Model reduction and validation for exterior flow problems - an HPC challenge

Vincent Heuveline[1] and Peter Wittwer[2]

[1] Numerical Methods and High Performance Computing (NUMHPC), University of Karlsruhe (TH), Germany
vincent.heuveline@rz.uni-karlsruhe.de
http://numhpc.rz.uni-karlsruhe.de

[2] Département de Physique Théorique
Université de Genève, Switzerland
peter.wittwer@physics.unige.ch

Key words: Navier-Stokes equations, artificial boundary conditions, computational fluid dynamics (CFD), high performance computing, model reduction

1 Introduction

There is an increasing interest in considering applications leading to exterior flow problems at Reynolds numbers of the order of one to several thousand. Specific examples of situations where such flows occur are the sedimentation of small particles in the context of climate prediction and the engineering of so-called micro-air vehicles (MAV). In the first example sedimentation speeds have to be computed accurately and in the second case the prediction of performance requires that the entire flow field is computed in details and that the hydrodynamic forces are determined with high precision.

It turns out that the numerical simulation for such problems, which can be formulated by means of a so-called exterior flow problem, is extremely CPU-demanding. For numerical purposes, when truncating the infinite exterior domain to a finite sub-domain, one is confronted to the problem of finding adequate artificial boundary conditions on the outer boundary of this domain.

In this paper we propose a numerical approach for the solution of so-called *high-fidelity models* which allow to validate reduced models in the context of exterior flow which can then be solved on standard workstation by means of adequate adaptive boundary conditions.

The solution of the *high-fidelity* CFD models relies on extremely CPU-time demanding computations which have been executed on HPC-Platform of more than 2000 processors leading to a peak performance of 15 TFLOP/s and an InfiniBand 4X DDR Interconnect. In the present work, we describe the considered numerical method and depict in more details the issues related to the parallelization toward an efficient use of the HPC-resources.

2 Problem formulation

Consider a rigid body that is placed into a uniform stream of a homogeneous incompressible fluid filling up all of $\mathbf{R}^3$. This situation is modelled by the stationary Navier-Stokes equations (tildes are used to indicate dimension-full quantities)

$$-\rho(\tilde{\mathbf{u}} \cdot \nabla)\tilde{\mathbf{u}} + \mu \Delta \tilde{\mathbf{u}} - \nabla \tilde{p} = 0 \ , \qquad \nabla \cdot \tilde{\mathbf{u}} = 0 \ , \tag{1}$$

in $\tilde{\mathbf{\Omega}} = \mathbf{R}^3 \backslash \tilde{\mathbf{B}}$, subject to the boundary conditions $\tilde{\mathbf{u}}|_{\partial \tilde{\mathbf{B}}} = 0$ and $\lim_{|\tilde{\mathbf{x}}| \to \infty} \tilde{\mathbf{u}}(\tilde{\mathbf{x}}) = \tilde{\mathbf{u}}_\infty$. Here, the body $\tilde{\mathbf{B}}$ is a compact set of diameter A containing the origin of the considered coordinate system, $\tilde{\mathbf{u}}$ is the velocity field, $\tilde{p}$ is the pressure and $\tilde{\mathbf{u}}_\infty$ is some constant nonzero vector field which we choose without restriction of generality to be parallel to the $\tilde{x}$-axis, *i.e.*, $\tilde{\mathbf{u}}_\infty = u_\infty \mathbf{e}_1$, where $\mathbf{e}_1 = (1, 0, 0)$ and $u_\infty > 0$. The density ρ and the viscosity μ, are arbitrary positive constants. From μ, ρ and u_∞ we can form the length $\ell = \mu/(\rho u_\infty)$, the so called viscous length of the problem. The viscous forces and the inertial forces are quantities of comparable size if the Reynolds number $Re = A/\ell$ is neither too small nor very large.

When solving the problem (1) numerically, one usually restricts the equations (1) from the exterior infinite domain $\tilde{\mathbf{\Omega}}$ to a sequence o bounded domains $\tilde{\mathbf{D}} \subset \tilde{\mathbf{\Omega}}$. In that context we study especially quantitatively the quality of the artificial boundary conditions proposed in [4] on the surface $\tilde{\Gamma} = \partial \tilde{\mathbf{D}} \setminus \partial \tilde{\mathbf{B}}$ of the truncated domain as a function of the domain size. It is important to note that the proposed artificial boundary conditions can be understood as numerical technique for model reduction. The derivation of these artificial boundary conditions relies on qualitative arguments related to the asymptotic behaviour of the velocity field in that context. Our goal in this paper is validate quantitatively the proposed approach for some canonical configuration.

On numerical point of view, this validation is highly CPU-time demanding since computation on very large computational domain are needed to obtain reliable reference data. For the 3D case the size of the computational domain needs to be typically more than hundred time bigger than the diameter of the considered body $\tilde{B}$.

