UNCECOMP International Conference on Uncertainty Quantification in Computational Sciences and Engineering

Parametric uncertainty quantification in the presence of modeling errors: Bayesian approach and application to metal forming

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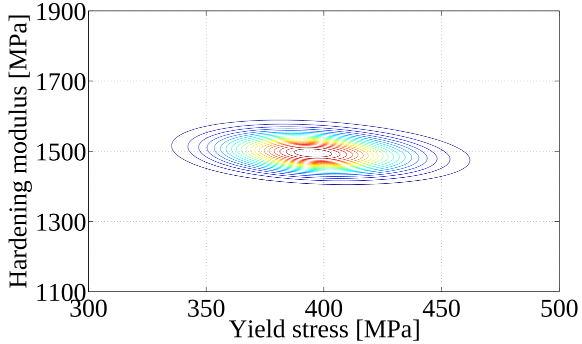
May 26, 2015

Motivation

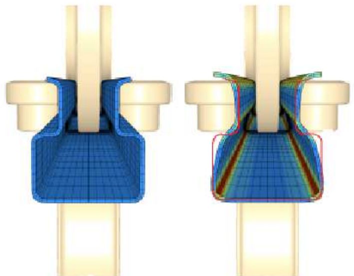
Data

h [MPa]	s [MPa]
1488	375
1485	403
1514	407
1500	377
...	...

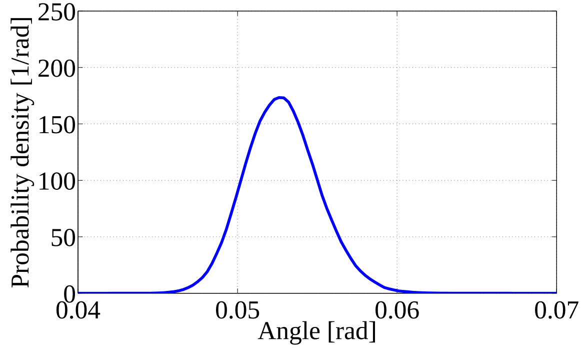
PDF of material properties



Engineering model



PDF of formed shape



Modeling errors due to data limitations

Modeling errors due to modeling simplifications

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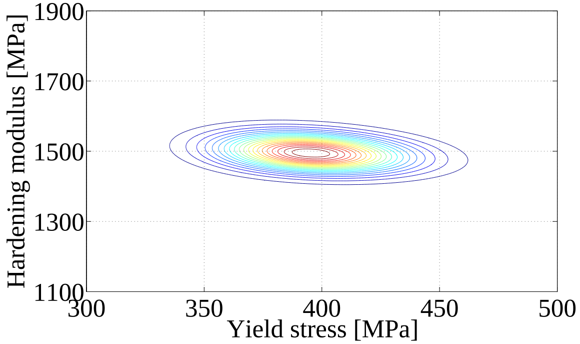
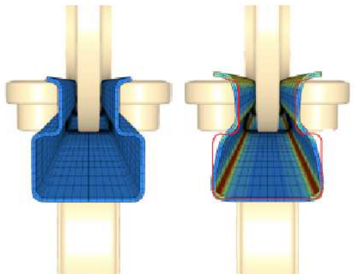
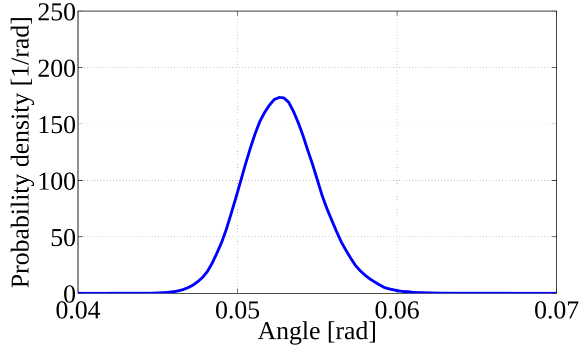


Engineering model



PDF of formed shape



Modeling errors due to data limitations

Modeling errors due to modeling simplifications

Outline

- Motivation.
- Outline.
- Methodology.
- Implementation.
- Application to metal forming.
- Conclusion.

Methodology

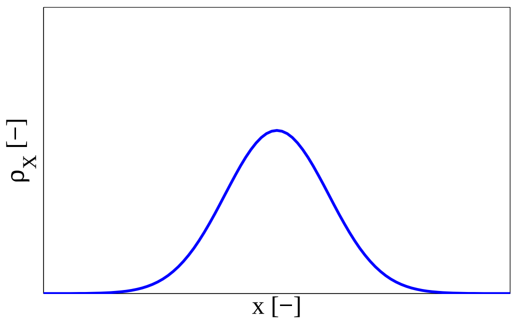
Model problem

$$\underbrace{\boldsymbol{y}}_{\text{output variables}} = \underbrace{\boldsymbol{g}}_{\substack{\text{engineering} \\ \text{problem}}} (\underbrace{\boldsymbol{x}}_{\text{input variables}})$$

Data

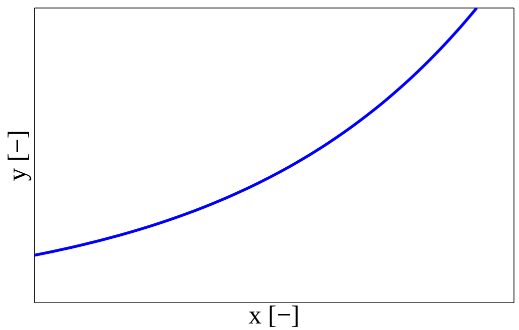
$\boldsymbol{x}_1^{\text{obs}}$
$\boldsymbol{x}_2^{\text{obs}}$
$\vdots$

PDF of input variables

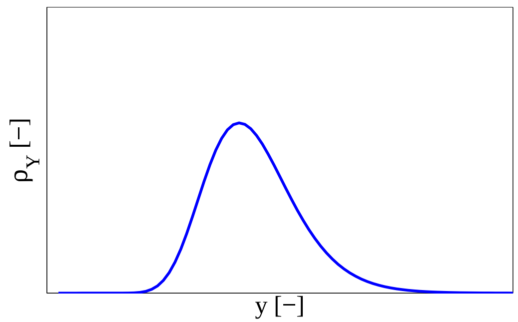


$\rho_{\boldsymbol{X}}(\boldsymbol{x}|\hat{\boldsymbol{p}})$

Engineering model



PDF of output variables



$\rho_{\boldsymbol{Y}}(\boldsymbol{y}|\hat{\boldsymbol{p}})$

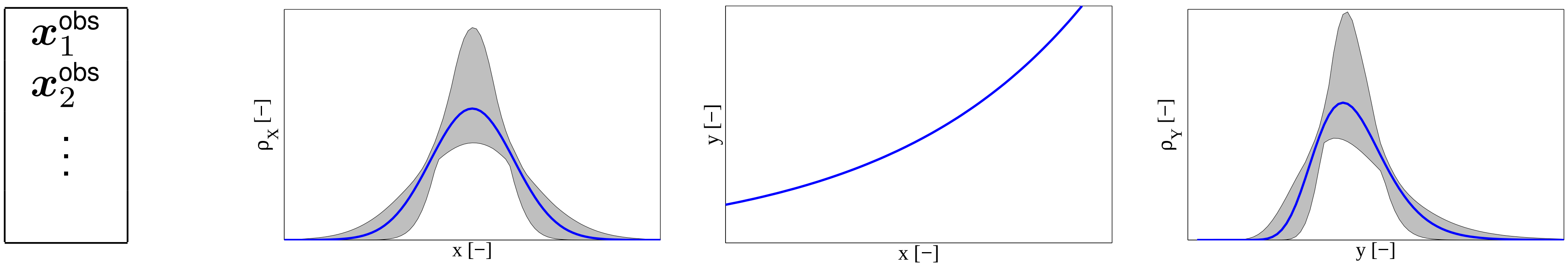
Bayesian methodology

Modeling errors due to data limitations are represented by inference of a **posterior PDF** for the parameters of the PDF for the input variables [Ghanem and Doostan, 2006; A, Ghanem, and Soize, 2010]:

$$\underbrace{\rho_{\boldsymbol{P}}^{\text{post}}(\boldsymbol{p})}_{\text{posterior PDF}} = \underbrace{c}_{\text{normalization constant}} \times \underbrace{\rho_{\boldsymbol{P}}^{\text{prior}}(\boldsymbol{p})}_{\text{prior PDF}} \times \underbrace{\prod_{k=1}^{\nu} \rho_{\boldsymbol{X}}(\boldsymbol{x}_k^{\text{obs}}|\boldsymbol{p})}_{\text{likelihood of parameters}}$$

This ultimately leads to **error bounds on the results of the parametric uncertainty analysis**.

