Efficient flow simulation on high performance computers

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Summary. In the last decades, tremendous progress has been made in the area of numerical methods and computer technology. This article gives an introduction to the recent lattice Boltzmann method for simulating the flow of incompressible fluids and shows its application to study the flow in the complex geometry of a randomly packed fixed bed reactor. In addition, general aspects of high performance computing are addressed, e.g. the efficient handling of large amounts of data produced during time-dependent simulations, the performance of recent commodity off-the-shelf (COTS) high performance computers and optimization strategies for them. Finally, the concept of the Federal State of Bavaria for the promotion of high performance techniques is summarized.

1 Introduction

Since more than two decades, the performance of computers is approximately increasing by one order of magnitude every five years. At the same time, the numerical algorithms and physical models have steadily been improved with respect to efficiency, applicability and validity. The acceleration obtained through improved or new numerical methods during the last 20 to 30 years (e.g. iterative methods for solving linear systems of equations, multi-grid methods and adaptive algorithms) therefore is in the same order of magnitude as the performance of the hardware increased. This means that by combining the latest numerical developments with the latest computer technology gives a boost of two orders of magnitude within five years. Thus nowadays the computational performance and the numerical methods are in principle available to allow numerical simulations of outstanding technical and scientific relevance.

However, to successfully tackle such questions, not only access to the hardware and numerical methods, but also several other aspects are of importance. First of all, the potential users have to know of the appropriate numerical
methods and the available performance of the computers. Next, the numerical methods have to be implemented efficiently, taking into account the special requirements of the hardware which shall be used later on. Luckily, several standards have successfully been established (e.g. MPI or OpenMP for parallelization) to make life easier, however, it is still worth to know as many details of the hardware (CPU, memory, network interconnect) as possible to obtain high performance. However, owing to the short live cycles of high performance computers it might be necessary to change the complete structure of the simulation program after only a few years again. In the CFD area, a certain number of commercial flow solvers is available on the market. These packages are feature rich and adapted to a large number of applications. However, their target platforms are often only desktop systems or small workstation clusters. Therefore, they are often only of limited used for outstanding grand challenge applications.

The computers available nowadays allow the computation of problems with a huge number of degrees of freedom within acceptable times. However, handling all the data in the pre- and post-processing can become a challenge, in particular the huge amount of data produced in the case of time-dependent simulations. Although much effort has been spent on pre-processing tools during the last decades, especially in the context of commercial CFD solvers, the pre-processing remains one of the most important and difficult as well as expensive and time-consuming steps of a CFD simulation. For the pre-processing as well as the analysis of the results, still a good knowledge of fluid mechanics and a good impression of the flow is necessary.

Among the many new developments in the CFD area during the last 15 years, the lattice Boltzmann method uses a completely different starting point compared to established CFD solvers. In addition, the method has several features (e.g. simplicity and efficiency while delivering similar accuracy as traditional methods) which make it very interesting for many applications, in particular flows in complex geometries or turbulent flows, although a number of important theoretical and methodological questions still have to be addressed.

Some of the aspects mentioned above, will be addressed in more detail in the remainder of the article which is structured as follows. In Sec. 2 the basics of the lattice Boltzmann method as well as some recent improvements of the method are summarized. As mentioned, the pre-processing is still one the most time consuming tasks of a CFD simulation. Therefore, several innovative ways of getting complex geometrical structures into the computer are briefly reviewed at the beginning of Sec. 3, with a special focus on the marker-and-cell voxel approach usually used with the lattice Boltzmann method. In the following, a focus on the simulation of transport processes in packed beds, as an example for the flow simulation in a complex geometry, will take place. First, the generation of the packing itself will be described (Sec. 3.1) before results of the actual flow simulation (Sec. 3.2) and a possibility of reducing the amount of data which has to be stored to analyze and visualize time de-