

Mathematical and Computational Materials Science
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**Real-time Bayesian data assimilation with
data-based model enrichment for the monitoring
of damage in materials and structures**

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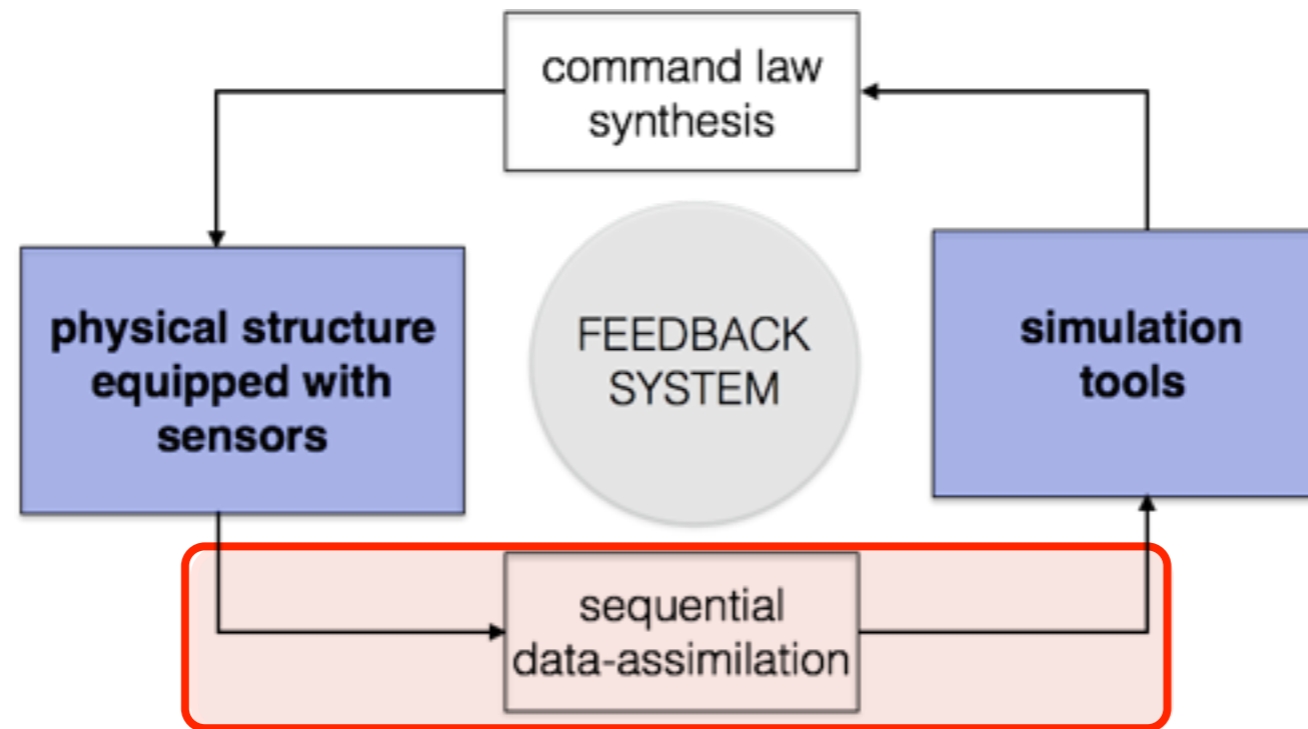


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Context

Dynamic Data-Driven Application Systems (DDDAS) [Darema 04]



*connected systems,
cyber-physics,...*



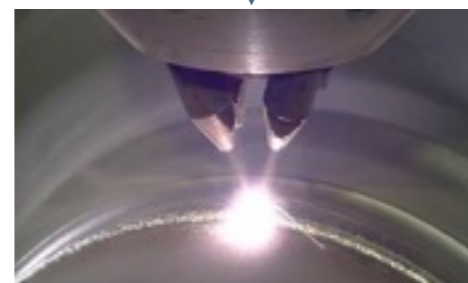
assisted surgery



renewable energy



building performance



manufacturing



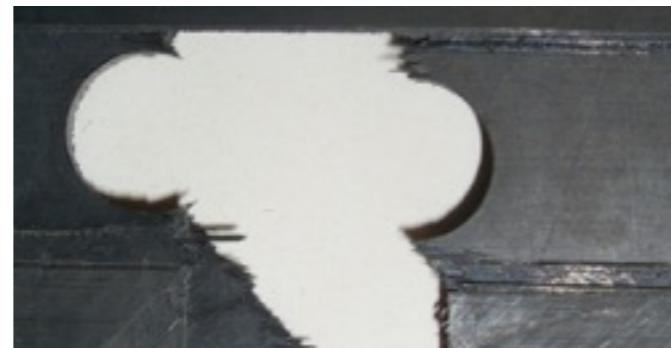
transportation



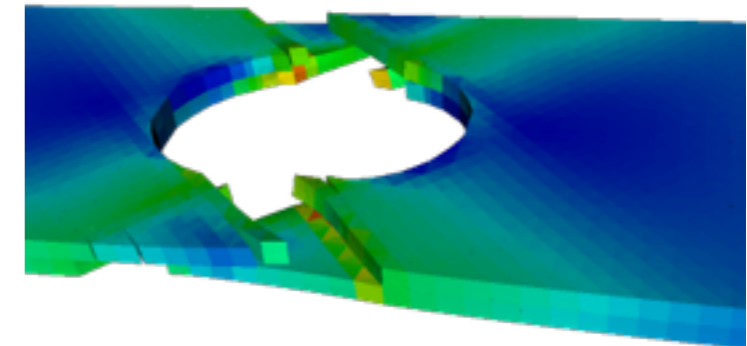
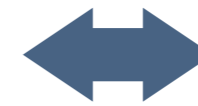
Context

- Application to **engineering structures** → **safety / reliability (degraded mode)**

*embedded strain sensors
(defects $\sim 1\text{mm}$)*



complex physics



predictive simulations

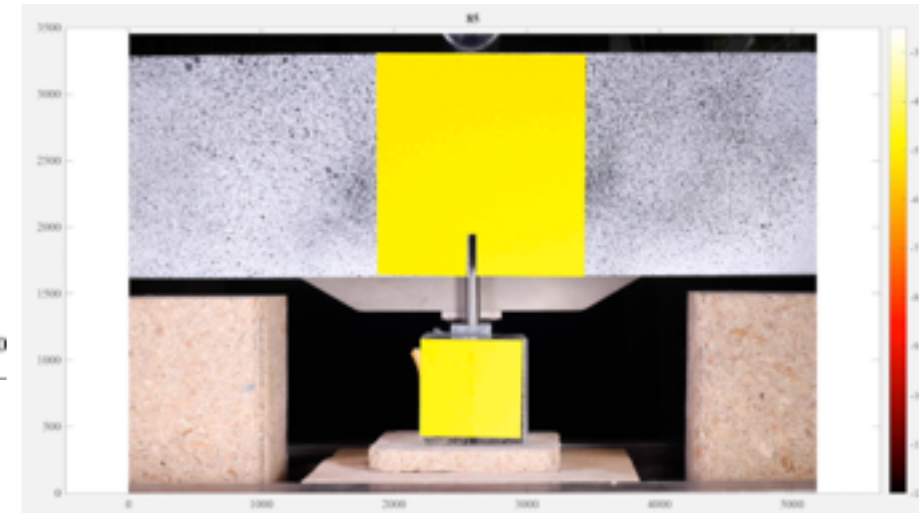
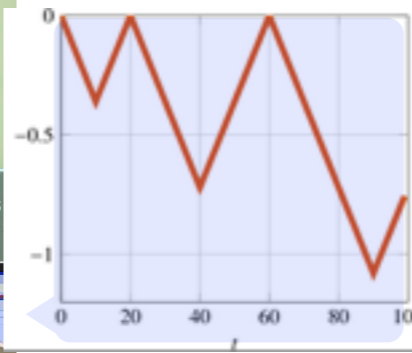
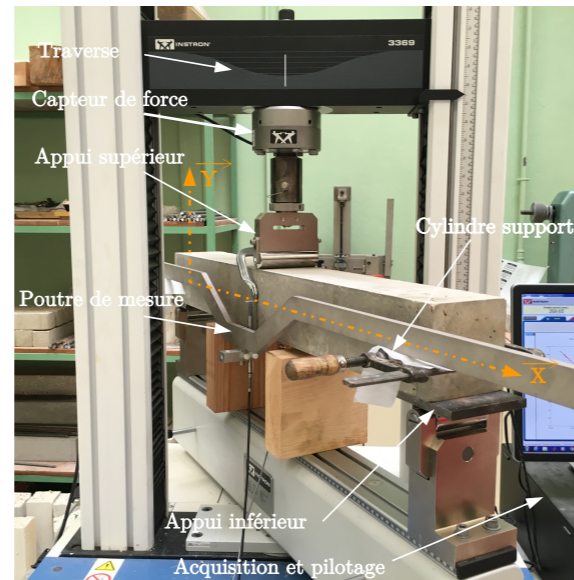
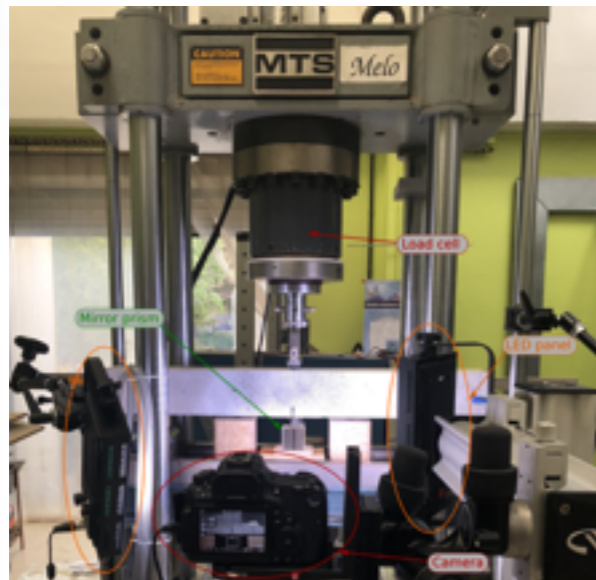
exploit the best of data & **material models**

GOAL: **dynamical model updating** from data assimilated on-the-fly

- for **complex nonlinear** large systems with **uncertain environment**
- in **real-time**
- from numerous, indirect and **noisy data** (images, optic fibers...)

Application of interest

→ structural integrity on a large-scale damageable concrete structure

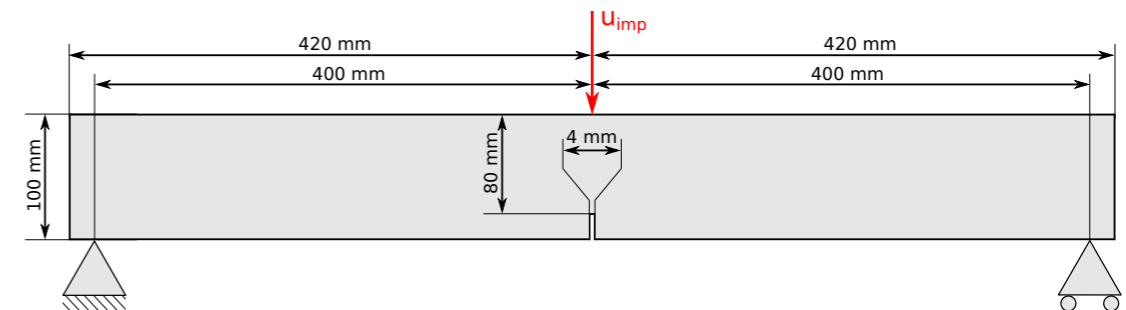
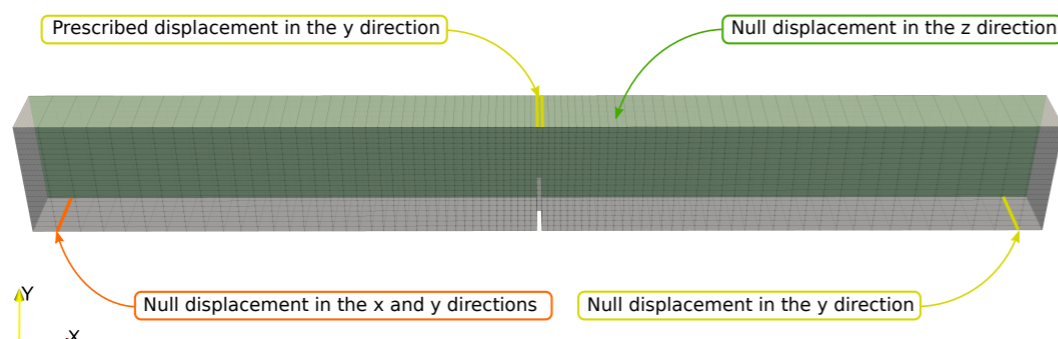
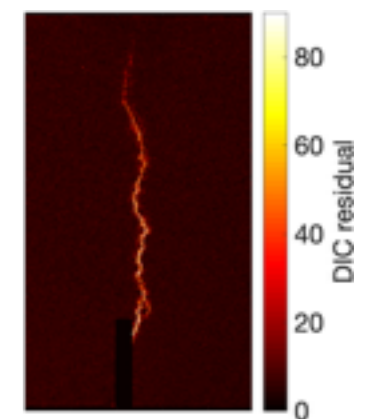


Digital Image Correlation (DIC)

→ DIC pictures taken every 5s, and post-processed with Corelli [Leclerc *et al.* 15]

→ prediction of crack propagation & failure (before the physics!!)

