DEISA Newsletter

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Direct numerical simulation of flow over a bump

Jean-Philippe Laval and Matthieu Marquillie, Laboratoire de Mécanique de Lille, France
Christian Stemmer, Technische Universität Munchen, Germany
Paolo Orland, Università di Roma La Sapienza, Italy
Lars Davidson and William K. Georges, Chalmers University of Technology, Gothenburg, Sweden
Philip Hancock, University of Surrey, UK

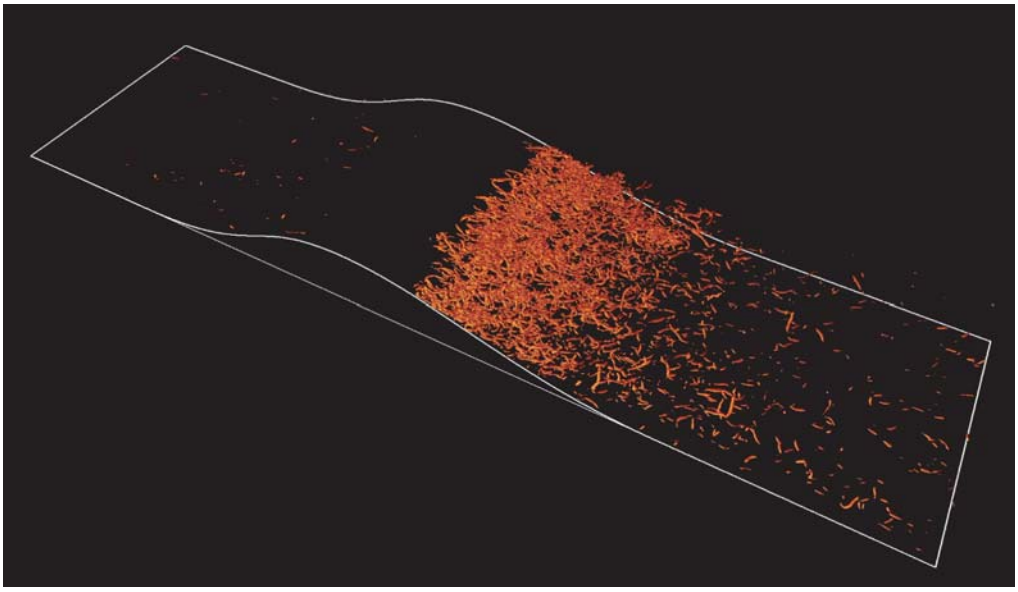

Fig. 1. Positive iso-contours of the Q-criterion ($Q = \|\Omega\|2- \|S\|2$, where Ω and S are respectively the vorticity tensor and the strain rate tensor) in the detection of coherent vortices on the lower wall of the simulation. Intense vortices are generated near the summit of the profile near the separation region of the turbulent boundary layer. The separation mechanisms will be investigated with respect to turbulent statistics.

Over the past half a century, a great deal has been learned about boundary-layer turbulence; however, all the existing models of the near-wall region are still empirical. The current project is linked to the objective of generating a database of high-quality DNS and conducting challenging experiments to improve the knowledge on and the modelling of near-wall turbulence.

A direct numerical simulation (DNS) of flow with an adverse pressure gradient was performed with a high Reynolds number, thanks to the large-scale supercomputing facilities available through the DEISA initiative. This type of simulation creates new opportunities for investigating three-dimensional wall turbulent structures. A more detailed characterization of these structures will be used to evaluate and improve turbulent models.

Understanding near-wall turbulence

Over the past half a century, a great deal has been learned about boundary-layer turbulence, both from the statistical and the structural points of view. Using the statistical approach, a wide range of boundary layers submitted to various favourable and adverse pressure gradients have been characterized experimentally. Nevertheless, all the existing models of the near-wall region are still empirical, and even the most sophisticated are not very successful in adverse pressure gradient situations. The current project is linked to the objectives of the European Project WALLTURB, which aims to generate a database of high-quality DNS and to conduct challenging experiments to improve the knowledge on and the modelling of near-wall turbulence. A DNS at a large Reynolds number can elicit information on 3D turbulent structures which is not directly available from the experiment.

Numerical simulations

The numerical code was used for a DNS of a similar flow at a lower Reynolds number. The incompressible Navier–Stokes equations are not solved in the curvilinear coordinate, but the partial differential equations are transformed using mapping. This leads to a modified system of equations which can be solved efficiently with smooth two-dimensional mapping. The code is parallelized in the spanwise direction using MPI routines. For space discretization, fourth-order central finite differences are used for the second derivatives in the streamwise direction. All the first derivatives of the flow quantities appear explicitly in the time-advancing scheme and the first derivatives in the streamwise direction are discretized using eighth-order finite differences. Chebyshev-collocation is used in the wall-normal direction. The transverse direction is assumed to be periodic and is discretized using a spectral Fourier expansion, the nonlinear coupling terms being computed using the conventional de-aliasing technique.

