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Physics-enhanced neural networks for equation-of-state calculations

Fast and accurate equation-of-state (EOS) data is of critical importance in the warm dense matter regime, for example as input to hydrodynamic codes used in inertial confinement fusion modelling. Since EOS data must be generated on-the-fly for many applications, a tabular approach based on interpolation of known data points is generally used. Alternatively, average-atom models are (in some cases) fast enough to generate on-the-fly EOS data in an *ab initio* way, i.e. without empirical inputs. In this presentation, we present a newly-developed method which can be considered a hybrid of these two approaches. In our method, we use data generated by average-atom models as input features to a neural network model [1], which is trained on the first-principles EOS dataset of Militzer *et al.* [2]. This approach has several advantages relative to using an unmodified average-atom model, and also compared to standard interpolation techniques.

[1] Callow, T. J., Kraisler, E., & Cangi, A. (2023). Physics-enhanced neural networks for equation-of-state calculations. arXiv preprint arXiv:2305.06856.
[2] Militzer, B., González-Cataldo, F., Zhang, S., Driver, K. P., & Soubiran, F. (2021). First-principles equation of state database for warm dense matter computation. Phys. Rev. E, 103(1), 013203

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