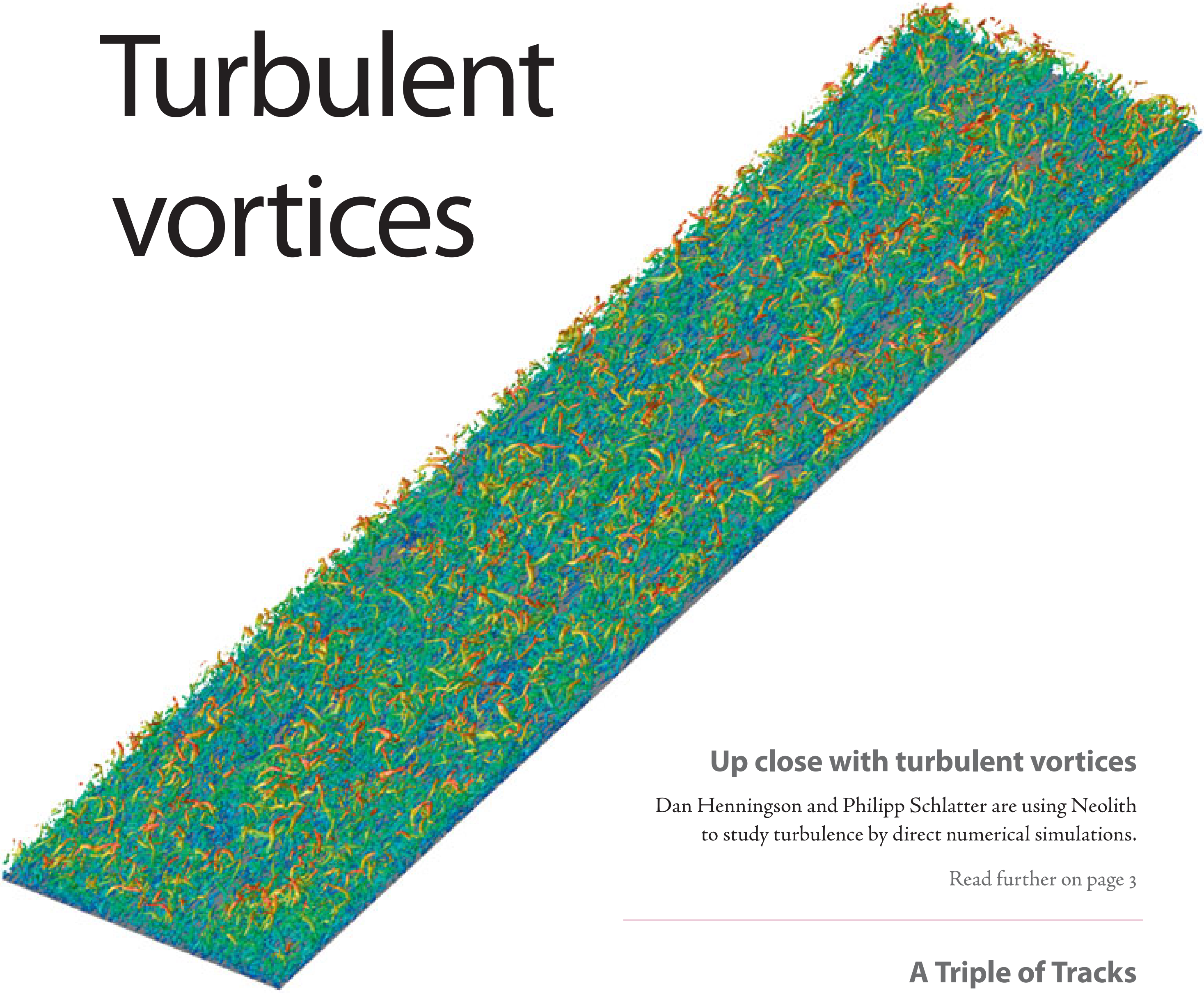
NSC
National Supercomputer Centre at Linköpings universitet

News
2008:4

Turbulent vortices



Up close with turbulent vortices

Dan Henningson and Philipp Schlatter are using Neolith to study turbulence by direct numerical simulations.

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A Triple of Tracks

NSC hosted the NSC'08 Storage workshop, SUNET TREFpunkt 19 and SUSEC Höstmöte in October.

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National research infrastructures are important

Recently, the Swedish government released the Research and Innovation Bill for the upcoming 4-year period (2009–2012). Good news is that for the first time in many years there is a significant increase of research funding. By 2012, the increase will be 5 billion SEK per year. Another good point is the emphasis on national research infrastructures. However, there is only a minor increase in funding for this sector (only 150 million SEK per year by 2012), which is nearly one order of magnitude less than what is needed. It is still a mystery how this gap should be bridged.

