Dynamic Kriging-assisted statistical calibration of material model

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Agenda

01

Problem statement:
Material parameters identification using uniaxial tensile testing data

02

Approach: Dynamic Kriging-assisted statistical calibration

03

Validation using a simplified easy-to compute model

04

Application to an industrial FE model

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Uniaxial tensile testing

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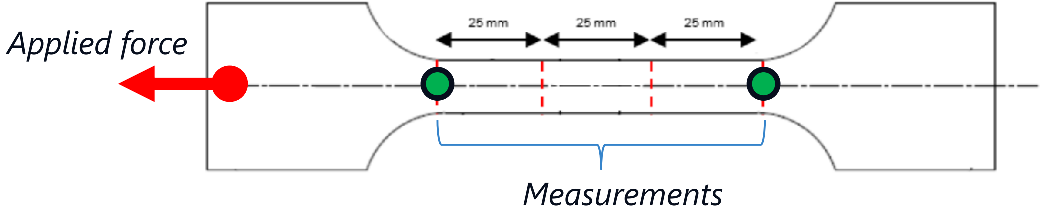
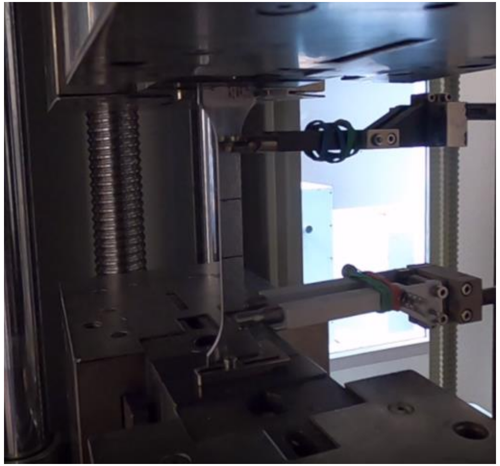
Uniaxial tensile testing

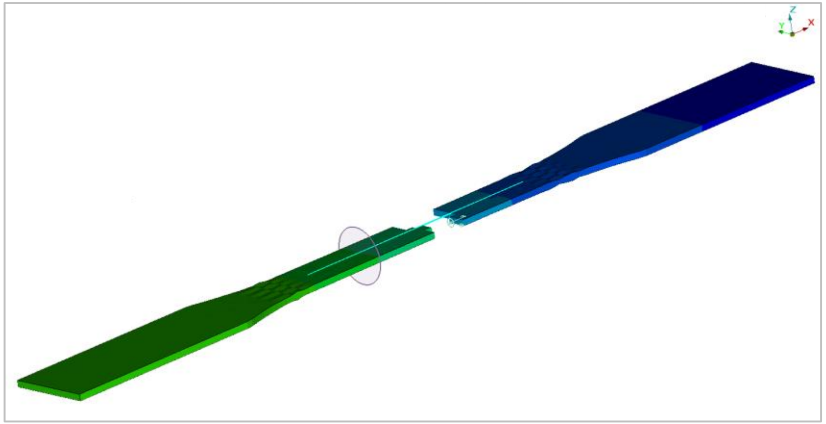


Type	Plate
Material	Aluminum
Designation	7075
Treatment	T6/T651
Specimen thickness	$12.5 \leq t \leq 25$

Physical test



FE simulation



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Johnson-Cook material model

Johnson-Cook plasticity model: $\sigma(\varepsilon_p) = Y + H\varepsilon_p^n$

Johnson-Cook failure model: $\varepsilon_{p,f} = D_1 + D_2 e^{D_3\eta}$

Model parameters vector: $\boldsymbol{\theta} = (Y, H, n, D_1, D_2, D_3)$

σ - stress
ε_p - plastic strain
$\varepsilon_{p,f}$ - plastic strain at failure
η - stress triaxiality