→ simulator using an isotropic damage model



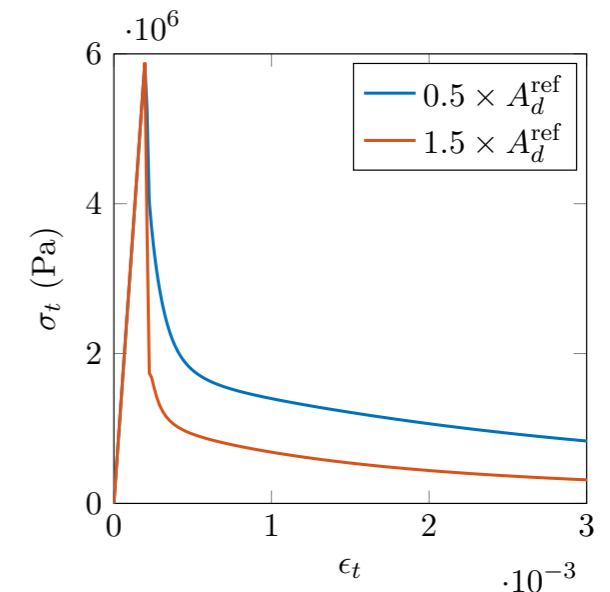
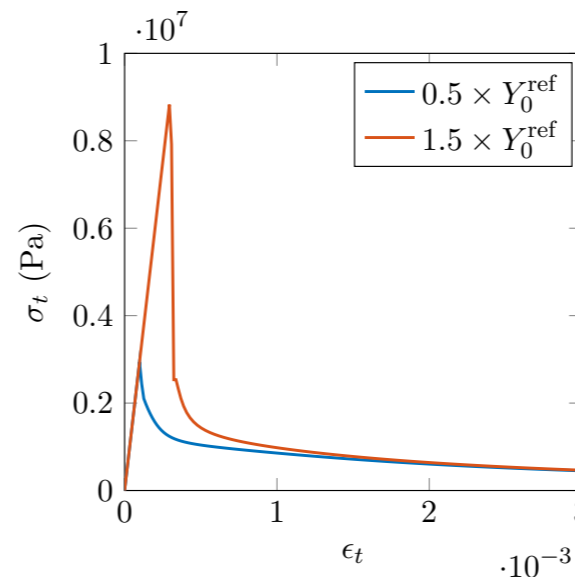
Objectives

$$\sigma = (1 - d)\mathbf{C}\epsilon \quad ; \quad d(Y, A_d, Y_0) = 1 - \frac{1}{1 + A_d(Y - Y_0)}$$

$Y = \frac{1}{2} \langle \epsilon \rangle_+ : \mathbf{C} : \langle \epsilon \rangle_+$ released energy rate

Y_0 initial threshold for damage initiation

A_d scalar brittleness (post-peak behavior)



→ **updating of parameters (Y_0, A_d) from data**

- robustness with uncertainties (measurement noise,...) → **Bayesian inference** [Kaipio & Sommersalo 04]
- real-time constraint → **Reduced Order Modeling (PGD)** [Chinesta *et al.* 14]
→ **Transport Map sampling** [El Moseley & Marzouk 12]
- model bias (BC, material (drying effects),...) → **online data-based correction**



Outline

1. Bayesian formulation with ROM

2. Real-time sampling using Transport Maps

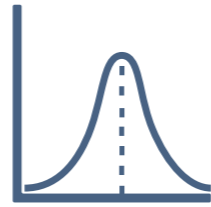
3. Model bias correction from data

4. Feedback control

Bayesian Formulation

Problem unknown

$$\pi(\mathbf{p}|\mathbf{d}^{\text{obs}})$$



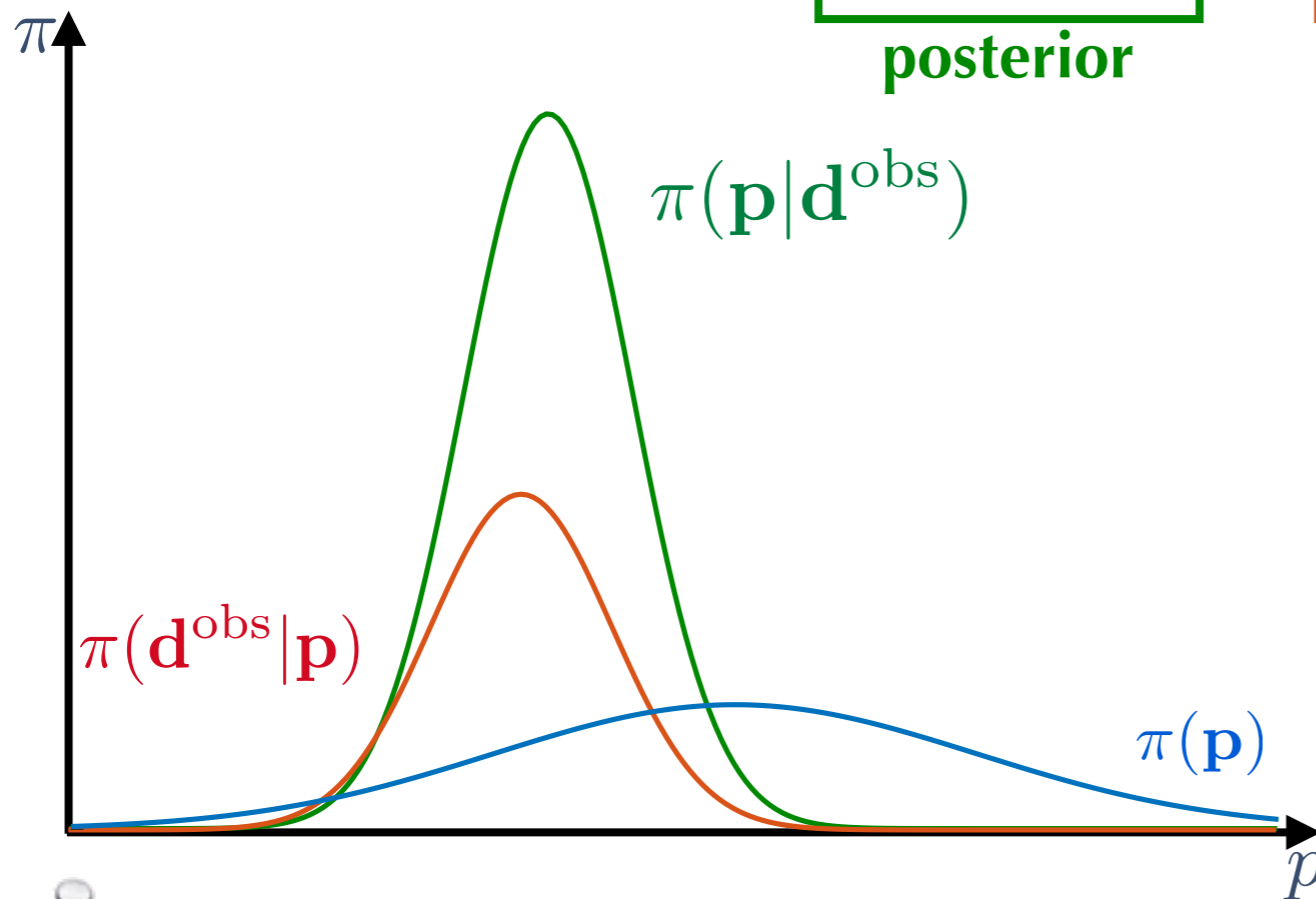
→ automatic regularization

→ natural framework to consider uncertainties

Bayes Theorem:

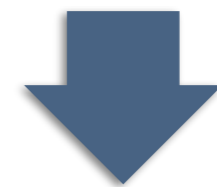
$$\pi(\mathbf{p}|\mathbf{d}^{\text{obs}}) \propto \pi(\mathbf{d}^{\text{obs}}|\mathbf{p}) \cdot \pi(\mathbf{p})$$

posterior
likelihood
prior



$$= \pi_{\text{meas}}(\mathbf{d}^{\text{obs}} - \mathbf{d}(\mathbf{p}))$$

if additive measurement noise



costly multi-query process

Sequential assimilation

$$\pi(\mathbf{p}|\mathbf{d}_1^{\text{obs}}, \dots, \mathbf{d}_i^{\text{obs}}) \propto \left(\prod_{j=1}^i \pi_{t_j}(\mathbf{d}_j^{\text{obs}}|\mathbf{p}) \right) \cdot \pi_0(\mathbf{p})$$

$$\pi_{t_j}(\mathbf{d}_j^{\text{obs}}|\mathbf{p}) = \pi_{\text{meas}}(\mathbf{d}_j^{\text{obs}} - \mathbf{d}(\mathbf{p}, t_j))$$

PGD Model Reduction

- ▶ modal description of multiparametric solution [Nouy 10, Chinesta *et al.* 14]
- ▶ low-rank canonical tensor format (separated variables)

$$\mathbf{u}_m(\mathbf{x}, t, \mathbf{p}) = \sum_{k=1}^m \Lambda_k(\mathbf{x}) \lambda_k(t) \prod_{i=1}^d \alpha_k^i(p_i)$$

- construction in the offline phase
- explicit dependency on parameters
- computed using the LATIN-PGD algorithm for nonlinear models [Vitse *et al.* 19]

→ straightforward model evaluation in the likelihood function

$$\mathbf{d}(\mathbf{p}, t) = \mathcal{O}(\mathbf{u}_m(\mathbf{x}, t, \mathbf{p})) \text{ [Berger } et al. 17, \text{ Rubio } et al. 18]$$

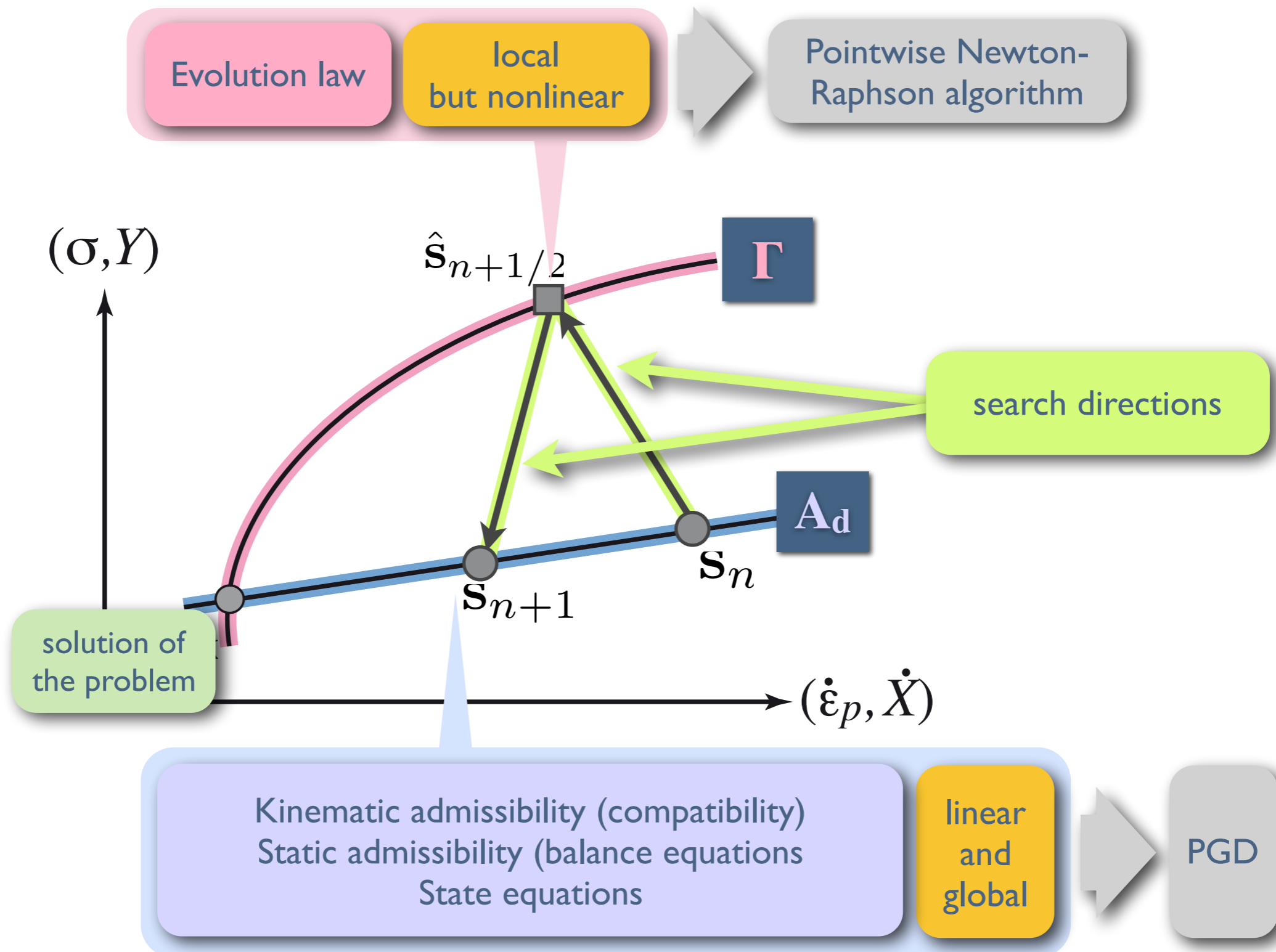
→ fast UQ on outputs of interest $q(\mathbf{p}) \approx \mathcal{Q}(\mathbf{u}_m(\mathbf{x}, t, \mathbf{p}))$

└→ samples $q_k = q(\mathbf{p}_k)$

Extension to NL problems

Use of the iterative LATIN-PGD algorithm [Ladevèze *et al.* 10]

→ *non-incremental iterative strategy*



PGD Modes

$$\mathbf{u}_m(\mathbf{x}, t, Y_0, A_d) = \sum_{k=1}^m \Lambda_k(\mathbf{x}) \lambda_k(t) \alpha_k^1(Y_0) \alpha_k^2(A_d)$$

