HPC – the Perspective of a CFD Practitioner

Antonio C.M. Sousa

Department of Mechanical Engineering
University of New Brunswick
Fredericton, NB
Canada E3B 5A3
(asousa@unb.ca)

Department of Mechanical Engineering
University of Aveiro
3810 – 193 Aveiro
Portugal
(antoniosousa@ua.pt)

The lecture will address the trends of the relation between Computational Fluid Dynamics (CFD), which is a subsection of Simulation-Based Engineering Science, and High Performance Computing (HPC) applications. This relation, at least in the recent past, has not been perceived as an easy one. In general, the engineering community have devoted little effort to the cause of HPC as compared to that of the science community, which have successfully argued that computational science is the third branch of science alongside theory and experiment. Computational engineering, in general, and CFD, in particular, as recognised in many studies conducted by leading scientific institutions, can benefit from HPC, even leading to generalized economic competitiveness.

After a brief introduction to CFD, it will be noted that HPC can be perceived, in what concerns CFD, in two categories: capability and capacity. It will be discussed why HPC CFD users, in general, aim to maximize one of these categories or their combination. Brief reference to traditional CFD methods, such as FDM, FEM and FVM, will be made; in addition, the potential impact of already well-established Particle methods, such as LBE, DVM, DPD, SPH, Monte Carlo (DSMC), and MD, will be analysed. It is interesting to note that some of these Particle methods have some advantages over the traditional methods; however, their commercialization has been minimal leaving their use only to the specialists. It will be highlighted the HPC needs are rather different for CFD codes main stages, namely: preprocessing, simulation (flow solution), and post-processing. Then the lecture will move to discuss the often asymmetric development relation between hardware and software. The hardware environment is changing at a fast pace primarily due to the increasing number of cores, soon the norm to be of the order of hundreds, and the extensive use of GPUs, which are designed for specific tasks. It will be reported, on the perspective of independent software vendors/developers, the strategies to adapt or develop software to run efficiently on the new architectures. Often, there is no awareness among the CFD users that many methodologies and code structures are 20 or more years old, and not easily adaptable to take advantage of the actual HPC available. Many fluid solvers deal with systems of non-linear equations, which are highly coupled creating a considerable difficulties in terms of data transfer. New programming skills strongly related to parallelism – skills that most CFD practitioners do not have, are a need, in fact, a must, to attain a new level of CFD computational performance. Even so, considerable caution is required when reprogramming as it may involve many millions of lines of computer code. The vendor/developer has to balance the efficiency of its ongoing operation with new advances in hardware.

The next big issue deals with the “democratisation” of HPC-CFD, or how it will be made available to small- to medium sized manufacturers for product improvement. Most of the times, this segment of the economic fabric does not have the required ingredients to make it work: money, in-house knowledge and medium-term strategy. However, there are a few hopeful signs of leadership from a few vendors, who, based on their own firsthand experience, are helping first time CFD customers to bridge the challenges that they face. Also, the new, on-demand cloud-based approach to CFD, although very incipient, has the potential of making significant inroads – leaving in the server huge data files is, *per se*, a considerable advantage.

The lecture will end by referring to a few engineering CFD capabilities, such as higher fidelity computational tools for turbulence and uncertainty quantification, which will require large HPC applications to provide for practical turnaround time in a production setting.