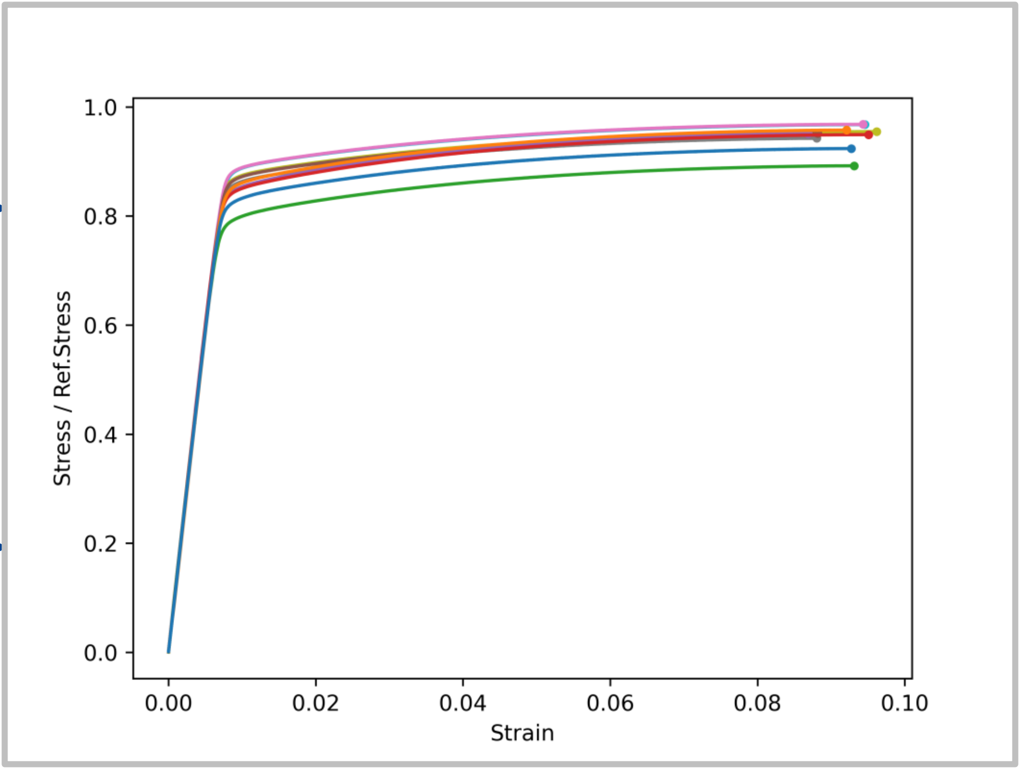
Model parameters identification

Physical experiment

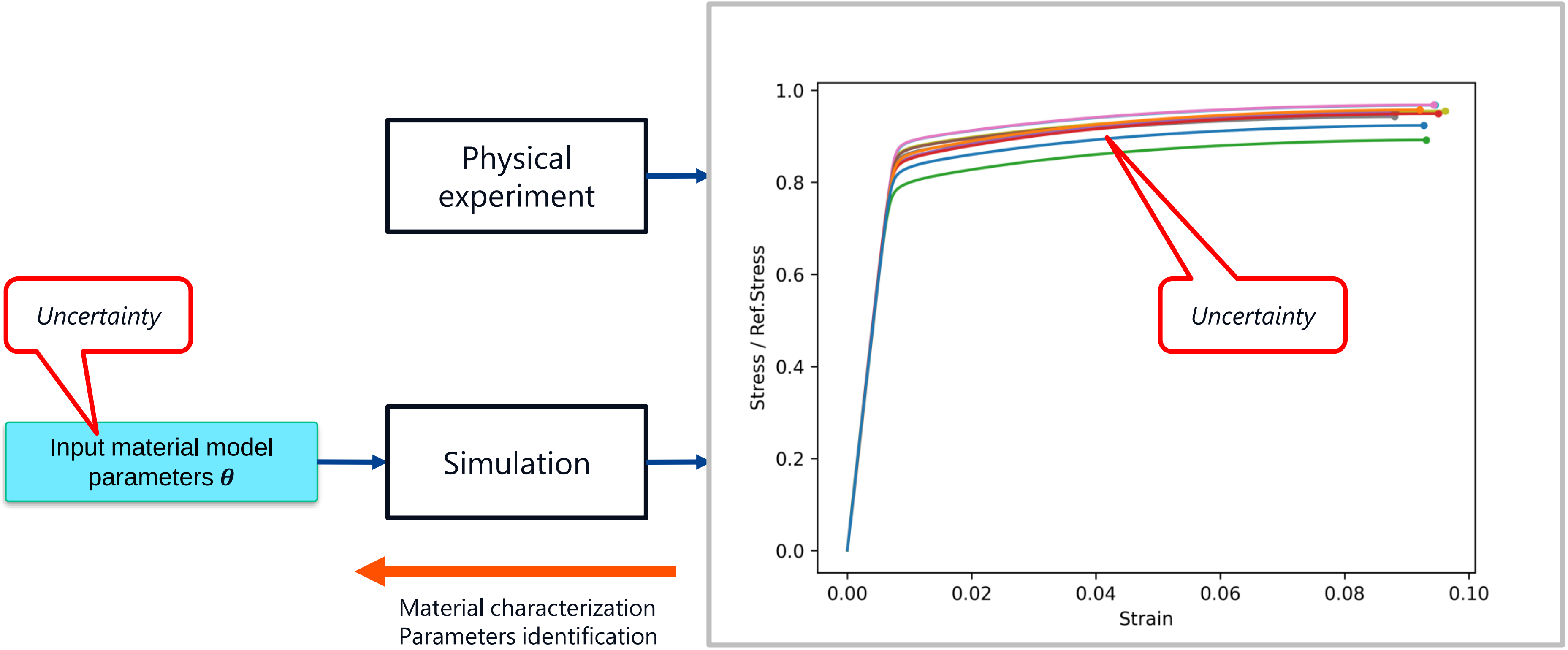
Input material model parameters $\boldsymbol{\theta}$

Simulation

Material characterization
Parameters identification



Model parameters identification



Goals

- Approximate the probability distribution of the material model parameters
  - Deterministic values: expectation or MAP estimator
  - Correlation between parameters
  - Uncertainty propagation in other model

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  - Direct approach is impossible (thousands of FE model evaluations)

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- Approximate the probability distribution of the material model parameters
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- Sample using MCMC
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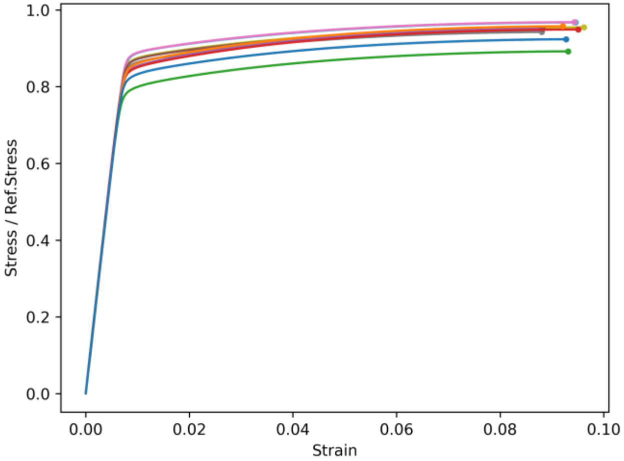
- Surrogate model for the posterior
  - Dynamic Kriging: minimize the number of model evaluations
  - Acquisition function exploring the high probability regions

Statistical calibration

Output vector and input parameters

- Output vector $\boldsymbol{y} := (\varepsilon_1, \ldots, \varepsilon_{N_{nodes}}, \sigma_1, \ldots, \sigma_{N_{nodes}})$