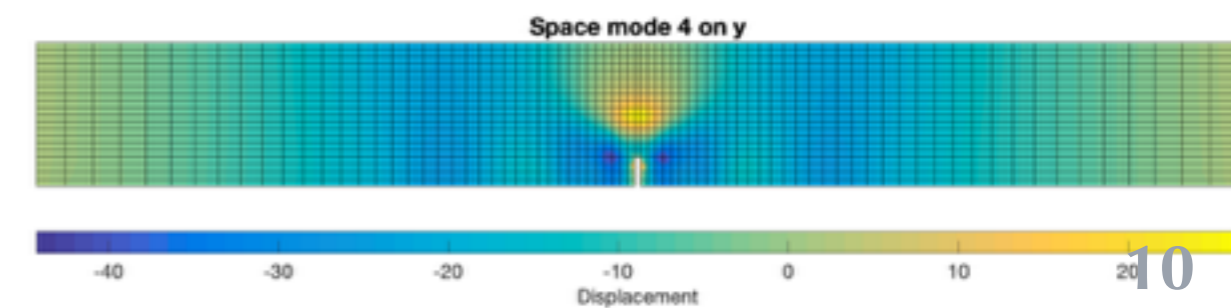
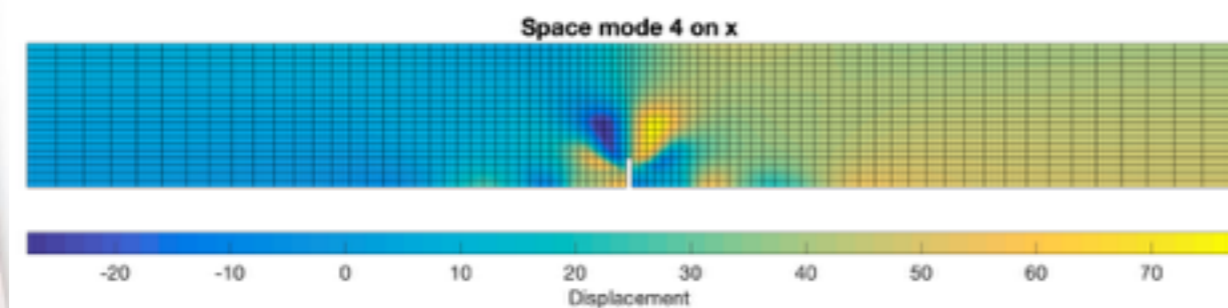
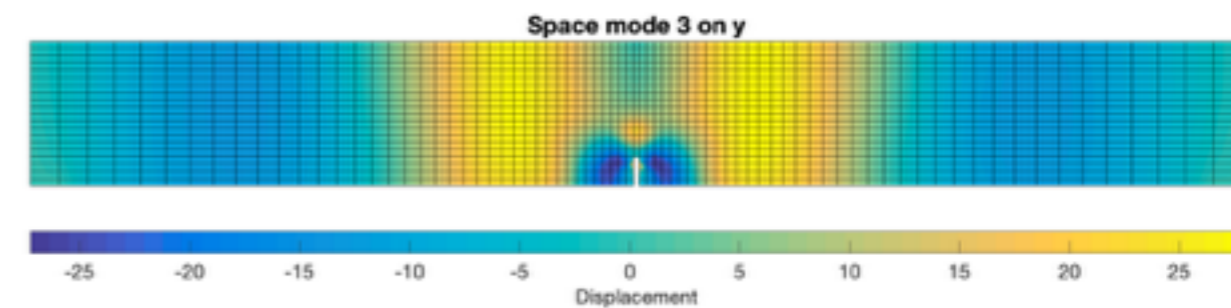
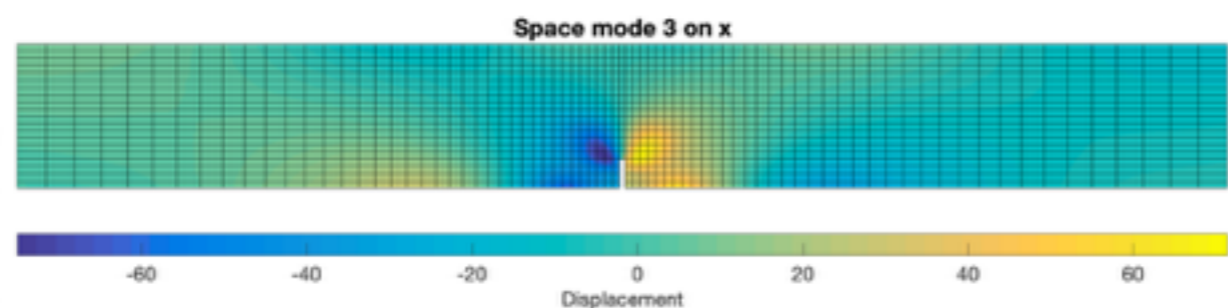
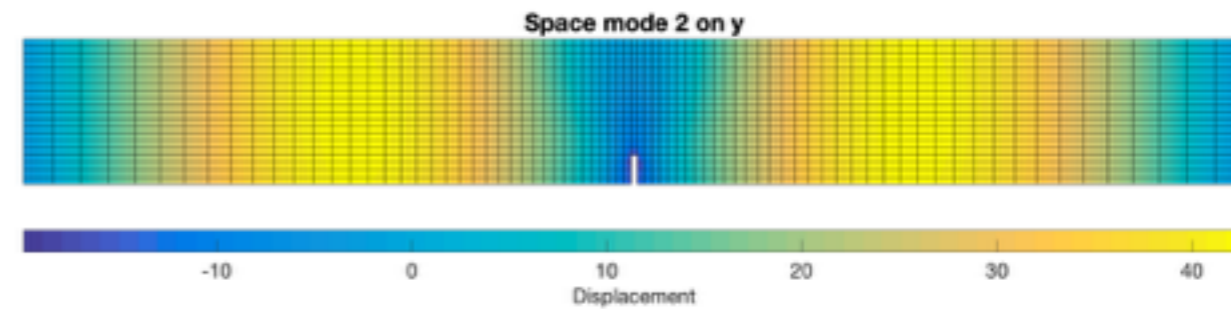
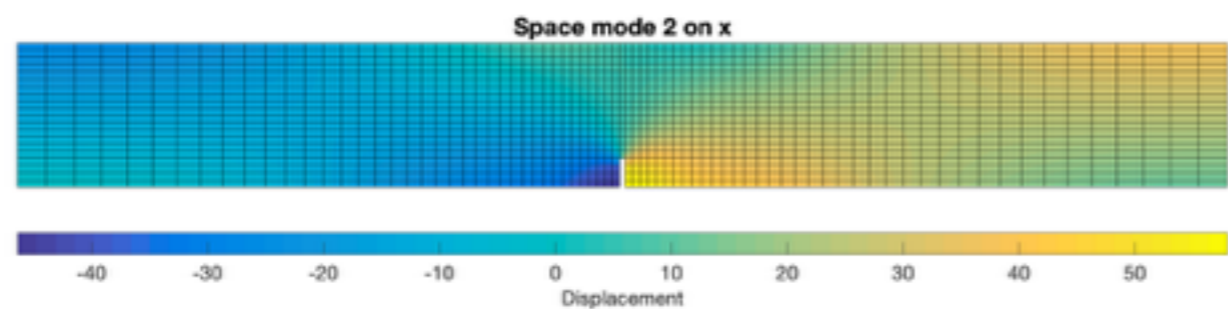
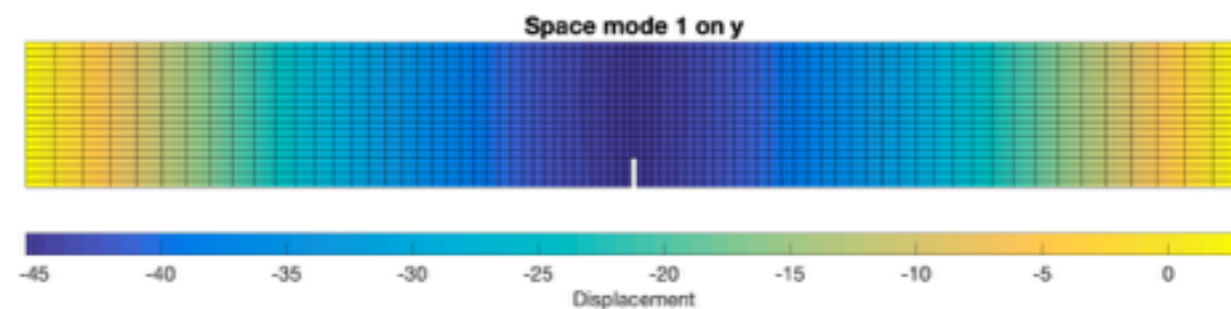
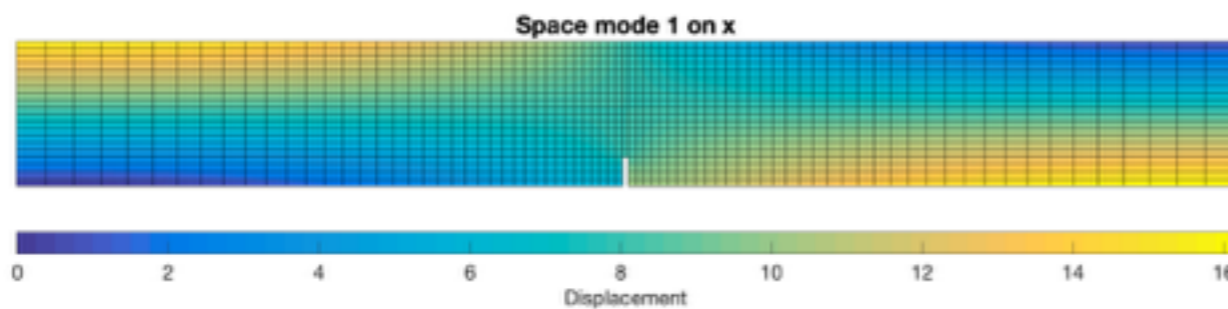
- Space modes Λ_k

100 loading steps

$$E = 30 \text{ GPa} \quad \nu = 0.23$$

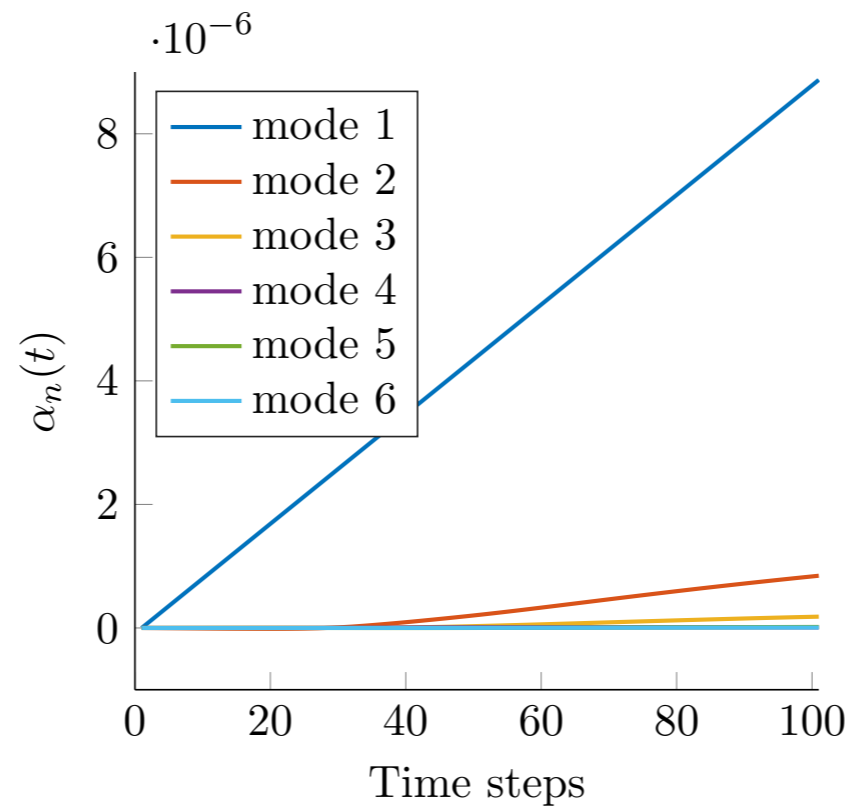
$$Y_0^{\text{ref}} = 216 \text{ J.m}^{-3}$$

$$A_d^{\text{ref}} = 2.25 \text{ J}^{-1}.\text{m}^3$$

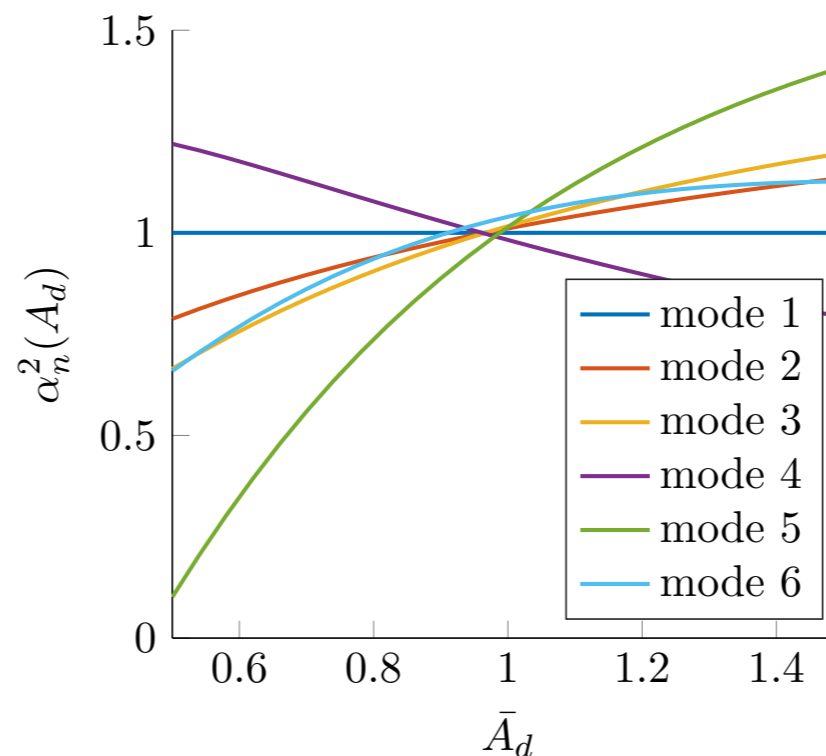
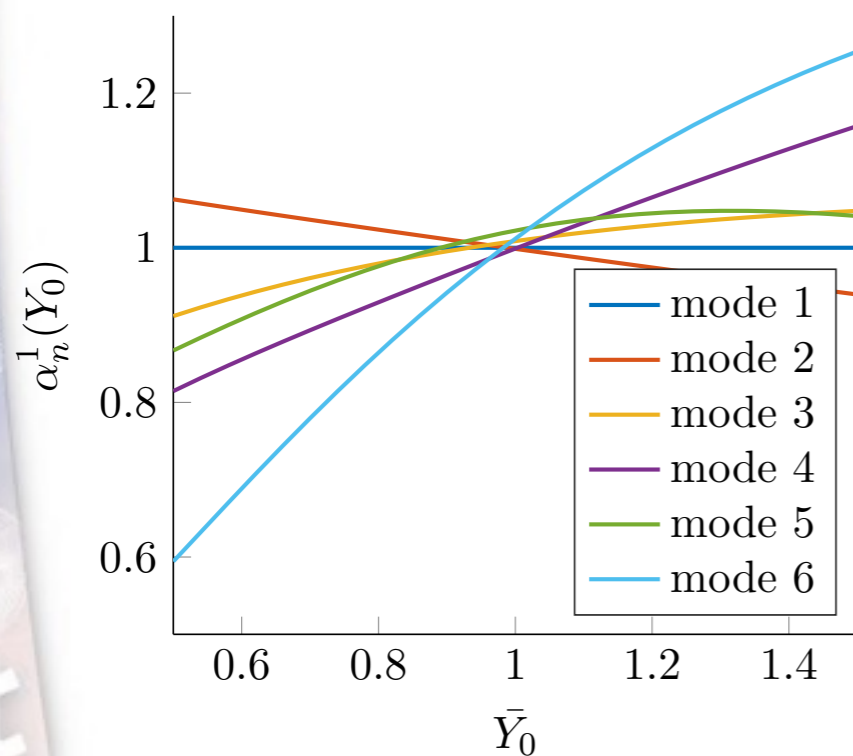


PGD Modes

- Time modes λ_k



- Parameter modes (α_k^1, α_k^2) (with $\bar{Y}_0 = Y_0/Y_0^{\text{ref}}$, $\bar{A}_d = A_d/A_d^{\text{ref}}$)