Data | PDF of input variables | Engineering model | PDF of output variables



$\rho_{\boldsymbol{X}}(\boldsymbol{x}|\boldsymbol{P})$ $\rho_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{P})$

Implementation

Sampling from posterior PDF

- Since the PDF of the input variables typically has multiple parameters, $\boldsymbol{p} = (p_1, \ldots, p_m)$, sampling from the posterior PDF is the challenging problem of sampling from a multivariate PDF.
- In [Ghanem and Doostan, 2006; A, Ghanem, and Soize, 2010], the sampling from the posterior PDF was effected by using Metropolis-Hastings and Gibbs Markov Chain Monte Carlo methods:

Given $\boldsymbol{p}^{(t)}$,

1. Generate $\boldsymbol{Q}_t \sim \pi_{\boldsymbol{P}}(\boldsymbol{q}|\boldsymbol{p}^{(t)})$
2. Take

$$\boldsymbol{P}^{(t+1)} = \begin{cases} \boldsymbol{Q}_t & \text{with probability } \upsilon(\boldsymbol{p}^{(t)}, \boldsymbol{Q}_t) \\ \boldsymbol{p}^{(t)} & \text{with probability } 1 - \upsilon(\boldsymbol{p}^{(t)}, \boldsymbol{Q}_t) \end{cases},$$

where

$$\upsilon(\boldsymbol{p}, \boldsymbol{q}) = \min\left(\frac{\rho_{\boldsymbol{P}}^{\text{post}}(\boldsymbol{q})}{\rho_{\boldsymbol{P}}^{\text{post}}(\boldsymbol{p})} \frac{\pi_{\boldsymbol{P}}(\boldsymbol{p}|\boldsymbol{q})}{\pi_{\boldsymbol{P}}(\boldsymbol{q}|\boldsymbol{p})}, 1 \right).$$

These Markov Chain Monte Carlo methods can be tedious to implement:

- effectiveness of proposal PDF in case of Metropolis-Hastings transitions,
- effectiveness of method for sampling from conditional PDFs in case of Gibbs transitions,
- burn-in length,
- ...

Sampling from posterior PDF (continued)

- We replace the Metropolis-Hastings or Gibbs MCMC with an alternative, less tedious to implement, **MCMC method based on an Ito SDE** that admits the posterior PDF as invariant PDF:

$$\begin{cases} d\boldsymbol{P}(t) = \boldsymbol{V}(t)dt \\ d\boldsymbol{V}(t) = -\boldsymbol{\nabla}_{\boldsymbol{p}}\phi(\boldsymbol{P}(t)) - \dfrac{1}{2}f_0\boldsymbol{V}(t)dt + \sqrt{f_0}d\boldsymbol{W}(t) \end{cases},$$

with the potential

$$\phi(\boldsymbol{p}) = -\log \rho_{\boldsymbol{P}}^{\text{post}}(\boldsymbol{p}),$$

and with the initial conditions

$$\boldsymbol{P}(0) = \boldsymbol{p}_0 \quad \text{and} \quad \boldsymbol{V}(0) = \boldsymbol{v}_0.$$

This method was introduced, although in another context, in [Soize, 2008]. It can be analysed mathematically and implemented numerically by using the available methods for Ito SDEs, and it has been shown to be very robust. We use the implicit backward-Euler time-stepping method.

Nonintrusive projection method

- Ghanem and Doostan[2006] used the intrusive projection method to propagate the uncertainties from the input variables through the engineering model to the output variables; A, Ghanem, and Soize[2010] used the Monte Carlo sampling method.

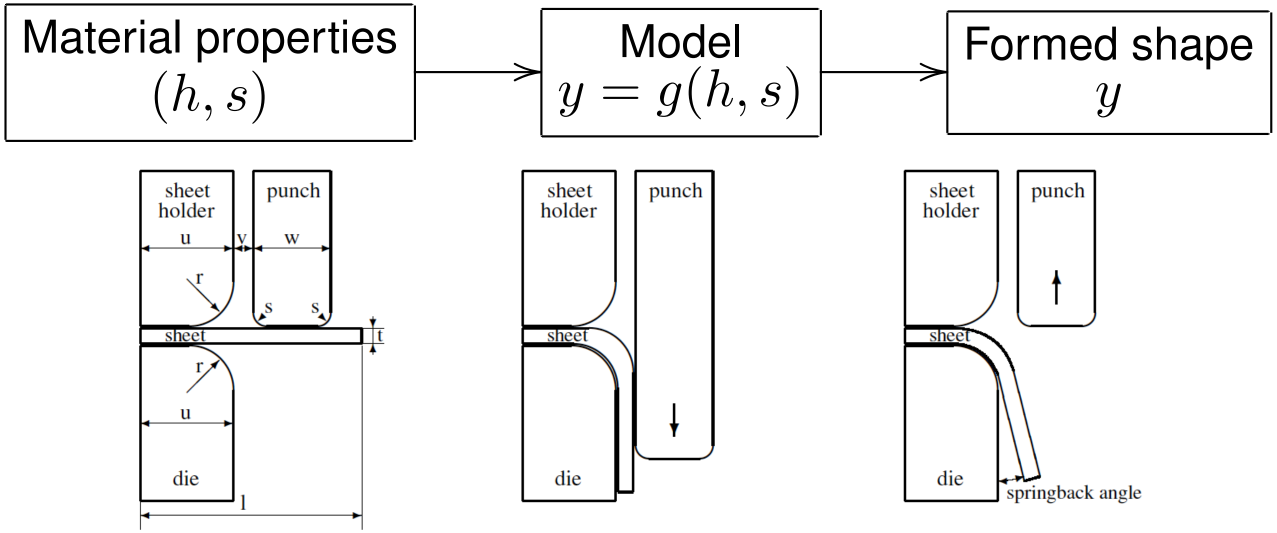
- We use the **nonintrusive projection method**, which, for sufficiently smooth and low-dimensional problems, combines the **efficiency** of projection with the **ease of implementation** of sampling. In particular, the nonintrusive projection method can be implemented as a wrapper around the engineering model, which must only be evaluated for a small number of values of its input variables.

- Once the surrogate model is available, it is used as an efficient substitute for the engineering model in the sampling-based approximation of statistical descriptors of the output variables:

$$\boldsymbol{Y} = \boldsymbol{g}(\boldsymbol{X}) \approx \boldsymbol{g}^r(\boldsymbol{X}) = \sum_{|\boldsymbol{\alpha}|=0}^{r} \boldsymbol{c}_{\boldsymbol{\alpha}} \boldsymbol{X}^{\boldsymbol{\alpha}}.$$

Application to metal forming

Engineering problem

- 

- Observed samples $(h_1^{\text{obs}}, s_1^{\text{obs}}), (h_2^{\text{obs}}, s_2^{\text{obs}}), \ldots, (h_\nu^{\text{obs}}, s_\nu^{\text{obs}})$.

