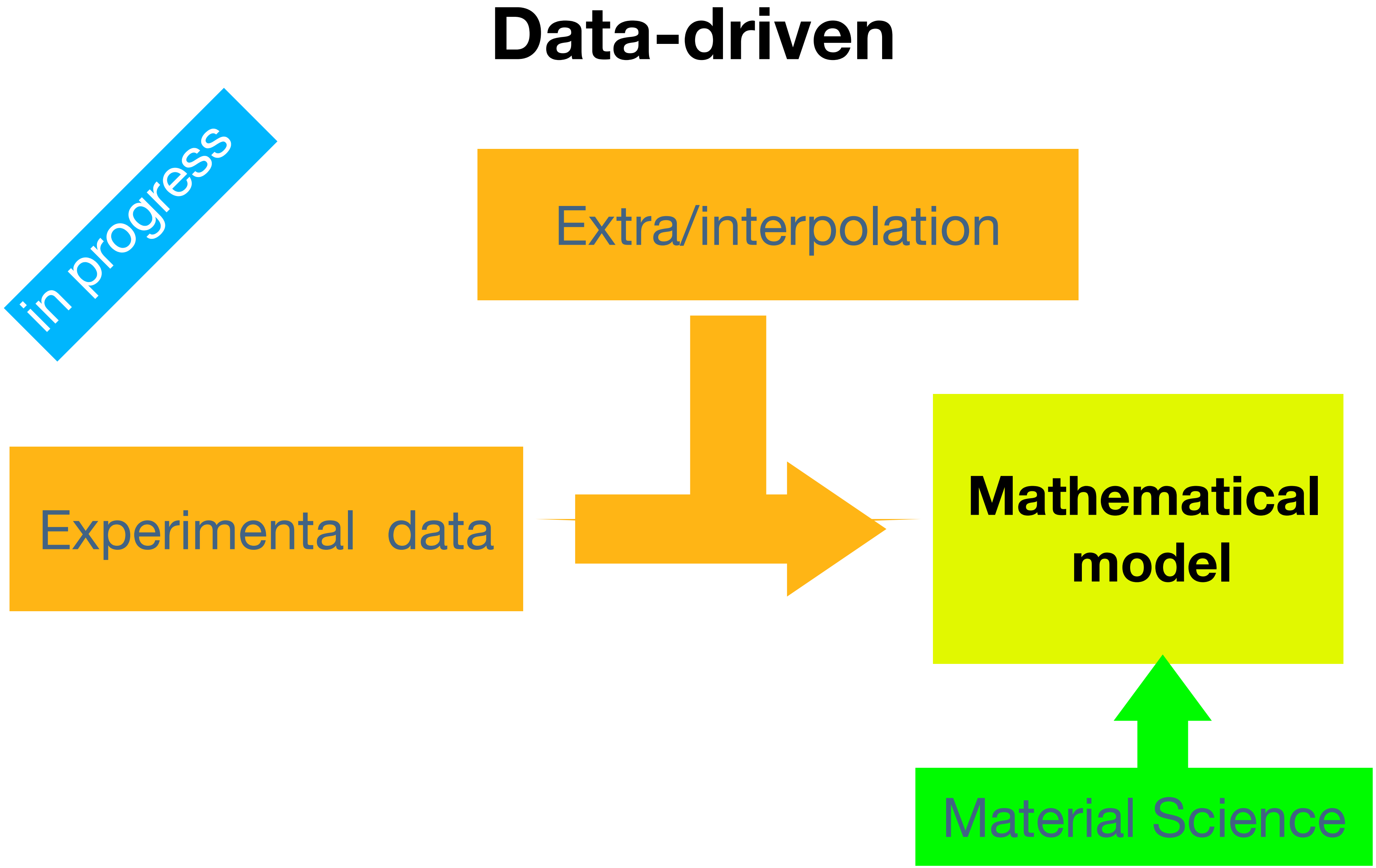


The Experimental Constitutive Manifold- The ECM-Tests





Data-driven modelling of materials



DD works in progress

- Data-driven approaches based on « 0 » physics

  material functional approach (exp. data ↑↑↑)

DD works in progress

- Data-driven approaches based on physics(at least partially)
  - Deep Neural Network (material functional approach: data↑↑↑)
  - Internal Variable Framework
    - GENERIC (hamiltonian-dissipative formulation)

      Ottinger-Grmela 97, Mielke 11
    - Experimental Constitutive Manifold

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Come back- Internal (hidden) variable approach

State $\mathrm{s} = (\dot{\varepsilon}^p, \dot{\mathbf{X}}, \boldsymbol{\sigma}, \mathbf{Y}) \in S^{[0,T]}$

X ,Y : additional internal hidden variables

State equations

$$\mathbf{Y} = \boldsymbol{\Lambda}\mathbf{X}$$

State evolution laws

$$\begin{bmatrix} \dot{\boldsymbol{\varepsilon}}_p \\ -\dot{\mathbf{X}} \end{bmatrix} = \mathbf{B}\left(\begin{bmatrix} \boldsymbol{\sigma} \\ \mathbf{Y} \end{bmatrix}\right)$$

X ,Y : not intrinsic

+ initial cond

Come back-
Internal (hidden) variable approach

- Additional internal variables : a choice

- Best choice (internal variable transformation)

Normal formulation X = Y (Ladeveze 1989,2020)

Stable materials

Come back-
Internal (hidden) variable approach

- **Viscoplasticity with one hidden internal variables $X \in \mathbb{R}^q$**

$$\boldsymbol{\varepsilon}_{p,p} = \boldsymbol{g}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

$$\boldsymbol{X}_{,p} = \boldsymbol{h}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

$$\dot{p} = f(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} \geqslant 0$$

$$\boldsymbol{X} = 0 \quad \boldsymbol{\varepsilon}_p = 0 \quad \text{at} \quad t = 0$$

