Abstract Habilitation thesis Etienne AHUSBORDE

Modeling and High Performance Numerical Simulation of Complex Fluid Flows

This dissertation aims at gathering some contributions of my research activity devoted to the development and implementation of mathematical and High Performance Computing (HPC) methods for modeling complex flows. Chapter 1 contains a detailed Curriculum Vitae and administrative data while Chapter 2 presents a general introduction.

Over the last decade, I have focused on two areas of research forming the two parts of this manuscript.

Part I concerns CFD simulations of incompressible flows for which a wide range of issues have been raised. One of the major difficulty when solving computationally the incompressible Navier-Stokes equations consists in ensuring the solenoidal constraint on the velocity. It can be done by the computation of a pressure field which will guarantee a solenoidal velocity field. From all the methods dealing with this point, we can sort them in two categories: exact (as Uzawa method) and approximative methods. Chapter 3 discusses several exact strategies to compute the 2D Stokes eigenvalue problem using spectral element methods. Among the approximative methods, pressure-correction schemes decouple the pressure from the velocity: pressure is treated explicitly in a first sub-step, and is corrected in a second one by projecting the predicted velocity onto an ad-hoc space during a pressure correction step. Chapter 4 proposes a new original method to compute the Hodge Helmoltz decomposition, drawing a parallel between this decomposition and the pressure correction step. In addition to the pressure correction scheme, the velocity-correction scheme switches the two sub-steps: a pressure prediction problem is solved, followed by a velocity correction step. Most of the studies made on these time-splitting methods consider only Dirichlet boundary conditions while few references deal with outflow boundary conditions. That is why Chapter 5 proposes a new numerical scheme treating outflow boundary conditions, for both pressure and velocity correction schemes. An additional issue on this theme concerns the computational geometry. When flows are calculated for complex geometries, one can either use a block-structured grid or an unstructured one. Chapter 6 describes a domain decomposition method to run the Navier-Stokes equations efficiently on non-matching and overlapping block-structured meshes. Chapter 7 describes how we developed a mesh partitioner to carry out HPC simulations on block-structured meshes.

Part II is dedicated to the modeling and finite volume numerical simulation of multiphase flows in porous media. Chapter 8 proposes a non exhaustive state of the art and the description of the environment DuMu^X in which we have been implementing and integrating all our developments for several years. Chapter 9 describes our main contributions concerning these methods and their implementations in a HPC context. We have been involved in the European project FORGE (Fate of Repository Gases) that aimed at studying gas migration in deep repository for radioactive waste. We participated to several benchmarks and we coupled DuMu^X with an upscaling strategy to treat the strong heterogeneities present in the nuclear waste disposal. Our method allowed to reduce drastically the 3D computational time, while producing results that were very close to those of the other participants. Since 2013, we have been interested in the numerical simulation of multiphase reactive flows. We started with a sequential scheme that consists in solving a two-phase compositional flow followed by a reactive transport problem. Several successive strategies involving significant developments have been considered to improve the resolution of the reactive transport problem. Nonetheless, sequential approaches can introduce splitting errors necessitating reduction for the time steps that can become prohibitive. As a consequence, we decided to complete our study by the development of fully coupled fully implicit strategies. Sequential and implicit strategies were validated through numerical benchmarks with applications to geological storage of CO_2 and nuclear waste. We present here a part of these results and focus on the comparison between sequential and global implicit approaches in terms of accuracy and computational time. Some parallel computations are also discussed.

Lastly, some concluding remarks and perspectives are formulated in Chapter 10.