- Experimental data : $\boldsymbol{y}_k^*, \; k = 1, \ldots, N_{obs}$

- Model parameters vector: $\boldsymbol{\theta} = (Y, H, n, D_1, D_2, D_3)$

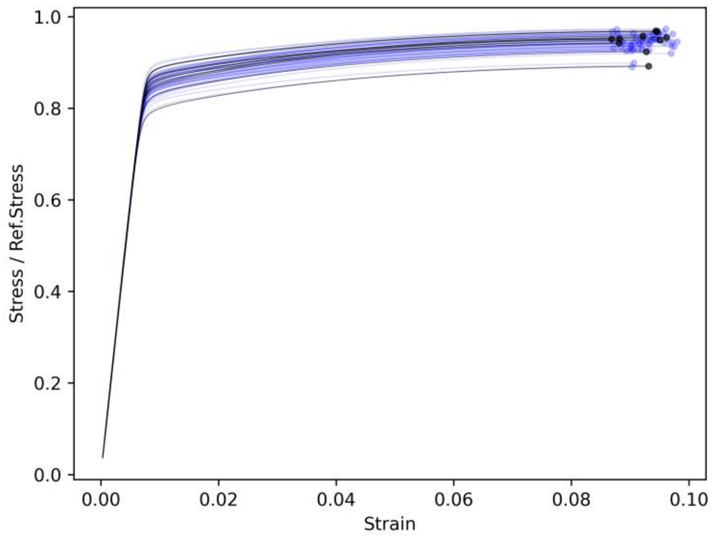
Probabilistic model for material response

Hypothesis: Output data (curve) ~ Gaussian process $\tilde{\boldsymbol{y}} \sim \mathcal{N}(\bar{\boldsymbol{y}}^*, VV^\top)$

$$\tilde{\boldsymbol{y}}(\boldsymbol{\eta}) = \bar{\boldsymbol{y}}^* + \boxed{V}\boldsymbol{\eta},$$

$$= \bar{\boldsymbol{y}}^* + \boxed{\frac{1}{\sqrt{N_{obs}}} \sum_{k=1}^{N_{obs}} (\boldsymbol{y}_k^* - \bar{\boldsymbol{y}}^*)}\eta_k$$

$\mathcal{N}(0,1)$



Experimental Data:	$\boldsymbol{y}_k^*,\ k = 1, \ldots, N_{obs}$
Data mean:	$\bar{\boldsymbol{y}}^* := \frac{1}{N_{obs}} \sum_{k=1}^{N_{obs}} \boldsymbol{y}_k^*$

Posterior

$$\tilde{\boldsymbol{y}} = \boldsymbol{f}(\boldsymbol{\theta}) + \boldsymbol{\xi}, \qquad \boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}, \Sigma), \qquad \Sigma^{\frac{1}{2}} = 0.05\,\mathrm{diag}\,\bar{\boldsymbol{y}}^*$$

$\mathcal{N}(\bar{\boldsymbol{y}}^*, VV^\top)$

our numerical model

model bias
(here simply iid Gaussian noise)

Posterior

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$\mathcal{N}(\bar{\boldsymbol{y}}^*, VV^\top)$

our numerical model

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(here simply iid Gaussian noise)

Posterior distribution:

$$p(\boldsymbol{\theta}|\boldsymbol{Y}^*) \propto e^{-\frac{1}{2}(\boldsymbol{f}(\boldsymbol{\theta})-\bar{\boldsymbol{y}}^*)^\top\left(\Sigma+VV^\top\right)^{-1}(\boldsymbol{f}(\boldsymbol{\theta})-\bar{\boldsymbol{y}}^*)}\,\pi_0(\boldsymbol{\theta}).$$

prior

Log-posterior:

$$J(\boldsymbol{\theta}) := -\frac{1}{2}\|\boldsymbol{f}(\boldsymbol{\theta}) - \bar{\boldsymbol{y}}^*\|^2_{(\Sigma+VV^\top)^{-1}} + \log \pi_0(\boldsymbol{\theta}) + const.$$

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Surrogate posterior

Log-normal Kriging metamodel for the posterior : $\hat{p}(\boldsymbol{\theta}) = e^{\hat{J}(\boldsymbol{\theta})}$

Gaussian process emulator of the log-posterior :

$$\underbrace{\hat{J}(\boldsymbol{\theta}) = \mu(\boldsymbol{\theta})}_{\text{Kriging mean}} + \underbrace{\sigma(\boldsymbol{\theta})}_{\text{Kriging variance}}\xi, \qquad \xi \sim \mathcal{N}(0,1)$$

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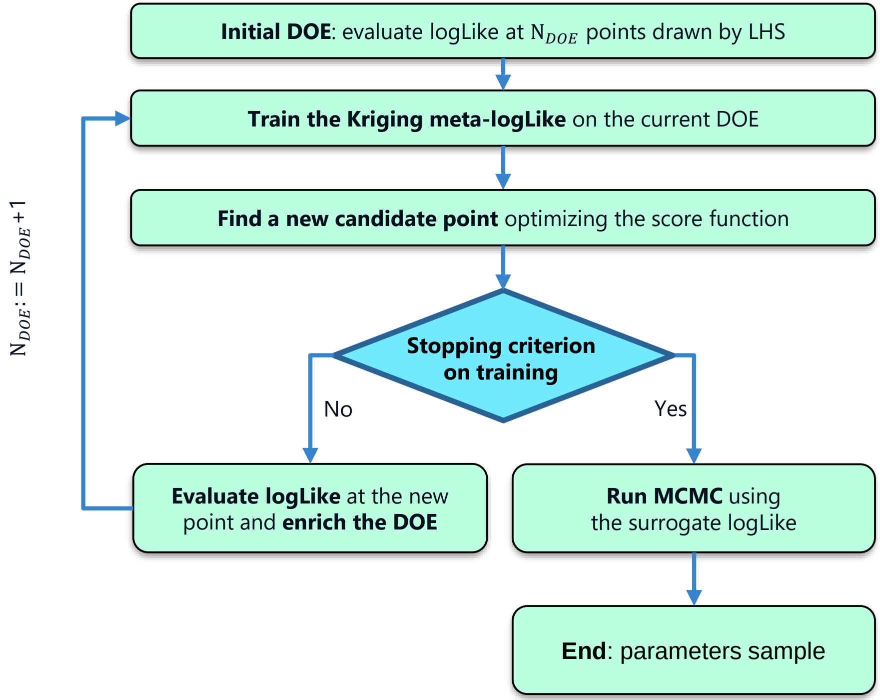
Choice for the prediction:

$$\hat{p}_{mean}(\boldsymbol{\theta}) = e^{\mu(\boldsymbol{\theta})+\frac{1}{2}\sigma^2(\boldsymbol{\theta})},$$

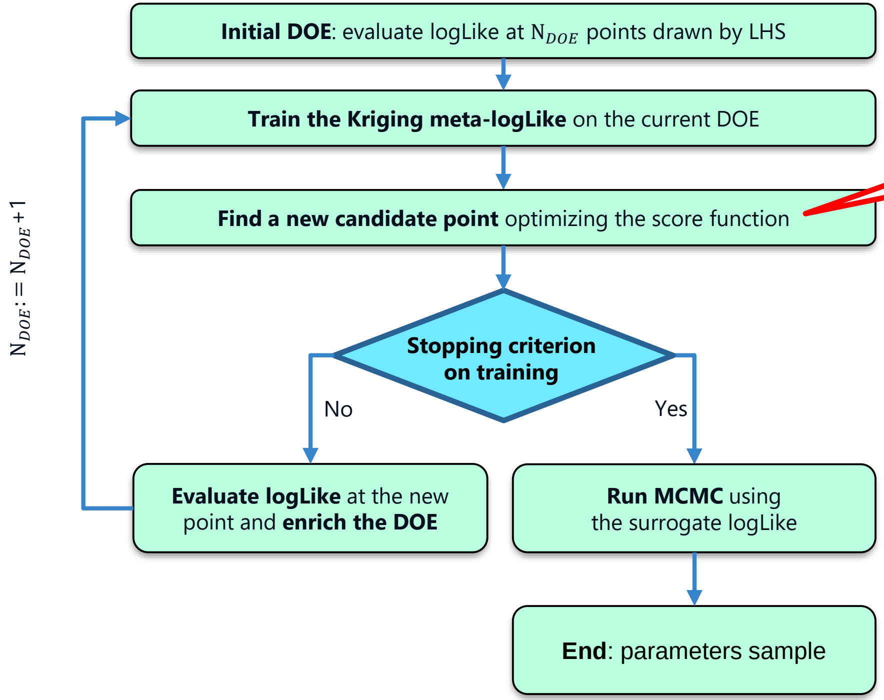
$$\hat{p}_{med}(\boldsymbol{\theta}) = e^{\mu(\boldsymbol{\theta})},$$

$$\boxed{\hat{p}_{mode}(\boldsymbol{\theta}) = e^{\mu(\boldsymbol{\theta})-\sigma^2(\boldsymbol{\theta})}.}$$