+ thermodynamics constraints

The Experimental Constitutive Manifold-Raw experimental data

- elasticity tensor

- a set of time-histories of pairs *inelastic strain rate / stress* : $\mathscr{H}^{(0,P)}$

written in term of **« material time »**

where $$p^i = \int_O^T |\dot{\boldsymbol{\varepsilon}}_p^i| dt$$ (cumulated inelastic strain)

ECM-definition : { $s_i(p) = (\boldsymbol{\varepsilon}_{p,p}, \boldsymbol{\sigma}, \dot{p})$ $i \in N(p)$; $p \in [0, P]$ **}**

The Experimental Constitutive Manifold-Fundamentals

internal variable framework

(Thermodynamic)

a structuring of ECM

The Experimental Constitutive Manifold-Fundamentals

- **Structuring of ECM with one hidden internal variables $X \in R^q$**

$$\boldsymbol{\varepsilon}_{p,p} = \boldsymbol{g}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

$$\boldsymbol{X}_{,p} = \boldsymbol{h}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

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$$\boldsymbol{X} = 0 \quad \boldsymbol{\varepsilon}_p = 0 \quad \text{at} \quad t = 0$$

for all given time-history $s_i(p) = (\boldsymbol{\varepsilon}_{p,p}, \boldsymbol{\sigma}, \dot{p})$ $i \in N(p)$; $p \in [0, P]$

+ thermodynamics constraints

The Experimental Constitutive Manifold-Fundamentals

- **Structuring of ECM with one hidden internal variables $X \in R^q$**

$$\boldsymbol{\varepsilon}_{p,p} = \boldsymbol{g}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

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$$\boldsymbol{X} = 0 \quad \boldsymbol{\varepsilon}_p = 0 \quad \text{at} \quad t = 0$$

only property
$\boldsymbol{g}, \boldsymbol{h}, f$: single-valued

+ thermodynamics constraints (case where dissipation is not measured)

$$Tr(\sigma\, \boldsymbol{\varepsilon}_{p,p}) - X \,.\, X_{,p} \geq 0 \qquad \dot{p} > 0$$

The ECM-Central Problem (the structured ECM)

to build X and q

specific tool inspired by classical Big Data techniques

ECM-potential **u**: if O(1) , no X

if not , X = arg min **u**

Our answer

Tool 1 - The ECM-Central Problem

Model problem

- « *Raw experimental* » *data* $\boldsymbol{\Sigma} \equiv \{(X,Y)^i | X, Y \in \boldsymbol{R}^n, i \in \boldsymbol{N}\}$

Z : internal (hidden) variable   spaces $\boldsymbol{\Sigma}_X, \boldsymbol{\Sigma}_Y, \boldsymbol{\Sigma}_Z$

- **Problem** : Find Z such f is a single-valued function

$$\underset{\boldsymbol{\Sigma}_X \times \boldsymbol{\Sigma}_Z}{f : (X^i, Z^i)} \rightarrow \underset{\boldsymbol{\Sigma}_Y}{Y^i} \quad \text{with} \quad \{(X^i, Y^i)\ i \in \boldsymbol{N}\}$$

Tool 1 - The ECM-Central Problem

- **Idea** (f : regular)

for $d^2(X^I, Z^I; X^j, Z^j) \leq \varepsilon^2 \Longrightarrow \alpha^{I\,j} = [\, d^2(X^I, Z^I; X^j, Z^j) \;-\; d^2(Y^I, Y^j)] \times 1/\varepsilon^2$

two cases

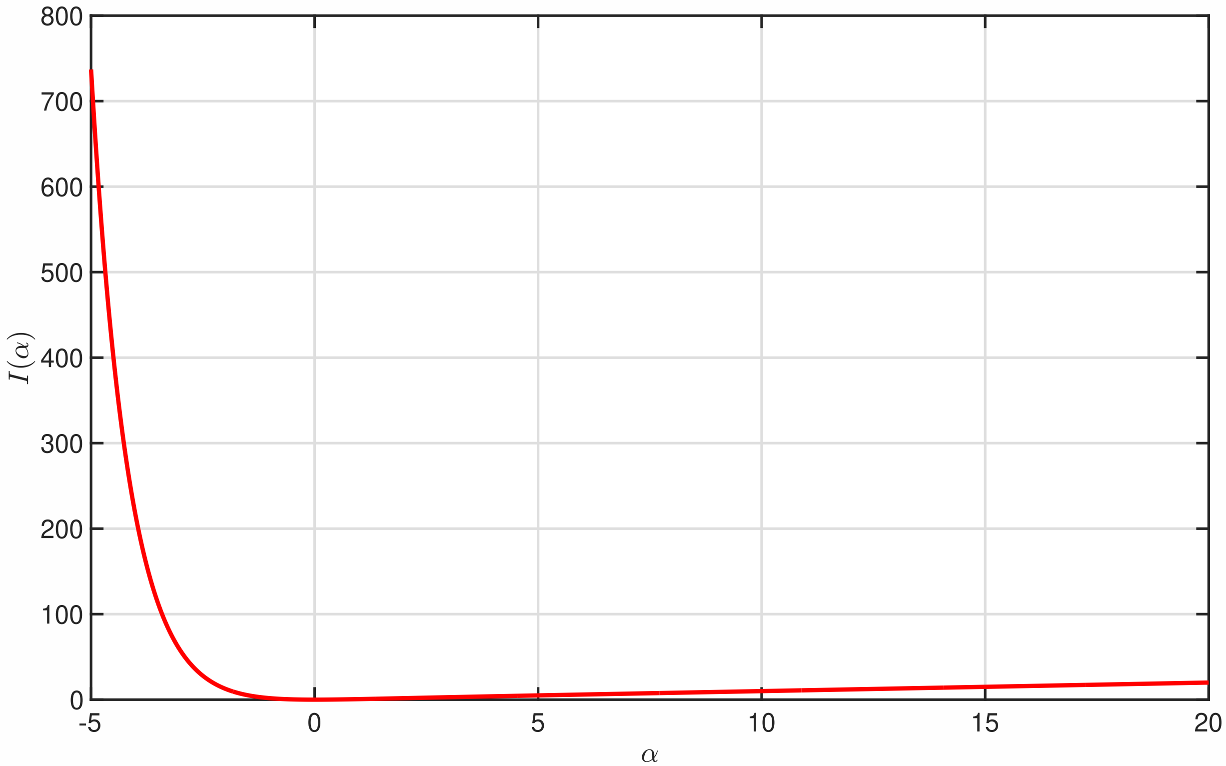
– $\alpha^{I\,j} = o\,(1)$ f: single valued

