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The effect of functionals on the Equation of State using Density Functional Theory cold curves ANN E. MATTSSON, JOHN H. CARPENTER, Sandia National Labs, NM — With increasing computer power more complicated systems can be investigated by modeling and simulation efforts. These demanding simulations put unprecedented strain on the Equation of State (EOS). EOS models that have been perfectly adequate for smaller simulations can fail in unexpected ways for these more challenging applications. With the aim of improving the EOS, models are often fitted to calculated data in parts of the parameter space where little or no experimental data is available. For example, data calculated with the Quantum Molecular Dynamics (QMD) technique may be used in the warm dense matter regime. In this paper we focus on another type of calculated data, cold curves calculated with Density Functional Theory (DFT). The ultimate accuracy of a DFT or QMD calculation, although QMD is not addressed here, is governed by the choice of approximation for the exchange-correlation energy functional that embodies all many-body effects. We will discuss how the accuracy of the approximate functionals, manifested in the calculated cold curves, translate into accuracy for the EOS in different parts of the parameter space.

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