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Spectral element solution of the Kohn-Sham atom KRISTOPHER ANDERSEN, High Performance Technologies, Inc / Naval Research Laboratory, NOAM BERNSTEIN, Naval Research Laboratory, JOHN PASK, Lawrence Livermore National Laboratory — Electronic structure calculations of atoms are important in nuclear physics, and are necessary input for most methods to construct first-principles effective potentials (i.e., pseudopotentials and projector augmented wave potentials). The standard method to solve the atomic problem within Kohn-Sham density functional theory is the shooting method. In this work, the more robust spectral element method is applied to the 1D atomic radial equation. The spectral element method provides a strict, upper-bound on the absolute error in the Kohn-Sham eigenvalues and wavefunctions enabling the solution to be converged to a well controlled accuracy. The results of this method are compared to the extensive "NIST Atomic Reference Data for Electronic Structure Calculations" database for elements H to U, providing a more rigourous assessment of this dataset than previously available.

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