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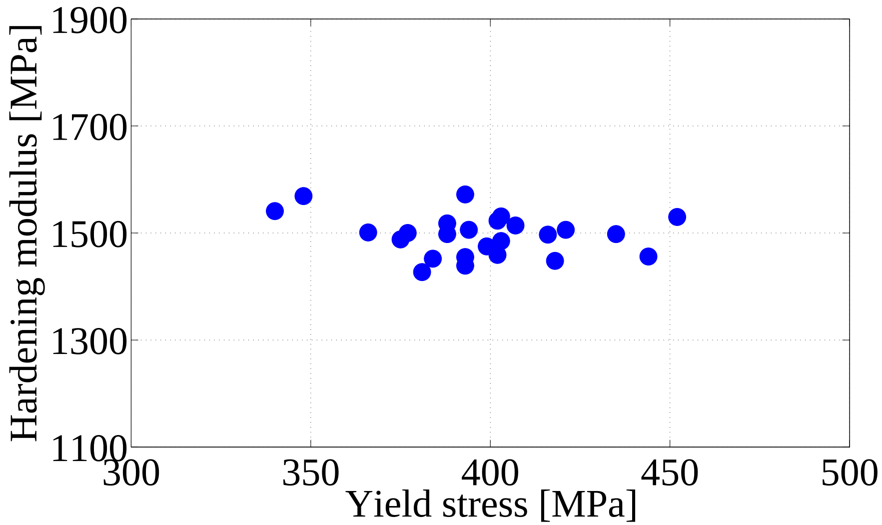
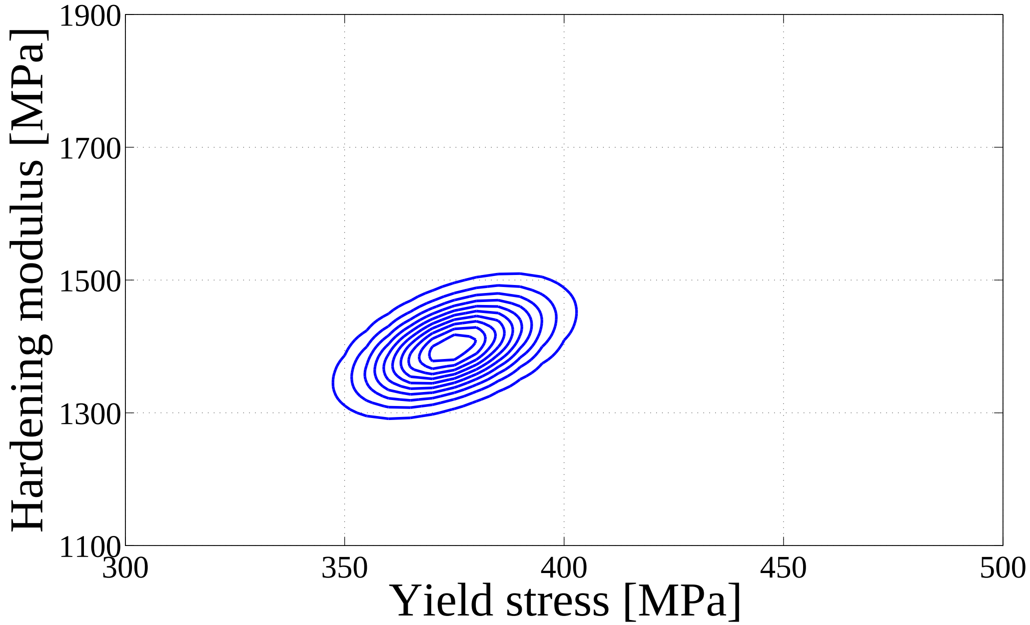


- Mechanics and physics impose that h and s be positive.

Characterization of uncertainties

- We select the bivariate gamma probability distribution

$$\rho_{(H,S)}(h,s|\underbrace{\overline{h},\sigma_H,\overline{s},\sigma_S,\rho}_{\text{parameters of the PDF}}) = \underbrace{\rho_\Gamma(h|\overline{h},\sigma_H)}_{\text{gamma marginal}}\underbrace{\rho_\Gamma(s|\overline{s},\sigma_S)}_{\text{gamma marginal}}\underbrace{\sigma\big(c_\Gamma(h;\overline{h},\sigma_H)c_\Gamma(s;\overline{s},\sigma_S);\rho\big)}_{\text{Gaussian copula}}.$$



- This probability distribution assigns vanishing probability to negative values of h and s.

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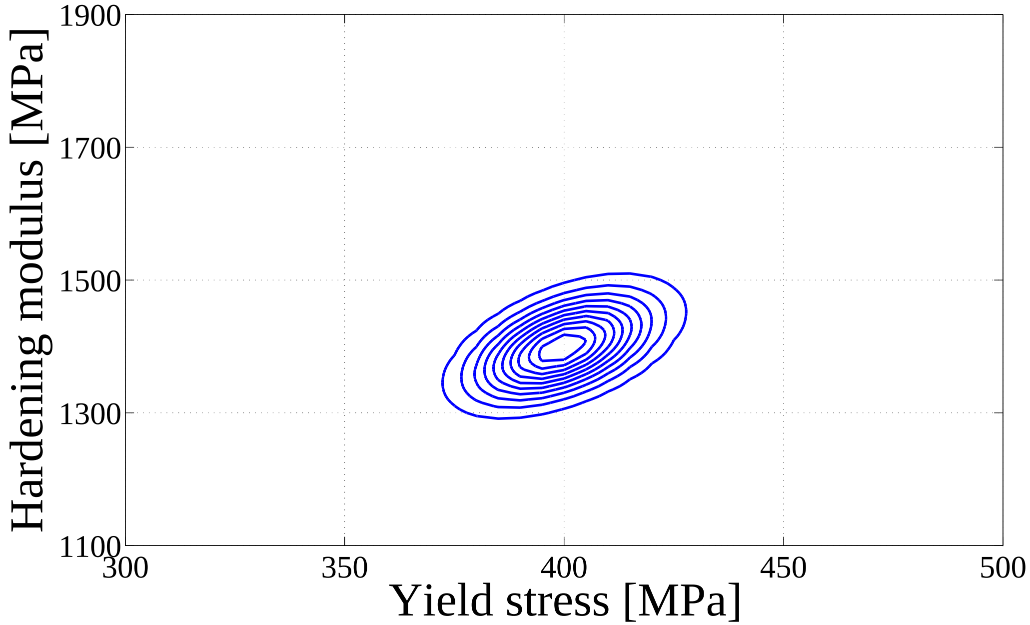

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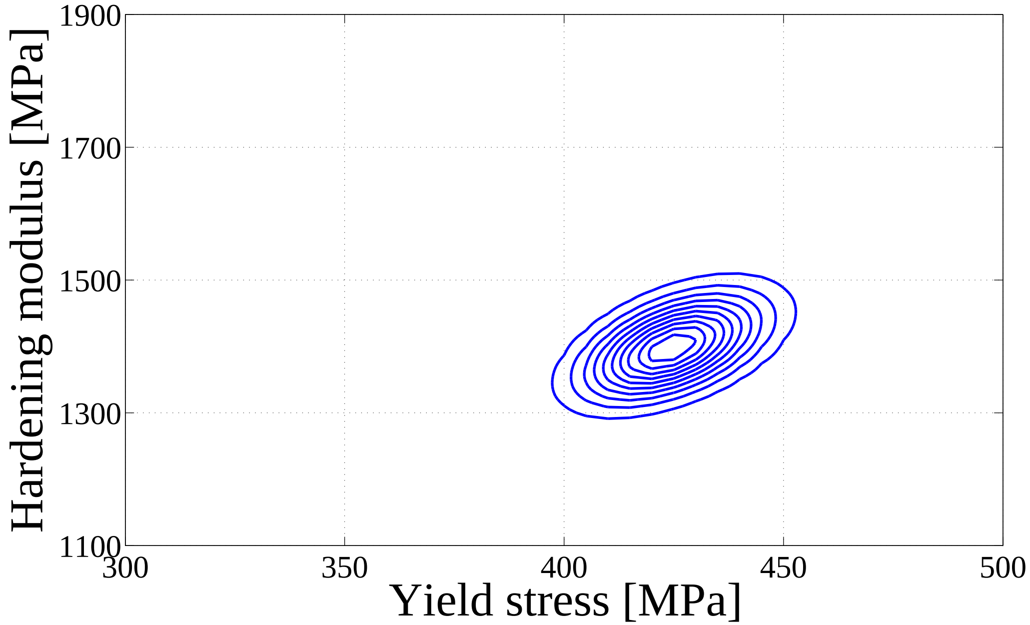

