Surrogate Model Creation for Constitutive Relations

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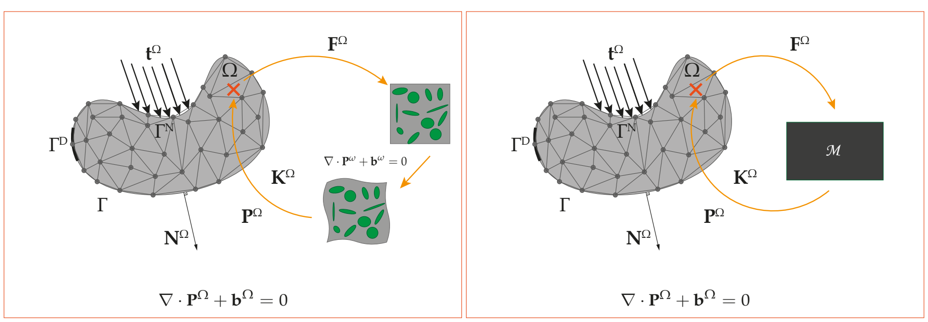
Various engineering applications rely on efficient, high-performance materials to overcome design challenges. This high performance can be achieved by engineering micro-heterogeneous materials also known as composites. Since the behavior of composites relies heavily on micro- scale interactions between different components, modeling macro-structures with fully-represented microscopic geometry is needed. Thus, the standard finite element modeling approach becomes im- practical. Computational homogenization, also known as concurrent finite element analysis (FE^2), is a method that is employed to model materials with distinct multi-scaled structures. FE^2 employs the concept of embedding a representative volume element (RVE), at each integration point of the macro-scale problem and obtaining the macroscopic constitutive behavior through homogenization, thus bypassing the need to develop a macro-scale constitutive model. Although it succeeds in up- scaling the microscopic material behavior accurately, this method comes with the major drawback of being computationally expensive due to its nested structure.



(a) FE^2 Framework

(b) FE^2 with Surrogate ML Model

Figure 1: Surrogate Constitutive Models for FE^2 Framework

Employing machine learning algorithms to create surrogate constitutive models for microscopic behavior is one possible approach [1] to accelerate the multi-scale simulations. This project aims to obtain a surrogate constitutive model with a given between macro-scale deformation Gradient Tensor $\mathbf{F}^\Omega$ and the macro-scale second Piola-

Kirchhoff Stress Tensor $\mathbf{S}^{\Omega}$ with additional other geometrical descriptors. In the end, you will be trying to solve a regression problem with F_{11}^{Ω}, F_{12}^{Ω},F_{22}^{Ω}, L, r and V_f as the features and the S_{11}^{Ω}, S_{12}^{Ω}, S_{22}^{Ω} as the labels. (Please, read [1] for the explanation of some of the notions you do not have a total grasp on now.) Note that, L is the height of the RVE, r is the radius of the circular inclusions in the RVE and the V_f is the volume fraction which indicates the percentage of the inclusions in the matrix of the composite material. The RVEs under investigation have inclusions modeled by Saint Venant-Kirchhoff and Neo-Hookean Materials. All the information related to the dataset generation can be found in the notebook. Finally, you can download the dataset from here. (Note that it is an xarray dataset so you will have to install xarray to your python environment.)

What you are expected to do is to create baselines of Gaussian Process Regression and Neural Network surrogates as done in [1]. You might want to start with the selections of [1] for start then, try to improve it by minor architecture and hyper-parameter changes (*e.g.* Looking at different kernels for GPR and width, depth, activation function for Multilayer Perceptron, etc.). After creating your baselines you are expected to implement **two different models** for the completion of this project. In other words, after establishing your baselines you will be trying to beat your baselines with other methods. (*e.g.* You can try to improve the test performance, decrease the number of training points (or decrease the number of gradient steps if you are doing, etc.) You should explain every decision that you made with the selected models explicitly and give the reasoning for those selections. But, before doing anything else try to understand your data (*e.g.* pre-process your data, etc.). If you have any questions regarding the project please reach out.

P.S. Try to be as fair as possible when you are making your comparisons. (*e.g.* Do not show your test data to your model, try to provide the same training points to all your models, etc.)

[Another] P.S. You should note that the best performance and algorithmic choices will be rewarded among groups given that the reasoning is explained properly and your results are reproducible.

References

[1] M. A. Bessa, R. Bostanabad, Z. Liu, A. Hu, Daniel W. Apley, C. Brinson, W. Chen, and Wing Kam Liu. A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality. *Computer Methods in Applied Mechanics and Engineering*, 320:633–667, 2017. ISSN 00457825. doi: 10.1016/j.cma.2017.03.037.