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Multiscale Hemodynamics Using GPU Clusters

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Abstract. The parallel implementation of MUPHY, a concurrent multiscale code for large-scale hemodynamic simulations in anatomically realistic geometries, for multi-GPU platforms is presented. Performance tests show excellent results, with a nearly linear parallel speed-up on up to 32GPUs and a more than tenfold GPU/CPU acceleration, all across the range of GPUs. The basic MUPHY scheme combines a hydrokinetic (Lattice Boltzmann) representation of the blood plasma, with a Particle Dynamics treatment of suspended biological bodies, such as red blood cells. To the best of our knowledge, this represents the first effort in the direction of laying down general design principles for multiscale/physics parallel Particle Dynamics applications in non-ideal geometries. This configures the present multi-GPU version of MUPHY as one of the first examples of a high-performance parallel code for multiscale/physics biofluidic applications in realistically complex geometries.

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1 Introduction

The behavior of blood in both capillaries and large coronary arteries has deep implications on the genesis of cardiovascular diseases such as atherosclerosis. Computational

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hemodynamics aims at studying flows in complex geometries, like those of blood vessels under stationary and pulsatile flow conditions. In the last few years, the study of hemodynamics has experienced an upsurge of activity due to the rapid advancement of methodological approaches and the availability of a steadily growing computing power, as also provided by high-performance commodity hardware, such as Graphics Processing Units (GPU). Blood is a complex fluid, composed of more than 99% in volume by two components, plasma and Red Blood Cells (RBC). Plasma is the solvent carrying simple Newtonian rheology, whereas RBCs play the role of basic building blocks, which are held responsible for shear-thinning and viscoelastic behavior. To the purpose of capturing the essence of blood dynamics, in particular close to the vessel walls and to morphological irregularities of the vessels, like the atherosclerotic plaques, it is imperative to look at the composite RBC-plasma system in its entirety, that is, by including the corpuscular nature of blood and evolve it concurrently with the continuum plasma component. For this reason, we adopt a multi-scale simulation approach that follows the two components on equal footing and in a concurrent fashion [2]. In our work, we leverage two distinct methods to handle plasma and RBCs and combine them in such a way to achieve a simple, yet effective, Janus-like representation of blood. Lattice Boltzmann (LB) is an efficient computational method to describe plasma as a fluid in the continuum within an Eulerian framework [3]. LB is a grid-based method, that uses a cartesian mesh and exchanges information related to the fluid among first and second mesh neighbors through the motion of fictitious molecules hopping and interacting on the sites of a regular lattice. LB shows an excellent scalability on high-end parallel computers that makes it very suitable for the simulation of large-scale systems, such as the complete coronary arterial system. Particle Dynamics (PD) is the method that handles the motion of suspended bodies in the Lagrangian (grid-free) framework. RBCs are represented as anisotropic particles that move, tumble and collide among themselves. RBCs are active scalars for the plasma, that is, they are responsible for a two-way exchange momentum with the solvent. The coupling is spatially local, rendering the concurrent evolution of plasma and RBCs an optimal choice for a bottom-up approach to the study of hemodynamics.

Coronary arteries constitute a system of interconnected vessels, presenting a non-trivial morphology (see Fig. 1), that surround the heart and carry oxygen to the heart muscle. The vessels are irregularly distributed in space and their layout calls for a highly sparse mesh to manage the active nodes only [4].

To reduce the time required for the simulation of the whole set of coronary arteries, it is mandatory to resort to parallel processing. To this purpose, we use a domain-decomposition scheme such that fluid and RBCs are handled on each subdomain by an individual processor. This aspect entails the first, coarse-grained level of parallelism, handled by conventional message-passing libraries, such as MPI [5]. The highly irregular shapes of the partitioned domains are obtained by specialized software packages, such as METIS [8] or SCOTCH [9], that produce quasi-optimal, from both the load-balancing and communication view points, partitionings. The migration and force calculation of RBC across multiple irregular domains requires the definition of *ad hoc* algorithms for