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Materials Modeling and the Integration Problem MATTHEW BURBIDGE, GUS HART, Brigham Young Univ - Provo — 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. Through the use of a simple toy problem, we will explain the fundamentals of the integration problem. Further, we will show that there is much room for improvement in current DFT codes (such as VASP). Using our toy problem we can get some insight as to what is going wrong. The resolution of this integration problem will result in millions of CPU hours saved for a typical computational materials scientist.

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