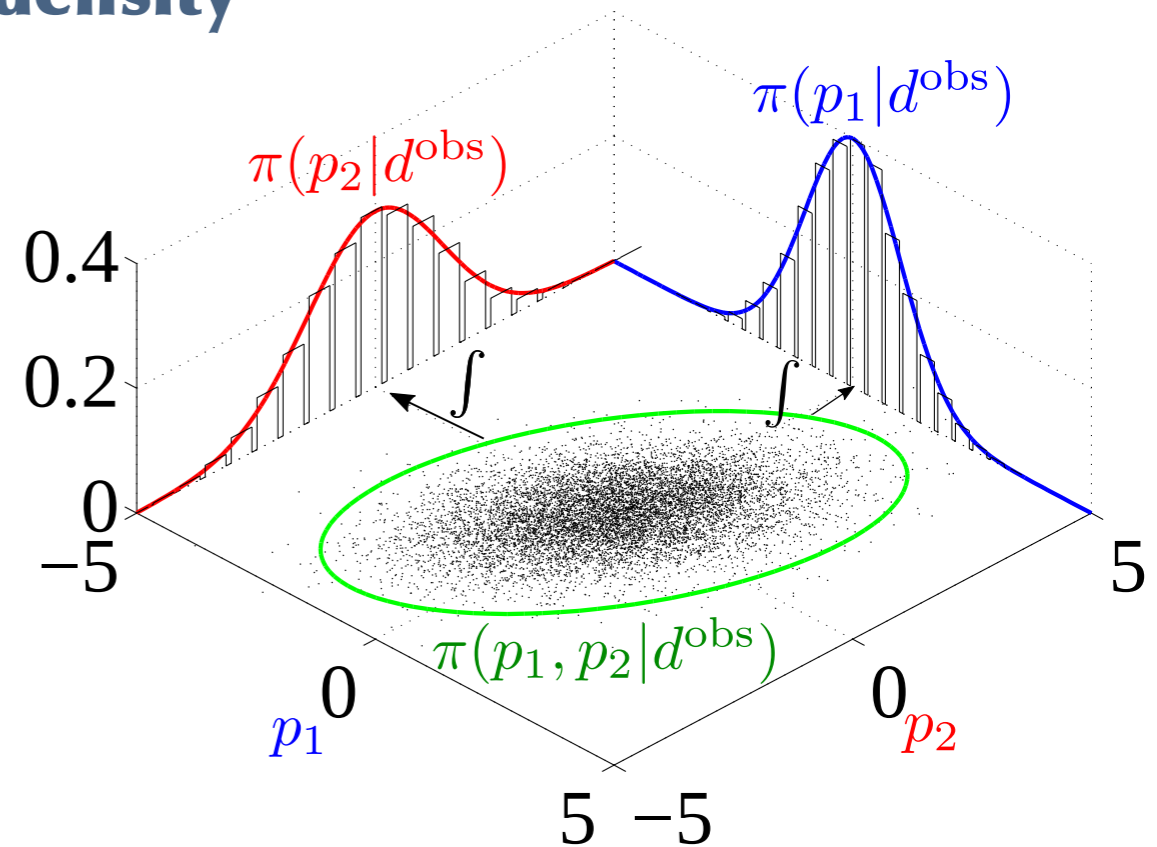
→ **1st mode = full elasticity**

Sampling of Posterior PDFs

Characterization of the posterior density

- Mean *a posteriori*
- Maximum *a posteriori*
- 1D Marginals
- Uncertainty propagation

➔ Need multi-dimensional integration



Monte-Carlo integration:

- Quantity of interest: $\mathbb{E}[h] = \int h(\mathbf{p})\pi(\mathbf{p})d\mathbf{p}$
- With samples $\mathbf{p}^{\{1, \dots, N\}} \sim \pi$: $\mathbb{E}[h] \approx \bar{h} = \frac{1}{N} \sum_{i=1}^N h(\mathbf{p}^i)$

➔ Need samples from posterior density

Sampling of Posterior PDFs

📌 Markov Chain Monte-Carlo (MCMC) method

• **small** proposal

• **large** proposal



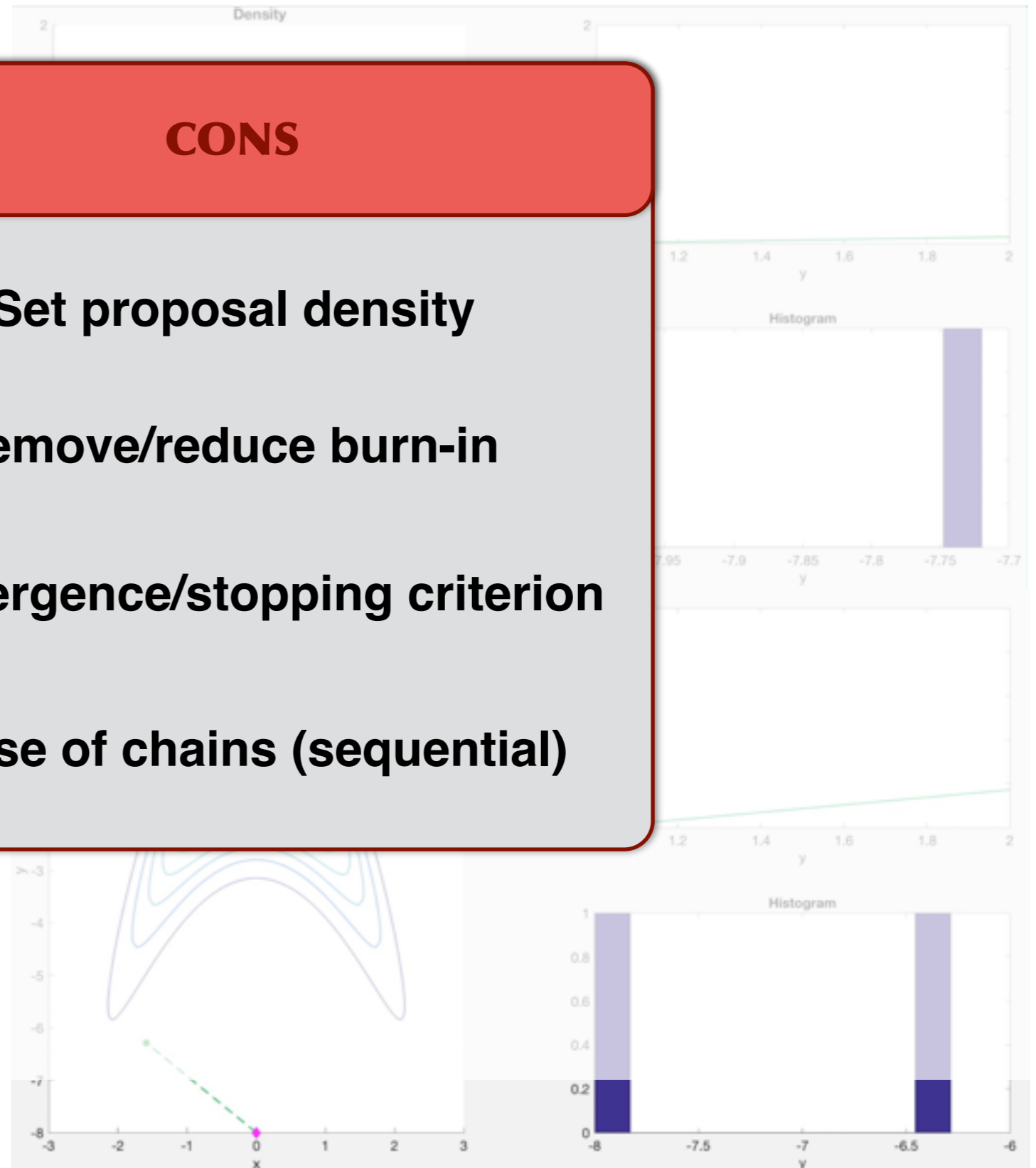
CONS

Set proposal density

Remove/reduce burn-in

Convergence/stopping criterion

Reuse of chains (sequential)





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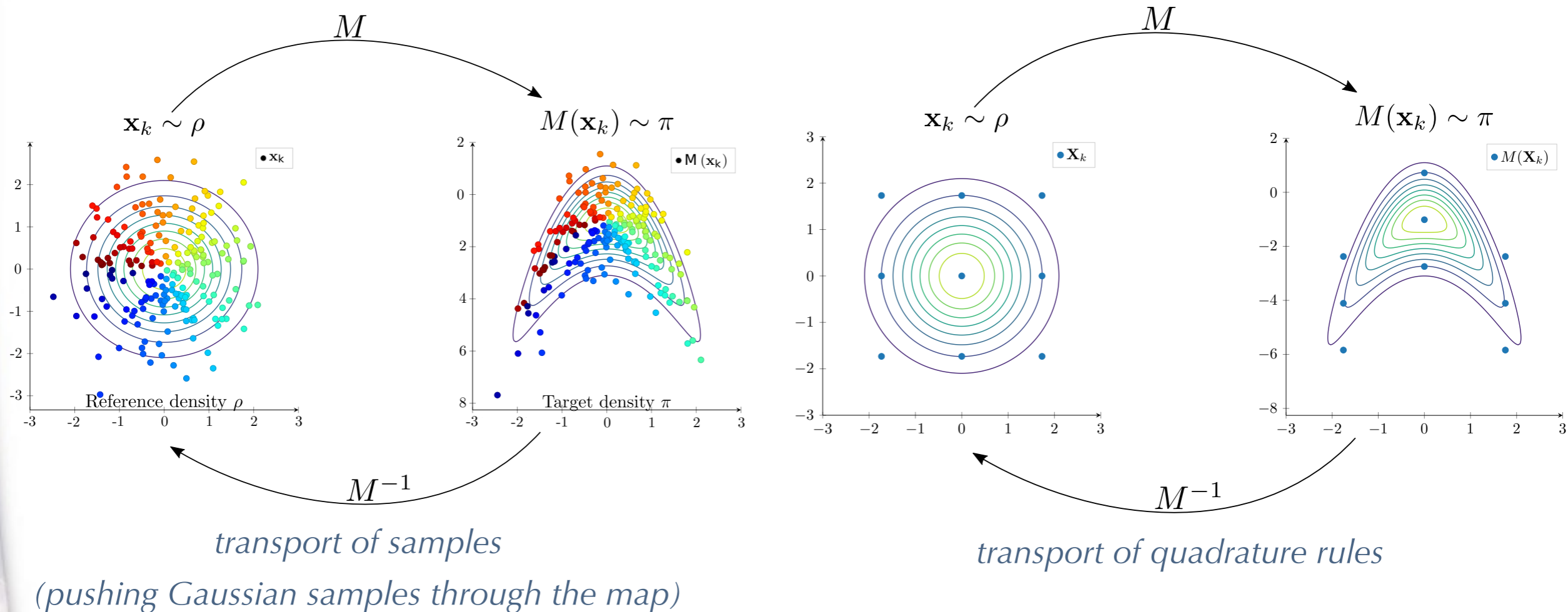
Transport Map Sampling

Transport Maps method [Villani 07, El Moselhy & Marzouk 12]

Transport integrals over the **target** density to integrals over a **reference** density

$$\int g d\nu_{\pi} = \int g \circ M d\nu_{\rho}$$

↓
deterministic application



→ computations (sampling, integration) performed in the reference space [Marzouk 16]

Transport Map Sampling

● Parametrization of Transport Maps

● Structure:

$$M(\mathbf{p}) = \begin{bmatrix} M^1(\mathbf{a}_c^1, \mathbf{a}_e^1, p_1) \\ M^2(\mathbf{a}_c^2, \mathbf{a}_e^2, p_1, p_2) \\ \vdots \\ M^d(\mathbf{a}_c^d, \mathbf{a}_e^d, p_1, p_2, \dots, p_d) \end{bmatrix}$$

Knothe-Rosenblatt rearrangements
(lower triangular monotonic maps)

- unique minimizer
- computational feasibility (inversion)
- optimality for a weighted metric
[El Moselhy & Marzouk 12]

● Parametrization:

$$M^k(\mathbf{a}_c^k, \mathbf{a}_e^k, \mathbf{p}) = \Phi_c(\mathbf{p})\mathbf{a}_c^k + \int_0^{p_k} (\Phi_e(p_1, \dots, p_{k-1}, \theta)\mathbf{a}_e^k)^2 d\theta$$

Φ_c, Φ_e : Hermite polynomials which given order

$\mathbf{a}_c, \mathbf{a}_e$: parameters

↳ obtained from minimization of Kullback-Liebler divergence

$$\mathcal{D}_{KL}(M_{\#}\nu_{\rho} || \nu_{\pi}) = \mathbb{E}_{\rho} \left[\log \frac{\nu_{\rho}}{M_{\#}^{-1}\nu_{\pi}} \right]$$

Transport Map Sampling

Minimization problem

$$\min_{\mathbf{a}_c^{1,\dots,d}, \mathbf{a}_e^{1,\dots,d}} \sum_{i=1}^N \omega_i \left[-\log(\tilde{\pi} \circ M(\mathbf{a}_c^{1,\dots,d}, \mathbf{a}_e^{1,\dots,d}, \mathbf{p}_i)) - \log(|\det \nabla M(\mathbf{a}_c^{1,\dots,d}, \mathbf{a}_e^{1,\dots,d}, \mathbf{p}_i)|) \right]$$

$$\tilde{\pi}(\mathbf{p}|\mathbf{d}^{\text{obs}}) = \pi_{\text{meas}}(\mathbf{d}^{\text{obs}} - u_m(\mathbf{p}))\pi(\mathbf{p}) \quad (\text{non-normalized pdf})$$

→ solved with gradient/Hessian information (BFGS,...)

→ partial derivatives explicitly recovered and stored in the **offline phase**

$$\frac{\partial^n \mathbf{u}_m}{\partial p_j^n}(\mathbf{x}, t, \mathbf{p}) = \sum_{k=1}^m \Lambda_k(\mathbf{x}) \lambda_k(t) \frac{\partial^n \alpha_k^j}{\partial p_j^n}(p_j) \prod_{\substack{i=1 \\ i \neq j}}^d \alpha_k^i(p_i)$$

↳ large speed-up for the computation of maps!!! [Rubio et al. 19]