Dynamic Kriging



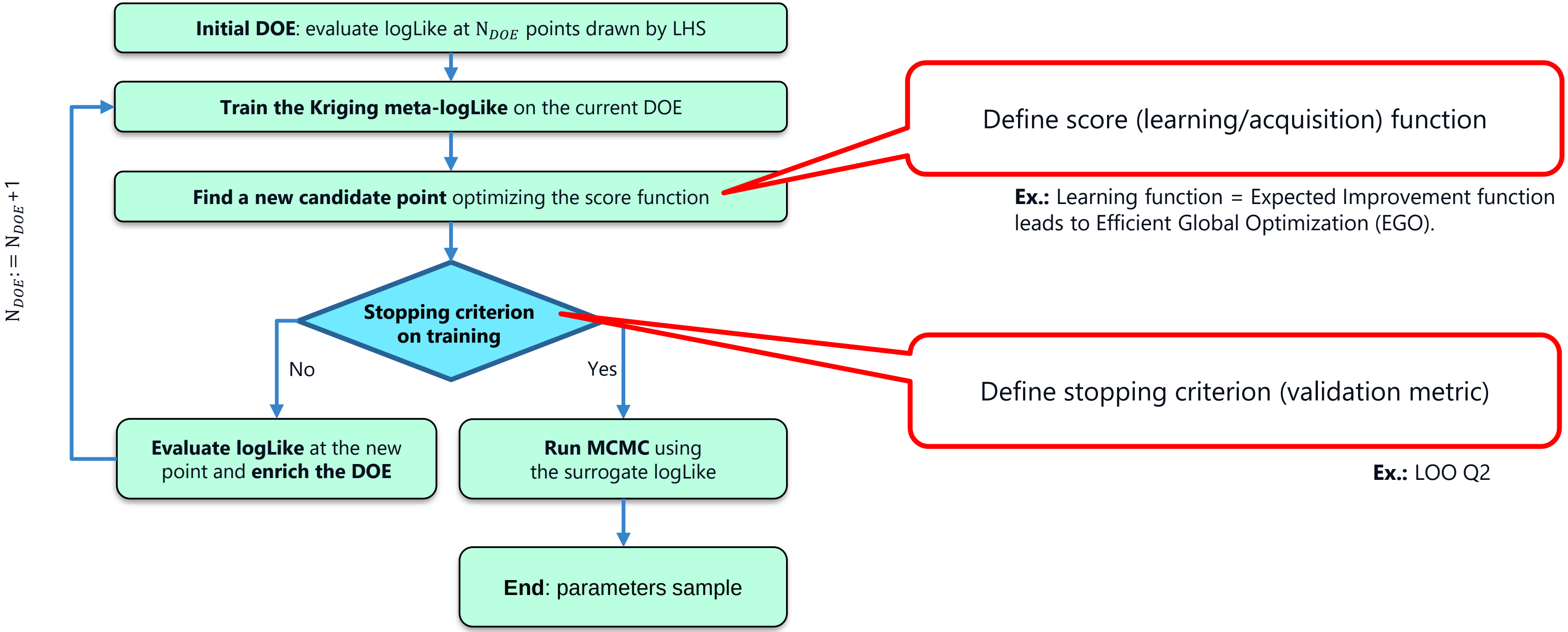
Dynamic Kriging



Define score (learning/acquisition) function

Ex.: Learning function = Expected Improvement function leads to Efficient Global Optimization (EGO).

Dynamic Kriging



Ex.: Learning function = Expected Improvement function leads to Efficient Global Optimization (EGO).

Ex.: LOO Q2

Dynamic Kriging: Learning (score/acquisition) function

Ex.: Learning function = Expected Improvement function leads to EGO. **Aim is the MAP point.**

Our aim is to explore the whole distribution (or at least the **high probability region**).

Learning function choice – Shannon entropy (as measure of uncertainty) of the log-normal process at a point:

$$\boxed{H(\boldsymbol{\theta}) = \mu(\boldsymbol{\theta}) + \log \sigma(\boldsymbol{\theta}) + const.}$$

Acquisition of a new DOE point:

$$\boldsymbol{\theta}^{new} = \arg\max_{\boldsymbol{\theta}} H(\boldsymbol{\theta}).$$

Dynamic Kriging: Stopping criterion

Validation metric (alternative to Q2) adapted for probability distributions.

Leave-One-Out version of (normalized) **Jensen-Shannon divergence** (JSD):

$$\boxed{D_{JS}(p,\hat{p}) = 1 - \frac{H_P + H_{\hat{P}}}{2H_M}}$$

$$H_P = -\frac{1}{N_{DOE}} \sum_{i=1}^{N_{DOE}} P_i \log P_i, \qquad H_{\hat{P}} = -\frac{1}{N_{DOE}} \sum_{i=1}^{N_{DOE}} \hat{P}_i \log \hat{P}_i \qquad H_M = -\frac{1}{N_{DOE}} \sum_{i=1}^{N_{DOE}} M_i \log M_i$$

$$P_i = \frac{p(\boldsymbol{\theta}_i)}{\sum_{i=1}^{N_{DOE}} p(\boldsymbol{\theta}_i)}, \qquad \hat{P}_i = \frac{\hat{p}_{loo}(\boldsymbol{\theta}_i)}{\sum_{i=1}^{N_{DOE}} \hat{p}_{loo}(\boldsymbol{\theta}_i)}, \qquad M_i = \frac{1}{2}(P_i + \hat{P}_i)$$

Validation using a simplified model

Easy-to-compute analytical model

Inputs to calibrate:

$$\boldsymbol{\theta} = (E, Y, H, n, D_1)$$

Uniform prior (heuristic)

Parameters	Lower bound	Upper bound
Yield stress E/E^{ref}	0.833	1.111
Yield stress Y/Y^{ref}	0.623	1.246
Hardening modulus H/H^{ref}	0.647	2.16
Hardening exponent n/n^{ref}	0.4	2
Failure parameter D_1/D_1^{ref}	0.566	1.132

Analytical model $\boldsymbol{f}(\boldsymbol{\theta})$

(simple in evaluation, so direct MCMC is feasible)

$$\sigma_{true}(\varepsilon_{true}) = \begin{cases} E\varepsilon_{true}, & \varepsilon_{true} \leq Y/E, \\ Y + H\left(\varepsilon_{true} - Y/E\right)^n, & \varepsilon_{true} > Y/E, \end{cases}$$

with $\varepsilon_{true} \in [0, D_1]$.

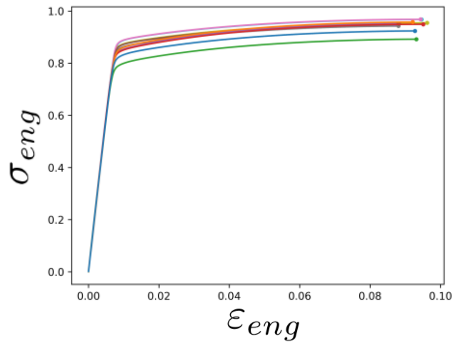
$$\sigma_{eng} = \frac{\sigma_{true}}{e^{\varepsilon_{true}} - \frac{1-2\nu}{E}\sigma_{true}},$$

