Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Density-to-Potential Inversions to Guide Development of Exchange-Correlation Approximations at Finite Temperature[1] DANIEL JENSEN, Center for Computing Research, Sandia National Laboratories, ADAM WASSERMAN, Purdue University, ANDREW BACZEWSKI, Center for Computing Research, Sandia National Laboratories — The construction of approximations to the exchange-correlation potential for warm dense matter (WDM) is a topic of significant recent interest. In this work, we study the inverse problem of Kohn-Sham (KS) DFT as a means of guiding functional design at zero temperature and in WDM. Whereas the forward problem solves the KS equations to produce a density from a specified exchange-correlation potential, the inverse problem seeks to construct the exchange-correlation potential from specified densities. These two problems require different computational methods and convergence criteria despite sharing the same mathematical equations. We present two new inversion methods based on constrained variational and PDE-constrained optimization methods. We adapt these methods to finite temperature calculations to reveal the exchange-correlation potential's temperature dependence in WDM-relevant conditions. The different inversion methods presented are applied to both non-interacting and interacting model systems for comparison.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94

Daniel Jensen
Center for Computing Research, Sandia National Laboratories

Date submitted: 09 Nov 2016 Electronic form version 1.4