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Improving Debye Scattering Calculation Time via Parallel Processing[1] ALEX MACH, ERIC MANDELL, Bowling Green State University — In today's world of ever increasing program execution intensity there is a need to find faster ways of processing information, often accomplished by switching to a multi-core or multi-CPU computer system. An example of a calculation that can transparently benefit is that of either x-ray or electron diffraction data, using an equation written by Debye. One problematic aspect of this calculation is that as the number of atoms in the atomic model increases, the time it takes to calculate the profile increases significantly. While this is normally not a problem when analyzing single crystals, it may be advantageous to some researchers to calculate data for a model that has nearly the same number of atoms as expected to contribute to x-ray or electron diffraction in experimental data (on the order of say 100,000 atoms). A model on this scale might examine subtle features in diffraction profiles, due to recurring relationships between adjacent crystals in a bulk material (i.e. faceting between graphene sheets). Here, improvements in calculation time are measured and compared for a single processor, a multi-CPU system, and a multi-core system using the Debye equation. We also examine differences between the multi-CPU and multi-core platforms.

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Eric Mandell
Bowling Green State University

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