– $(-\alpha^{I\,j}) \gg 1$ f: multi valued

Tool 1 - The ECM-Central Problem

- **Univocity indicator** (variant of Kullback-Leibler divergence)

  - $I(\alpha) = (\exp(-\alpha)-1)(-\alpha)$: convex,positive,« linear » for $\alpha \geq 0$



$\alpha \in [-\infty, +\infty]$

  - $\mathbf{u}(Z) = \sum_{i \in \mathbf{N}} \sum_{j \in \mathbf{N}} P^{ij} I(\alpha^{ij})$

Tool 1 - The ECM-Central Problem

separator $P^{ij} = \Gamma_{ij} \; / \; \left(\sum_{j \in \mathbf{N}} \Gamma_{ij} \right)$

where $\Gamma_{ij} = \exp\left(- d^2(X^i, Z^i; X^j, Z^j) \,/\, \varepsilon^2 \right)$

$$d\,(X^i, Z^i; X^j, Z^j) = O(\varepsilon) \Leftrightarrow \quad P^{ij} = O(1)$$

otherwise $\quad P^{ij} \sim 0$

Application

$\varepsilon = 2/100$ ($N_{\text{neighbors}} \sim 10$)

Tool 1 - The ECM-Central Problem

Construction of the internal variable Z

$$f : (X^i, Z^i) \to Y^i$$
$$\boldsymbol{\Sigma}_X \times \boldsymbol{\Sigma}_Z \quad \boldsymbol{\Sigma}_Y$$

- $\boldsymbol{\Sigma} \equiv \{(X, Y)^i | X, Y \in \boldsymbol{R}^n, i \in \boldsymbol{N}\}$
- Unknowns : Z , $\boldsymbol{\Sigma}_Z$
- Tools: $P^{ij}(X^i, Z^i ; X^j, Z^j)$; $\mathbf{u}(X, Z; Y)$

$$Z = \underset{Z'}{\arg\min}\ \mathbf{u}(X, Z'; Y)$$

Z : modulo a X-function

additional constraints

Tool 1 - The ECM-Central Problem

- **ECM -potential ($X \in R^q$) : a solution**

$$\left(X_i(p) \in \mathbf{R}^q;\ i \in \mathbf{N}(p);\ p \in [0, P] \right) = \arg\min_{X'} \mathbf{u}(X')$$

stiff minimization problem : (augmented lagrangian, PGD)

Tool 1 - The ECM-Central Problem

- **Solution with one hidden internal variables $X \in R^q$**

$$\boldsymbol{\varepsilon}_p^{i},\ \boldsymbol{\varepsilon}_{p,p}^{i},\ \boldsymbol{X}^{i},\ \boldsymbol{X}_{,p}^{i},\ \sigma^{i},\ \dot{\boldsymbol{p}}^{i},\ \boldsymbol{p}^{i} \qquad i \in \mathbf{N}$$

+ thermodynamics constraints (case where dissipation is not measured)

$$Tr(\sigma^{i}\boldsymbol{\varepsilon}_{p,p}^{i}) - X^{i}.X^{i}_{,p} \geq 0 \qquad \dot{p}^{i} > 0$$

Tool 2 : interpolation

ECM : set of particular experimental data

Inter/extrapolation

Ext (ECM) : practical mathematical model

available data ↗↗↗

still very limited

Tool 2 : interpolation

- **Interpolation based on RKHS** (Reproducing Kernel Hilbert Space)

  (Belkin 2018 ,Rieger -Zwicknagl 2010,Narcowick et al 2004,…)

  — Gaussian kernel : $\exp(\ -\beta\ d^{2}(\ X,\ X_{,})\ \ )$

  — among efficient interpolation methods for regular functions

  exponential convergence in term of the fill distance h

  $$h = \underset{(\sigma,X)\in \mathbf{D}}{\mathrm{Max}}\ \underset{(\sigma_i,X_i)\in \mathbf{D_N}}{\mathrm{Mini}}\ d(\ \sigma\ ,X;\ \sigma_i\ ,X_i)$$

  — reproduce « exactly » given experimental data

Tool 2 : interpolation

Example : construction of the elasticity domain : $p = f(\sigma, X)$ $\dot{p} > 0$

data (experimental points)

$$(\sigma, X, p)^i \quad i \in I_+ = (i \,;\, \dot{p}^i > 0)$$

> 0

interpolation $p = f(\sigma, X) = \underline{t}^T [\,\mathbf{G} + \mu\, \mathbf{1}]^{-1} \underline{g}(\sigma, X) \qquad \mu > 0$

where $G_{ij} = \exp(-\beta\, d^2(\sigma^i, X^i; \sigma^j, X^j))$

$\underline{t}_i = p^i$

$\underline{g}_i(\sigma, X) = \exp(-\beta\, d^2(\sigma, X; \sigma^i, X^i))$

Tool 2 : interpolation

- **Finally** : Ext(**ECM**)

$\boldsymbol{g},\boldsymbol{h},f$: interpolated functions

$$\boldsymbol{\varepsilon}_{p,p} = \boldsymbol{g}(\boldsymbol{\sigma},\boldsymbol{X},p) \quad \dot{p} > 0$$

$$\boldsymbol{X}_{,p} = \boldsymbol{h}(\boldsymbol{\sigma},\boldsymbol{X},p) \quad \dot{p} > 0$$

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+ thermodynamics constraints (case where dissipation is not measured)

$$Tr(\sigma\, \boldsymbol{\varepsilon}_{p,p}) - X \,.\, X_{,p} \geq 0 \qquad \dot{p} > 0$$