$$\varepsilon_{eng} = e^{\varepsilon_{true}} - 1.$$

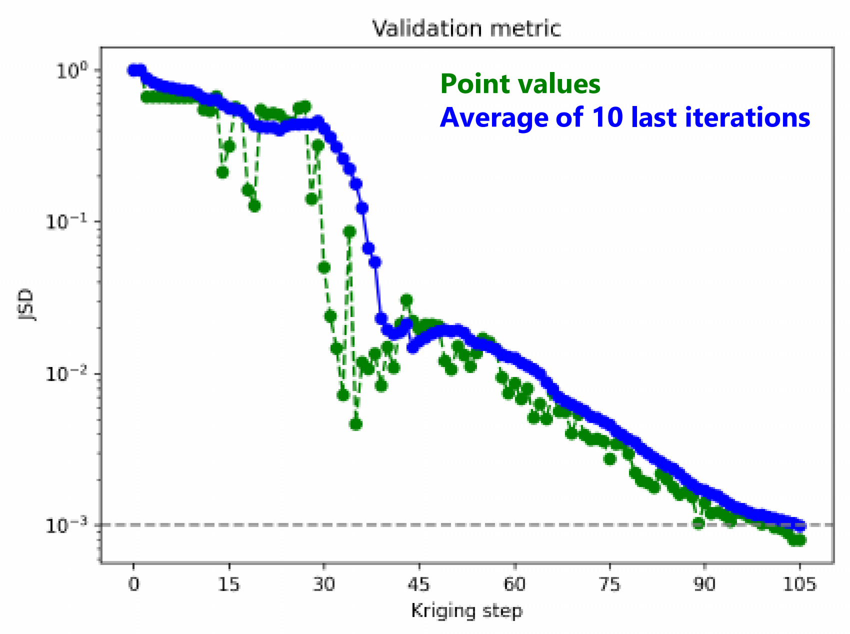
5 parameters simplified Johnson-Cook material model

Outputs to compare with data:

$$\sigma_{eng}, \varepsilon_{eng}$$



Dynamic Kriging procedure



Surrogate model implementation:

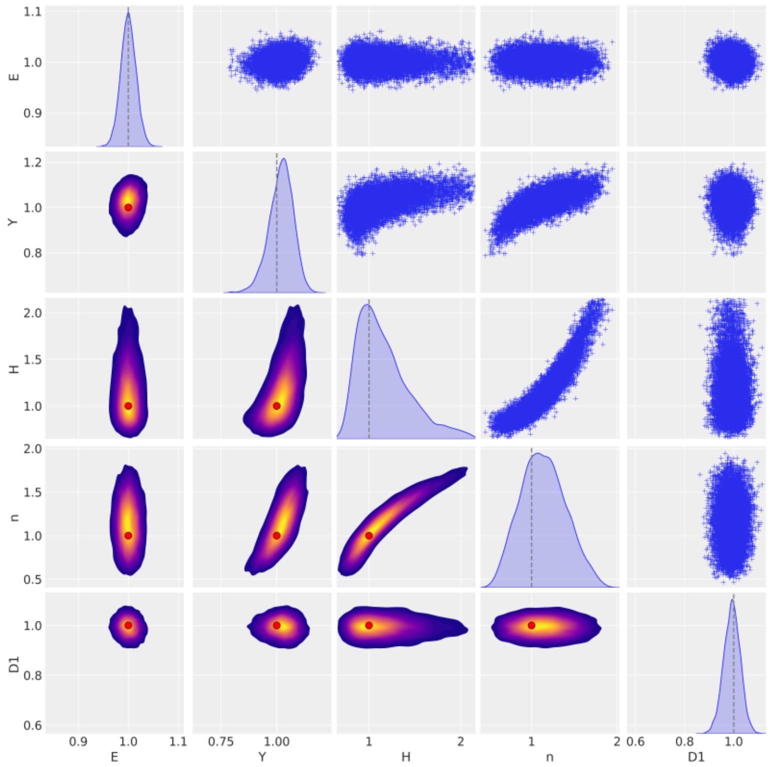
- *OpenTURNS*
- Matérn 5/2 covariance
- Zero trend

True posterior vs. Surrogate posterior

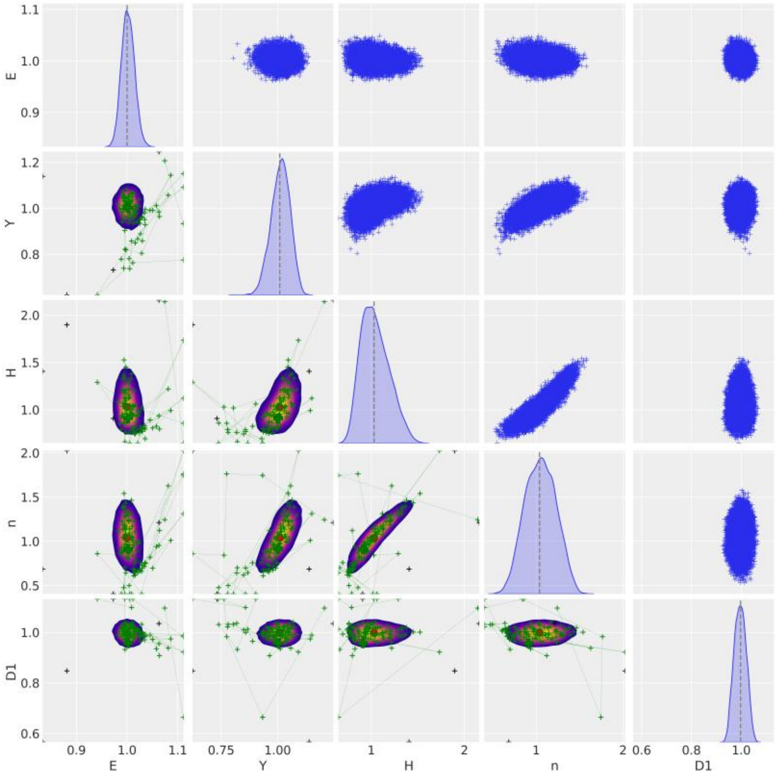
Initial DOE (*MaxPro*) of size = 5
Dynamically added points

Sampling : *SMC*

** Reference values = Ground truth MAP*



Ground truth posterior



Surrogate posterior

MAP estimator

Parameters	Lower bound	Upper bound	Surrogate MAP
Yield stress E/E^{ref}	0.833	1.111	0.999
Yield stress Y/Y^{ref}	0.623	1.246	1.009
Hardening modulus H/H^{ref}	0.647	2.16	1.03
Hardening exponent n/n^{ref}	0.4	2	1.04
Failure parameter D_1/D_1^{ref}	0.566	1.132	0.997