National research infrastructures, such as SNIC (Swedish National Infrastructrure for Computing), which NSC is part of, are of fundamental importance for Swedish researchers and necessary for allowing Swedish scientists to perform frontline research. Furthermore, these infrastructures are needed for Nordic and European large-scale collaborations.

Recently, a conference was held on E-science and research infrastructures, hosted by Sweden as part of the current presidency in the Nordic Council of Ministers. The conference attracted a large interest with close to 200 attendees, reflecting the great importance for these fundamental research instruments. At the conference, several statements regarding needs, plans and opportunities for the near future were agreed upon, cf. http://www.vr.se.

E-science is a new term reflecting the new dimension created by using modern information technology to tackle scientific problems of a complexity that otherwise would be impossible. E-science also enables long-distance collaborations and utilisation of distributed data resources. E-science will contribute to fundamental improvements in many scientific disciplines and it is important that Sweden is well equipped in this area.

Finally, I would like to thank all users, collaborators and co-workers at NSC for an eventful and interesting 2008 and wish you all a Merry Christmas and a Happy New Year 2009.

BENGT PERSSON, DIRECTOR OF NSC

Neolith on the Grid

With our continuing efforts to facilitate the use of our resources, we now offer the possibility to submit jobs over the grid to our largest resource – Neolith. During the development and testing of the grid interface Carsten Müller from the Department of Materials Chemistry at Uppsala University have helped us as a test user.

Carsten has been using the ARC middleware for three years to run jobs on the grid and has this to say: The largest advantage with the grid is that you don't need to keep track of your files over several different filesystems. You just keep them on your own workstation and you can still easily submit your job to any machine. The downside is that debugging your applications becomes harder, also, if you need to compile your programs at the resource this becomes harder as well since you can not log in directly and do testing.

With these benefits and limitations of running jobs on the grid, it is preferable to run jobs that uses preinstalled software that is being exposed over the grid. We currently only have Gaussian set up in this way on Neolith, but if you need other software, please do not hesitate to contact us.

Currently we will handle requests on a case by case basis, so if you have an account on Neolith and would like to run jobs over the grid with Gaussian or any other software, please do not hesitate to contact us at NSC by e-mail to: support@nsc.liu.se.

DANIEL JOHANSSON

November 2008 TOP500 List Released at SC08

The Roadrunner system at Los Alamos, first to cross the 1 petaflop/s line when it achieved first place in June, defended its leading position with a slightly improved 1.105 petaflop/s result. It was chased by Oak Ridge's Cray XT5 system named Jaguar, which became the second petaflop system at 1.059 petaflop/s.

NSC's Neolith cluster at position 55 also has an improved result (47.0 teraflop/s), enabling it to regain its position as the fastest Swedish academic resource, leaving HPC2N's Akka a few steps behind at position 59. A Swedish government agency still has the fastest resource in Sweden, now at position 18 in the list.

Pär Andersson at NSC has combined the TOP500 list with population statistics from dbpedia.org. The US tops the list at 36.6 kiloflop/s per capita. Sweden claims second place at 29.8 kflop/s per capita, while Weta Digital secures third place for New Zealand at 25.6 kiloflop/s per capita.

For more details on the TOP500 list, see http://www.top500.org/lists/2008/11

KENT ENGSTRÖM

Up close with turbulent vortices

In our everyday live, we are constantly surrounded by fluids, be it gaseous air or liquid water. Under certain simplifying circumstances, the motion of such fluids can be described by a comparably simple set of equations, derived from the basic Newton laws of mechanics. These so-called Navier-Stokes equations, known already for over a century, are nowadays accepted to accurately predict most of the relevant physical phenomena occurring in fluid mechanics. In this case, the fluid properties and the scales of the problem can be described with one single non-dimensional number, the famous *Reynolds number*, which can be viewed as the ratio between inertial and viscous effects. Nevertheless, exact solutions to the Navier-Stokes equations are known for only a few specific cases. The reason is mainly given by the strong nonlinearity of the equations, and the difficulty of specifying boundary conditions. This nonlinearity is also at the root of one of the most intriguing features of flows: *Turbulence*. This ubiquitous flow state is characterised by a seemingly random, highly unsteady and swirly motion of the fluid, extending from very large scales (on the order of the considered domain) down to extremely small scales (smaller than micrometers on, for instance, a commercial airplane at cruising speed). Since no complete theory of turbulence is available, basic research in turbulence relies heavily on either experimental studies in wind tunnels or the direct numerical simulation (DNS) of turbulent flows; direct in the sense that all arising length and time scales are fully resolved on the computational grid. In particular DNS bears many advantages compared to experiments, e.g. that the full time-dependent velocity field with many statistical quantities is available for analysis, and that boundary conditions can be specified accurately. However, the number of degrees of freedom necessary for realistic flow setups are extremely large [1], in particular as the Reynolds number is large. The larger the Reynolds number, the larger is the range of scales present in the flow. The increase in computer power, though, allows us now for the first time to consider flows numerically that have previously only existed in laboratories.