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Construction of the ECM Illustration

- Elasto-plastic materials
- Plane stress problems
- « Experimental data » : simulated

Construction of the ECM Illustration-The Central Problem

- **Structuring of ECM with one hidden internal variables $X \in R^q$**

$$\boldsymbol{\varepsilon}_{p,p} = \boldsymbol{g}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

+ thermodynamics constraints

$$\boldsymbol{X}_{,p} = \boldsymbol{h}(\boldsymbol{\sigma}, \boldsymbol{X}, p) \quad \dot{p} > 0$$

$$p = f(\boldsymbol{\sigma}, \boldsymbol{X}) \quad \dot{p} > 0$$

$$\boldsymbol{X} = 0 \quad \boldsymbol{\varepsilon}_p = 0 \quad \text{at} \quad t = 0$$

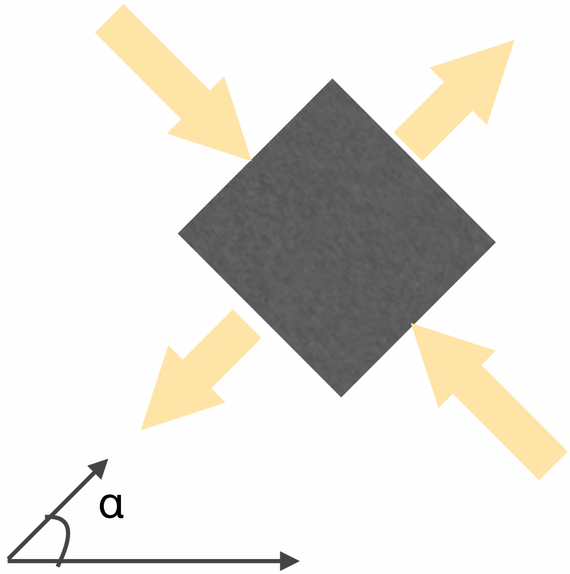
Domain of elasticity : star-shaped

$D(p) = \{\lambda\,(\boldsymbol{\sigma}, \boldsymbol{X});\ \lambda \in [0,1],\ p = f(\boldsymbol{\sigma}, \boldsymbol{X})\ \ \dot{p} > 0\}$

Material Science

Construction of the ECM

Illustration : Experimental data



Biaxial tests

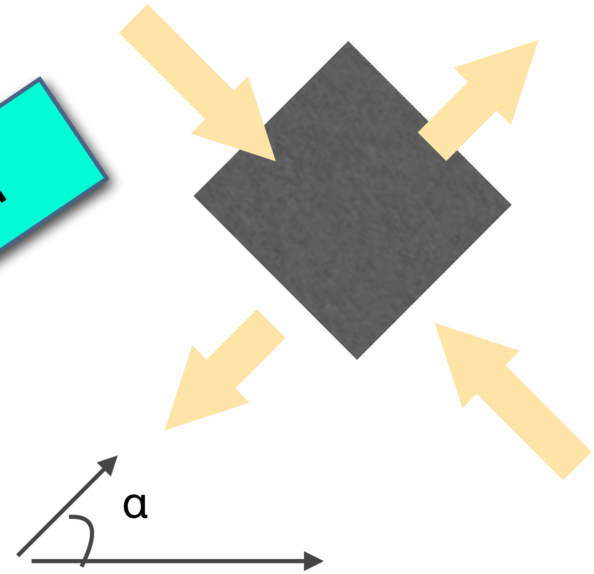
Direction: <u>m</u>(α) α ∈[-45°,+45°]

Biaxiality coef: (α) a ∈[-1,+1]

Construction of the ECM

Illustration : Experimental data

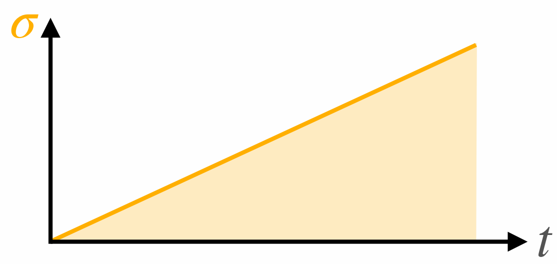
Isotropic material



Biaxial tests

Test program I $\mathscr{H}_P(0,P)$:proportional monotonous loadings

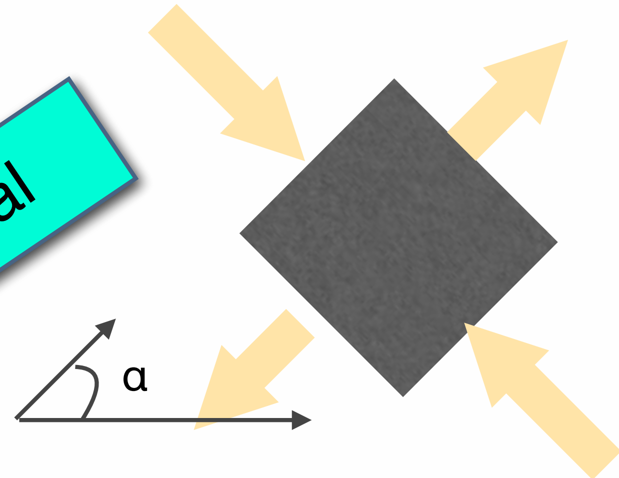
$\alpha = 0$; $\sigma_{nn} \geq \sigma_{tt}$ $\sigma_{tn} = 0$



Construction of the ECM

Illustration : Experimental data

Isotropic material

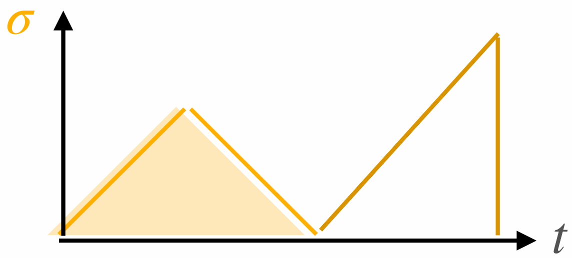


Biaxial tests

Test program 2 $\mathcal{K}_{NP}(0,P)$: non-proportional monotonous loadings

$p \in [0, P/2] \quad \alpha \in (-45°,+45°) \quad a \in [-1,+1]$

$p \in [P/2, P] \quad \alpha = 0 \; ; \; \sigma_{nn} \geq \sigma_{tt} \quad \sigma_{tn} = 0$



