## Surrogate Model Creation for Constitutive Relations

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March 27, 2022

Various engineering applications rely on efficient, high performance materials to overcome de- sign challenges. This high performance can be achieved by engineering microheterogenous materials also known as composites. Since the behavior of composites relies heavily on micro- scale interactions between different components, modeling macrostructures 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<sup>2</sup>), is a method that is employed to model materials with distinct multi-scaled structure. FE<sup>2</sup> 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.

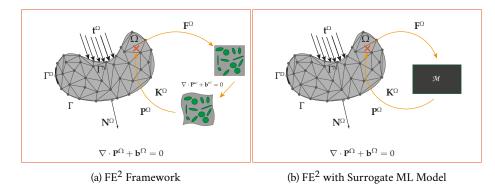


Figure 1: Put your caption here

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

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Kirchhoff Stress Tensor  $\mathbf{S}^{\Omega}$  with additional other geometrical descriptors. In the end, you will be trying to solve a regression problem with  $F_{11}^{\Omega}$ ,  $F_{12}^{\Omega}$ ,  $F_{22}^{\Omega}$ , L, r and  $V_f$  as the features and the  $S_{11}^{\Omega}$ ,  $S_{12}^{\Omega}$ ,  $S_{22}^{\Omega}$  as the labels. 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 inclusion modeled by Saint Venant-Kirchhoff Material. 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.

## 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.