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A Universal Kohn-Sham Density Functional Theory Approach for Warm Dense Matter[1] ALEXANDER WHITE, LEE COLLINS, Los Alamos National Lab — Understanding many processes depends strongly on microscopic physics modeling of warm dense matter (WDM) and hot dense plasma. This regime challenges both experiment and analytical modeling, necessitating predictive *ab initio* atomistic computation, typically based on quantum mechanical Kohn-Sham Density Functional Theory (KS-DFT). However, cubic computational scaling with temperature and system size prohibits the use of DFT through much of the WDM regime. A recently-developed stochastic approach to KS-DFT can be used at high temperatures, with the exact same accuracy as the deterministic approach, but the stochastic error can converge slowly and it remains expensive for intermediate temperatures. We have developed a universal mixed stochastic-deterministic algorithm for DFT at any temperature. This approach leverages the physics of KS-DFT to seamlessly integrate the best aspects of these different approaches. We demonstrate that this method significantly accelerated self-consistent field calculations for temperatures from 3 to 50 eV, while producing stable molecular dynamics and accurate diffusion coefficients. LA-UR-20-22738

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