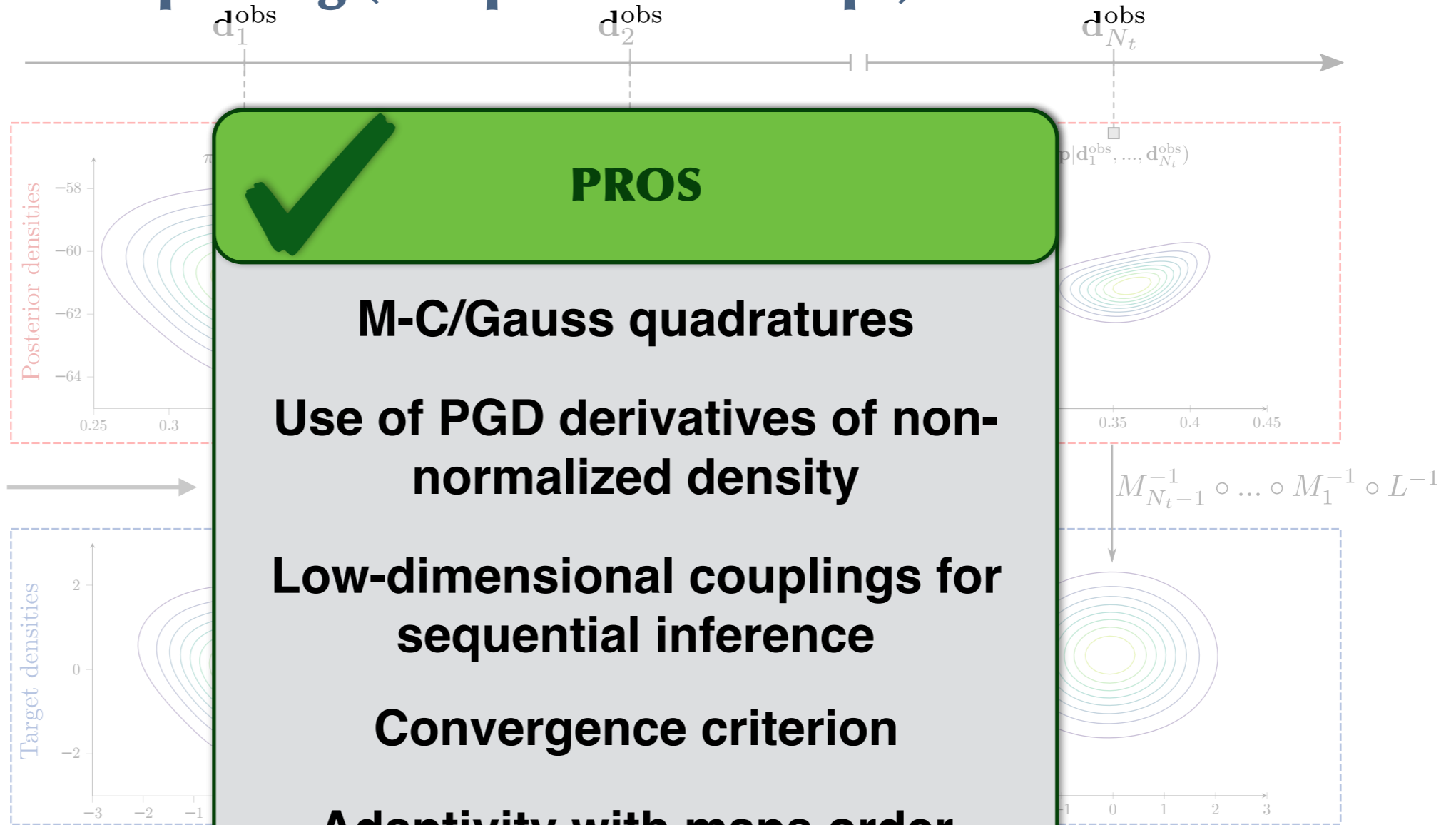
Variance diagnostic [Spantini et al. 18]

$$\epsilon_\sigma = \frac{1}{2} \text{Var}_\rho \left[\ln \frac{\nu_\rho}{M_\#^{-1} \nu_\pi} \right]$$

- sampling error estimate
- clear convergence criterion
- adaptive strategy on map order

Transport Map Sampling

Sequential updating (composition of maps)



PROS

- M-C/Gauss quadratures
- Use of PGD derivatives of non-normalized density
- Low-dimensional couplings for sequential inference
- Convergence criterion
- Adaptivity with maps order
- Deterministic computations

constant CPU cost

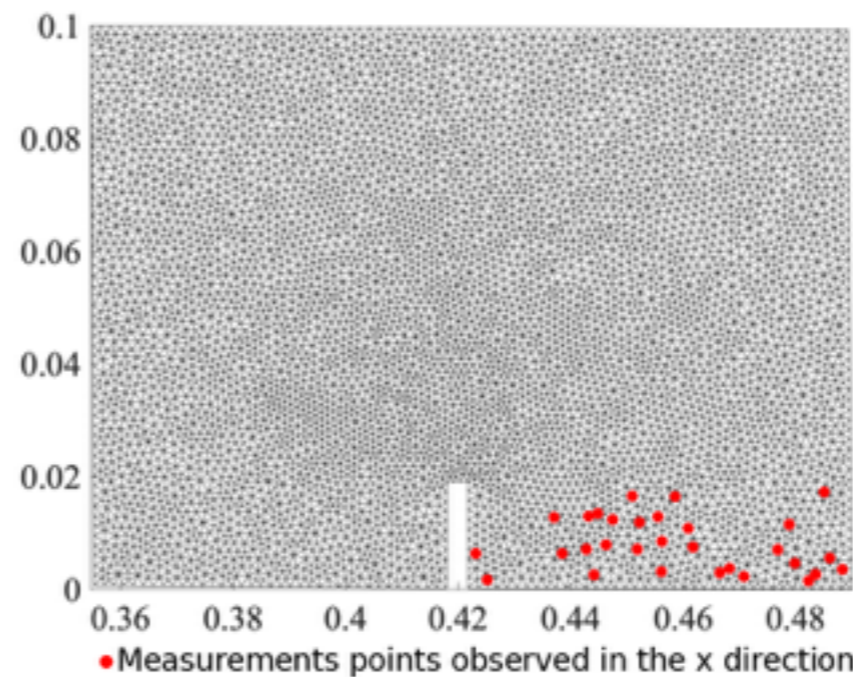
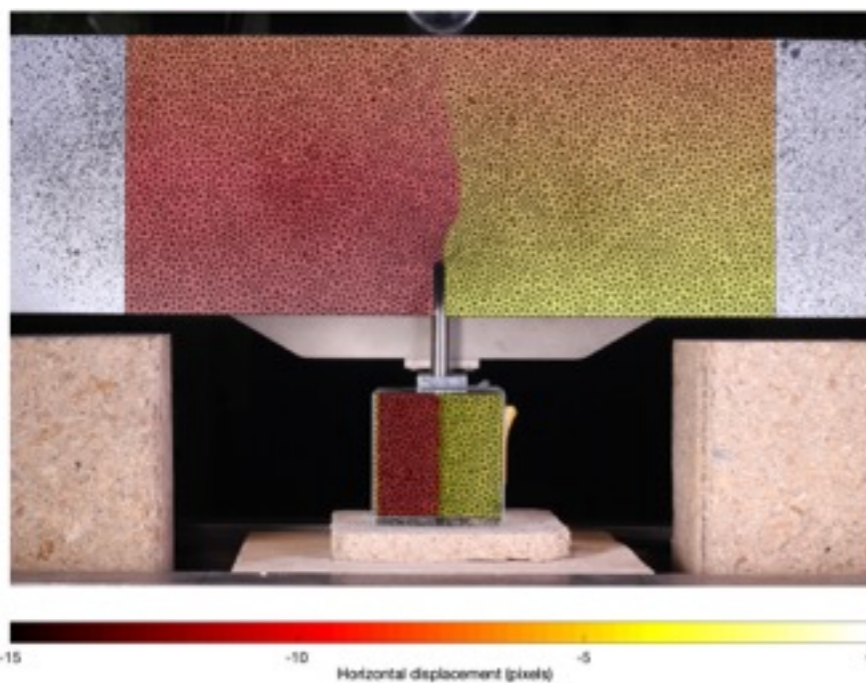
Results

Assimilation with Transport Maps & PGD

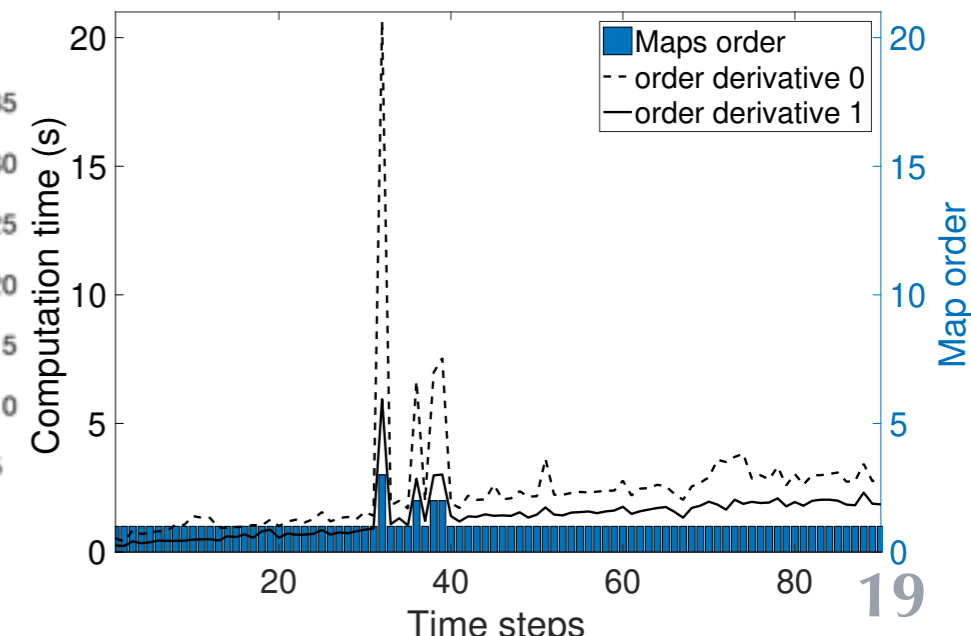
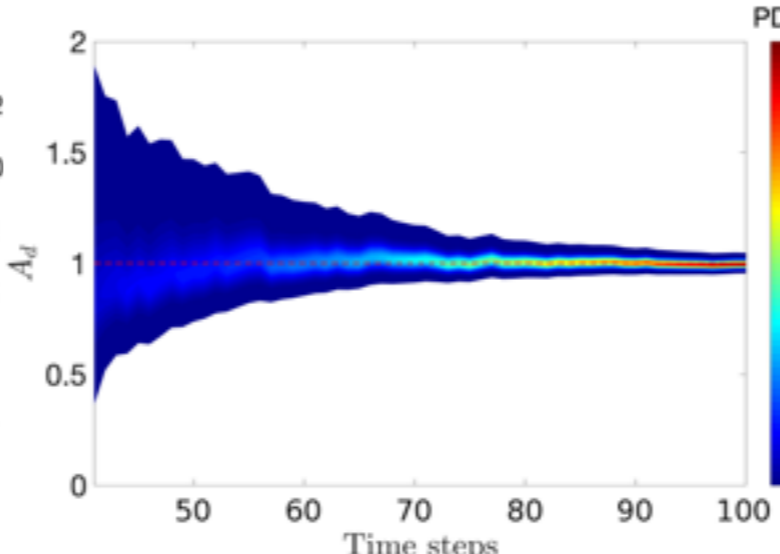
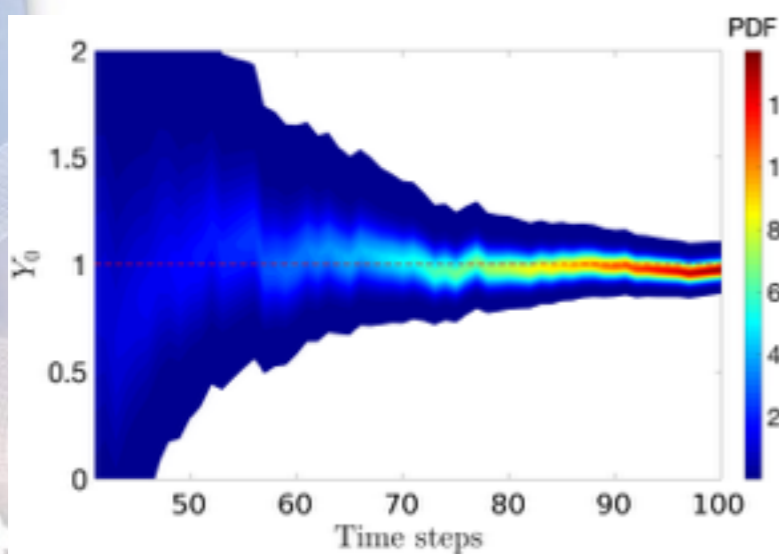
$$\pi(\bar{Y}_0, \bar{A}_d | \mathbf{d}_1^{\text{obs}}, \dots, \mathbf{d}_i^{\text{obs}}) \propto \prod_{j=1}^i \pi(\mathbf{d}_j^{\text{obs}} | \bar{Y}_0, \bar{A}_d) \cdot \pi_0(\bar{Y}_0, \bar{A}_d)$$

$$\epsilon_\sigma = 10^{-3}$$

PGD approximation with $m = 6$



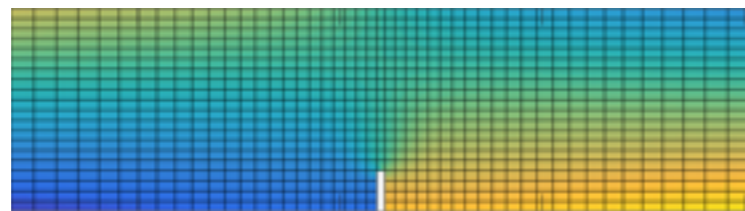
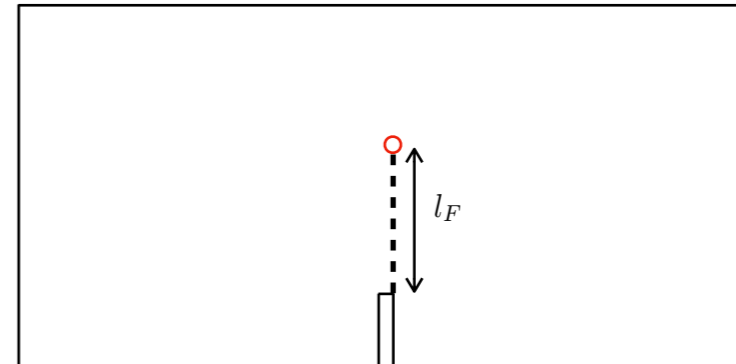
selection of most relevant DIC data (sensitivity analysis)



Post-processing

Kinematic bridge between damage & fracture mechanics

● **Goal:** Predict the final crack propagation:

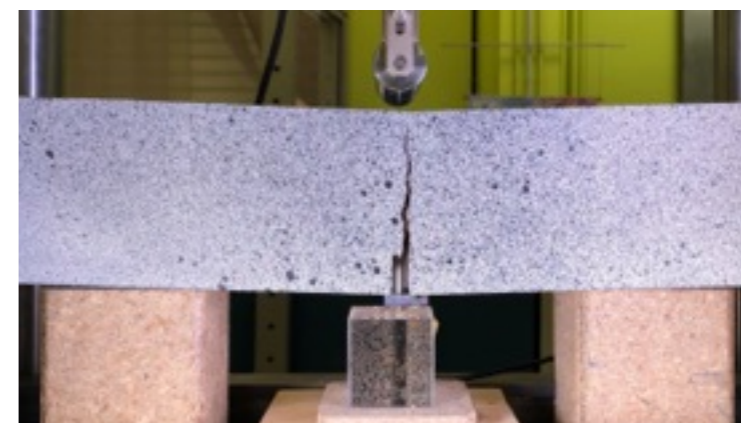
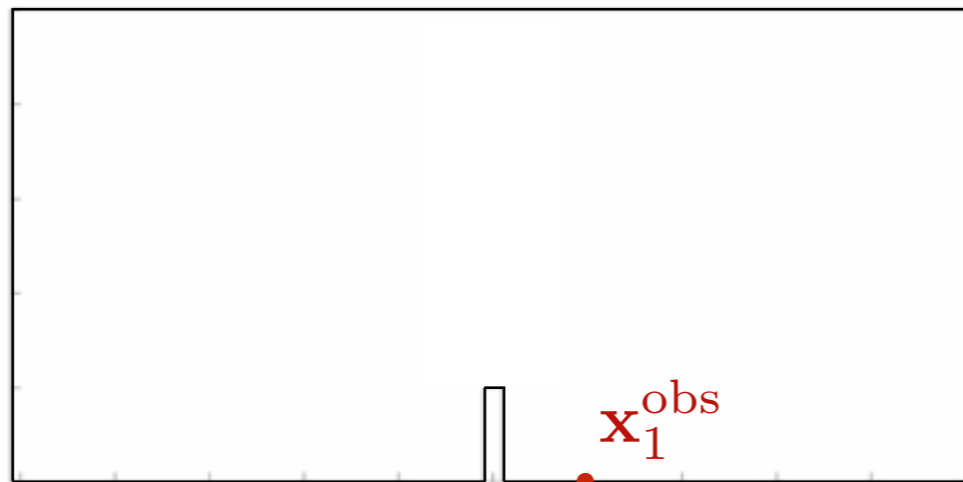


$$\mathbf{u}_{\text{PGD}}(\mathbf{x}, t_F, Y_0, A_d)$$



$$\mathbf{u}_{\text{SVD}}(\mathbf{x}, l)$$

$$\mathbf{x} = \mathbf{x}_1^{\text{obs}}$$

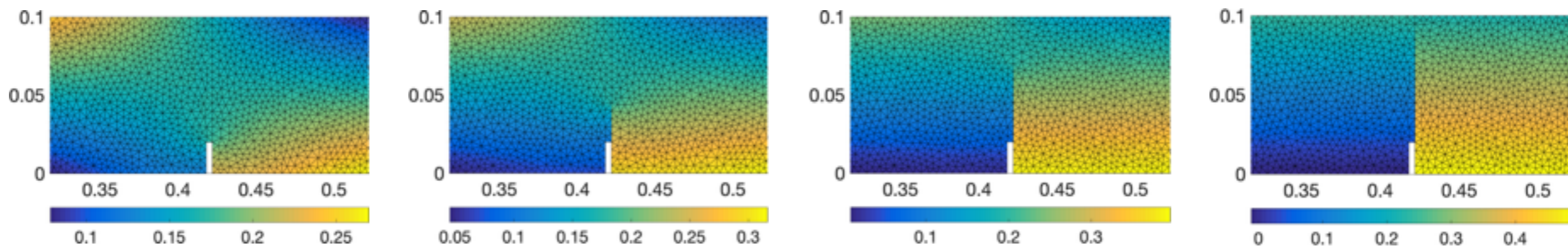


● Bayesian bridge: $\pi(l) = \pi_u(u^{\text{SVD}}(l)) \cdot \pi_{\text{pr}}(l)$

Results

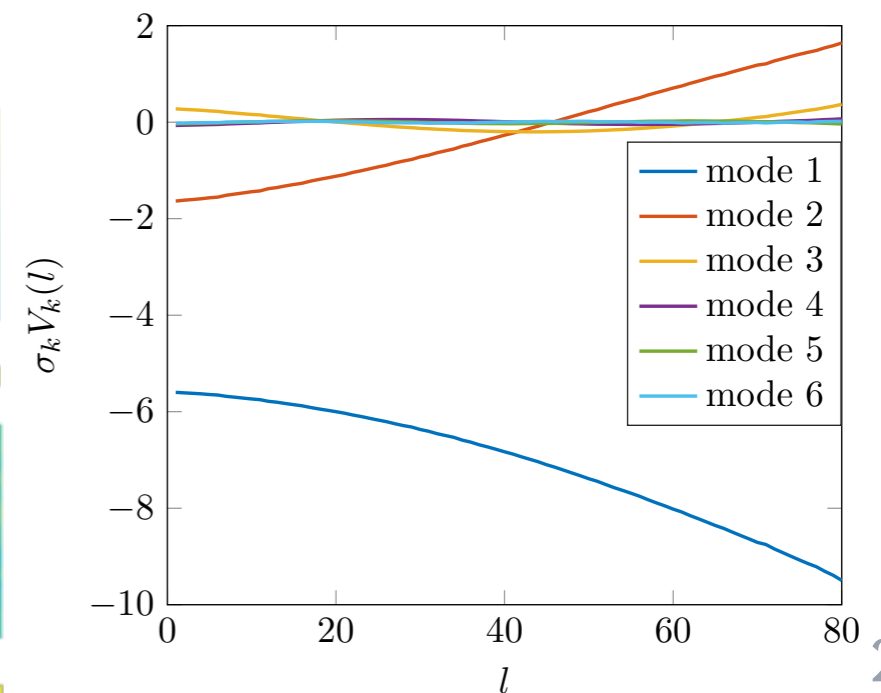
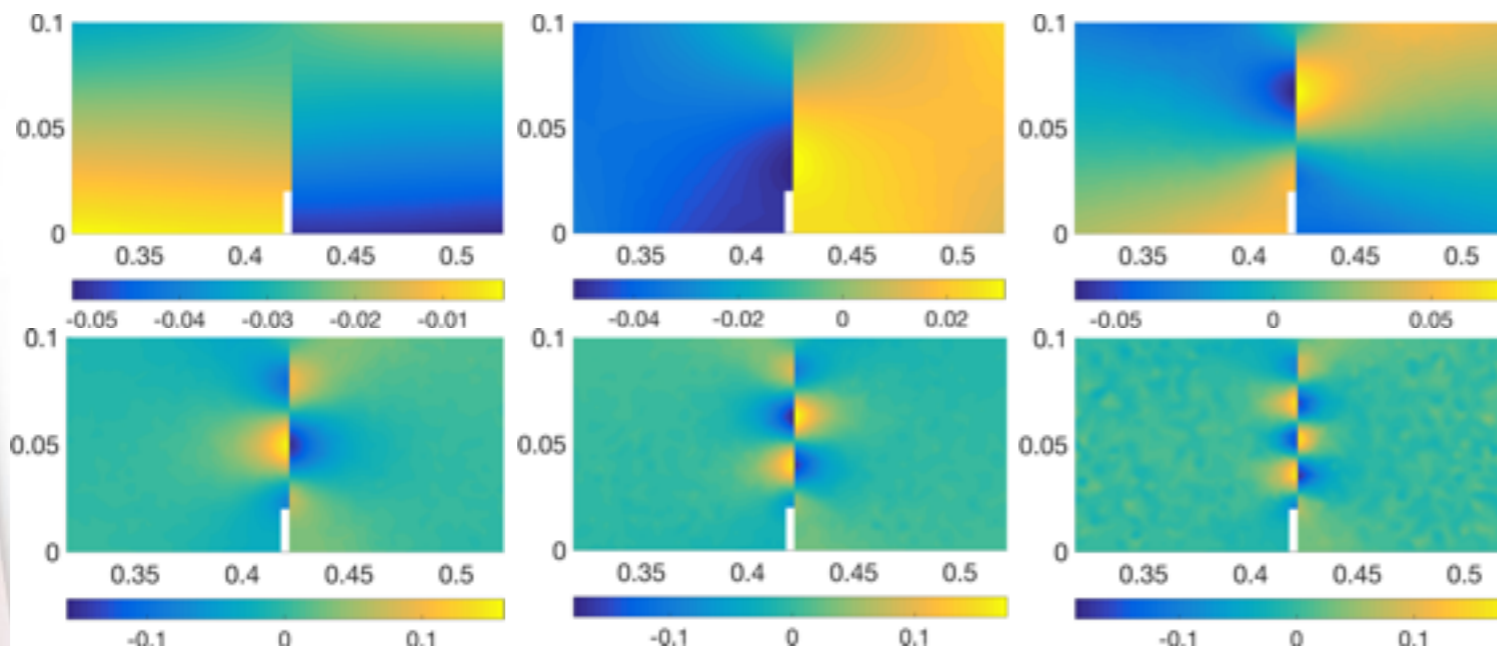
Kinematic bridge between damage and fracture mechanics

→ post-process of elastic solutions with varying crack length l (unit loading)



$$l \in \{0, 1, 2, \dots, 79\} \longrightarrow \mathbb{Y} = \{\mathbf{Y}_1, \dots, \mathbf{Y}_{80}\} \longrightarrow \mathbb{Y} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

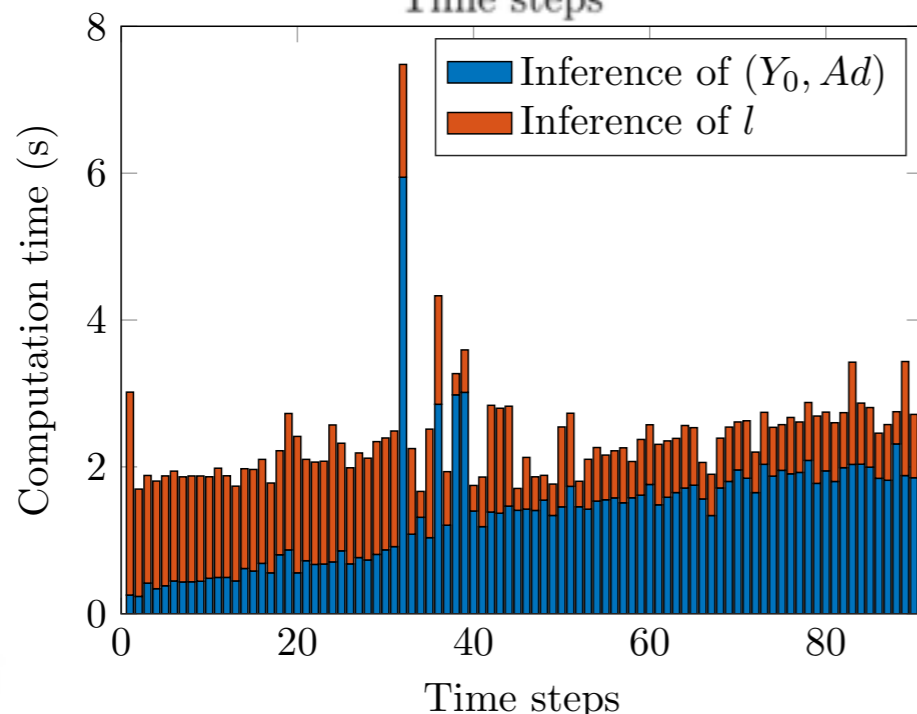
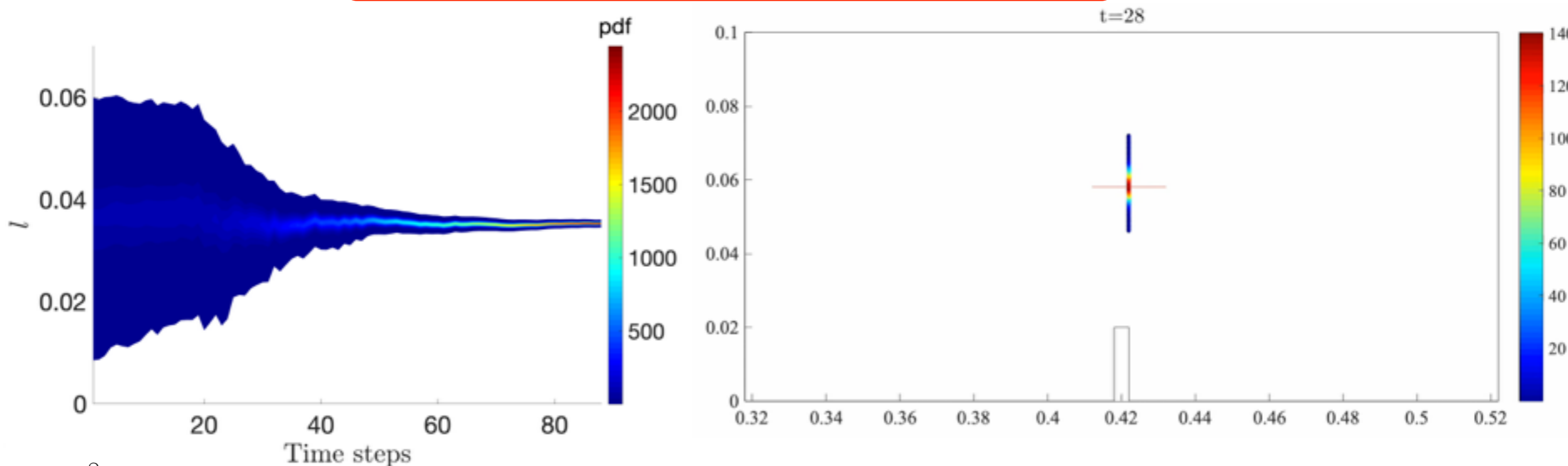
$$\mathbf{u}_{\text{SVD}}(\mathbf{x}, l) = \sum_{k=1}^{N_{\text{SVD}}} \sigma_k \mathbf{u}_k(\mathbf{x}) v_k(l) \quad (\text{meta-model constructed in the offline phase})$$



Results

On-the-fly prediction of the final crack length l_T

$$\pi(l_T) = \pi_u(\mathbf{u}^{\text{SVD}}(l_T)) \cdot \pi_0(l_T)$$



→ can be considered as real-time

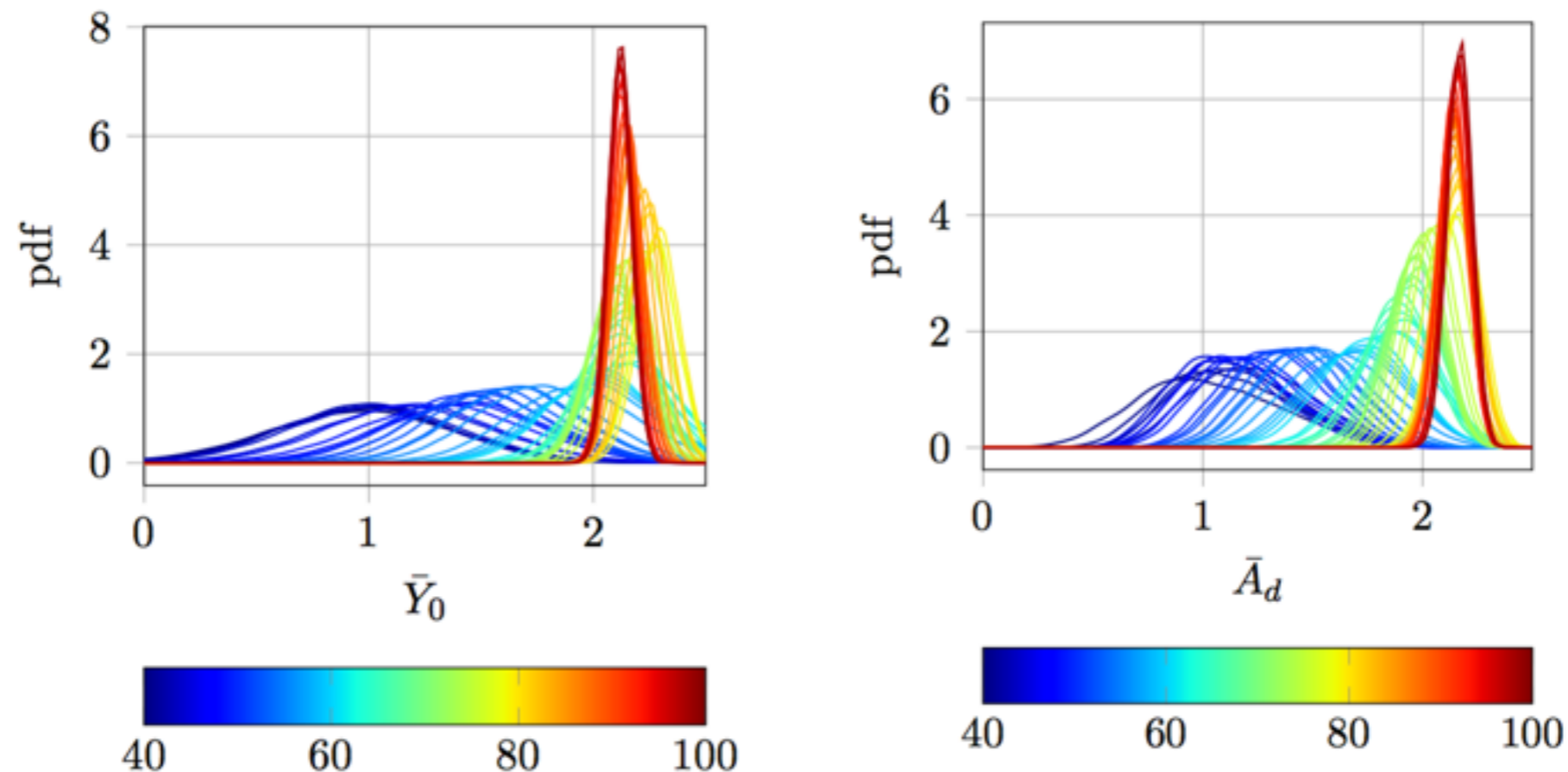


Outline

- 1. Bayesian formulation with ROM**
- 2. Real-time sampling using Transport Maps**
- 3. Model bias correction from data**
- 4. Feedback control**

