Coffee Talk #7

July 5, 2022

Ozgur Taylan Turan

On-the-fly Construction of Surrogate Constitutive Models for Concurrent Multiscale Mechanical Analysis Through Probabilistic Machine Learning[1]

[1] I. Rocha, P. Kerfriden, and F. van der Meer (Jan. 2021). "On-the-Fly Construction of Surrogate Constitutive Models for Concurrent Multiscale Mechanical Analysis through Probabilistic Machine Learning". In: *Journal of Computational Physics: X* 9, p. 100083. ISSN: 25900552. DOI: 10.1016/j.jcpx.2020.100083

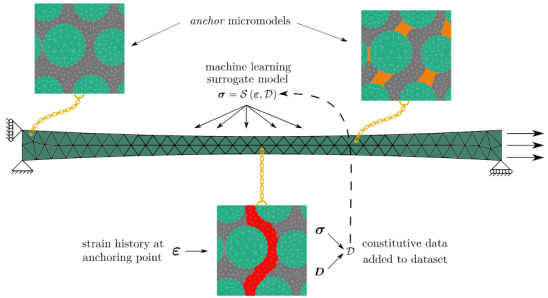
Why this paper?

- Cool application of ML with active learning?

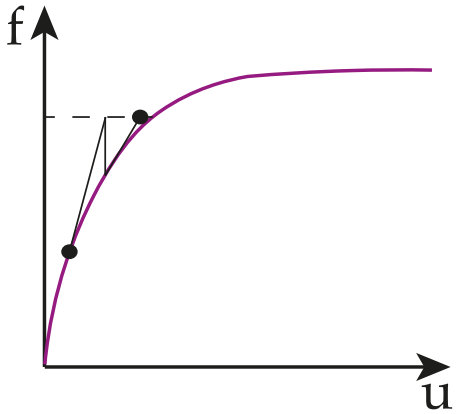
Preliminary Info

Multiscale Modeling

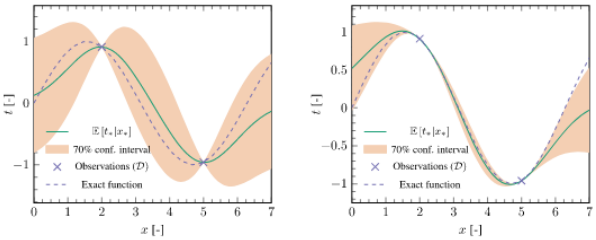
- $\text{div}(\sigma) = 0$ and
- $\epsilon = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathsf{T}})$ where the interest lies:
- $\sigma = \mathcal{M}(\epsilon)$



- Gaussian Process Regression with *derivative* information.
- Application is 3-dimensional, but independent GP's are utilized.



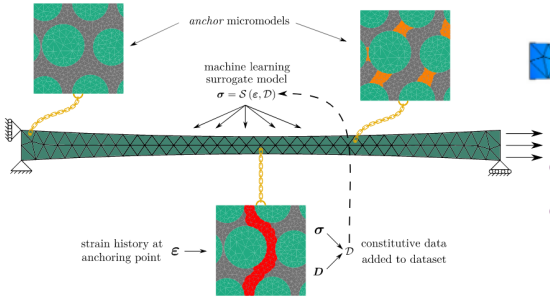
- Gaussian Process Regression with *derivative* information.
- Use all data to adjust the kernel hyper-parameters.



(a) Only target observations

(b) Target and derivative observations

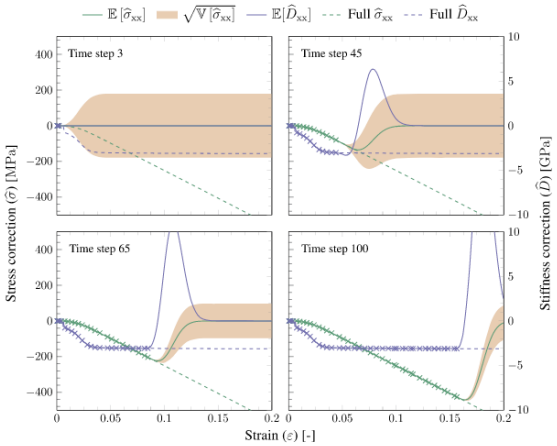
What is the main idea?



- Solve the simplest problem!
- With k-means clustering find anchor points

What is the main idea?

- As you go along check your prediction variance
- $\gamma = \max_i^3(\sqrt{\mathbb{V}[\sigma_i]})$



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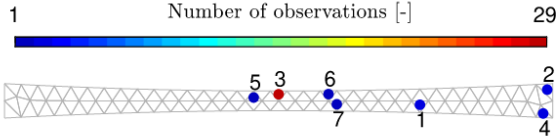
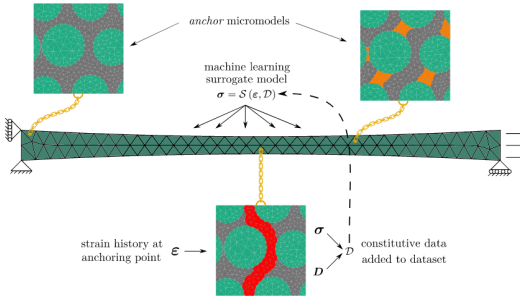
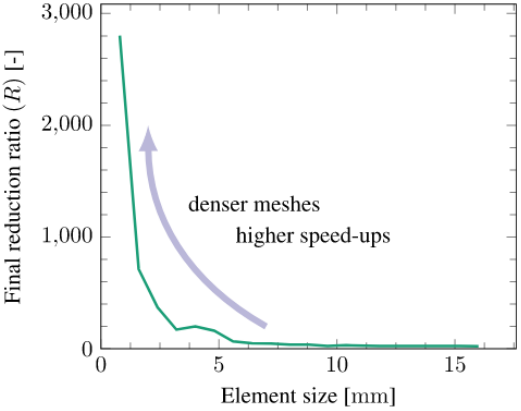


(a) $k = 1$

Result-A

$$R := \frac{n_{\text{full}}}{n_{\text{gpr}}}$$





Conclusions

- Speed ups with the combination of ml and direct numerical solvers
- A bit fragile system as most of the information needed by the direct numerical solver comes from the surrogate models.

THANKS!