To illustrate the general appearance of turbulence, consider the flow of a simple fluid along a flat plate, forming a so-called *turbulent boundary layer*. This setup can be considered a simplified version of the outer flow along airplane wings or ship hulls, and is a standard test case for experimentalist, turbulence modellers and theoreticians. In Figure 1, a snapshot of the vortical structures inside such a boundary layer is presented. This picture is taken from one of the largest DNS so far, which we recently performed within our research group utilising our highly parallelised simulation code based on a fully spectral discretisation method [2, 3]. The snapshot clearly shows the appearance of turbulent structures of various sizes and shapes, densely populating the turbulent region close to the rigid surface. In particular, very close to the wall fine-scale streamwise elongated structures are visible, termed wall-layer streaks. These fine structures are believed to be the backbone of the regeneration process in turbulence. However, farther away from the wall larger structures exist, sometimes resembling vortex rings in a cross-stream plane, so-called hairpin vortices. It is the interaction and characterisation of such structures that is still fairly unclear, however believed to be essential for a full understanding of wall turbulence and, as mentioned below, crucial for a potential control of turbulence.

In contrast to the instantaneous chaotic appearance of turbulence given in Figure 1, Figures 2 and 3 show statistical (averaged) quantities measured from our DNS; the skin friction coefficient c_f and the shape factor H_{12} are shown and compared to recent experimental results obtained in the MTL wind tunnel at KTH. In particular c_f is of tremendous engineering importance since it provides a measure of the drag exerted by the plate which in turn allows for example the calculation of the number of passengers in an airplane with modified wing design. H_{12}, on the other hand, provides a measure for the internal shape of the boundary layer, and turns out to be a very sensitive

SC08 in Austin

With over 10000 participants, this year's SC08 in Austin, Texas, was the largest to date. It also celebrated the 20th anniversary of the Super Computing, SC, conferences with a historical exhibition. The local newspaper aptly described the conference as "Geek-o-Rama", "the NASCAR of computing" and the county fair of high-tech. Five NSC employees traveled to the event that took place November 15–21.

It's hard to summarize all the thoughts provoked by exhibitors, talks, BoFs and chance meetings during the week. There was a lot of talk about GPGPU acceleration (unfortunately, there was less talk about successfully ported applications with good performance gains). Tools for performance optimization and parallel debugging were hotter than the last few years. Not surprisingly, "green computing" continues to be important, with a lot of talk about performance per Watt. On top of that, of course there was a lot of new, improved products to view.

Austin proved to be a very nice city. The hotels and the conference venue were all within walking distance. We can also reveal there are some great restaurants to dine at, and if you are a live music aficionado, you certainly don't want to miss 6th Street.

Kent Engström

quantity when assessing various (experimental, numerical and theoretical) data sets. One of the most remarkable results pertaining to turbulent boundary layers is illustrated in Figure 3: The averaged wall-normal profile of the streamwise velocity, scaled in so-called wall units (the "plus" signs on the variables). It turns out that the velocity profile exhibits a unique shape consisting of a linear region close to the wall (viscous sublayer), followed by a logarithmic behaviour and finally the so-called wake region. These components together, going back to the pioneering work of the Hungarian physicist Theodore von Kármán, are usually termed the *"law of the wall"*. Both Figures 2 and 3 clearly show that the present DNS agrees very well with experimental results for the same flow case at the same Reynolds number. Therefore, the present results allow the uncertainty of various boundary layer quantities (skin friction etc.) to be drastically reduced, and furthermore allows for a cross-validation of both experimental techniques and simulation results.

Understanding the structures and dynamics of turbulent flows is strongly related to two other disciplines in fluid dynamics in which our group is active: The study of the stability of a given flow to disturbances, i.e. *transition to turbulence*, and, in particular for technical applications, to take the step from studying the flow to actively change and change a flow.