Bias Effects

- ▶ use of a surrogate PGD model with $m = 3$



- influence limited during first time steps (elasticity with 1st mode alone)
- divergence of the sequential data assimilation procedure (shifted marginals)
- use of error estimates or high-fidelity models often not possible
[Calvetti *et al.* 18]

Bias Correction

- **data-based enrichment**, comparing predicted outputs and actual data
- defined dynamically and in a stochastic setting
extension of PBDW/hybrid twins [Maday et al. 15, Chinesta et al. 18]

🔊 Stochastic residual (computable)

$$\mathbf{B}(\mathbf{x}^{\text{obs}}, t_i) = \mathbf{d}_i^{\text{obs}} - \mathbf{e}_{\text{meas}} - \mathcal{M}(\mathbf{x}^{\text{obs}}, t_i, \mathbf{p})$$

↙ spatial coordinates of measurement points

🔊 Corrected model

$$\mathcal{M}^{\text{corr}}(\mathbf{x}^{\text{obs}}, \mathbf{p}, t_{i+1}) = \mathcal{M}(\mathbf{x}^{\text{obs}}, \mathbf{p}, t_{i+1}) + \hat{\mathbf{B}}_{i \rightarrow i+1}(\mathbf{x}^{\text{obs}})$$

extrapolated model bias
(Gaussian pdf)

↳

$$\pi(\mathbf{d}_{i+1}^{\text{obs}} | \mathbf{p}) = \pi_{\hat{B}}(\mathbf{d}_{i+1}^{\text{obs}} - \mathcal{M}(\mathbf{x}^{\text{obs}}, \mathbf{p}, t_{i+1}))$$

Bias Correction

📌 Extrapolation procedure

- ▶ linear independent extrapolation of mean and standard deviation of $\mathbf{B}(\mathbf{x}^{\text{obs}}, t_i)$
→ no physics consideration / inconsistent results (noise extrapolation)
- ▶ global linear extrapolation involving physics (filtering noise)

$$\mathbb{B}_{\text{mean}} = [\text{mean}(\mathbf{B}(\mathbf{x}^{\text{obs}}, t_1)), \dots, \text{mean}(\mathbf{B}(\mathbf{x}^{\text{obs}}, t_i))] \quad \mathbb{B}_{\text{std}} = [\text{std}(\mathbf{B}(\mathbf{x}^{\text{obs}}, t_1)), \dots, \text{std}(\mathbf{B}(\mathbf{x}^{\text{obs}}, t_i))]$$



SVD decomposition (+truncation)

$$\mathbb{B}_{\text{mean}} = \mathbf{U}_{\text{mean}} \mathbf{D}_{\text{mean}} \mathbf{V}_{\text{mean}}^T \quad \mathbb{B}_{\text{std}} = \mathbf{U}_{\text{std}} \mathbf{D}_{\text{std}} \mathbf{V}_{\text{std}}^T$$

→ linear extrapolations of time SVD modes: $\hat{\mathbf{V}}_{\text{mean}} \quad \hat{\mathbf{V}}_{\text{std}}$

↳ use of the Sequential-Karhunen-Loeve (SKL) method [Ross et al. 08]
fast SVD decomposition of $[\mathbf{M}_{[1,i-1]} \quad \mathbf{M}_i]$ knowing that of $\mathbf{M}_{[1,i-1]}$

→ recovery of $\hat{\mathbf{B}}_{i \rightarrow i+1}(\mathbf{x}^{\text{obs}})$ with truncated SVD

Indication on Model Bias

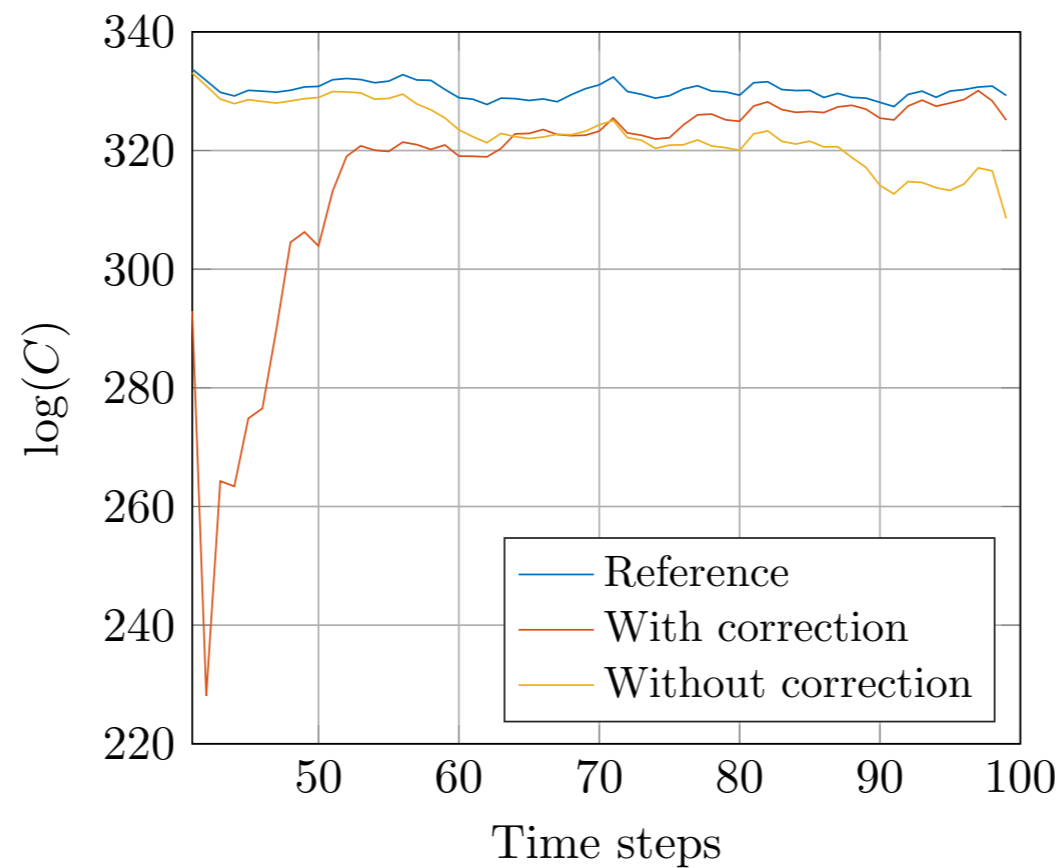
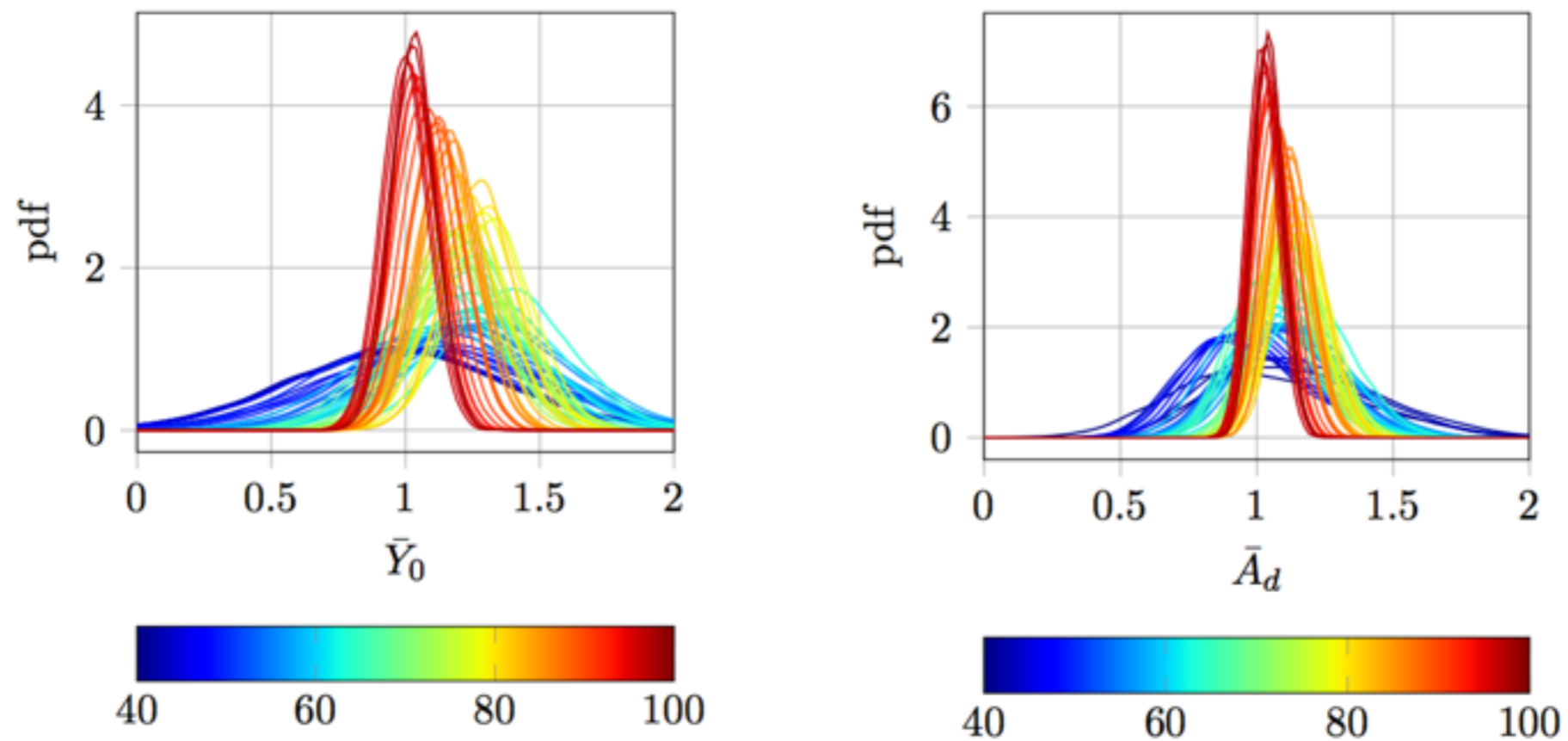
$$\pi(\mathbf{p}|\mathbf{d}^{\text{obs}}) = \frac{1}{C} \pi(\mathbf{d}^{\text{obs}}|\mathbf{p}) \cdot \pi_0(\mathbf{p})$$

$$C = \int \pi(\mathbf{d}^{\text{obs}}|\mathbf{p}) \cdot \pi_0(\mathbf{p}) d\mathbf{p} = \pi(\mathbf{d}^{\text{obs}}) \text{ : model evidence}$$
$$= \exp \left(\mathbb{E}_\rho \left[\log \left(M_{\#}^{-1} \pi \right) - \log(\rho) \right] \right) \text{ [El Moselhy \& Marzouk 12]}$$

└─ decreases when the model becomes inaccurate

- evolution of C monitored along the assimilation process
- implementation of the correction **when C drops drastically**
- if model inaccurate in a given time range, corresponding maps removed

Results

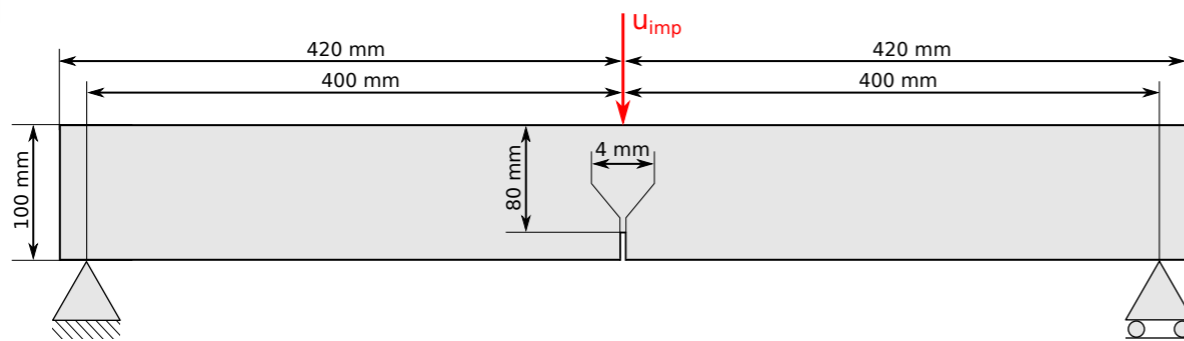
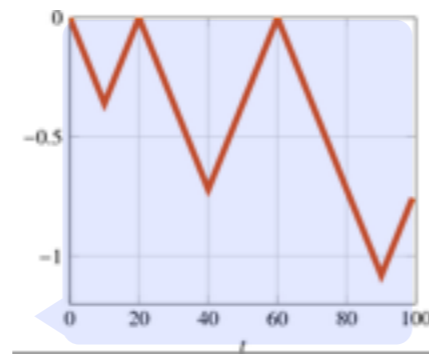




Outline

- 1. Bayesian formulation with ROM**
- 2. Real-time sampling using Transport Maps**
- 3. Model bias correction from data**
- 4. Feedback control**

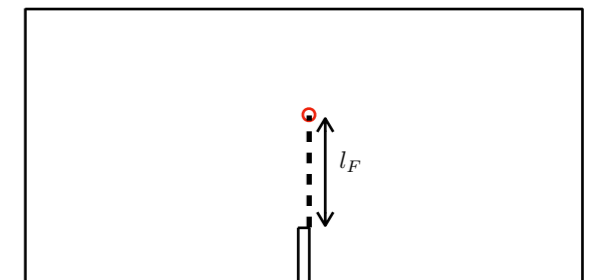
Control example



● **Goal:** Control the final length of the crack (at the end of the loading history)

