

Abstract Submitted
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A simple spline solution to a 50 year old problem JEREMY JORGENSEN, BYU — As increasingly complex issues confront humanity (nuclear waste management, efficient fuel cells, water purifying systems, etc) it is progressively more important to find solutions. There are materials yet to be discovered that could solve these problems. Computers and density functional theory (DFT) enable scientists to predict new materials. Speeding up these codes would have a real impact on materials development. Modern DFT programs perform a slowly converging numeric integration. We plan to replace the current integration method, a standard rectangle method, by spline interpolation. This will increase computation speeds by up to 5,000%, which will boost data processing speeds and increase the likelihood of novel materials being discovered.

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