A tool for accelerating material calculations through the generation of highly efficient k-point grids TIM MUELLER, PANDU WISESA, Johns Hopkins University — The calculation of many material properties requires the evaluation of an integral over the Brillouin zone, which is commonly approximated by sampling a regular grid of points, known as k-points, in reciprocal space. We have developed an automated tool for generating k-point grids that significantly accelerates the calculation of material properties compared to commonly used methods. Our tool, which is being made freely available to the public, is capable of generating highly efficient k-point grids in a fraction of a second for any crystalline material. We present an overview of our method, benchmark results, and a discussion of how it can be integrated into a high-throughput computing environment.

Tim Mueller
Johns Hopkins University