

Load balancing with p4est for Short-Range Molecular Dynamics with ESPResSo

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Abstract. For short-range molecular dynamics (MD) simulations with heterogeneous particle distributions that dynamically change over time, highly flexible and dynamical load balancing methods are mandatory to achieve good parallel scalability. Designing and implementing load balancing algorithms is complex, especially for existing applications which were not designed to support arbitrary domain decompositions. In this paper, we present our approach to incorporate general domain decompositions and dynamic re-balancing into the existing MD software package ESPResSo. We describe the relevant interfaces and abstractions which enable us to reuse the physics algorithms in ESPResSo, without major re-implementations. As proof-of-concept, we show the implementation of a domain decomposition based on space-filling curves and a dynamic re-balancing mechanism using an enhanced version of the p4est library. The results indicate that our load balancing mechanism is capable of reducing the imbalance amongst processes and the total runtime of simulations in simple and complex scenarios. At the same time, the implementation of models and solvers in ESPResSo remains largely unchanged.

Keywords. Load balancing, distributed memory parallelization, domain decomposition, space-filling curves, molecular dynamics

1. Introduction

Short-range molecular dynamics (MD) [1,2] is an important simulation method in computational sciences. For example, in [3] it is used in conjunction with dynamic binding of particles to study the agglomeration of soot particles. To reduce the complexity of calculating the interactions for N particles to $\mathcal{O}(N)$, the so-called Linked-Cell method [4,5] is employed. The simulation of large amounts of particles still requires parallelization based on a domain decomposition approach, which is known to be scalable beyond other approaches for distributed memory parallelization, like atom or force decomposition [6]. However, we need sub-domains with more complex shapes than cuboids and suitable load balancing algorithms to address inhomogeneities of the particle distribution in space and time. In [7], we theoretically assess how to cope with inhomogeneities and iden-

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