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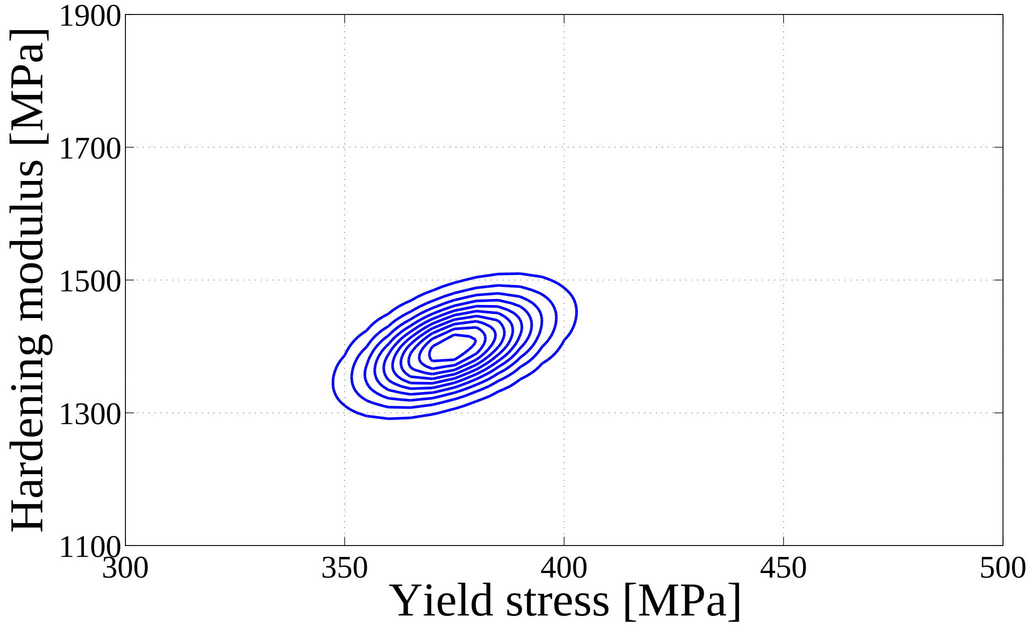

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Application to metal forming

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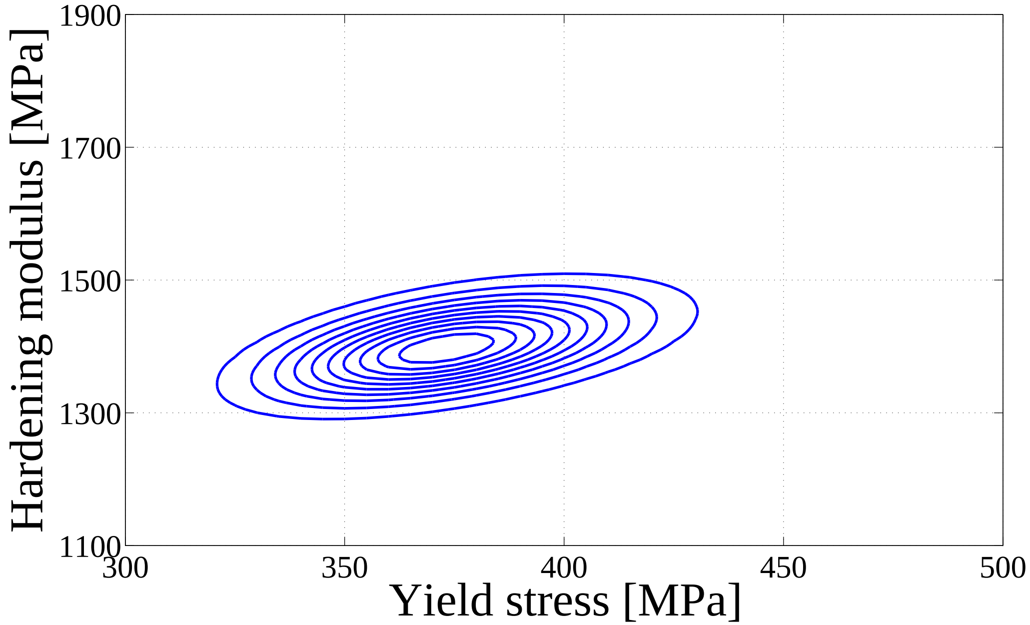

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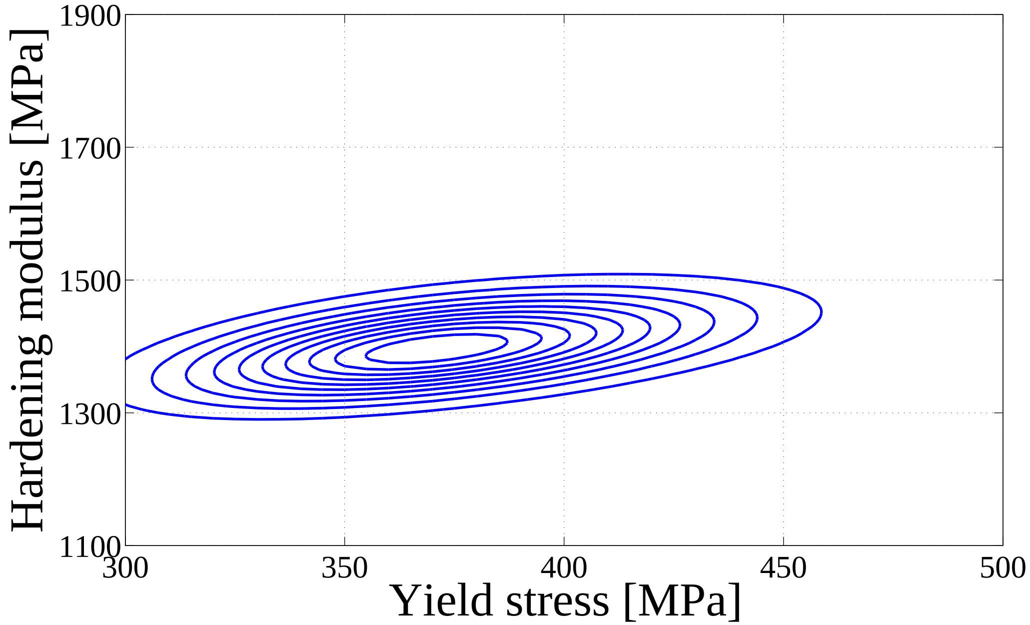

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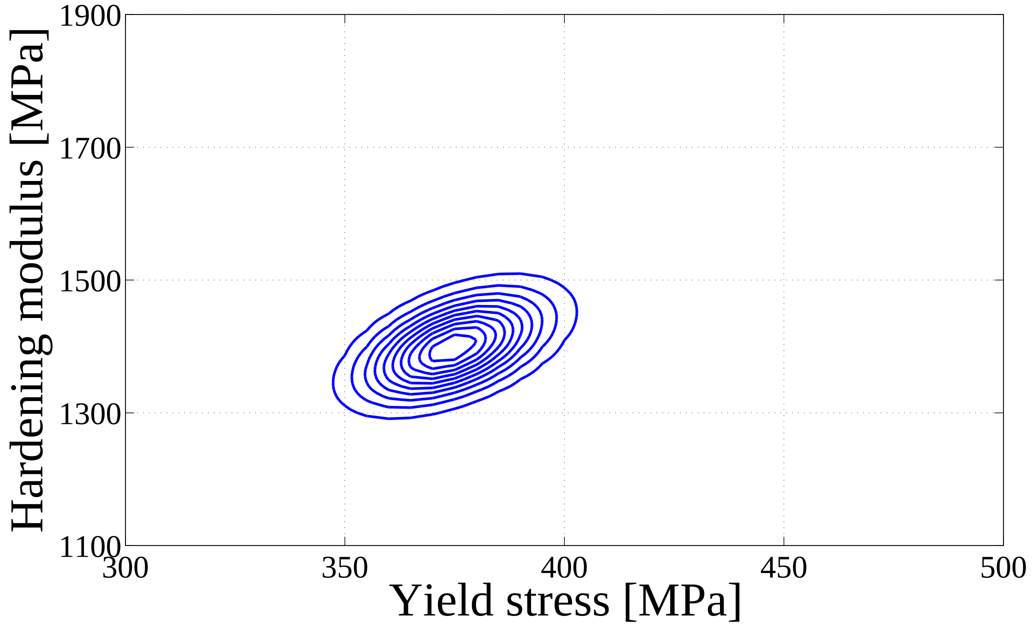

