MERGING LATTICE BOLTZMANN AND PARTICLE METHODS FOR MULTISCALE SIMULATIONS AT THE PHYSICS AND BIOLOGY INTERFACE

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Summary We provide a brief account of the Lattice Boltzmann-Particle Dynamics multiscale procedure for the simulation of complex states of flowing matter at the interface between physics, chemistry and biology.

1 INTRODUCTION / BACKGROUND

In the last three decades, mesoscale methods have witnessed a major progress for the simulation of complex flowing systems at the interface between physics, chemistry and biology. In particular, such methods prove very effective in bridging the computational gap between continuum theory, say fluid and solid mechanics, and atomistic methods. Among others, the Lattice Boltzmann (LB) method has gained a prominent role thanks to its flexibility to incorporate microscale physics by suitable coupling with particle-based methods, the so-called LBPD (Lattice Boltzmann-Particle Dynamics) multiscale paradigm. Most importantly, LBPD has proven capable of preserving the outstanding LB amenability to parallel computing also in the presence of complex fluid-particle interactions and geometries of real-life complexity. In this paper, we shall provide a cursory account of the LBPD paradigm, along with a brief illustration of its major achievements so far, as well as an outlook of its groundbreaking applications once Exascale computing is available.
2 METHODOLOGY

The LBPD paradigm combines a lattice version of Boltzmann’s kinetic equation for the fluid with a particle representation of suspended bodies within the fluid. The latter can cover a wide variety of objects, ranging from rigid particles (colloids), biopolymers, membranes and other deformable bodies. The LB and PD components communicate through forces exerted by particles on the fluid and vice versa. The proper management of the corresponding hand-shaking procedures demands highly advanced parallel programming techniques, especially in the case of complex geometries. Among others, overlapping communication with computation proves vital to attain sustained parallel performance on massively parallel computers.

3 NUMERICAL RESULTS

The LBPD paradigm has been implemented in the multiscale/physics code MUPHY, which has been in use for more than a decade to simulate a variety of complex multiscale flows, such as blood flow in the arterial system at red-blood-cell resolution, the translocation of biopolymers through cell membranes, protein crowding and aggregation within the cell (for a review see [3]). These applications have attained a sequence of remarkable parallel performances, culminating with the 20 Pflops/s on the Titan supercomputer for the 2013 Gordon-Bell edition. MUPHY is currently being extended to include multiphase and multicomponent flows for the design of mesoscale porous materials at nanometric resolution.

4 CONCLUSIONS

The LBPD paradigm shows potential to provide access to a new level of complexity in the description of phenomena occurring at the physics-chemistry-biology interface. For instance, once Exascale performance is available, it may permit the direct simulation of full biological organelles, as well as the design of new mesoscale materials at nanometric resolution. To achieve such goals, however, highly advanced parallel programming techniques must be deployed.

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