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Why do calculations of metals converge so slowly?[1] GUS HART, JEREMY JORGENSEN, WILEY MORGAN, HAYDEN OLIVER, PARKER HAMILTON, Brigham Young University — Calculating the energy of a metal from "first principles" requires a three-dimensional integration of a multivalued function over an irregular domain (the "Fermi surface"). The numerical convergence of this integral is not only extremely slow but is also very irregular. We will give simple examples demonstrating the source of the difficulty and explain what strategies might be effective to combat the problem. We will show data on real materials and discuss why this problem is so central to computational materials science.

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