Automated variance-based sensitivity analysis of a heterogeneous atomistic-continuum system

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Abstract. A fully automated computational tool for the study of the uncertainty in a mathematical-computational model of a heterogeneous multi-scale atomistic-continuum coupling system is implemented and tested in this project. This tool can facilitate quantitative assessments of the model's overall uncertainty for a given specific range of variables. The computational approach here is based on the polynomial chaos expansion using projection variance, a pseudo-spectral method. It also supports regression variance, a point collocation method with nested quadrature point where the random sampling method takes a dictionary of the names of the parameters which are manually defined to vary with corresponding distributions. The tool in conjunction with an existing platform for verification, validation, and uncertainty quantification offers a scientific simulation environment and data processing workflows that enables the execution of simulation and analysis tasks on a cluster or supercomputing platform with remote submission capabilities.

Keywords: Heterogeneous multi-scale model, Sensitivity analysis, Computational science, Atomistic and continuum coupling, Molecular dynamics simulation, Finite element method, Coupling simulation, High performance computing

1 Introduction

Evidently, many scientific and research fields use sensitivity analysis for their critical application and computational programs, where an automated method which can lead to highly accurate diagnosis and analysis of the level of uncertainty affected by either mathematical modelling or programming aspect can be used to reduce uncertainties quicker and more cost effective. To monitor and challenge such problem that has attracted increased attention in recent years, this study aimed to construct a general automated platform that not only can remove some unnecessary steps to solve the problem through automating the process but also it can accelerate the analysis by enabling the execution of simulation and analysis tasks on a cluster or supercomputing platform.

With particular attention to the problems, this project's special focus was analysing a publicly available open-source code SCEMa (see Fig. 1) (https://GitHub.com/UCL-CCS/SCEMa). The selected code here [6] was a heterogeneous multi-scale scientific simulation model. It’s highly non-linear stress/strain behaviour which is the result of a coupling of an atomistic and a continuum system made this code an attractive candidate for characterizing, tracing, and managing statistical uncertainty analysis. Here, to facilitate uncertainty quantification, the analysis and sampling methods that was applied to the problem was based on polynomial chaos expansion. Although other existing approaches such as metropolis-hastings, quasi monte carlo sampler and stochastic collocation sampler could be also applied to the problem of uncertainty quantification. To measure sensitivity across the whole varying input space, the known direct variance-based method of sensitivity, so called Sobol first-order sensitivity index and total-effect index (see Fig. 2 and Fig. 3) were considered.

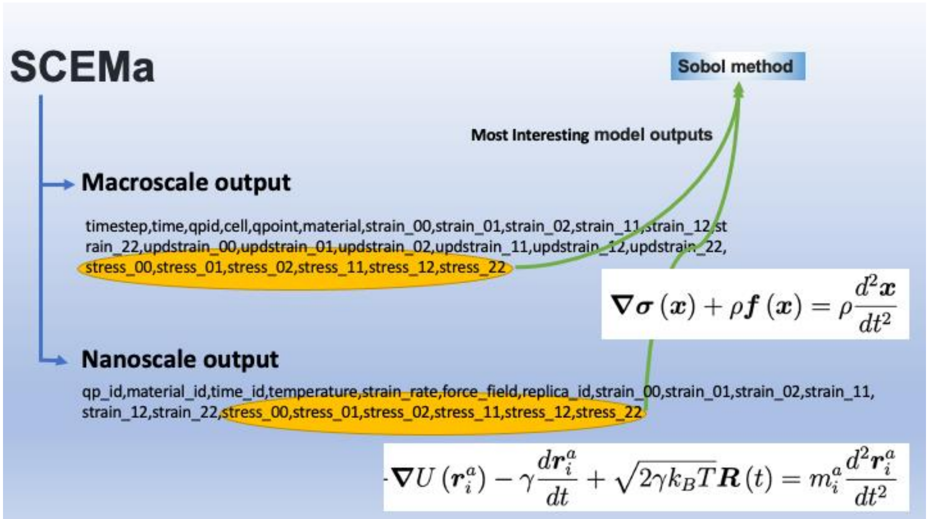

Fig. 1. SCEMa (Simulation Coupling Environment for Materials), a heterogeneous multiscale method implementation

