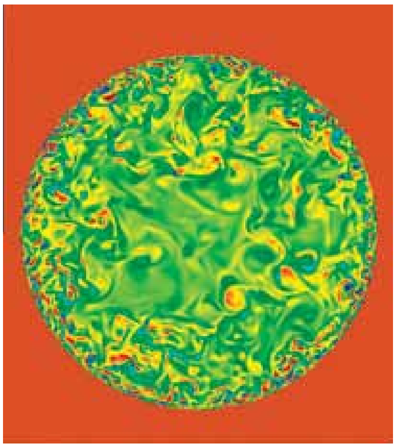
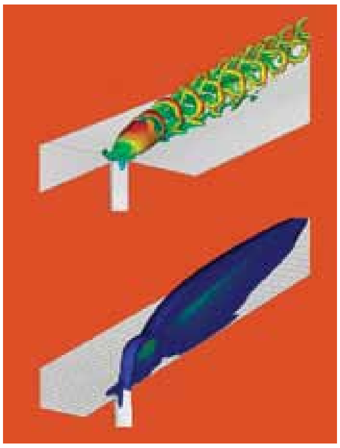
CRESTA

LARGE-SCALE FLUID DYNAMICS SIMULATIONS – TOWARDS A VIRTUAL WIND TUNNEL





> "Since every simulation is inherently imperfect, you will want to continue to increase the physics fidelity of any advanced code, be it in physics, chemistry, climate modeling, biology, or any other application domain. So you will always have — and Mother Nature demands that you will always have — a voracious appetite for more and more powerful computational capabilities."

– William Tang, Princeton Plasma Physics Laboratory and Princeton University INCITE IN REVIEW

“Advanced simulation is viewed as critical in bringing new reactor technology to fruition in an economical and timely manner.”

– Paul Fischer,Argonne National Laboratory INCITE IN REVIEW

Today numerical modelling is one of the major tools in scientific and engineering work. It allows to investigate and understand a variety of physical phenomena occurring in our environment giving the possibility to design efficient tools and devices we need in our everyday lives.

Computational fluid dynamics (CFD) is used to analyse complex physical phenomena taking place in liquids and gases in a variety of problems considering systems as simple as pipes and as complex as nuclear reactors. It helps designers in a wide range of applications starting from building quiet air conditioning and ending with more fuel efficient airplanes, or safer and more reliable power plants.

There is a large number of diverse processes related to fluid dynamics and heat transfer that have to be taken into consideration while modelling practical engineering interesting problems. Nek5000 in one of the CFD codes capable of performing efficiently such simulations in a complex geometries. Nek5000 is developed at Argonne National Laboratories (USA) and has a long history in the high-performance computing community, including winning the 1999 Gordon Bell Award. It is used by a number of different research groups around the world with the main application areas in reactor thermal-hydraulics, combustion, oceanography, vascular flow modelling, aeronautics and astrophysics.

Nek5000 is especially well-suited for modelling the time-dependent transport problems having minimal dissipation, for which a proper treatment of the small scale flow structures is essential, as errors accumulated at small scales may become dominant when propagated through large computational domains over long integration times. This requirement gives an important constraint for a minimal number of the grid points used in the setup, which defines the eventual size of the simulation. The computational capabilities of recent supercomputers and scalability of CFD codes limit the simulation size and thus the set of problems that can be studied.

Our goal is a virtual wind tunnel – a numerical environment capable of performing high resolution direct numerical simulations of practical engineering problems with a level of detail and accuracy comparable to “real” experiments. As it gives possibility to study flow interactions in previously impossible ways, it could replace in the future a typical experiment. Its important advantage is the use of sophisticated numerical tools, e.g. global linear stability analysis which allows for the identification of the driving mechanism of flow instabilities. It can give designers essential information for their work, but is based on computationally intensive solution of the eigenvalue problem, and requires sufficient massively parallel computing resources. Therefore, as a real experiment requires a high-quality laboratory, the virtual wind tunnel is in the realm of exascale computing which is required when it comes to the modelling of the realistic, interesting problems.

At present, Nek5000’s design enables large-scale parallelism scaling up to a million processes. However, fast evolution of modern HPC architectures sets new challenges for developing new algorithms and implementations. Those challenges are tackled by CRESTA and Nek5000 is one of the applications in this project with KTH (Sweden) being the responsible application partner.