Construction of the ECM
Illustration

- « **Experimental** » **data :** generated by a plasticity model with isotropic and kinematic hardening

test program 1 $\mathscr{H}_P(0,P)$: Proportional monotonous loadings

+

test program 2 $\mathscr{H}_{NP}(0,P)$: Nonproportional biaxial tests

~ ~

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Number of tests : 340

Construction of the ECM
Illustration

- « **Experimental** » **data :** generated by a plasticity model with isotropic and kinematic hardening

test programs 1+2 : $\mathscr{H}_{P}(0,P) + \mathscr{H}_{NP}(0,P)$

$$\mathbf{u(\,0\,) = 10^{100} \gg 0(1)}$$

$$\mathbf{u(\,\varepsilon_p\,) = 4{,}3 \approx 0(1)}$$

ECM equivalent to a plasticity model

with isotropic and kinematic hardening

Construction of the ECM
Illustration

- « **Experimental** » **data :** generated by the plasticity model of Chaboche-Marquis

test programs 1+2 : $\mathscr{H}_P(0,P) + \mathscr{H}_{NP}(0,P)$

$$\mathbf{u(\varepsilon_p) = 4{,}3 \approx 0(1)}$$

$$\boldsymbol{\varepsilon}_p \neq \mathbf{X}_{CM}$$

Construction of the ECM
Keypoint 1

Keypoint 1 : ECM-Identification— Test number ?

Construction of the ECM
Keypoint 1

Example : construction of the elasticity domain : $p = f(\sigma, X)$ $\dot{p} > 0$

Test Programmes 1 and 2

Total number of tests : 25 , 340

Discretized admissible domain (p,σ,X) : 20^7 points

25 tests : 25 X 80 = 2000 experimental points

Construction of the ECM
Keypoint 1

Example : construction of the elasticity domain : $p = f(\sigma, X)$ $p > 0$

Verification guide

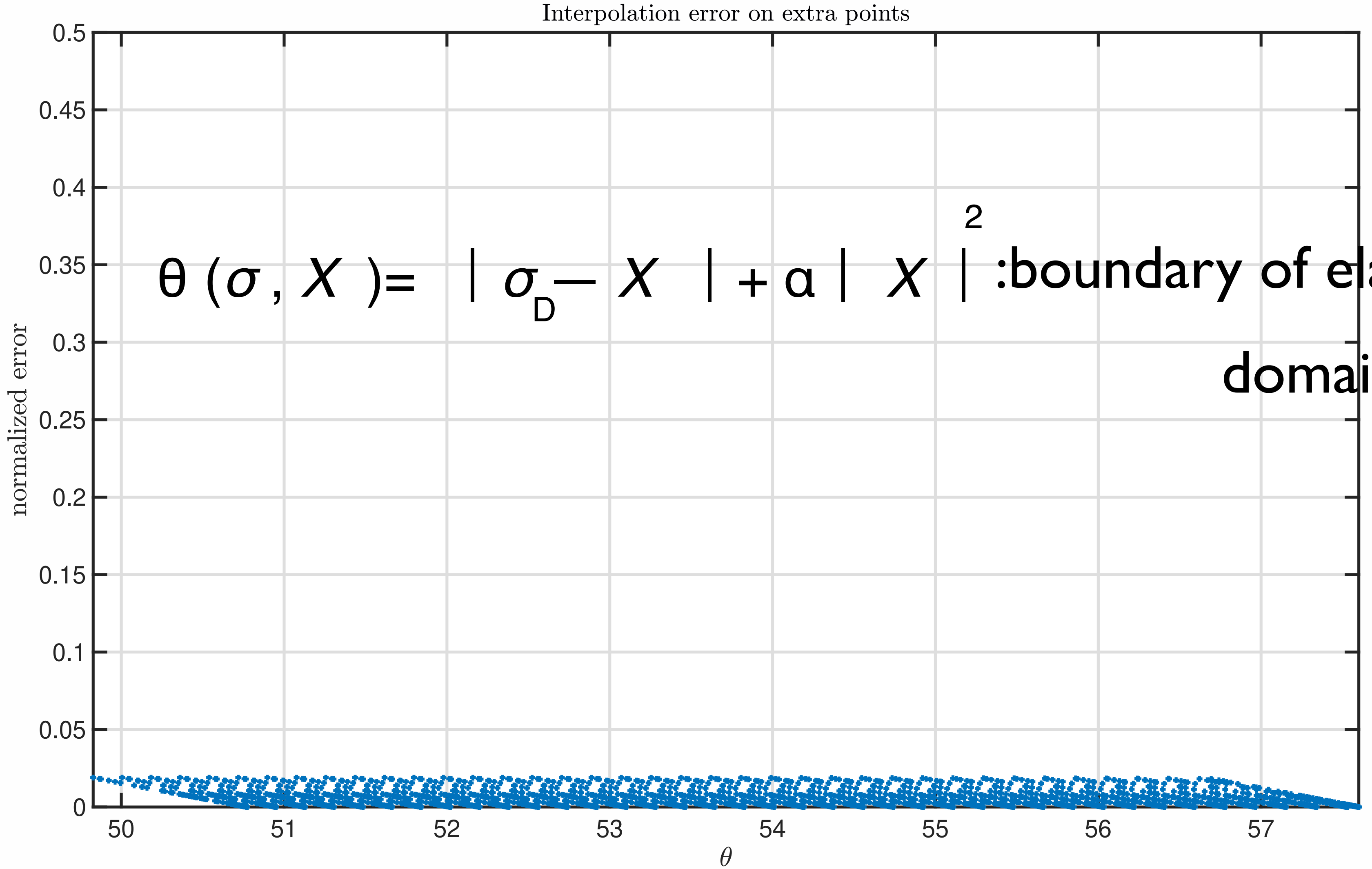
— Material Science $\Longrightarrow$ an ellipsoid

$$\theta(\sigma, X) = |\sigma_D - X| + \alpha |X|^2$$

— error $= \operatorname*{Max}_{J \in \text{reference points}} |\theta^J - \text{interpolated}(\theta)^J|$