** Reference values = Ground truth MAP*

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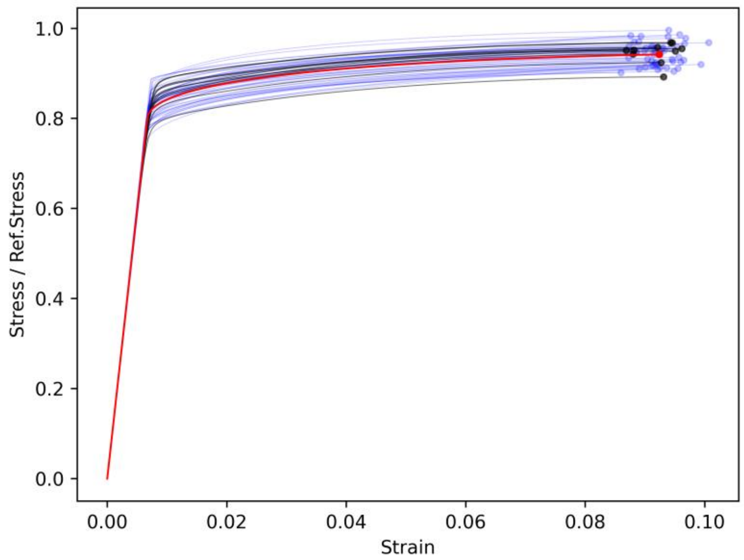
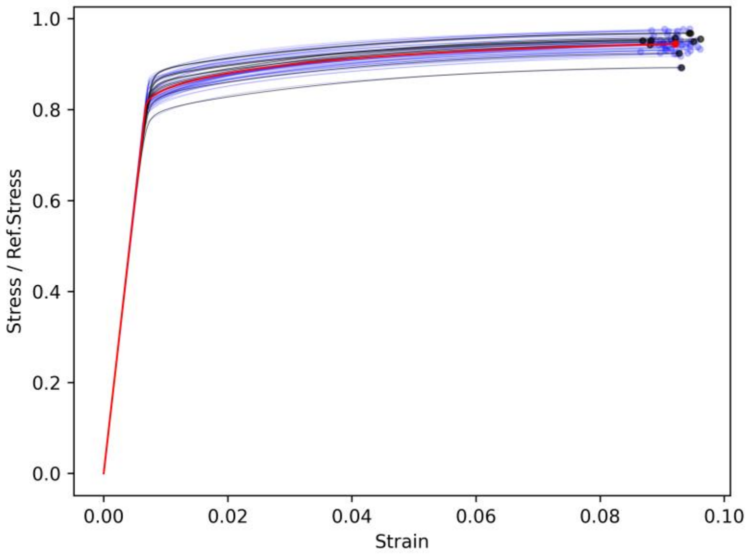
Material response samples



True posterior: **50 MCMC samples**, **MAP**, **10 data curves**



Surrogate posterior: **50 MCMC samples**, **MAP**, **10 data curves**

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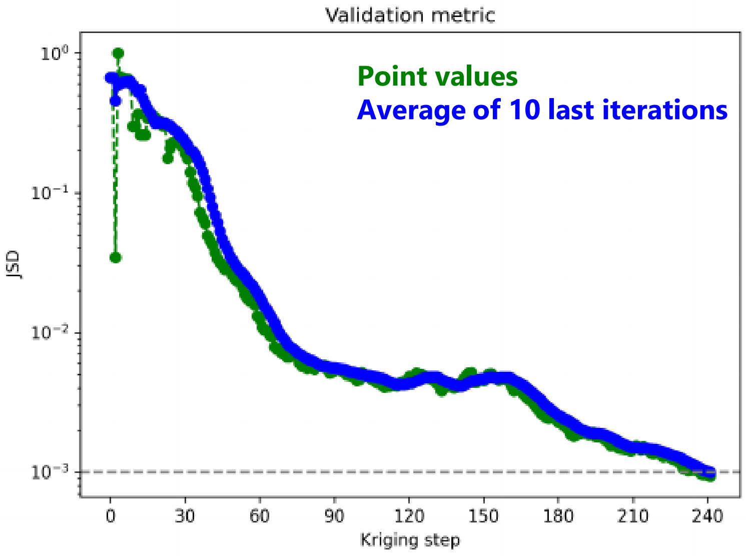
Application to the FE model

Dynamic Kriging for FE model

- FE model (*OpenRadioss*):
  - ~1000 nodes
  - Runtime ~ 3 min

- 6 parameters Johnson—Cook material model:
  - 3 plastic parameters (Yield stress, Hardening modulus and exponent)
  - 3 failure parameters (D1, D2, D3)

