Seminário
20 de Agosto de 2014

Hybrid Coupling Schemes in Computational Fluid Dynamics

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Local: Anfiteatro Escadinha - Fac. de Engenharia
Horário: 16:00 às 18:00

Abstract: Computatonal fluid dynamics is a wide field. A huge variety of demanding applications require different computational tools to allow for exploration and investigation of complex flow phenomena. Choosing a single "standard" method to tackle a specific problem is often a difficult task: multiple length and temporal scales, numerical accuracy and efficient (e.g. massively parallel) algorithms are classical ingredients that need to be considered in this choice. Since not every problem can be grouped into a particular solver's "favourite problems" due to this diversity of challenges, a combination of different computational methods may therefore represent a convenient approach. In my talk, I want to focus on three flow models – the incompressible Navier-Stokes model, the Lattice Boltzmann method and molecular dynamics – and two respective coupling approaches to combine them. This allows to cover a wide range of length and temporal scales.

First, I discuss details of coupling Navier-Stokes and Lattice Boltzmann solvers. Based on na optimisation procedure, steady-state scenarios in two and three dimensions are presented, including discussion of the numerical accuracy and performance of the coupling scheme. Second, in order to walk further down the scales, I present a coupling tool for combining mesh-based fluid solvers (such as Lattice Boltzmann or Navier-Stokes solvers) and molecular dynamics. The tool allows for flexible coupling of various codes, hiding the coupling algorithmics from both coarse-grained and molecular dynamics software. I give details on software decisions, point out the capabilities of the approach and demonstrate its features for massively parallel Lattice Boltzmann-molecular dynamics simulations.