

Abstract Submitted  
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**Experiences in Automated Calibration of a Nickel Equation of State** JOHN H. CARPENTER, Sandia National Laboratories\* — Wide availability of large computers has led to increasing incorporation of computational data, such as from density functional theory molecular dynamics, in the development of equation of state (EOS) models. Once a grid of computational data is available, it is usually left to an expert modeler to model the EOS using traditional techniques. One can envision the possibility of using the increasing computing resources to perform black-box calibration of EOS models, with the goal of reducing the workload on the modeler or enabling non-experts to generate good EOSs with such a tool. Progress towards building such a black-box calibration tool will be explored in the context of developing a new, wide-range EOS for nickel. While some details of the model and data will be shared, the focus will be on what was learned by automatically calibrating the model in a black-box method. Model choices and ensuring physicality will also be discussed.

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