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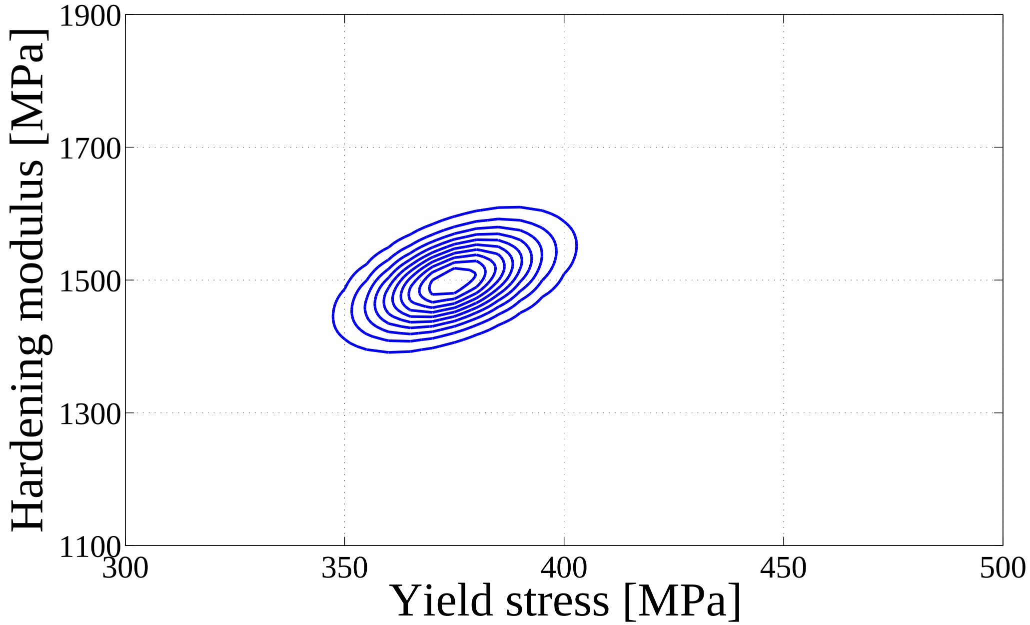

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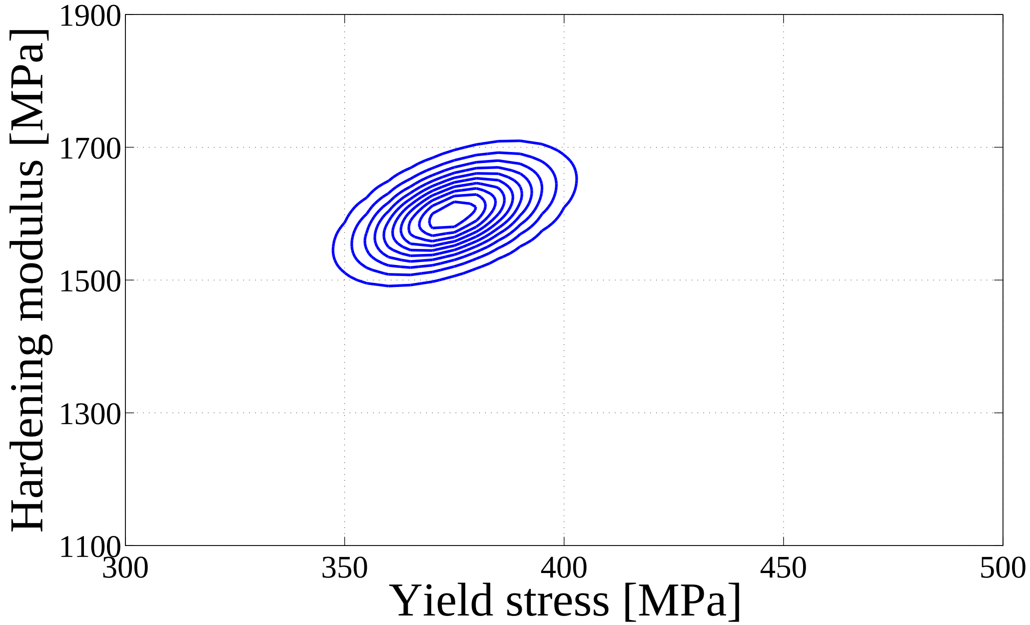

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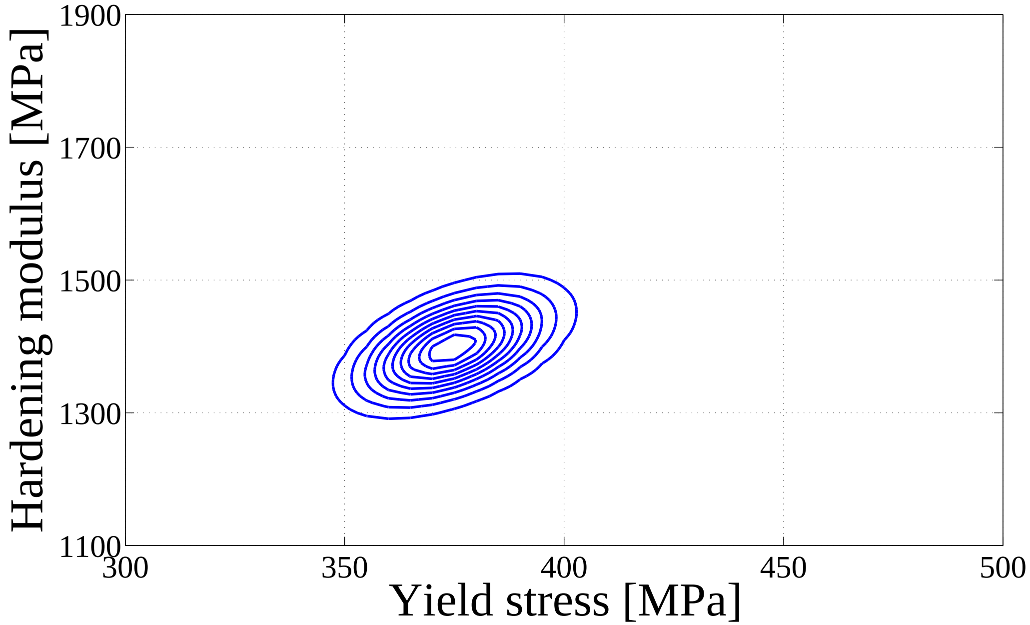

