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Qeios

Peer Review

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

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The manuscript presents a novel and timely contribution to uncertainty-aware modeling of the Equation of State (EOS) for gold by employing an Error-in-Variables Gaussian Process (EIV-GP) framework. The approach innovatively integrates first-principles Density Functional Theory (DFT) data with a probabilistic machine learning model that accounts for uncertainties in both inputs and outputs. The emphasis on decomposing and quantifying multiple sources of uncertainty is a valuable step forward in EOS modeling, with potential relevance beyond the specific system studied.

The reviewers were largely enthusiastic about the methodology and scientific direction of the work. In particular, the use of Gaussian Processes (rather than neural networks) was appreciated for its interpretability and probabilistic treatment of uncertainty. The paper also stands out for its attempt to systematically incorporate and trace input uncertainties through to EOS predictions.

That said, there are a few areas requiring improvement before the manuscript can reach its full impact:

1. Contextualization within Prior Work

There is an opportunity to more clearly position this work in the context of related efforts, especially the GPz framework developed by Almosallam and others, which similarly models multiple sources of uncertainty and has been successfully applied in astrophysics and HEDP. A comparison—either theoretical or empirical—would strengthen the manuscript's claims of novelty.

2. Scalability and Computational Feasibility

While the authors acknowledge the cubic scaling of standard GPs, they stop short of offering a concrete path forward. Given the growing size of high-fidelity datasets, discussion of sparse approximations or

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inducing-point methods would be valuable. Citing examples like GPz's O(N) scaling could ground this discussion in practical relevance.

3. Quantitative Evaluation

The comparisons with legacy EOS tables (e.g., L790/Y790) are qualitative. Including quantitative metrics such as RMSE, confidence interval overlap, or statistical tests (e.g., KS test) would substantiate claims of improved accuracy or uncertainty modeling.

4. Clarity and Completeness of Presentation

The manuscript could benefit from reorganization or refinement in several sections:

Clearly define datasets, training inputs, inferred parameters, and error sources early in the methods section.

Table III, which presents uncertainty components, would benefit from a discussion of cumulative uncertainty or sensitivity analysis.

The iterative algorithm in the appendix should be explained more transparently, ideally with pseudocode.

Figures comparing model predictions to experiment (e.g., Hugoniot plots) can include experimental error bars for context.

5. Broader Impact and Future Use

Adding even a brief vision statement—e.g., on using GP-EOS models for forward uncertainty propagation or experimental design—would make the work's implications more tangible.

Summary

This is a promising and well-executed study that tackles a meaningful problem at the intersection of computational physics and statistical learning. The reviewers found it to be novel, rigorous, and potentially impactful, but also identified several areas—especially around clarity, comparative context, scalability, and quantitative rigor—where improvements are needed.

If these revisions are addressed, the manuscript would represent a valuable contribution to uncertainty quantification in EOS modeling and could set a precedent for broader applications in physics-informed machine learning.

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Declarations

Potential competing interests: No potential competing interests to declare.