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Parallel Molecular Dynamics with Irregular Domain Decomposition

Mauro Bisson[1,*], Massimo Bernaschi[2] and Simone Melchionna[3,4]

[1] *Department of Computer Science, University of Rome "Sapienza", Italy.*
[2] *Istituto Applicazioni Calcolo, Consiglio Nazionale delle Ricerche, Rome, Italy.*
[3] *Institute of Material Sciences and Engineering, École Polytechnique Fédérale de Lausanne, Switzerland.*
[4] *CNR-IPCF, Istituto Processi Chimico-Fisici, Consiglio Nazionale delle Ricerche, Rome, Italy.*

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Abstract. The spatial domain of Molecular Dynamics simulations is usually a regular box that can be easily divided in subdomains for parallel processing. Recent efforts aimed at simulating complex biological systems, like the blood flow inside arteries, require the execution of Parallel Molecular Dynamics (PMD) in vessels that have, by nature, an irregular shape. In those cases, the geometry of the domain becomes an additional input parameter that directly influences the outcome of the simulation. In this paper we discuss the problems due to the parallelization of MD in complex geometries and show an efficient and general method to perform MD in irregular domains.

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Key words: Molecular dynamics, irregular domain decomposition, parallel algorithms, hemodynamics.

1 Introduction

Molecular Dynamics (MD) is a very popular simulation method to study many-body systems by looking at the motion of N individual particles. In essence, MD tracks the motion of particles whose trajectories are the result of forces mutually exerted among them. The temporal propagation of the particle positions obeys Newton's equations of motion, by applying a time-discretization procedure of the differential equations followed by an integration in time [1,2].

*Corresponding author. *Email addresses:* bisson@di.uniroma1.it (M. Bisson), massimo@iac.rm.cnr.it (M. Bernaschi), simone.melchionna@epfl.ch (S. Melchionna)

Since its inception, MD has benefited from several algorithmic advances that nowadays permit the simulation up to billions of particles with $\mathcal{O}(N)$ complexity. Multiple techniques for Parallel Molecular Dynamics (PMD) have been put forward over the years. In particular, PMD has now reached a high degree of efficiency when dealing with regular geometries, that is, with bulk systems whose computational domain can be subdivided in terms of cubes, slabs, or other regular subdomains. Several implementations of PMD are freely available and run on both supercomputers, such as the IBM Blue Gene, and high-performance commodity hardware, such as clusters of Graphical Processing Units (GPUs). Among the most popular packages are NAMD [3] and LAMPPS [4], softwares that are known to scale over thousands of processors. Moreover, we recall ACEMD, a production bio-molecular dynamics software specially optimized to run on NVIDIA GPUs [5]. Finally, AMBER [6] is another molecular simulation program featuring NVIDIA GPU acceleration support [7].

Recently, there has been growing interest in employing MD for the multi-scale simulation of particles suspended in a fluid. In the multi-scale framework, solute particles are handled according to the conventional MD scheme whereas the solvent is handled by means of conventional fluid dynamics solvers, such as the popular Lattice Boltzmann (LB) method. The non-conventional aspect of the multi-scale approach enters in the coupling between scales, an aspect that takes into account the physical level of both the solute, the solvent and their mutual interaction. In the case of the LB-MD multi-scale system, such design involves the kinetic level to account for the microdynamics of the solvent. As a result, the LB-MD method enjoys the same $\mathcal{O}(N)$ complexity of stand-alone MD for systems with uniform distribution of solute particles.

In the last few years, our group has been devising and deploying multi-scale methods to study the transport of molecular systems [9] and, more recently, the suspension of red blood cells, an important topic in computational hemodynamics [10]. The latter constitutes a strategic field since it allows to understand the physical behavior of blood from a bottom-up standpoint, that is, by following the motion of red blood cells and plasma. The wealth of information accessible from the multiscale approach and the ensuing biomedical implications are beyond question.

When simulating large cardiovascular systems, the typical geometrical layout consists of several interconnected blood vessels spreading in space with an irregular pattern. Consequently, a parallel algorithm for both the LB and MD components needs to account for the geometric sparsity of the vasculature. The optimal approach to parallelism is to decompose the computational space into subdomains where the fluid and the particles are handled on the same footing. In this way, the solution of the fluid-dynamic equations, the calculation of inter-particles and fluid-particle interactions are mostly local on the processor responsible for the subdomain.

A possible approach to handle complex cardiovascular systems could be, by analogy with large scale stand-alone PMD in a simple regular box, to use a decomposition into box-shaped subdomains. Such approach is highly discouraged since it leads to poorly balanced subdomains, both in terms of number of active (from the fluid dynamics view-