2 Computational approach

The implementation of the uncertainty quantification tool FabSCEMa (https://github.com/UCL-CCS/FabSCEMa) proceeded with regards to FabSim, an automation toolkit for complex simulation tasks (https://github.com/djgroen/FabSim3), EasyVVUQ, a python library designed to facilitate verification, validation and uncertainty quantification (VVUQ) for a wide variety of simulations (https://github.com/UCL-CCS/EasyVVUQ) and also other existing toolkits under VECMA Toolkit (https://www.vecma-toolkit.eu/). To facilitate uncertainty quantification of the Heterogeneous Multi-scale scientific simulation models, SCEMa code, it was necessary to execute the programs on heterogeneous computing resources such as traditional cluster or supercomputing platform (this work used extensively the ARCHER2 UK National Supercomputing Service). The main reason for this limitation lies in the fact that the sampling space was very large and execution of such multiple simulations almost impossible on any local development machine.

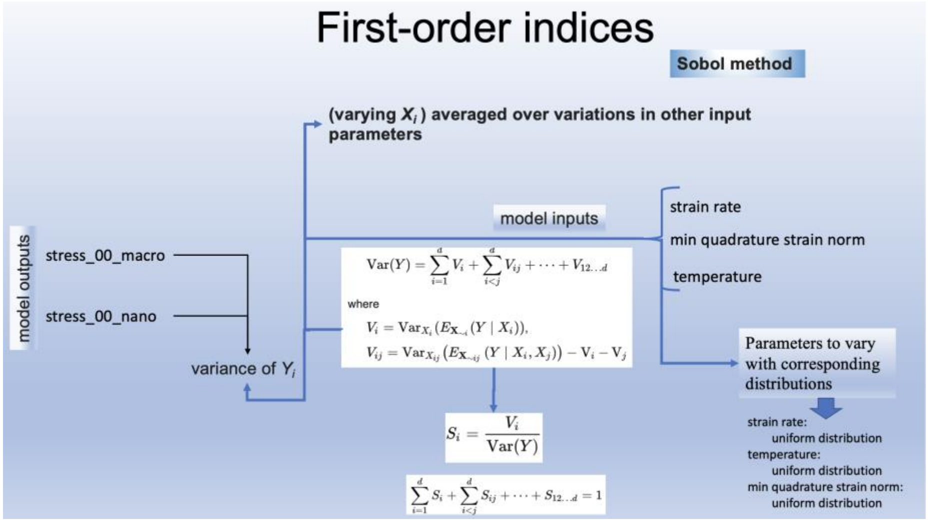

Fig. 2. Sobol first-order indices

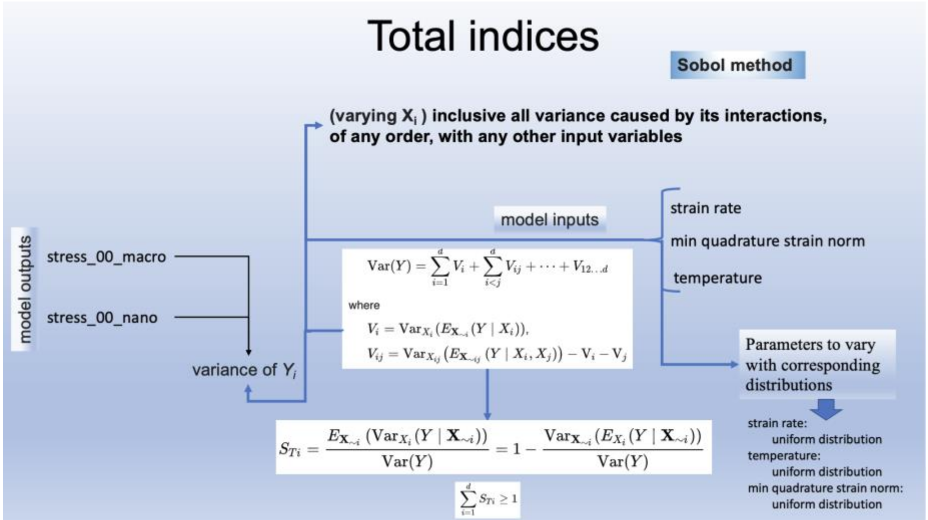

Fig. 3. Sobol total indices

3 Results

Figures 4 and 5 show a visual comparison between first order and total order sensitivity indices based on polynomial chaos expansion, polynomial order 2 and polynomial order 3. Here the tool, we have implemented in this study, after simulating SCEMa code (running several samples with different topologies) uses the normal stress predictions (stress_00_macro and stress_00_nano), which are the result of macro and nano (the atomistic and a continuum) simulation outputs, as especially selected multiple outputs which are analysed through independent sensitivity analyses

[3,4]. The model multiple inputs (a tensor of uncertain model inputs) are strain rate, min quadrature strain norm and temperature (see Fig. 2 and Fig. 3) where the corresponding distributions are based on uniform distribution.