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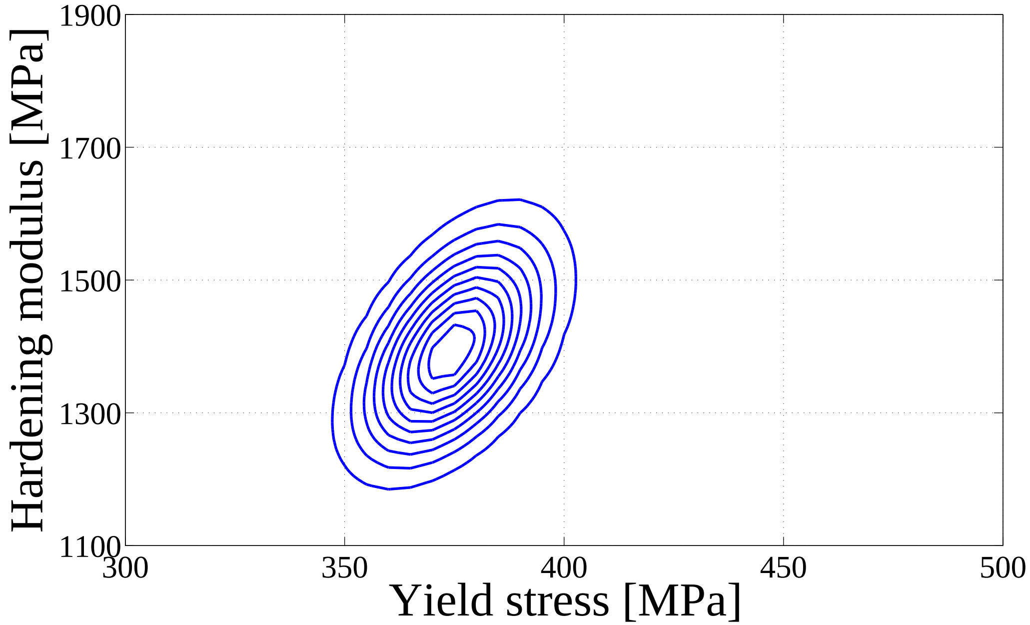

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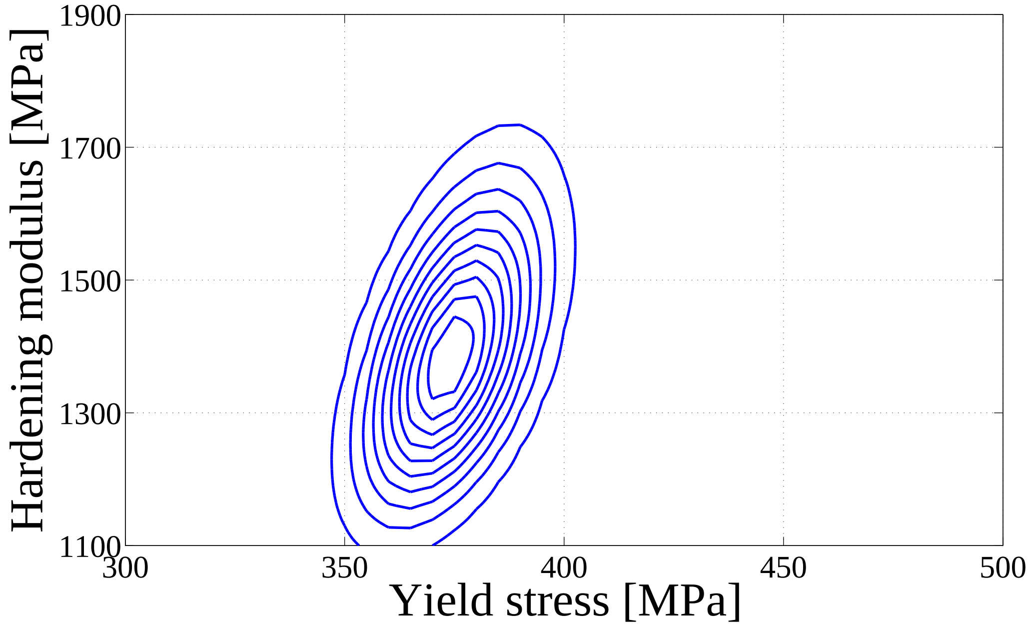

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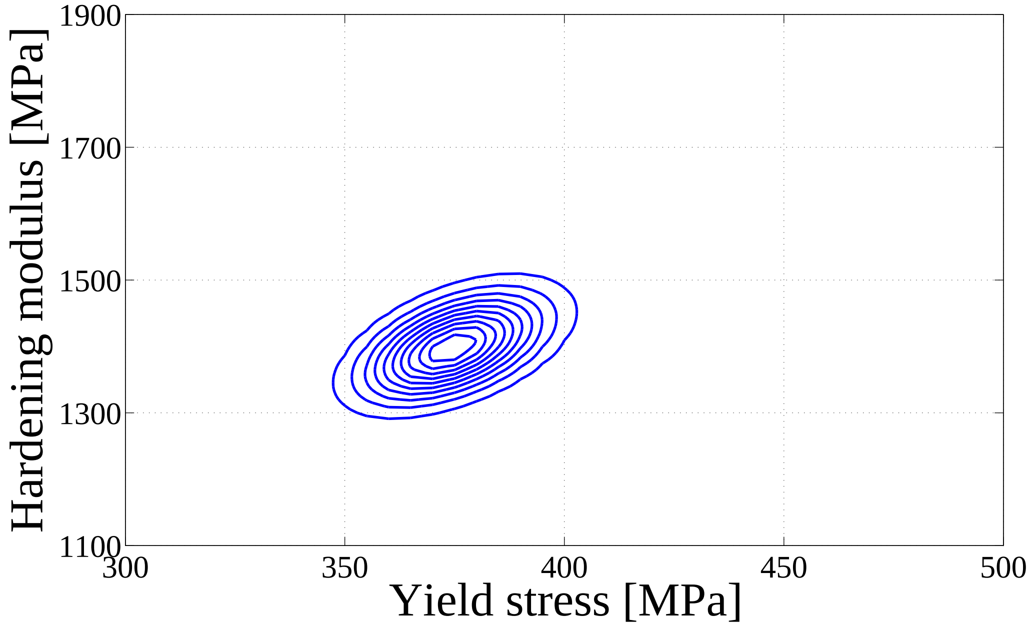

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Application to metal forming

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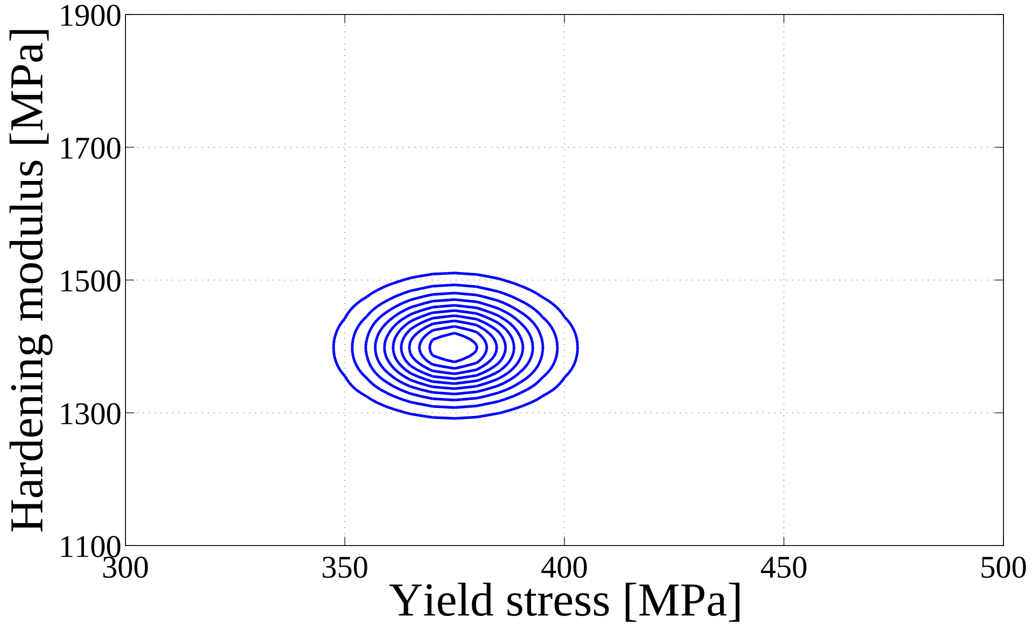

