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Fitting Classical Forcefields Programmatically for Application in Molecular Dynamics Simulations

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Experiments rely on models and theory to study the properties of physical systems. Consequently, computer experiments or simulations complement experiments and have enabled theoretical studies of properties of physical systems through the implementation of models and theory. Interatomic potentials have been successfully applied to computational studies involving up to millions of atoms. Obtaining interatomic potentials for a particular material typically involves fitting parameters of an analytical function such as the Buckingham to reproduce experimental properties of that material. Finding good parameters out of billions of possible parameter combinations makes obtaining good interatomic potentials very time-consuming and could take up to a year or more. We have recently developed a program which greatly simplifies the process of fitting Buckingham interatomic potentials and greatly reduces fitting time to a few weeks. The program implements the OpenMPI framework enabling it to run on high-performance computing systems on any number of processors. The core of the fitting algorithm is an error variable akin to a cost function in machine learning which allowed to program to intuitively optimize the interatomic potential parameters. When compared to experimental properties, preliminary fitting performed on cubic Li2O with space group FM3-M yielded percentage differences of -0.59 % for lattice parameters a, b, and c, -0.04 % for the bulk modulus, 0.00 %, 0.00 %, -63.39 % for the elastic constants C12, C12 and C44, and -29.35 % the static dielectric constant. These results were obtained by running the program on 24 processors for 4 days on a high-performance computing system.

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