Automated Generation of Highly Accurate, Efficient and Transferable Pseudopotentials

Rachael Hansel$^1$, Alan Tackett$^2$, and D. Greg Walker$^{1,3}$

$^1$Interdisciplinary Materials Science, Vanderbilt University,
$^2$Advanced Computing Center for Research & Education, Vanderbilt University,
$^3$Department of Mechanical Engineering, Vanderbilt University
Nashville, TN, USA

A genetic algorithm was used to automate the search for optimized pseudopotential parameters. Genetic algorithms (GA) have been used extensively to solve complex engineering problems with coupled parameters and multiple-minima design spaces. These algorithms can be highly parallelized and are extremely powerful due to the ability to automate the exploration of extremely large search spaces. This proof-of-concept study shows that combining GA with \textit{ab-initio} simulations can produce a Pareto set of pseudopotentials. This family of solutions demonstrates the trade-off between accuracy and computational efficiency. The two objectives chosen were accuracy (compared to a validated work of Holzwarth et. al\textsuperscript{1}) and the number of Gflops required for crystal structure calculation. To encourage potential transferability, each element was optimized in three different lattices: 1) nitrogen in GaN, AlN, and YN, 2) oxygen in NO, ZnO, and SiO$_4$, and 3) fluorine in LiF, NaF, and KF. The optimal solutions generated here are equivalent in accuracy and required significantly less computational work than the validated data of Holzwarth et al\textsuperscript{1}. Ultimately, the work presented here shows that GAs can successfully be used to generate a family of highly accurate, efficient, and transferable pseudopotentials.