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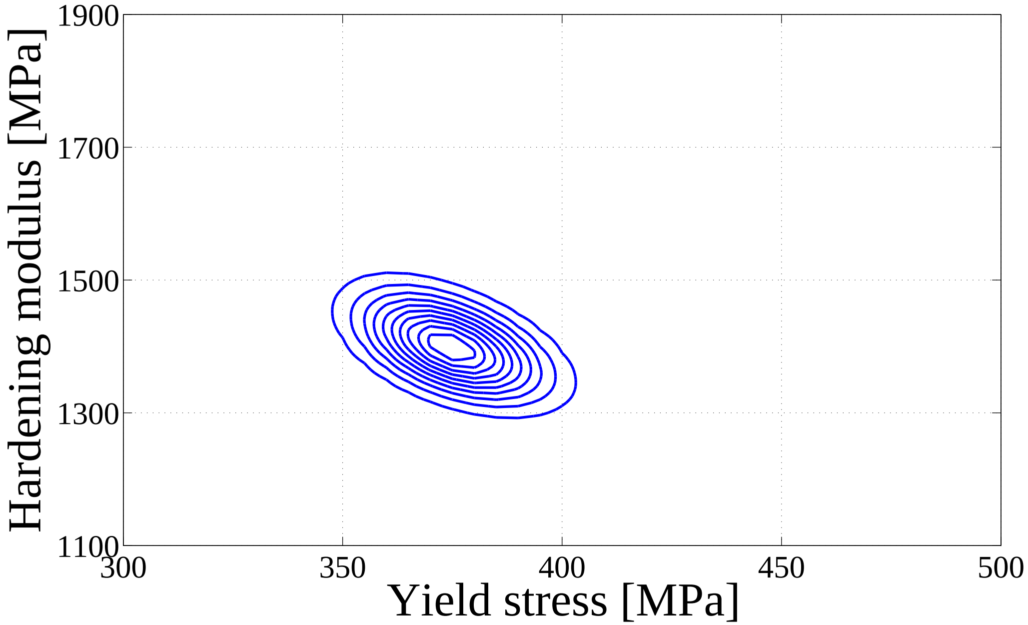

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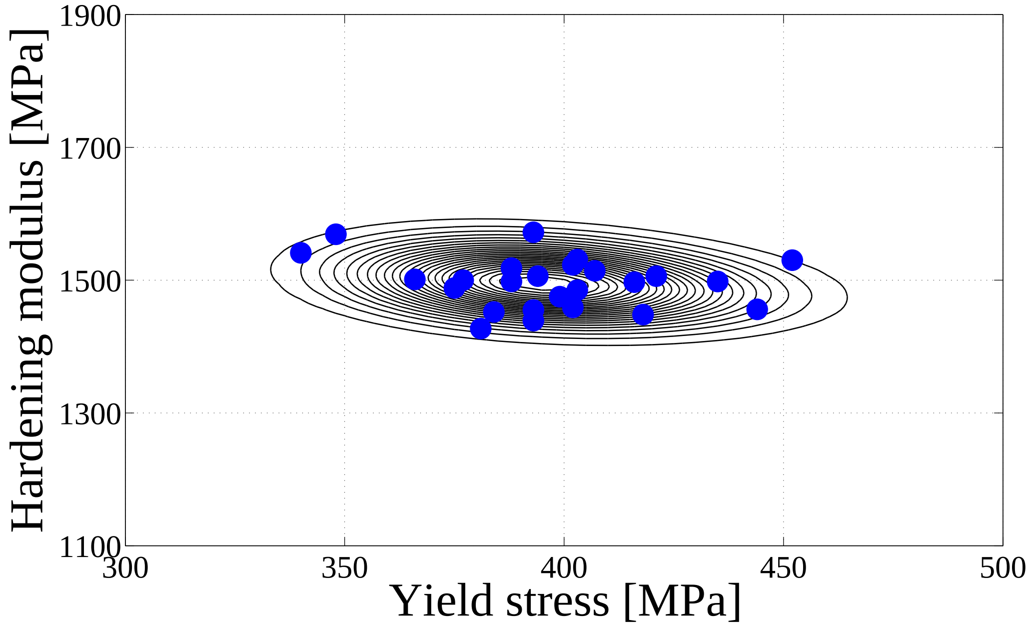
Characterization of uncertainties (continued)

- We estimate adequate values for the parameters of the bivariate gamma probability distribution by using the method of maximum likelihood as follows:

$$(\hat{\overline{h}}, \hat{\sigma}_H, \hat{\overline{s}}, \hat{\sigma}_S, \hat{\rho}) = \text{solution of} \max_{(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho)} l(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho),$$

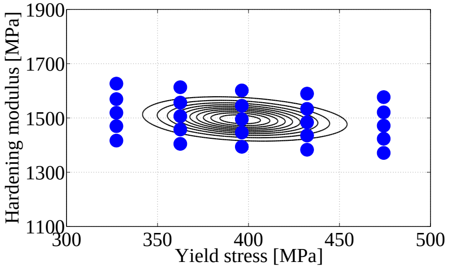
where the likelihood of the parameters $\overline{h}$, σ_H, $\overline{s}$, σ_S, and ρ is given by

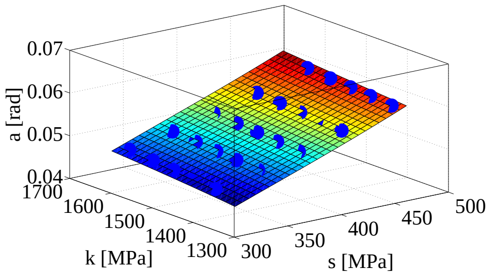
$$l(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho) = \prod_{k=1}^{\nu} \rho_{(H,S)}(h_k^{\text{obs}}, s_k^{\text{obs}} | \overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho).$$

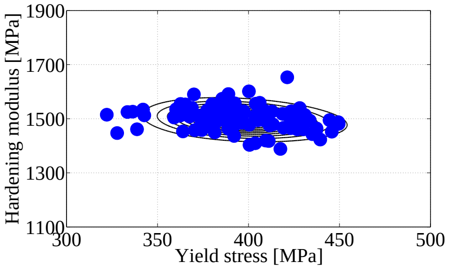


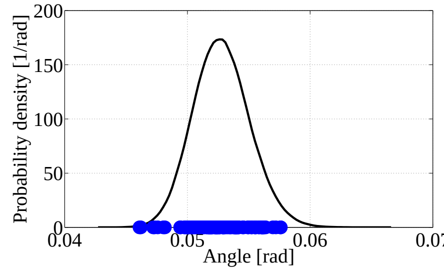
Application to metal forming

Nonintrusive projection method

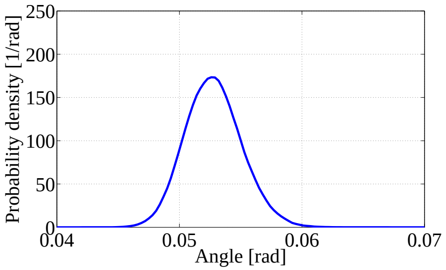








Propagation and sensitivity analysis of uncertainties



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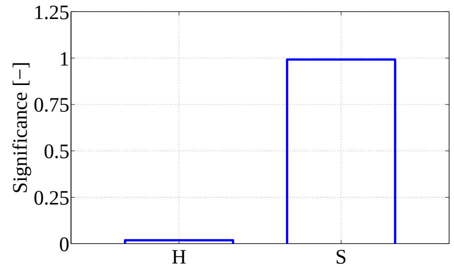


Sensitivity analysis.

Bayesian methodology

- Modeling errors due to the finite length of the data set are represented by inference of a **posterior PDF** for the parameters of the PDF for the hardening modulus and the yield stress:

$$\rho^{\text{post}}(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho) = c \times \rho^{\text{prior}}(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho) \times \prod_{k=1}^{\nu} \rho_{(H,S)}(h_k^{\text{obs}}, s_k^{\text{obs}} | \overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho).$$

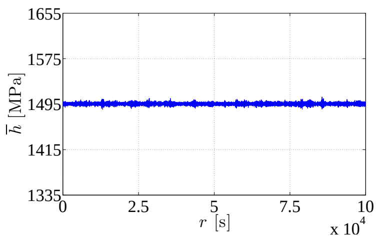
- We use a **noninformative prior** PDF:

$$\rho^{\text{prior}}(\overline{h}, \sigma_H, \overline{s}, \sigma_S, \rho) \sim \frac{1}{\overline{h}} \times \frac{1}{\sigma_H} \times \frac{1}{\overline{s}} \times \frac{1}{\sigma_S} \times \sec(\rho)^2.$$

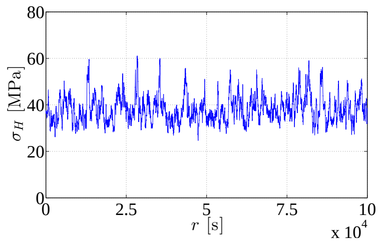
This prior PDF is uniform on the linear space of values that is obtained by transforming the parameters from their nonlinear space of values to a corresponding linear space of values through the bijections $\log(\overline{h})$, $\log(\sigma_H)$, $\log(\overline{s})$, $\log(\sigma_S)$, and $\tan(\rho \times \frac{\pi}{2})$, respectively.