Construction of the ECM
Keypoint 1

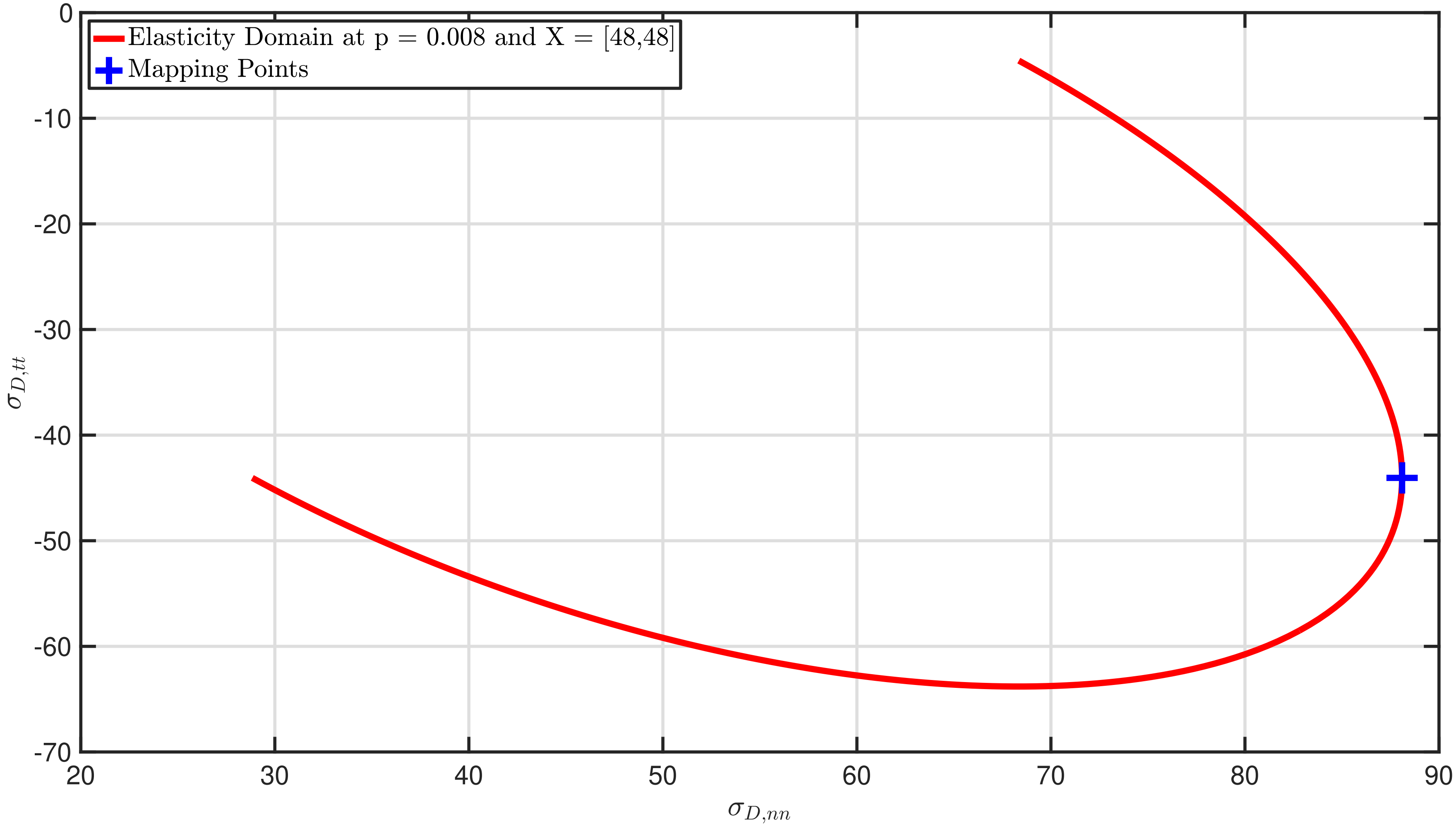
Total number of tests : 25



$$\theta(\sigma, X) = |\sigma_D - X| + \alpha |X|^2$$:boundary of elasticity domain

Construction of the ECM

Keypoint 1



Construction of the ECM

Keypoint 1

Total number of tests : 25 , 340

Similar Ext(ECM)

Keypoint 2: Learning process

Construction of the ECM

Keypoint 2

LEARNING

Experimental data ↗

↓

Hierarchical ECM

hidden variable number ↗

Construction of the ECM Illustration

- « **Experimental** » **data :** generated by the plasticity model of Chaboche-Marquis

test programs 1+2 : $\mathscr{H}_{P}(0,P) + \mathscr{H}_{NP}(0,P)$

FIRST STAGE

$\mathbf{u(\varepsilon_p) = 4{,}3 \approx 0(1)}$

first hidden internal variable

$\mathbf{X^1 = \varepsilon_p}$

Construction of the ECM
Keypoint 2

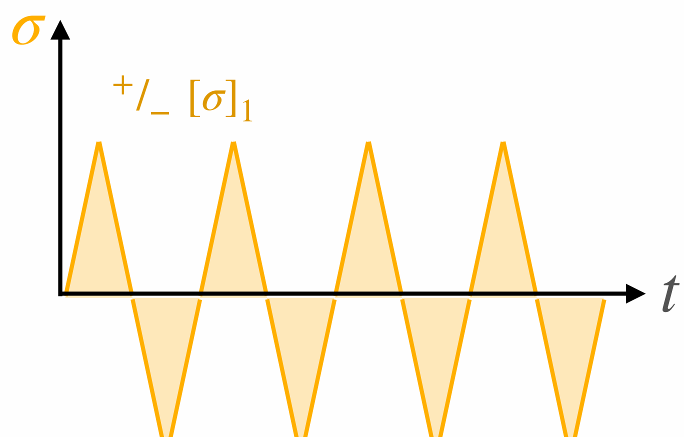
- « **Experimental** » **data :** generated by the plasticity model of Chaboche-Marquis