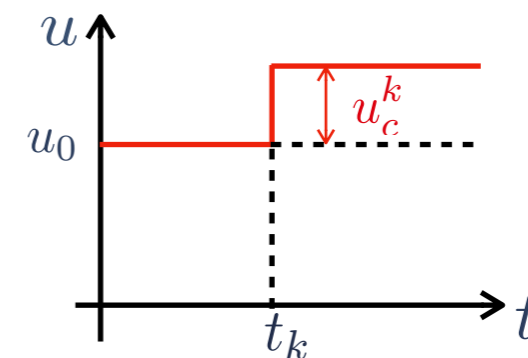
● Quantity of interest:

$$q = \text{mean}[l_F(T, \mathbf{p}, u)] - 3 \cdot \text{std}[l_F(T, \mathbf{p}, u)]$$



● Objective: $q_{obj} = 1$ (probability to be after prescribed position = 0.99)

● Control variable: magnitude of each loading cycle



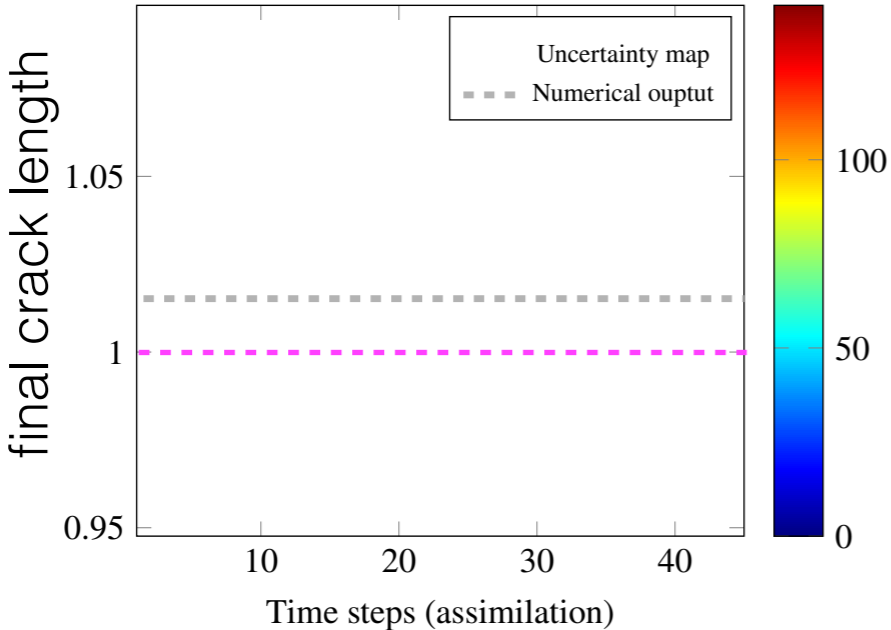
● Computation of the control variable \longrightarrow simple

propagating uncertainty on parameters through the PGD model & TM sampling 30

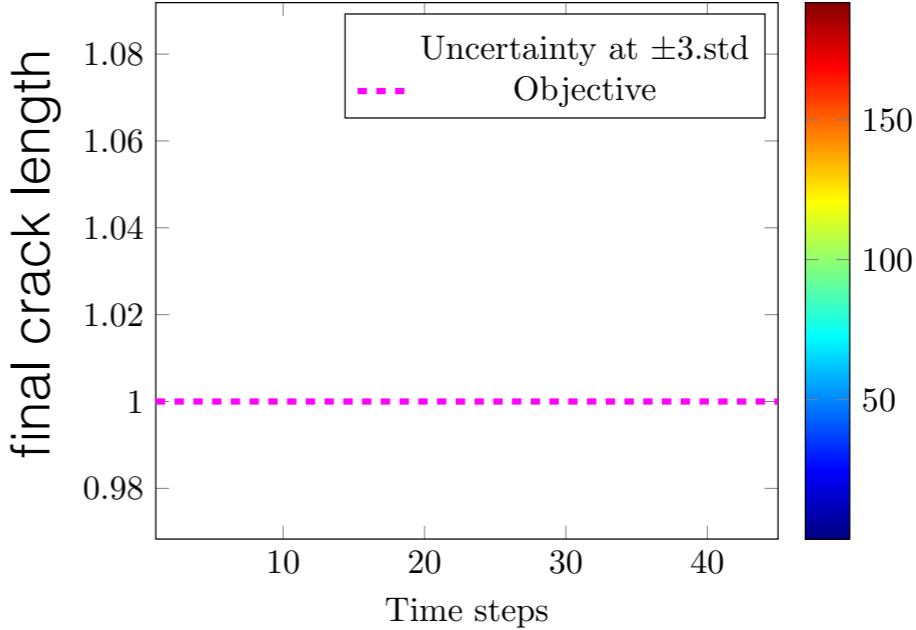
Control example

Results

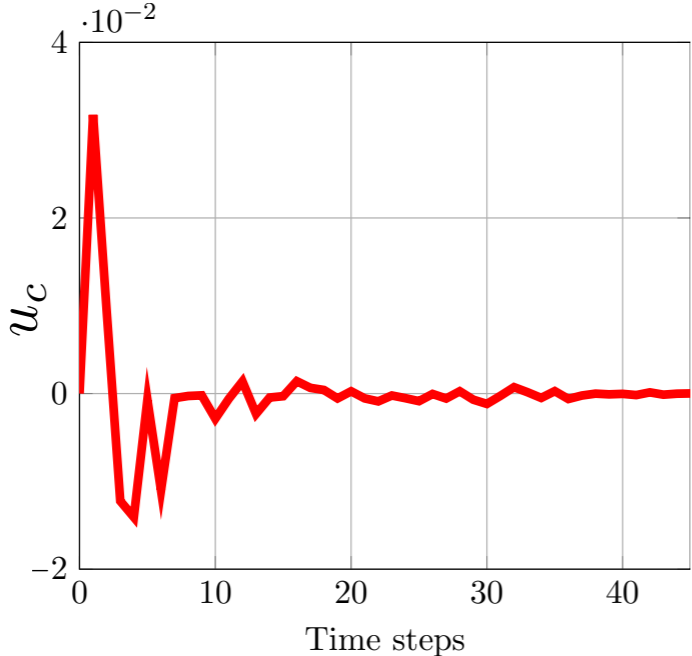
Without control:



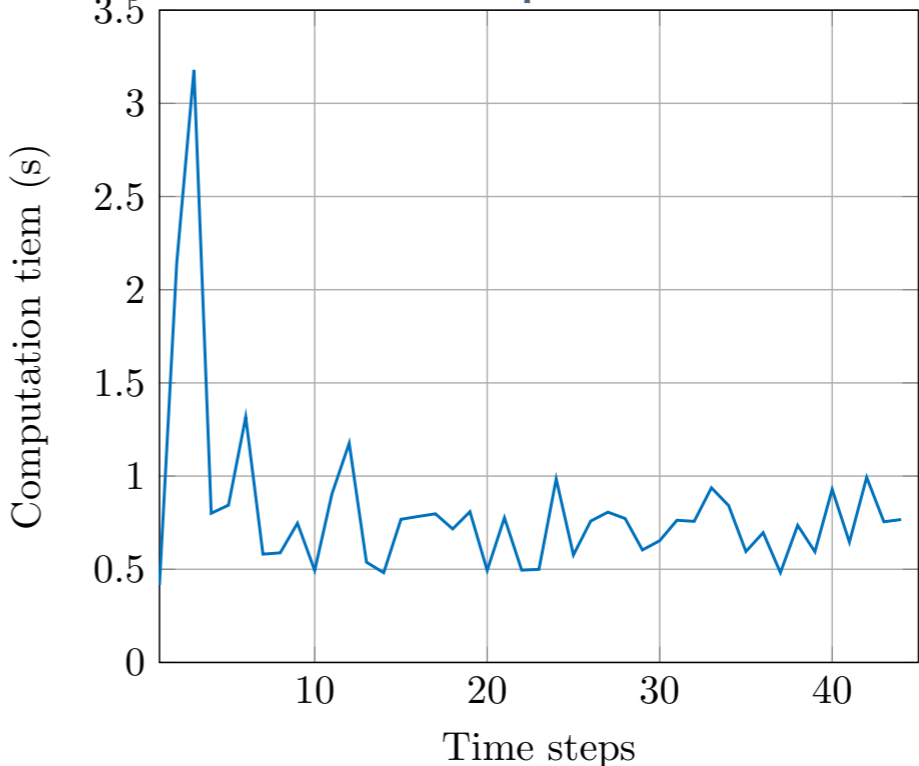
With control:



Command:



Total computation time:



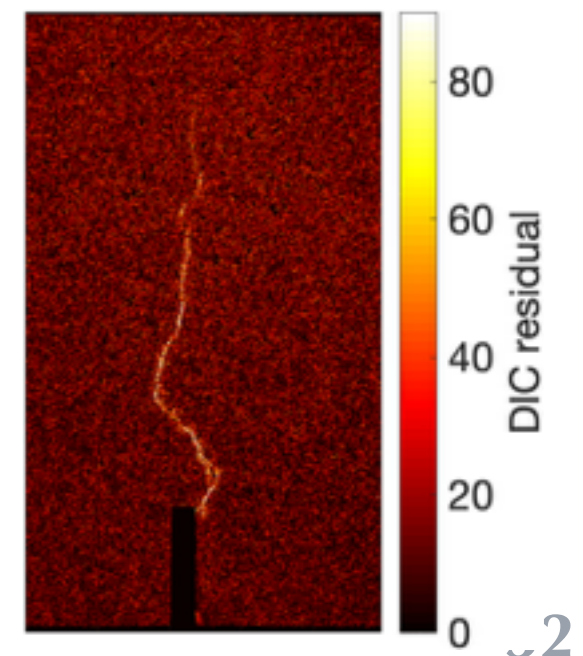
Conclusions & Prospects

Conclusions:

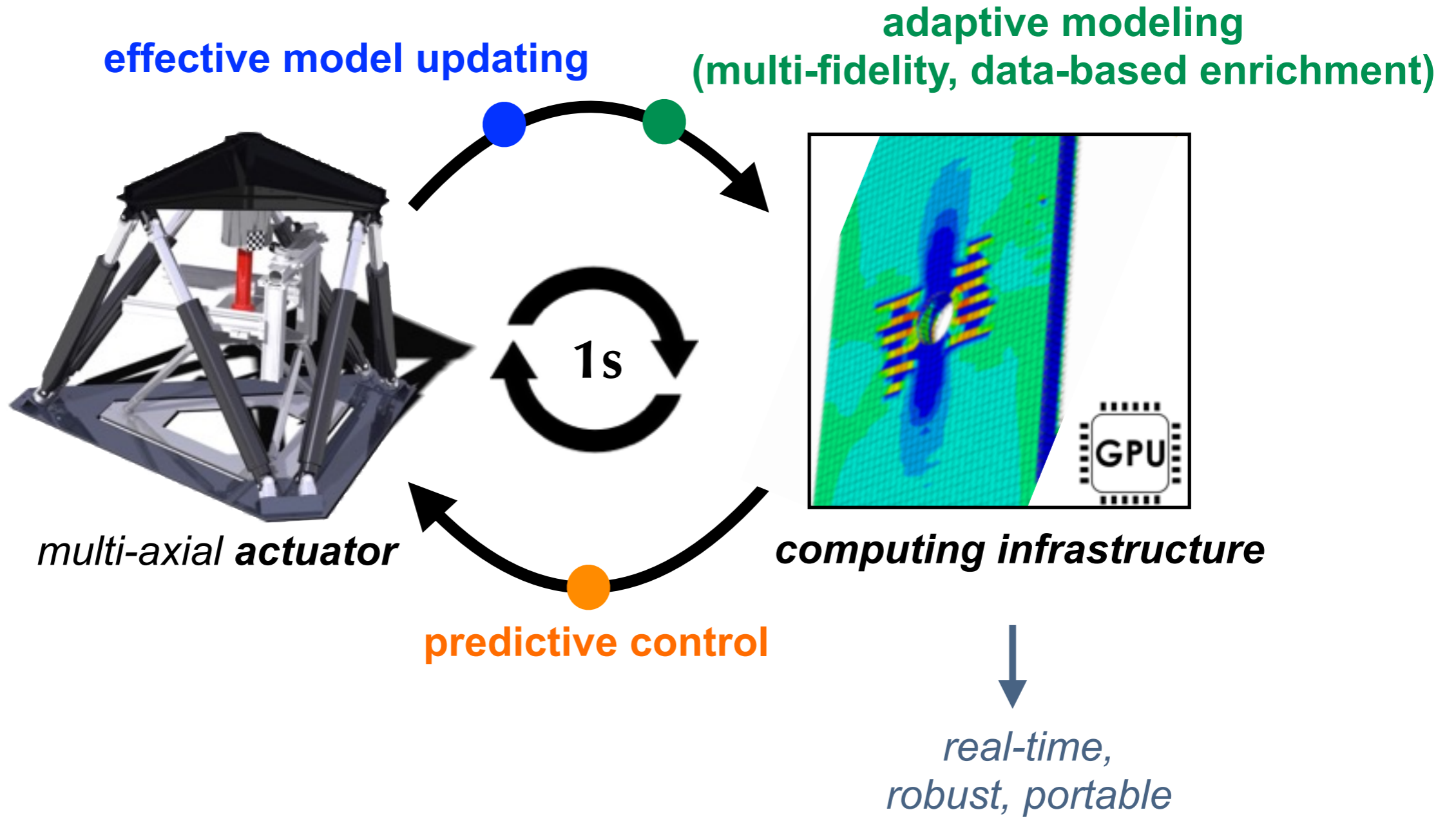
- Transport Maps allow deterministic computations to characterize posteriors
- A constant CPU cost is involved along the sequential updating
- PGD allows to get fast computations
- Consistent procedure for modeling error (bias) correction
- Application on a nonlinear damage problem (single crack)

Prospects:

- Improve automatic order adaptivity of maps in TM sampling
- Regression of the maps composition
- Improve the description of crack propagation
- More complex constitutive models (e.g. composites)
- Investigate high-dimension problems (field identification)
- System control with UQ (damage)
- Interpret model enrichment (learning/mining)



New Project



➔ SMART ENGINEERING STRUCTURES

Thank you!!

- P-B. Rubio, F. Louf, L. C., Fast model updating coupling Bayesian inference and PGD model reduction, *Computational Mechanics*, 62(6):1485-1509 (2018)
- P-B. Rubio, F. Louf, L. C., Transport Map sampling with PGD model reduction for fast dynamical Bayesian data assimilation, *International Journal for Numerical Methods in Engineering*, 120:447-472 (2019)
- P-B. Rubio, L. C., F. Louf, Real-time Bayesian data assimilation with data selection, correction of model bias, and on-the-fly uncertainty propagation, *Comptes-Rendus de l'Académie des Sciences, Mécanique*, 347:762-779 (2019)
- P-B. Rubio, L. C., F. Louf, Real-time data assimilation and control on mechanical systems under uncertainties, *Advanced Modeling and Simulation in Engineering Sciences*, accepted (2021)