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Long range forces in a performance portable Molecular Dynamics framework

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Abstract. Molecular Dynamics (MD) codes predict the fundamental properties of matter by following the trajectories of a collection of interacting model particles. To exploit diverse modern manycore hardware, efficient codes must use all available parallelism. At the same time they need to be portable and easily extendible by the domain specialist (physicist/chemist) without detailed knowledge of this hardware. To address this challenge, we recently described a new Domain Specific Language (DSL) for the development of performance portable MD codes based on a "Separation of Concerns": a Python framework automatically generates efficient parallel code for a range of target architectures.

Electrostatic interactions between charged particles are important in many physical systems and often dominate the runtime. Here we discuss the inclusion of long-range interaction algorithms in our code generation framework. These algorithms require global communications and careful consideration has to be given to any impact on parallel scalability. We implemented an Ewald summation algorithm for electrostatic forces, present scaling comparisons for different system sizes and compare to the performance of existing codes. We also report on further performance optimisations delivered with OpenMP shared memory parallelism.

Keywords. Molecular Dynamics, Electrostatic, Ewald Summation, Domain Specific Language, Parallel Computing

1. Introduction

Molecular Dynamics (MD) codes are well established computational tools for predicting the behaviour of complex physical, chemical and biological systems. They can be used to replace expensive laboratory experiments or to perform simulations in experimentally inaccessible areas of parameter space. Classical MD codes model a material by following a large number N of interacting particles, which obey Newton's laws of motion. Since statistical fluctuations are suppressed with inverse powers of N, to overcome finite size effects and to study increasingly

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