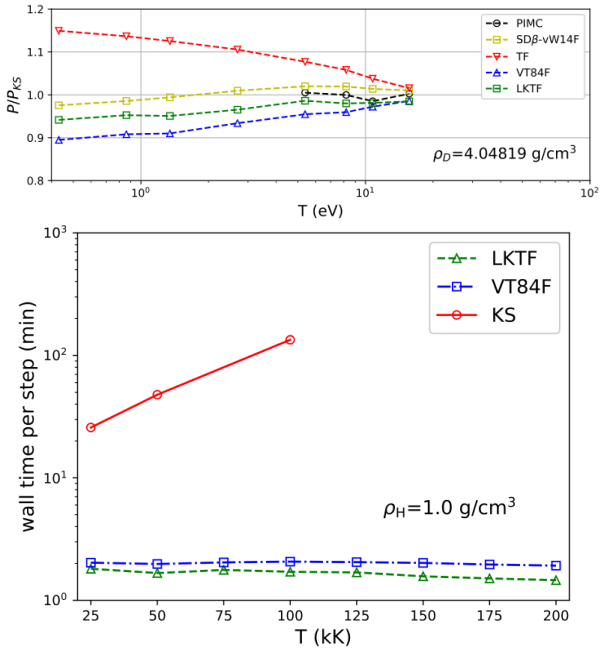
Accelerating Extreme-Condition System Simulations



Upper: LKTF gives superior pressure accuracy compared to path integral Monte Carlo (PIMC) than our previous VT84F & other, more expensive functionals. Lower: The cost per step stays the same vs. conventional Kohn-Sham that scales cubically with system size and T.

K. Luo, V.V. Karasiev, and S.B. Trickey, Phys. Rev. B **101**, 075116 (2020)

Work was performed at Univ. Florida

Scientific Achievement

Successful extension of best current zero-temperature orbital free density functional to high temperature & pressure simulations

Significance and Impact

Big reduction in computational cost to simulate planetary interiors & other highly compressed materials with little accuracy loss ⇒ deeper, broader study of important exotic systems affordable on university-scale machines

Research Details

- Extended zero-temp "LKT" functional developed in this project [Phys. Rev. B **98,** 041111(R) (2018)] to T>0 with technique developed here to give "LKTF" (free energy)
- LKT is best 1-point functional today for use with local pseudopotentials (unavoidable in orbital-free DFT) & almost as good as far more costly 2-point functionals
- LKTF maintains that superiority for systems in extreme conditions