Large amount of data recorded for future analysis

In this project, a single DNS of channel flow over a smooth profile was performed at a Reynolds number $Re_T = 600$ at the inlet of the simulation domain. The inlet conditions were generated from a precursor DNS of flat channel flow. The smooth profile at the lower wall was duplicated from a similar experiment at the Laboratoire de Mécanique de Lille.

The computations were performed at HLRS (Germany) with 8 nodes (64 processors) of NEC-SX8 and required a total of 380GB of memory for a physical space resolution of 2304x384x576. With these parameters, the averaged performances of the code reached 9 GFlops per processor. In order to adapt the mesh to the dissipation scales, the grid was densified in the downstream part of the bump. After reaching a stationary state, a total of 5TB of raw data were recorded in order to compute high order statistics of the turbulence along both the flat wall and the curved wall. The time evolution of coherent structures, such as vortices, was also recorded and will be analyzed in the separation region.

Towards ITER on Supercomputers

Damien Lecarpentier

The GYROKINETICS project was carried out in 2006 and 2007 by researchers from the Max Planck Institute for Plasma Physics at Garching, Germany, and the Ecole Polytechnique Fédérale of Lausanne, in Switzerland. Using DEISA's resources under the DECI and the JRA3 frameworks, the project team further developed the gyrokinetic simulation approach to plasma turbulence, which is expected to help improve the performance of magnetic confinement fusion devices.

"Magnetic confinement fusion has the potential to provide a substantial proportion of the world's energy needs in the 21st century – and beyond – in a safe and environmentally friendly way", says Frank Jenko, researcher at the Max Planck Institute for Plasma Physics and member of the GYROKINETICS project.

"Its realization is, however, hampered by the complex behavior of hot collisionless plasmas (ion gases) in strong magnetic fields. Such plasmas are subject to temperature and density gradient driven microturbulence, which determines the energy and particle transport across flux surfaces and hence the minimum size of a burning plasma. Turbulence, thus, limits the so-called energy confinement time, keeping the plasma from reaching a state in which external heating becomes dispensable", he explains.

"Gaining a thorough theoretical understanding of turbulent transport is, therefore, crucial for improving the performance of magnetic confinement fusion devices, and constitutes one of the key goals in modern fusion research".

Understanding turbulent transport through gyrokinetic simulation

"Simulations are necessary if we are to understand and control plasma microturbulence. However", Jenko continues, "because fusion plasmas are virtually collisionless, a three-dimensional (i.e. in space) fluid description must, in principle, be abandonned, in favor of a six-dimensional (i.e. in phase space) kinetic one".

"Fortunately, several processes on very small spatio-temporal scales – such as the gyrating motion of the particles around magnetic field lines – can be removed, analytically, from the basic equations, thus making the problem five-dimensional. This reduces the computational requirements by many orders of magnitude, without sacrificing accuracy. This approach is called gyrokinetics, which gave the present project its name".

"Over the last few years, several massively parallel gyrokinetic codes, capable of solving nonlinear gyrokinetic equations, have been developed throughout the world, and they have matured to a point at which direct comparisons with experimental data are becoming feasible", Jenko notes.

During the project, Frank Jenko and his colleagues used, in particular, two state-of-the-art gyrokinetic plasma turbulence codes, which were independently developed at the two participating institutions, and which were based on complementary numerical approaches.

These two codes are the "particle-in-cell" ORB5 code, which computes the trajectories of large ensembles of marker particles, and the CFD-type GENE code, which represents the particle distribution functions on a fixed grid in phase space.

"Given that the simulation of turbulence in magnetized plasmas represents a major challenge at the forefront of computational plasma physics, a dual approach like this seemed particularly appropriate. By benchmarking the results of both codes, we expected to both gain more insight into the behaviour of these different numerical methods and to maximize the reliability of the physical results that were obtained", Jenko explains.

Simulations with unprecedented levels of resolution were realised

For the project, the gyrokinetic plasma turbulence codes ORB5 and GENE were adapted to the DEISA environment within the JRA3 framework, and were then ported to the SGI Altix system.

The DEISA infrastructure also provided the researchers with computational resources in order to realise their simulations.