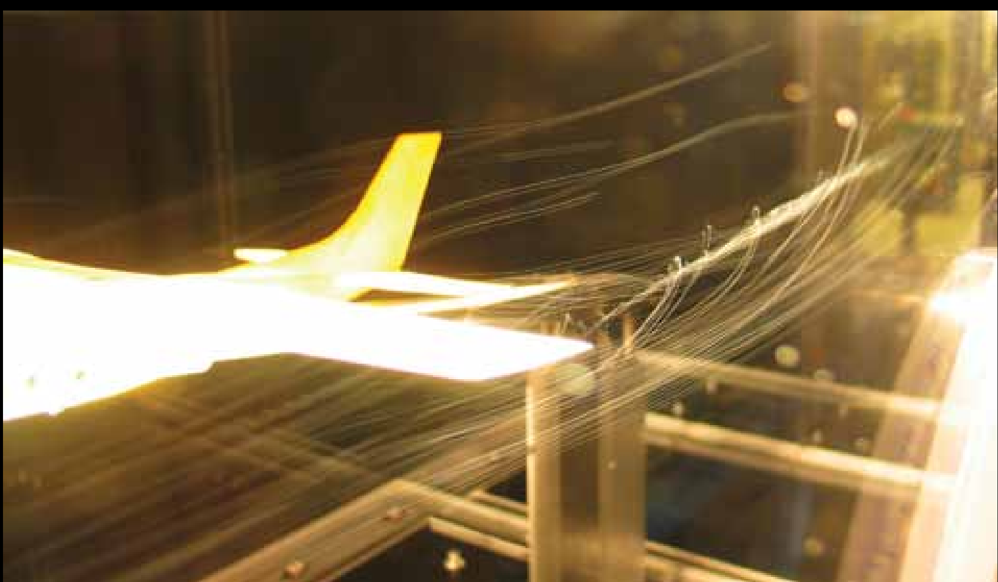
SEVENTH FRAMEWORK PROGRAMME

CFD modelling concerns many different aspects of our everyday life. Weather forecasting or wind farm design are just two of many applications. Another one is the simulation of the vortex structure of the wind flow around a skyscraper.

As an important trend in modern HPC architectures is the introduction of so-called accelerators: the main effort within CRESTA is devoted to the adaptation of Nek5000 for GP-GPU acceleration using OpenACC. It explores the tensor-product operator evaluation, which is one of the most computationally intensive parts in Nek5000, and allows for fast executions of small matrix-matrix multiplication on GPU. In the first step the simplified version of Nek5000 called NekBone was successfully ported to multi-GPU systems giving both very good speedup in comparison with the CPU-only code, and a good parallel scaling with 68% full scale parallel efficiency for 16 thousand GPU nodes. This result marked the starting point for the more challenging adaptation of Nek5000 itself, including preconditioners etc. The current implementation gives 1.59 speedup of the multi-GPU version (512 GPUs) compared to CPU-only code (512 nodes with 8192 cores), but there are a number of promising improvements that are currently explored. Test were performed on the Cray XK7 system Titan with Nvidia Kepler K20x GPUs.

Our ability to model diverse problems of practical engineering interest grows with increasing computational power. Previously, computational domains for simulations including transition to turbulence on an air foil could cover only a small fraction of the whole wing. Now, on our way towards a virtual wind tunnel, we are able for the first time to perform fully three-dimensional numerical simulation on the whole wing profile.

In the virtual wind tunnel we can study flow interaction in the way impossible to achieve in experiment. It gives very high level of detail at every simulation time, and allows to extensively study flow dynamics using advanced tools. For example, in an unstable configuration of a jet of fluid exiting through the nozzle and interacting with surrounding cross-flow we can identify the so-called core of the instability, i.e. the region in the flow most sensitive to perturbations. Such an experiment relies on a modification of the equations, and are thus impossible to perform in reality.