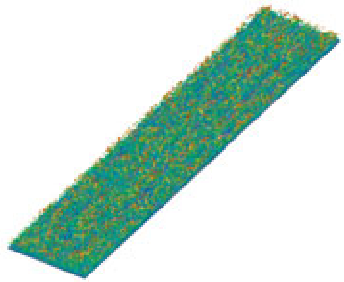

Fig. 1: Visualisation of the flow structures in a fully turbulent boundary layer developing above a solid wall; the flow is from lower left to upper right. Isocontours of the λ_2 vortex-identification criterion are shown with the colour code indicating the distance from the wall. The shown section of an instantaneous velocity field covers about one fifth of the total spatial simulation extent; measured in viscous (wall) units, the shown size is about 12000x2500, corresponding to an area of no more than 5mm by 1mm on a wing of a commercial airplane at cruising speed.

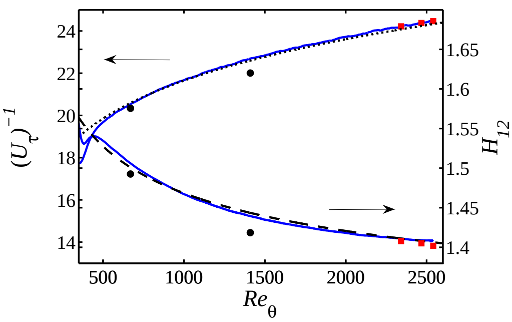

Fig. 2: Integral averaged quantities of a turbulent boundary layer relevant for engineers and designers of e.g. airplane wings. The characteristic skin friction coefficient $U_\tau / U_\infty = (c_f/2)^{1/2}$ (left axis) and the shape factor H_{12} are shown as a function of the downstream distance, measured in the Reynolds number Re_θ. An excellent agreement with both empirical correlations (black lines) and recent KTH experiments (red squares) can be observed. The solid circles correspond to older simulation data [4]. The unpublished experimental data is obtained in the MTL wind tunnel at KTH, courtesy Ramis Örlü.

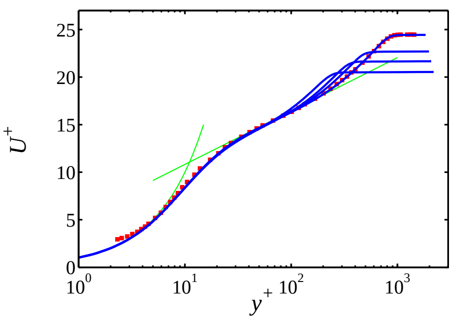

Fig. 3: The mean streamwise velocity profile U^+ as a function of the wall distance y^+ for four increasing Reynolds numbers. The agreement with experiments performed at KTH (red squares, courtesy Ramis Örlü) at Re_θ=2500 is excellent. The two green lines indentify the famous *"law of the wall"* with the linear and logarithmic behaviour.

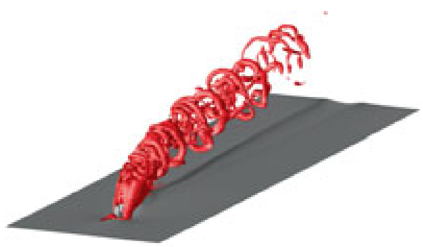

Fig. 4: Transitional flow structures caused by a jet emanating into a laminar boundary layer ("jet in crossflow" configuration, [5]), similar as smoke leaving a smoke stack. The red isosurfaces are the λ_2 vortex-identification criterion, whereas the gray surface corresponds to a low streamwise velocity value close to the flat plate. The flow in the jet is dominated by strong ring-like vortices periodically generated close to the nozzle ("vortex shedding").

LISA'08 in San Diego

Compared to SC08, LISA'08 has a broader scope, encompassing System Administration of any Large Installation of (usually Linux and Unix) computers. A NSC staff member was there and reports:

- Most people at the conference were U.S. residents, naturally. But the unproportionally big attendance from Norway and Sweden, together approximately five percent of the participants, was noted.
- Last year a group of computer scientists was commissioned to review a number of electronic voting machines, in actual use in California. I heard a talk about the results, that was a veritable horror story of security problems!
- A number of system configuration tools was presented and there still is not a clear winner. At NSC we have recently begun to use one of them: Puppet.
- The old Linux/Unix tool "top" has begotten a child, "topnet", that for each process presents also the amount of net traffic that the process generates. It looks very promising as another tool for debugging network problems, so I will examine it further.
- It was great, meeting so many other sysadmins!