"We were granted something in the order of 400,000 CPU-h", notes Jenko. "With that

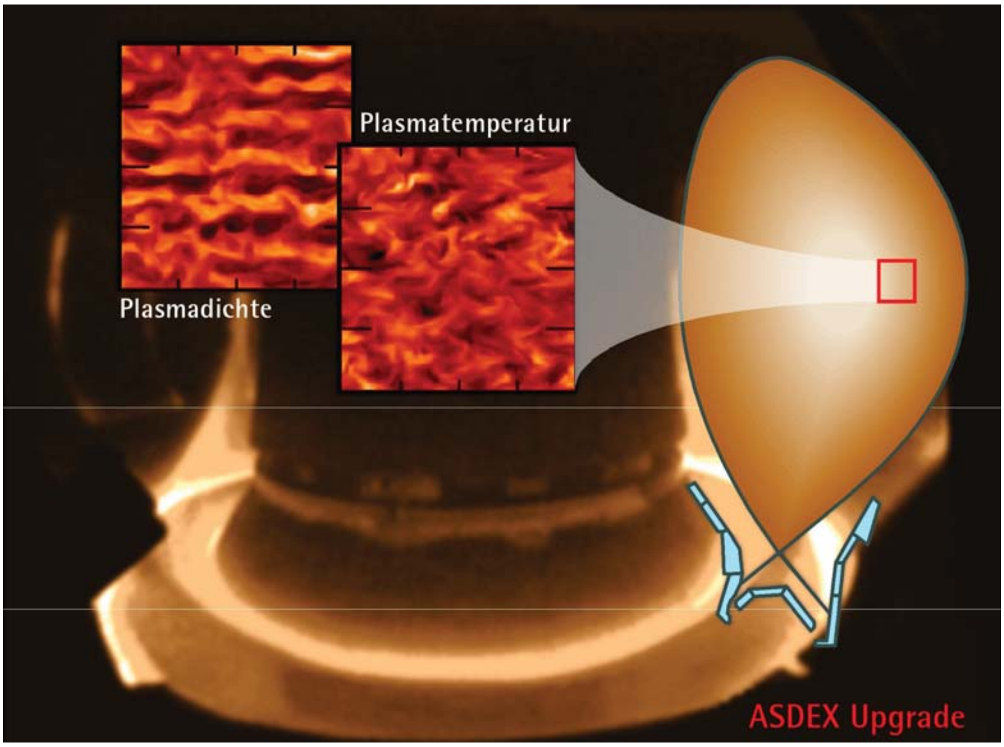

Fig. 2. Interior view of the fusion experiment ASDEX-Upgrade during a plasma discharge together with two contour plots from gyrokinetic simulations, demonstrating turbulent behaviour.

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budget, we were able to perform a number of simulations with GENE and ORB5, and thus to assess the role of fluctuations on very small spatio-temporal scales (smaller than the ion gyroradius and the ion transit time)".

"These scales had been neglected in previous studies, but there has been increasing evidence both from theory and experiment over the last few years that they can play an important role and should be retained in the analysis. Our simulations were some of the largest achieved to date in computational fusion research, with an unprecedented level of resolution", he adds.

"As a result, we were able to show that certain small-scale turbulent processes can make substantial – and even dominant – contributions to the overall heat transport carried by the plasma electrons. It turned out, in particular, that there often tends to be a scale separation between ion and electron thermal transport. While the former is usually carried more or less exclusively by long wavelength fluctuations, a substantial proportion of the latter can be carried by much smaller scales

According to the research team, these findings represent an important new insight into the physics of turbulent transport in magnetized plasmas, and will have important implications for future full-torus simulations of large fusion devices, such as the International Thermonuclear Experimental Reactor ITER.

Virtual fusion experiment: the ultimate goal

For qualitative progress in the theoretical understanding of turbulence in fusion devices, and in the capability to quantitatively predict its consequences, supercomputers – as instruments of numerical modelling – are absolutely essential. Research on magnetic confinement fusion has already moved away from the semi-empirical and predominantly experiment-driven approach to one based on numerical modelling. These changes suggest that experiments might one day be replaced entirely by simulations.

"Our ultimate goal is to conduct "virtual fusion experiments", says Jenko, "in which simulations are so realistic that they could almost come to replace experiments".

