

Abstract Submitted
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Enhancements to the k -point grid server: generating highly efficient grids through the use of informatics PANDU WISESA, WAN WAN, TIM MUELLER, Johns Hopkins University — Calculating material properties often involves using a grid of points, commonly known as k -points, to approximate an integral over the Brillouin zone in reciprocal space. The choice of grids directly affects the computational resources consumed and accuracy of the calculation. Finding a grid that minimizes computational cost for a desired level of accuracy can be computationally expensive, but we have facilitated the process by creating a publicly-available k -point grid server backed by a database of hundreds of thousands of efficient, pre-calculated k -point grids. We estimate that for well-converged calculations these grids on average reduce the resources consumed by approximately half while maintaining the same level of accuracy. We discuss recent updates to the server and how to make use of them, including new features and support for additional software packages.

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