$$\boldsymbol{\theta} = (Y, H, n, D_1, D_2, D_3)$$



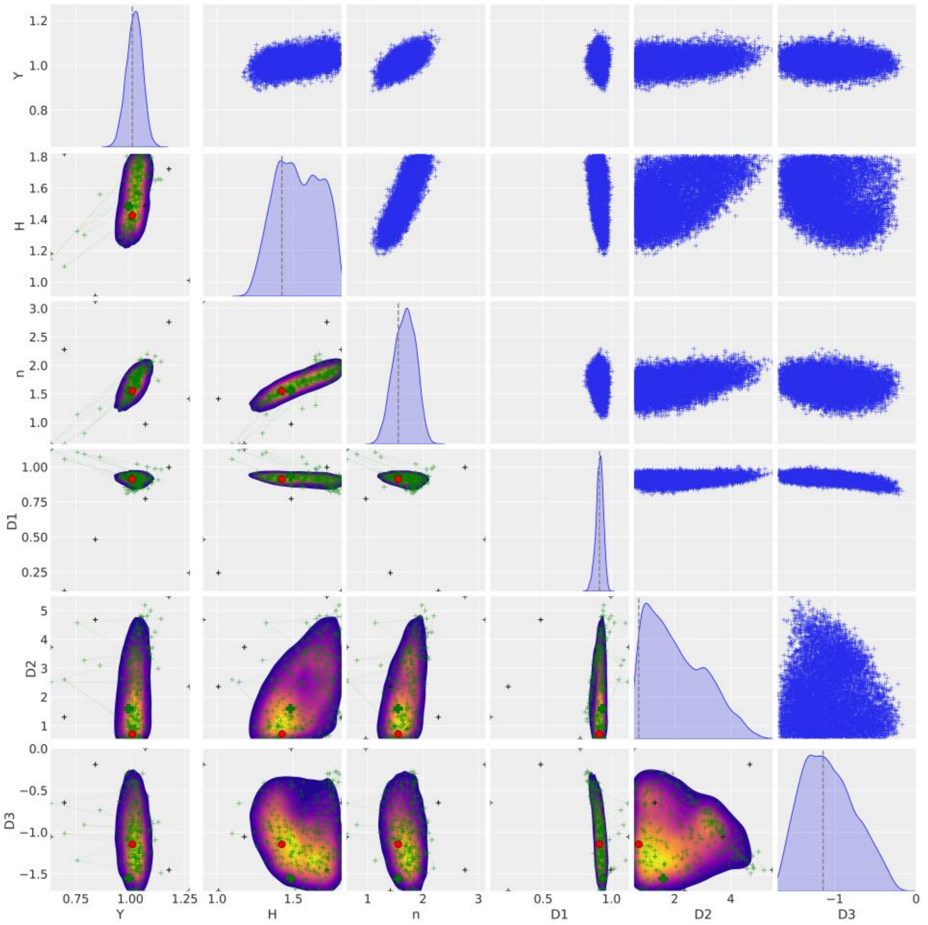
Surrogate posterior

- 6 parameters Johnson—Cook material model.
- Uniform prior (heuristic).

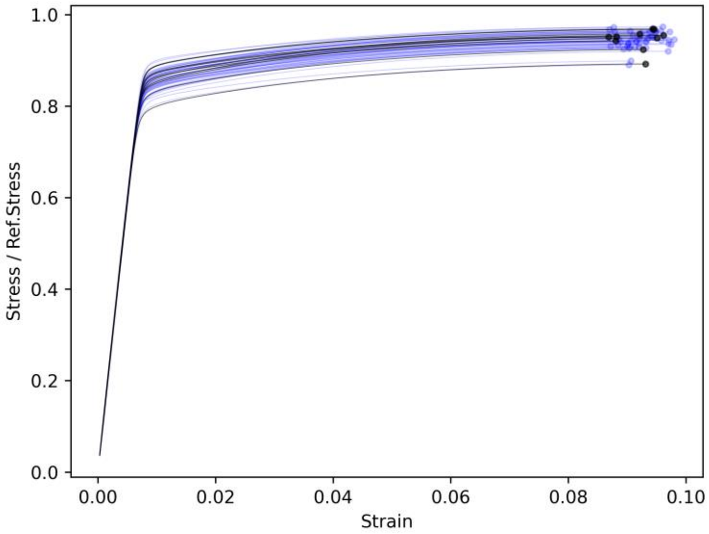
Parameters	Lower bound	Upper bound	Surrogate MAP
Yield stress Y/Y^{ref}	0.635	1.27	1.009
Hardening modulus H/H^{ref}	0.9	1.8	1.425
Hardening exponent n/n^{ref}	0.625	3.125	1.55
Failure parameter D_1/D_1^{ref}	0.113	1.13	0.91
Failure parameter D_2/D_2^{ref}	0.55	5.5	0.716
Failure parameter $D_3/\lvert D_3^{ref}\rvert$	-1.7	0	-1.14

** Reference = Fixed nominal parameters values*

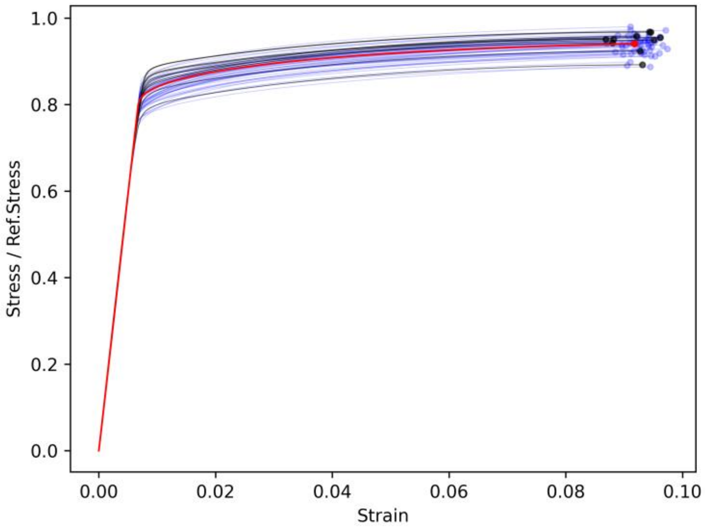
Initial DOE size = 6
Dynamically added points



Material response samples



Reference (Gaussian response model): **50 samples**, **10 data curves**



Surrogate: **50 MCMC samples**, **MAP**, **10 data curves**

Conclusion & Perspectives

- Surrogate posterior distribution
  - Dynamic DOE procedure
  - Entropy-based acquisition function to explore high probability region
  - Validation metric based on Jensen-Shannon divergence
  - Validation using a simplified model

- Uncertainty quantification of the material model parameters
  - MAP estimator
  - Correlation between parameters
  - MCMC sampling from the surrogate

- *Perspectives:*
  - Model bias identification
  - Error analysis

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