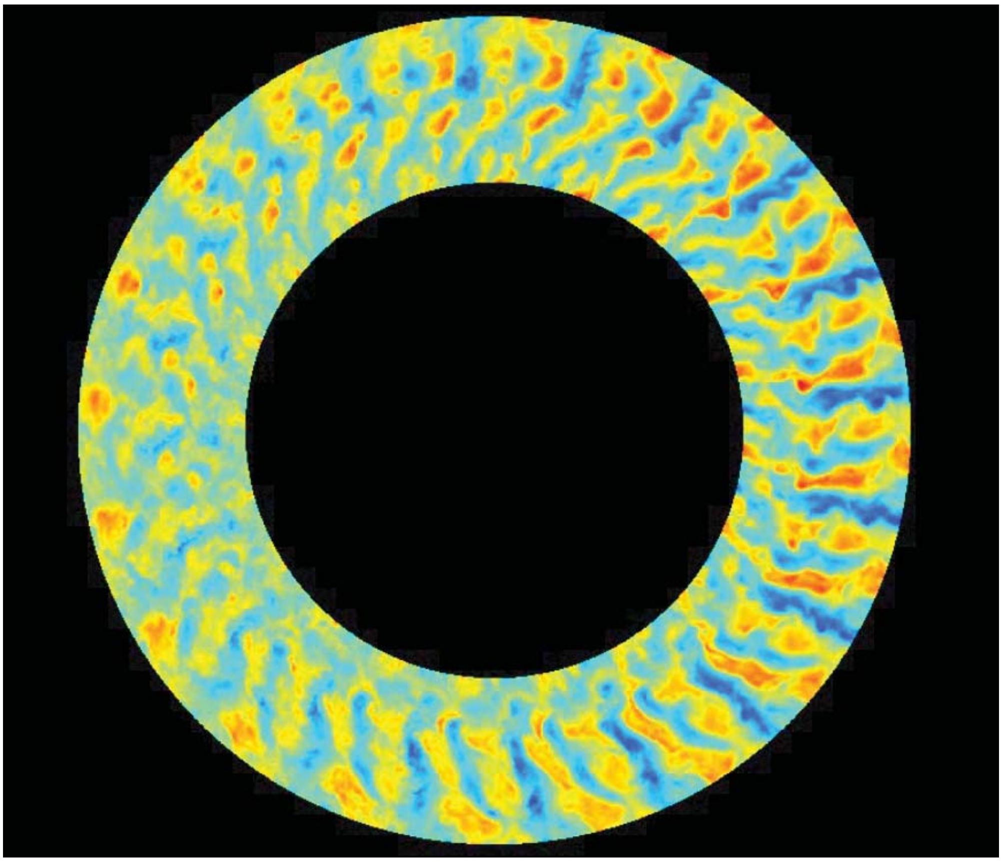

Fig. 3. Snapshot from a GENE simulation depicting turbulent transport in the interior of a fusion experiment.

Fig. 4. Frank Jenko, researcher at the Max Planck Institute for Plasma Physics and memeber of the GYROKINETICS project .

"The aim of the GYROKINETICS project was to take significant steps in that direction, by extending the scale range far beyond that used in past studies. Virtual fusion experiments remains, however, many years away", Jenko acknowledges.

"To reach this goal, the range of spatio-temporal scales will have to be extended, and a number of additional physical effects will have to be included, gradually establishing computational gyrokinetics as a reliable tool for analyzing and optimizing actual experiments".

"Significant code development will be required and supercomputers will have to become much more powerful still. Comprehensive gyrokinetic simulations of a device like ITER will require Petascale or even Exascale supercomputers", he points out.

"Given their ambitious goals and enormous resource demands, pushing both the software and the hardware they employ to their very limits, computational fusion physicists throughout Europe will always be eager to work with the latest generation of supercomputers. In this context, DEISA provides an excellent framework. It is likely to be instrumental in providing the fusion community with reliable predictive simulations of turbulent transport in fusion plasmas, thus helping to improve the performance of magnetic fusion devices, " Jenko concludes.

DEISA PRACE Symposium 2009
“HPC Infrastructures for Petascale Applications”
11-13 May, 2009, Amsterdam

PRELIMINARY PROGRAMME

Monday, May 11 (13:00 – 18:00)

Welcome

“Global Perspectives 1”
Mario Campolargo, EU
Ed Seidel, NSF, US
Ryutaro Himeno, RIKEN, JP
and more N.N.

Tuesday, May 12 (9:00 – 18:00)

“Global Perspectives 2”
Kostas Glinos, EU
Achim Bachem, PRACE
Stefan Heinzel, DEISA
John Towns, TeraGrid, US

“Science Communities”
Climate Research: Sylvie Joussaume, France
Cosmology: Carlos Frenk, UK
Fusion Research: Frank Jenko, DE
Life Sciences: Peter Coveney, UK

“PRACE Perspectives“
Directions in HPC Technology
Survey of HPC Systems and Applications in Europe
Training and Education for Petascale Computing

“DEISA Extreme Computing 1”
Speakers from different areas of science from all over Europe

Evening Conference Dinner

Wednesday, May 13 (9:00 – 13:00)

“DEISA Extreme Computing 2”
Speakers from different areas of science from all over Europe

Closing remarks

The registration is now open:
http://www.deisa.eu/news_press/symposium