

Abstract Submitted  
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**Functional derivatives for multi-scale modeling** SAMUEL REEVE,  
ALEJANDRO STRACHAN, Purdue Univ — As we look beyond petascale computing and towards the exascale, effectively utilizing computational resources by using multi-fidelity and multi-scale materials simulations becomes increasingly important. Determining when and where to run high-fidelity simulations in order to have the most effect on a given quantity of interest (QoI) is a difficult problem. This work utilizes functional uncertainty quantification (UQ) for this task. While most UQ focuses on uncertainty in output from uncertainty in input parameters, we focus on uncertainty from the function itself (e.g. from using a specific functional form for an interatomic potential or constitutive law). In the case of a multi-scale simulation with a given constitutive law, calculating the functional derivative of the QoI with respect to that constitutive law can determine where a fine-scale model evaluation will maximize the increase in accuracy of the predicted QoI. Additionally, for a given computational budget the optimal set of coarse and fine-scale simulations can be determined. Numerical calculation of the functional derivative has been developed and methods of including this work within existing multi-fidelity and multi-scale orchestrators are explored.

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