Qeios

Peer Review

Review of: "Development of an Uncertainty-Aware Equation of State for Gold"

Stephen Andrews[1]

1. Los Alamos National Laboratory, Los Alamos, United States

REVIEW OF "DEVELOPMENT OF AN UNCERTAINTY-AWARE EQUATION OF STATE FOR GOLD"

The authors present a study where a Gaussian Process (GP) is trained on a set of high-fidelity simulations and experimental data in order to construct an uncertainty-aware Equation of State (EOS) for gold across a wide regime of thermodynamic states. The paper is well-written and thorough, and the findings are well-supported by the methods and results. There were some areas where the methodology could have been presented more clearly, and these are highlighted in the comments below:

Section II - The authors should clarify exactly which parameters are being inferred in the GP and where the uncertainties are included. Perhaps an equation or table could be used to clarify this. Some questions that arise are:

- How many different data sets make up the training data, y?
- What are these datasets, and how many measurements do they contain?
- What are the input parameters for the training data, X?
- What are the errors in the input dimensions, sigma_x?

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- What are the hyper-parameters in the GP kernel that are being trained?

Most of these questions are answered in the text but were difficult to find. The presentation could be enhanced by clearly defining them in this section.

Section IV - The choice of the magnitudes of the uncertainties in the data is central to your assessment of uncertainty in the free energy surface. The text in this section describes a rigorous approach to understanding these uncertainties, but there is not a clear connection between the approach described in the text and the numbers in table III. The authors should either enhance their discussion of how these numbers were obtained or make more explicit reference to existing practices that can quantify the uncertainty in the predictions of these codes.

Section V.C - The experimental data (from ref 13 at least) are provided with experimentally measured uncertainties. The paper could be greatly enhanced if the uncertainties in the Hugoniot prediction were compared to the experimental uncertainties. Perhaps some statistical test (maybe Kolmogorov-Smirnov) could be performed to see if the uncertainties in the prediction are similar to the experimentally measured uncertainties.

Conclusions - The authors highlight that GPs have challenges training with very large datasets. It is not clear how large the dataset was for this study. Could the authors describe how large the dataset was and what the computational effort was when training the GP?

Appendix - On page 24, the 3rd equation starting with log(P(y|X,theta)). For clarity, could you replace K with K(X,theta)? That would highlight how the hyper-parameters affect the posterior probability that is being maximized.

Overall comment: The ultimate goal of an EOS should be to use it in some sort of calculation. The authors should describe in more detail how a GP model of the free energy surface could be incorporated into existing codes to assess how uncertainty in the EOS affects predictive capability.

General comments

- The authors should describe the table names "U790" and "L790", first shown in Figure 7, earlier in the text. It was unclear what these terms meant when they were first discussed.
- This may be beyond the authors' control and dictated by the journal style, but it would be ideal if the equations were numbered in the manuscript.
- The authors make frequent use of strong adverbs in their writing, i.e., "We have meticulously integrated ... ", "... meticulously examining its behavior", etc. The authors' arguments are convincing enough without needing to add these superfluous adverbs.

Declarations

Potential competing interests: No potential competing interests to declare.