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**Can k-point integration for metals be dramatically improved?** GUS HART, JEREMY JORGENSEN, Brigham Young University, PRIYA GOPAL, Central Michigan University, MARCO BUONGIORNO-NARDELLI, University of North Texas — Our group has spent hundreds of millions of cpu hours calculating the energies of different materials and their competing structures. The energy of the occupied electron states is a small part of the total energy of a given material, but electron energy accounts for almost all of the numerical error in these calculations (at least in metals). Current methods of integrating electron band energies are simple (usually rectangle rule + smearing) but converge very slowly, requiring many, many k-points, even for simple metals. But integration approaches with better convergence rates, such Gauss quadrature, are hard to utilize. Because of the multivalued nature of electron bands (leading to crossings, kissings, etc.) standard interpolation methods are ineffective. We will discuss a number of improvements we have made and discuss a possible solution to the interpolation problem.

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