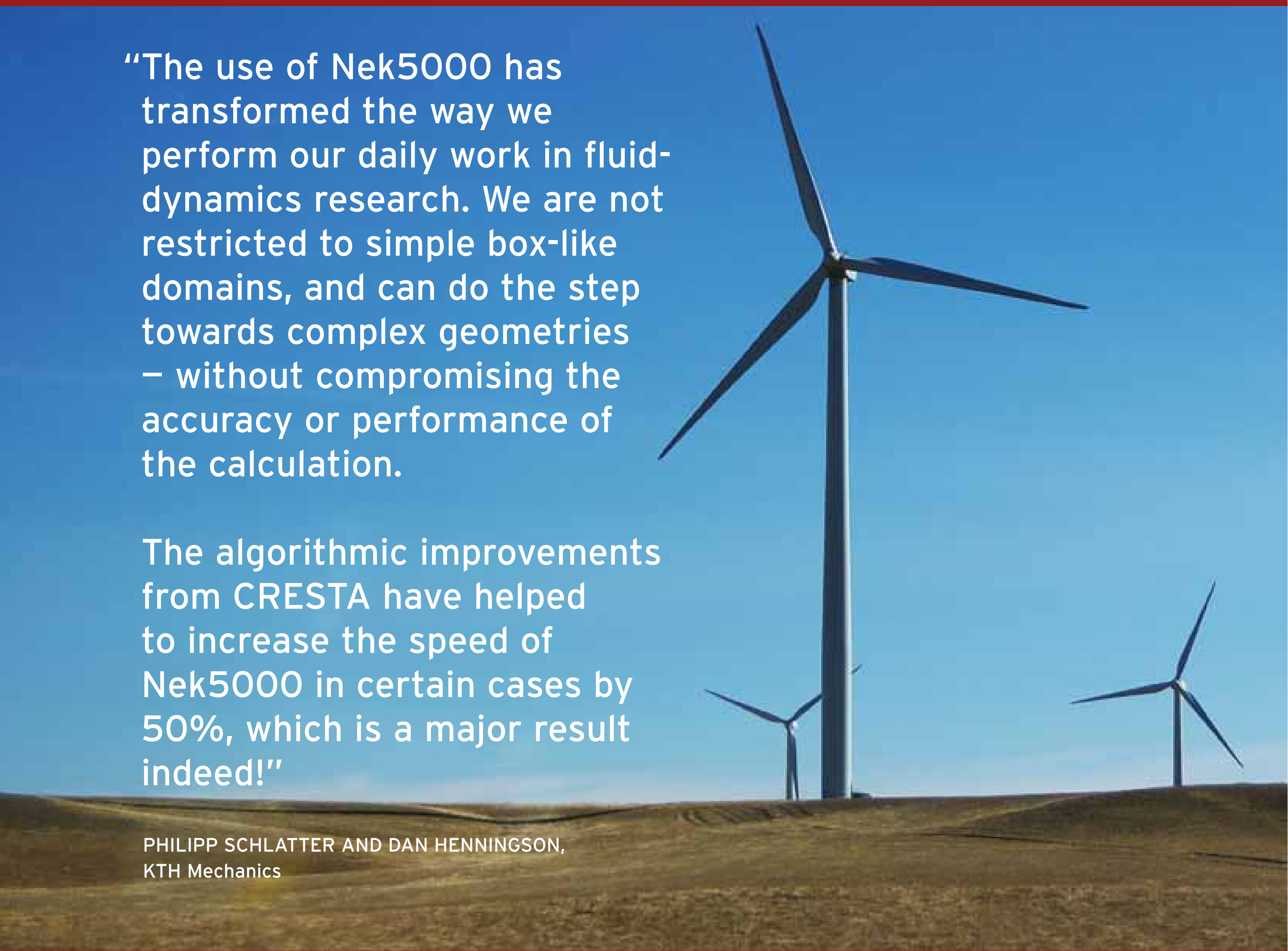


The same computational kernel was also investigated in the context of modern CPU architectures. An assembly level vectorisation using SIMD instructions was developed in collaboration between Nek5000 and GROMACS communities. It doubled the performance of matrix-matrix multiplication on the CPU and gave 15% gain in the execution time of the whole application.

The second CRESTA activity is to incorporate Adaptive Mesh Refinement (AMR) in the Nek5000 algorithm. It allows to dynamically control the computational error and thus to minimise it during the simulation by proper adaptation of the grid. AMR can be considered as an essential feature for large-scale, computationally expensive simulations as it improves considerably the efficient use of resources, simplifies significantly the grid generation and ensures the correctness of the calculated results. The main challenge is the negative effect of AMR on the code scalability, as the communication pattern gets more complex, and the whole simulation has to be properly reinitialised every time the mesh is adjusted. The preliminary results obtained for three-dimensional heat transfer problem and two-dimensional flow past cylinder are very promising.

An essential feature of modern CFD codes is their parallel scaling, which is prerequisite for an effective usage of parallel supercomputers. A successful porting of the kernel NekBone to multi-GPU systems gives 68% full scale parallel efficiency for 16 thousand GPU nodes.

Work done within CRESTA provides benefit to the whole Nek5000 community showing the way towards exascale and delivering specific code implementations, that can be run on future HPC systems.



"The use of Nek5000 has transformed the way we perform our daily work in fluid-dynamics research. We are not restricted to simple box-like domains, and can do the step towards complex geometries – without compromising the accuracy or performance of the calculation.

The algorithmic improvements from CRESTA have helped to increase the speed of Nek5000 in certain cases by 50%, which is a major result indeed!"

PHILIPP SCHLATTER AND DAN HENNINGSON, KTH Mechanics

The CRESTA project receives funding from the EU's Seventh Framework Programme (FP7/2007-2013) under the grant agreements nr. 287703.