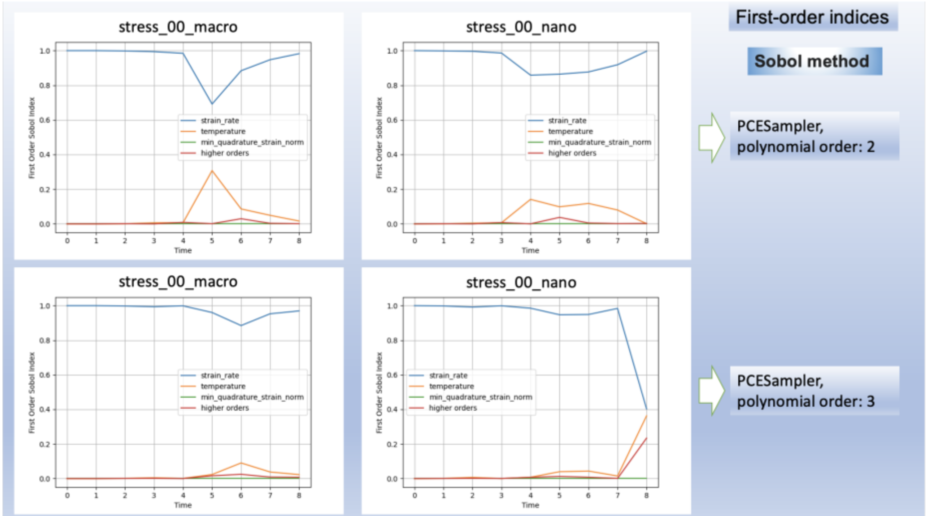

Fig. 4. Sobol first-order sensitivity indices based on polynomial chaos expansion, polynomial order 2 and polynomial order 3

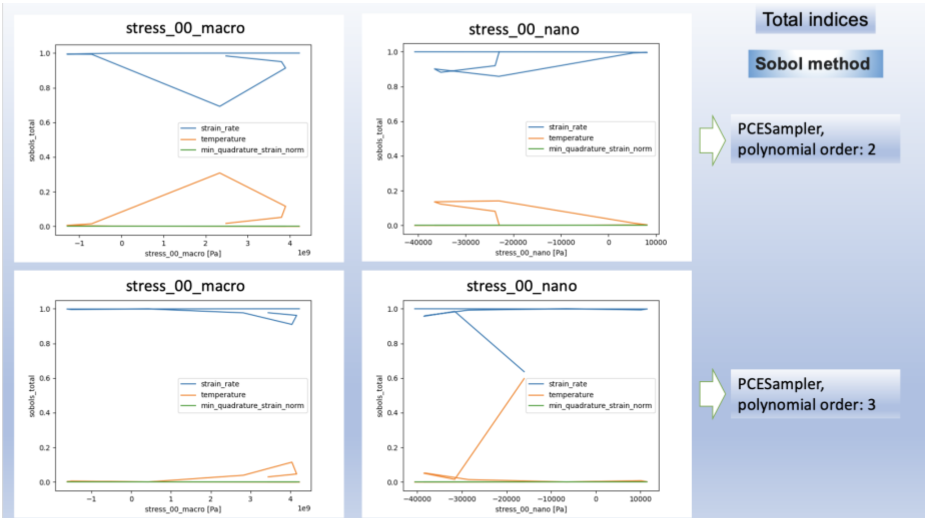

Fig. 5. Sobol total sensitivity indices based on polynomial chaos expansion, polynomial order 2 and polynomial order 3

4 Conclusion

In this study, we demonstrated an automated computational tool for the study of the uncertainty in a mathematical-computational model of a complex coupling system. Here the developed fully automated analysis method tool can be easily modified and applied to any other complex simulation system where it can provide an accurate detailed knowledge of the uncertainty with regards to analysis and sampling methods such as polynomial chaos expansion in a relatively short period of time. This tool is not dependent on the number of input-output parameters that are used in the uncertainty quantification algorithm. The visual results, the visual picture of the importance of each variable in comparison to the output variance, can help researchers/experts easily interpret wide and varying data.

Acknowledgments

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