Bayesian methodology (continued)

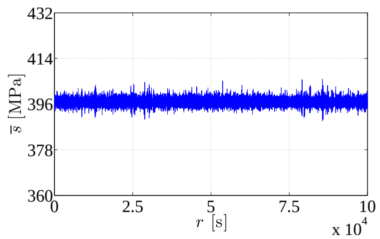
- Sampling from posterior PDF by using **MCMC method based on Ito SDE**:



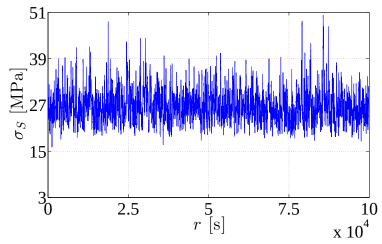
$\overline{h}$.



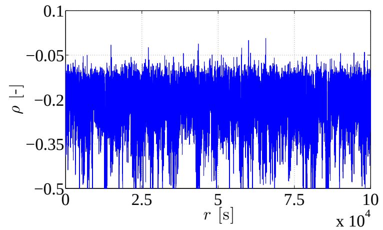
σ_H.



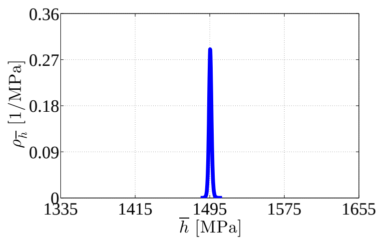
$\overline{s}$.



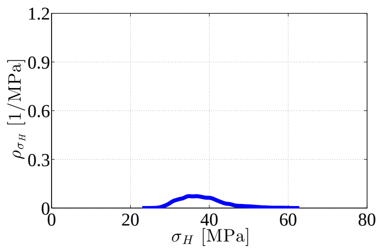
σ_S.



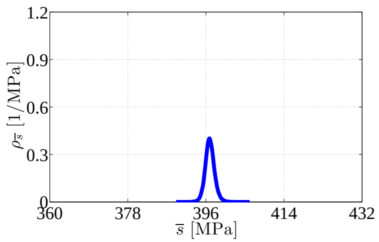
ρ.



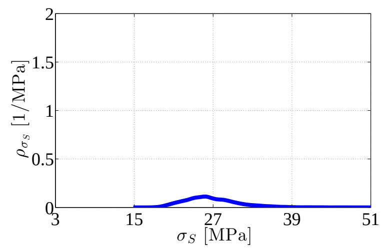
$\overline{h}$.



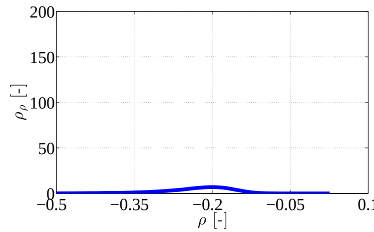
σ_H.



$\overline{s}$.



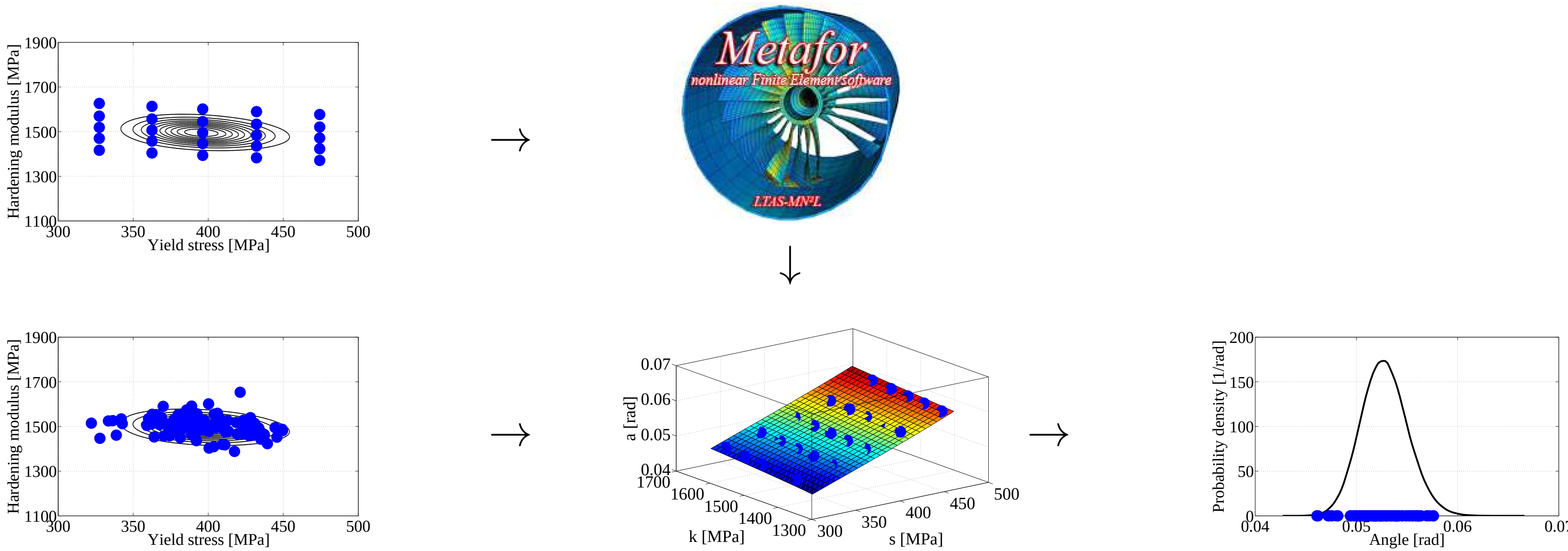
σ_S.



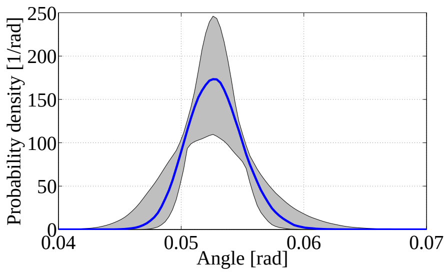
ρ.

Bayesian methodology (continued)

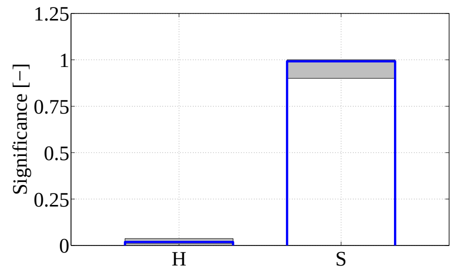
- Nonintrusive projection method:



- Propagation and sensitivity analysis of uncertainties:



Propagation.



Sensitivity analysis.

Conclusion

- Modeling errors due to data limitations and modeling simplifications can affect parametric uncertainty quantification.

- We revisited the Bayesian methodology, which allows modeling errors due to data limitations to be represented by inferring a posterior PDF for the parameters of the PDF for the input variables. This ultimately leads to error bounds on the results of the parametric uncertainty quantification.

- The novelties introduced in this presentation concern the implementation:
  - sampling from the posterior PDF by means of an MCMC method based on an Ito SDE,
  - nonintrusive projection method.

- We demonstrated the proposed framework on an application relevant to metal forming.

- A direction for future work is in representing in addition the impact of modeling errors due to modeling simplifications, thus ultimately leading to a comprehensive error budget.

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