SECOND STAGE

additional test program 3

Cycling loading (4 cycles): $p \in [0, P]$

$\alpha = 0$ $a \in [-1,+1]$



Construction of the ECM
Keypoint 2

- « **Experimental » data :** generated by the plasticity model of Chaboche-Marquis

$$u(X^1) = 10^{20} \gg 1$$

$$X^1 = \varepsilon_p$$

NEW ECM

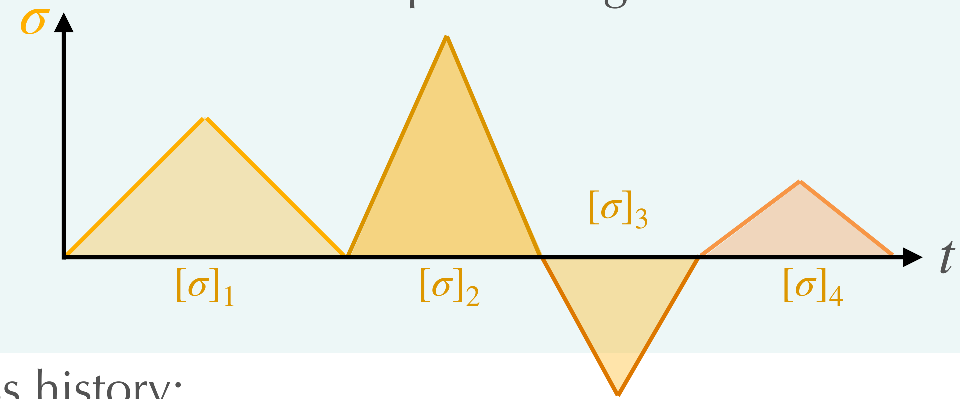
$$u(X^1, X^2) = 3{,}4 \approx 0(1)$$

New ECM equivalent to the plasticity model of Chaboche-Marquis

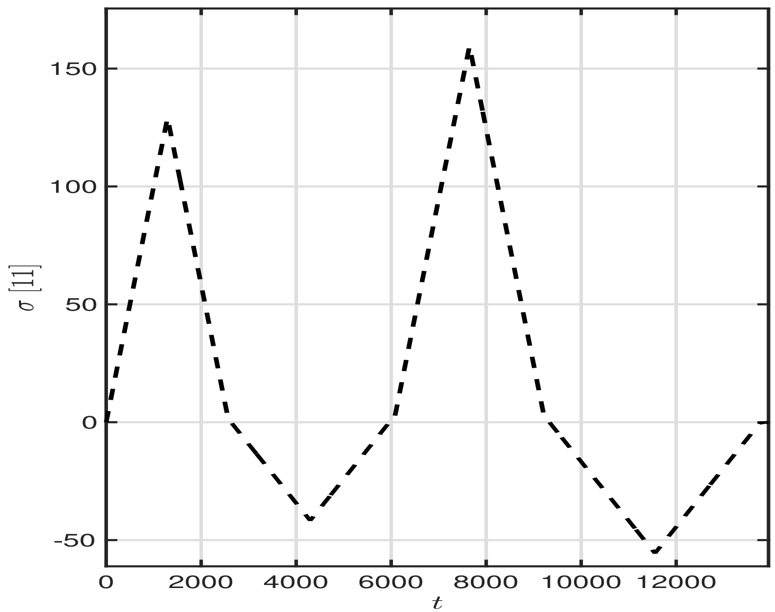
Data-driven computation

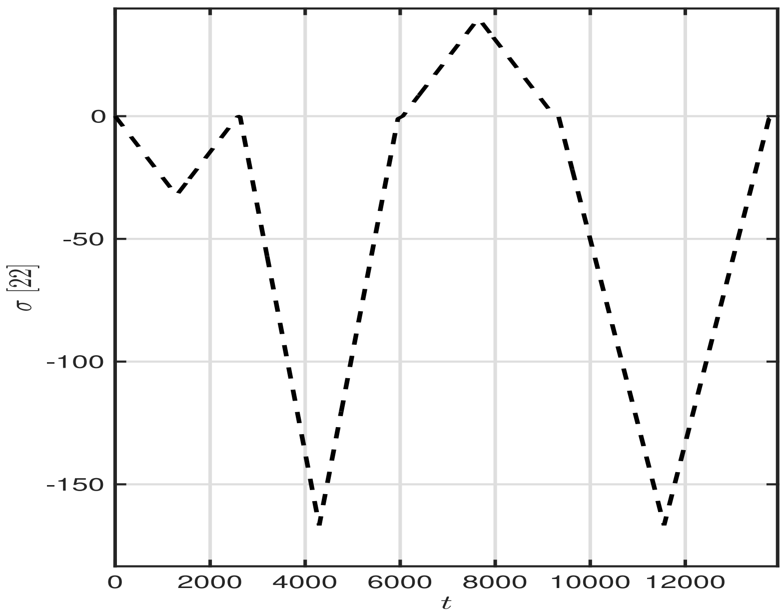
New loading scenario:

Four-steps loading



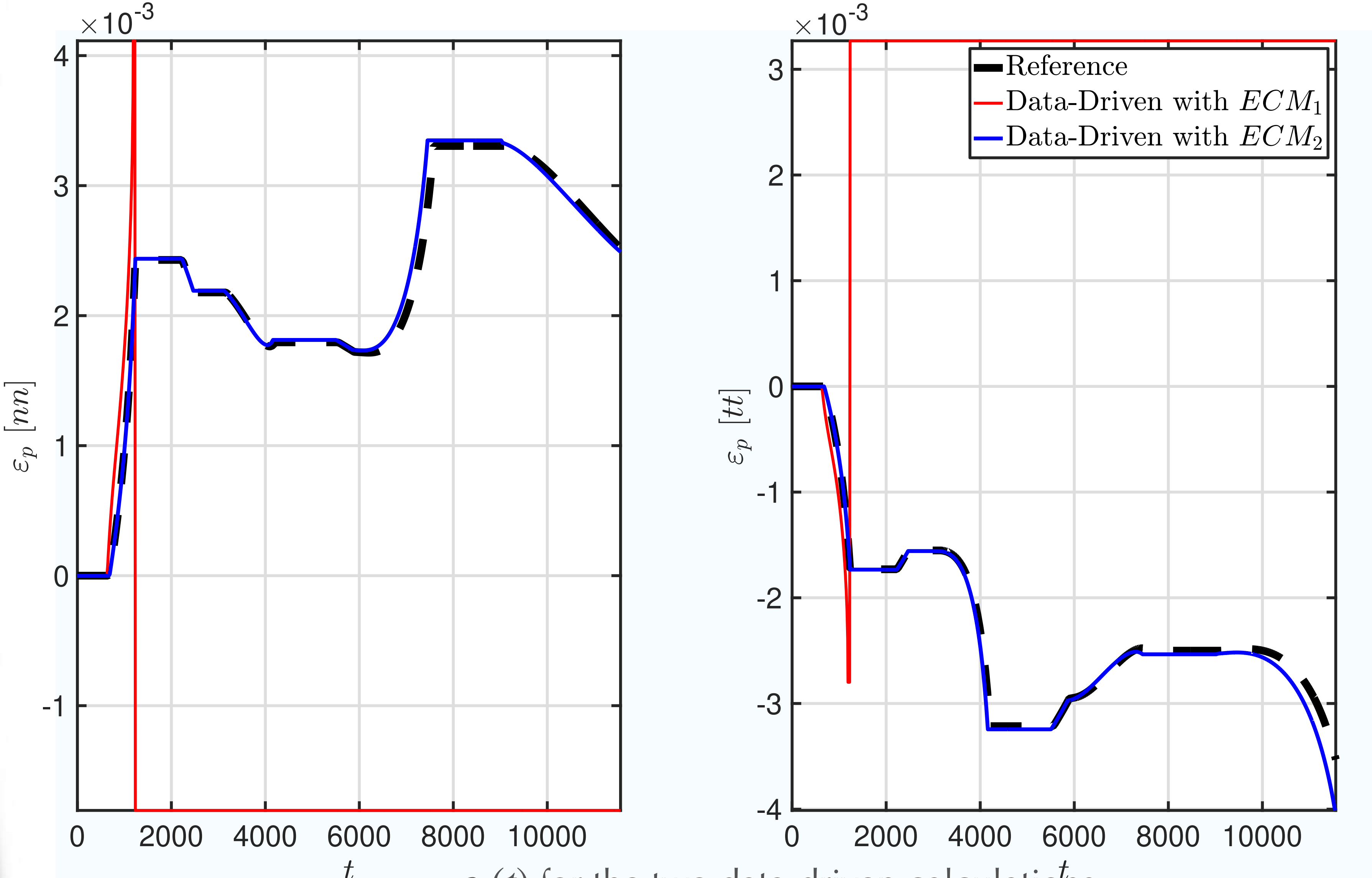
Prescribed stress history:





Construction of the ECM

Data-driven computation



$\varepsilon_p(t)$ for the two data-driven calculations

ECM1 : X^1 ECM2: X^1, X^2

Construction of the ECM
Keypoint 3

Keypoint 3: Validation

Ext(**ECM**) = { experimental test $s_i(p)$ $i \in N(p)$; $p \in [0, P]$ }

+ Interpolation

$$s_i(p) = (\boldsymbol{\varepsilon}_{p,p}, \boldsymbol{X}_{,p}, \boldsymbol{\sigma}, \boldsymbol{X}, \dot{p})_i$$

Construction of the ECM

Keypoint 3

Computed solution with Ext(**ECM**)

$s(p)\ p \in [0, P]$

:

close or not to the true material response ?

Data-driven interest

Criterium : « distance » to experimental data

$$e = \max_{p \in [0, P]} \left[\min_{i \in N(p)} d(s(p), s_i(p)) \right]$$

experimental test $s_i(p) = (\boldsymbol{\varepsilon}_{p,p}, \boldsymbol{X}_{,p}, \boldsymbol{\sigma}, \boldsymbol{X}, \dot{p})_i$

CISM motus

OUTLINE

Data-driven computation(material)

1. Today approach in computational solid mechanics

2. Data-driven computational approaches (complex nonlinear materials)

3. A DD approach for complex materials with memory: basic features and numerical tools

4. A DD approach for complex materials with :illustrations

5. Conclusion

CONCLUSION-potential applications

- The proposed data driven approach :

A new way in Material Science to build constitutive material

Two stones

The ECM-Central Problem

+

A Classical Interpolation Procedure

Hierarchical ECM with $\mathbf{X}^1 = \boldsymbol{\varepsilon}_p$

The end

thank you

CONCLUSION-potential applications

- **Solutions to situations for which Material Science classical approach fails or does not work well**

—easy correction or extension a first model

(addition of phenomena, modification of ambient conditions)

Example :

Extension Plasticity Model $\Longrightarrow$ Viscoplastic Model (ECM)

$$\dot{P} = f(\lambda(\sigma, X), p)$$

interpolation of few experimental tests

CONCLUSION-potential applications

— To build explicit homogenized model from a microstructure

FE-simulation of experimental tests on the Representative Element Volume (microstructure time/space)

« Experimental » data

Data-driven material model:ECM

The end

thank you

Data-driven modelling of materials

Deep Neural Network

a working solution
learning : parameters↗
test number?
verification/validation ?

Physics-compatible
hidden variable framework

a working solution
Interpolation: classical
(RKHS,RBF,..)
learning : hidden variables↗
verification/validation ++++