Fig. 1. Streamlines around the body at $Re = 1$ for the exterior flow problem 1.

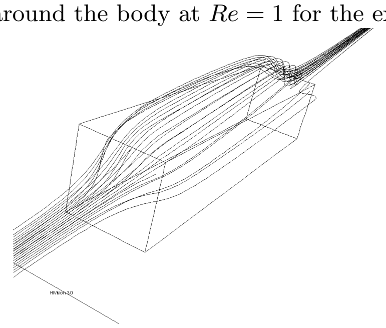
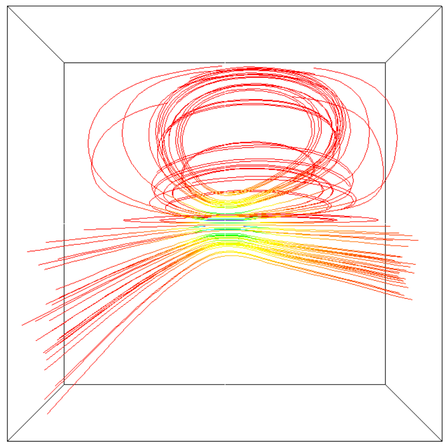


Fig. 2. Streamlines upper half: typical nonphysical back-flow when imposing constant homogeneous boundary conditions. Streamlines, lower half: no back-flow is created imposing the proposed artificial boundary conditions.



3 Solution process on HPC-Platform

In order to solve equation (1), we consider a discretization based on conforming mixed finite elements with continuous pressure. This discretization starts from a variational formulation of the system of equations (1) on a bounded domain $\mathbf{D} \subset \mathbf{R}^3$ containing the body $\mathbf{B}$. The corresponding nonlinear algebraic systems are solved implicitly in a fully coupled manner by means of a damped Newton method. The linear subproblems occuring in each nonlinear steps are solved by the *Generalized Minimal Residual Method* (GMRES) preconditioned by means of multigrid iterations.

This preconditioner, based on a new multigrid scheme oriented towards conformal higher order finite element methods, is a key ingredient of the overall solution process. Two specific features characterizing the proposed scheme are: domain decomposition method for the smoother and a parallelization of the overall scheme by means of a dedicated local blocking strategy.

The implementation of the overall solver is part of the software project HiFlow (www.hiflow.de) which is a multipurpose Finite-Element package with a strong emphasis in computational fluid dynamic. It is developed in C++ and its design takes great advantage of the object oriented concepts and of the generic programming capabilities offered by this language.

For the partitioning of the computational domain, the considered decomposition scheme relies on the package ParMetis (Parallel Graph Partitioning and Fill-reducing Matrix Ordering). Further the data structure for the large sparse matrices are handled in the framework of the software package PETSc (Portable, Extensible Toolkit for Scientific Computing).

For all computations the used parallel computer is an HP XC4000 system which is a massively parallel distributed memory computer with 772 nodes all in all. All nodes (without the fileserver nodes) consist of AMD Opteron processors with a frequency of 2.6 GHz. All nodes have local memory, local disks and network adapters. A single compute node has a theoretical peak performance of 20.8 GFLOPS and 41.6 GFLOPS respectively, i.e. the theoretical peak performance of the whole system is 15.7 TFLOPS. The main memory above all compute nodes is somewhat more than 12 TB. Additionally special nodes are attached as file servers to the cluster to support a fast and scalable parallel filesystem. All nodes are connected by an InfiniBand 4X DDR Interconnect that shows a high bandwidth of about 1600 MB/s and a low latency.

The extremely CPU-time demanding computations allow to validate the proposed approach for model reduction by means of artificial boundary conditions. The needed computation would not be feasible without an efficient and extensive use of an HPC-platform. When compared with the results obtained using traditional homogeneous boundary conditions, the computation times considered the reduced model are typically reduced by several orders of magnitude.

References

1. S. Bönisch, V. Heuveline, and P. Wittwer. Adabtive boundary conditions for exterior flow problems. *Journal of Mathematical Fluid Mechanics*, 7:85–107, 2005.
2. S. Bönisch, V. Heuveline, and P. Wittwer. Second order adaptive boundary conditions for exterior flow problems: non-symmetric stationary flows in two dimensions. *Journal of mathematical fluid fechanics*, 8:1–26, 2006.
3. V. Heuveline. On higher-order mixed FEM for low Mach number flows: Application to a natural convection benchmark problem. *Int. J. Numer. Math. Fluids*, 41(12):1339–1356, 2003.
4. P. Wittwer. Leading order down-stream asymptotics of stationary Navier-Stokes flows in three dimensions. *Journal of Mathematical Fluid Mechanics*, 8:147–186, 2006.