4CF14-2014-000189

Abstract for an Invited Paper
for the 4CF14 Meeting of
the American Physical Society

Rectangles Stink: Numerical Integration in DFT Codes[1]

GUS HART, Brigham Young University

The 1998 Nobel prize was given to Kohn and Pople for their development of Density Functional Theory. DFT allows one to do quantum-mechanical calculations for materials and has been developed into a powerful computational tool. Typical DFT calculations require a numerical integral over the electron states in the material. Even though this integral is a small piece of the overall calculation, it is a primary source of error when the material is metallic. Metals are particularly problematic for the basic rectangle integration rules used in DFT codes. I'll give a pedestrian review of DFT calculations, a basic introduction to numerical integration, and finish with a demonstration of a new integration method for metals. Improving the current integration method should lead to a 5000% speedup in typical calculations.

[1]ONR N00014-13-1-0635 (MURI)