LENNART KARLSSON

Flow control could potentially be used to reduce the drag of bodies thereby bringing down the fuel consumption of airplanes or cars. An example of a flow undergoing transition is given in Figure 4, obtained by DNS [5], again using our in-house simulation code [2]. A jet of fluid is released through a nozzle in the wall into a laminar cross flow. This flow configuration is usually referred to as "jet in crossflow" and appears in many technical applications such as fuel injection or smoke stacks. Depending on the various parameters describing the system, the fluid emanating from the nozzle is deflected, and clear ring-like instabilities emerge, which eventually lead to a breakdown of the initially ordered flow. One of the open questions to be answered here is the origin and characterisation of the growing instability, and as to how the breakdown could be increased or decreased, depending on the desired application.

The DNS presented in this article all rely on fine grid resolution and large integration times. For example, the boundary layer simulation presented in Figures 1–3 employs a total of approximately 10^9 (spectral) grid points, running on 256-1024 processors at both NSC Neolith and PDC Hebb for a duration of many weeks. Consequently, turbulence simulations require large computational resources, with efficient processors and – more importantly – a fast network. In that sense, the NSC Neolith system is very suitable for this type of applications. Furthermore, the recently installed system Ekman/Vagn as a collaboration between NSC and PDC, will provide us with the opportunity to study various transitional and turbulent phenomena in much greater detail.

PHILIPP SCHLATTER
AND DAN S. HENNINGSON

LINNÉ FLOW CENTRE,
KTH MECHANICS

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[3] Q. Li, P. Schlatter and D.S. Henningson, Spectral Simulations of Wall-Bounded Flows on Massively-Parallel Computers, *Tech. Rep.*, KTH Mechanics, 2008.
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Philipp Schlatter received a PhD in Fluid Mechanics at ETH Zürich (Switzerland) in 2005. Thereafter, he moved to KTH, first as a Göran Gustafsson Postdoc, and after 2007 as a Forskarassistent funded by VR. He is also engaged as Director of Studies in the KTH Computational Science and Engineering Centre (KCSE).

Dan Henningson received a PhD in Mechanics at KTH 1988 after which he was an assistant professor in the Mathematics Department at MIT. In 1999 he became a professor of Fluid Mechanics at the Department of Mechanics KTH. From 2005 he is the head of that department. He is also the director of the Linné Flow Centre.

A Triple of Tracks

Large scale storage is currently a rapidly expanding area in Sweden and northern Europe. In October, NSC hosted the NSC'08 Storage workshop with focus on two important areas for High Performance Computing: small fast storage and large safe storage.

The latest developments in file systems such as Lustre, GPFS and other were presented with emphasis on HPC needs. We were also informed about the current status and plans regarding HPC storage in Norway and Finland. The organisation of the Swedish Database Infrastructure Committee (DISC) was presented, as well as laws and regulations regarding large databases.

Simultaneously with the NSC'08 Storage track, SUSEC held its autumn meeting, gathering IT security staff from Swedish universities, university colleges and related organisations. After that, the baton was passed on to SUNET, which held its 19th SUNET TREFpunkt meeting for networking staff from SUNET connected organisations.

We would like to take this opportunity to thank all the speakers for their contributions to the three tracks.

The programmes and the presentations for all three tracks are available at http://www.nsc.liu.se/nsc08/

TOM LANGBORG

UPCOMING EVENTS

PRACE Petascale Computing Winter School

February 10 – 13, 2009, Athens, Greece.
http://www.prace-project.eu/events/prace-winter-school-february-9-13-athens-greece

HPCA-15; 15th International Symposium on High-Performance Computer Architecthure

February 14 – 18, 2009, Raleigh, North Carolina, USA.
http://www.comparch.ncsu.edu/hpca/index.html

PPoPP 2009; 14th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming

February 14 – 18, 2009, Raleigh, North Carolina, USA.
http://ppopp09.rice.edu

PerCom-09; IEEE Intl Conference on Pervasive Computing and Communications

March 16 – 20, 2009, Dallas, USA.
http://www.percom.org

HP-Cast NTIG (Nordic Technical Interest Group in HPC using HP clusters)

Preliminary date: March 24 – 25, 2009, CSC, Finland.

ACM International Conference on Computing Frontiers

May 18 – 20, Ischia, Italy.
http://www.computingfrontiers.org/2009

IPDPS-09: IEEE International Parallel and Distributed Processing Symposium

May 25 – 29, 2009, Rome, Italy.
http://ipdps.org

HiCOMB 2009 8th IEEE International Workshop on High Performance Computational Biology

May 25, 2009. Rome, Italy.
http://www.hicomb.org

ICS'09: 23rd International Conference on Supercomputing

June 9 – 11, 2009, New York, USA.
http://www.ics-conference.org

ISC'09: International Supercomputing Conference

June 23 – 26, Hamburg, Germany.
http://www w.isc09.org

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