Abstract Submitted
for the 4CF17 Meeting of
The American Physical Society

Making materials prediction faster: Choosing integration grids to leverage symmetry PARKER HAMILTON, GUS HART, WILEY MORGAN, RODNEY FORCADE, Brigham Young Univ - Provo — In material science, calculations often use complex integrals. These integrals can be expensive and time consuming because the function being integrated is difficult to model. The function does however have symmetry points that can reduce the total number of points needed to perform the integral. It follows that the more symmetries a grid shares with the original function, the easier the integral becomes. We have developed a method to exhaustively enumerate the symmetry preserving grids related to the parent function. This method allows for the generation of a new grid for each parent function that preserves the symmetry of the parent function.

Parker Hamilton
Brigham Young Univ - Provo

Date submitted: 22 Sep 2017 Electronic form version 1.4