NSC News
2009:2
National Supercomputer Centre at Linköpings universitet

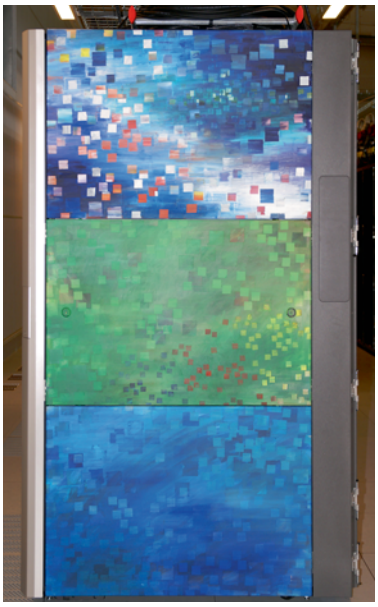
20 YEARS IN HPC 1989–2009

Blood Flow Simulations

Large Eddy Simulations in Biofluid Mechanics

Professor Matts Karlsson and co workers at Linköpings universitet use Large Eddy Simulations to study turbulence in blood flow.
A factor that may increase the risk for cardiovascular diseases.

Read further on page 3



Vernissage in the computer hall

NSC has started to artistically decorate its systems.
The first to be decorated was Bore/Gimle with a painting by the artist Kristin Winander.

Read further on page 5

New projects and New systems

This spring has been a hectic and interesting period for us at NSC with planning work for new systems including necessary extension of the capacity of our computer hall, enabling the hosting of the new capacity system and the future system for material science research. We have also inaugurated a painting decorating our system Bore/Gimle used by SMHI (please see separate note). Furthermore, the new four-year EU-project IS-ENES on infrastructure for climate research was launched in March 2009 with a large kick-off meeting in Paris. For NSC, it will include new tasks on code optimisations for parallel systems and development of distributed storage for climate applications. Therefore, we have recruited two scientific programmers, that will start at NSC after the summer. Furthermore, to accomplish the extended services at NSC, we are currently in the process of recruiting also additional system manager(s) to NSC.

It is interesting to notice that in the recent SNAC application round, there was a substantial over-application for computational time at the large SNIC systems. For instance, Neolith at NSC was over-sought by a factor of 4. This shows that the needs for high-performance computational (HPC) resources are increasing at a higher pace than previously was anticipated. It reflects that HPC is spreading into more scientific disciplines and to an increasing number of researchers. Furthermore, the last years' valuable additions to the SNIC resources have enabled researchers to ask scientific questions at new exciting levels.

With this in respect, it is quite timely that NSC is currently procuring a large capacity system that will provide valuable computer power both to local users and to national users with SNAC allocations. We plan for having the new system in operation during autumn. This procuration is for the first time made together with three other SNIC centres (UPPMAX in Uppsala, C3SE in Gothenburg, and LUNARC in Lund), also investing in new hardware. The combined procuration gives advantages in visibility towards the vendors and benefits for the centres in increased collaborations and knowledge exchange.

At NSC, we are currently preparing for the annual conference NSC'09 that we arrange 13–15 October. This year, when NSC is celebrating its 20 year anniversary, the theme is code optimisation for large scale parallel systems. The conference will include a PRACE code-porting workshop and the yearly SNIC interaction. We wish you all very welcome to Linköping for this traditional HPC event. More details will follow on our web site.

Finally, I would like to wish all users and colleagues at NSC a pleasant and relaxing summer!

BENGT PERSSON, NSC DIRECTOR

IS-ENES

The EU project IS-ENES, InfraStructure for the European Network for Earth System Modelling, was started in March 2009. On 30–31 March, all 18 partners from 10 countries met in Paris for a large kick-off meeting with presentations of the different workpackages and initial discussions on the work to be performed. The project will last for 4 years. Among the partners we find the leading European meteorological institutes, including SMHI, and major research groups in meteorology and climatology. Furthermore, together with NSC two additional super-computing centres are participating – BSC (Barcelona Supercomputing Centre) and DKRZ (German High Performance Computing Centre for Climate- and Earth System Research), which will give valuable contacts of mutual interest. One task to be performed at NSC is optimisation of climate code for new massively parallel systems. Another task is development of distributed storage solutions for climate data including long-term support of these services. Participation in IS-ENES will bring new important knowledge to NSC, which will be of value not only for this project but also for other scientific areas where NSC is providing computational resources and when developing storage solutions for SNIC users. Two scientific programmers are now recruited to NSC for performing these tasks. They will add valuable competence to NSC and help users also in other scientific areas.

The IS-ENES project members at the kick-off meeting in Paris

Large Eddy Simulations in Biofluid M

The proportion of older persons in the communities of the western world is rapidly increasing, and cardiovascular disease is the number one cause of death and the most serious health threat (National Center of Health Statistics and National Heart Lung and Blood Institute, USA). One reason for this is that specific pathophysiological mechanisms that cause cardiovascular disease in older individuals are superimposed on heart and vasculature that have been modified by an evolving aging process. Thus, changes in the cardiovascular structure and function in subjects with cardiovascular disease are not solely due to the disease per se, but reflect age-disease interactions.

Turbulence in the arterial blood flow may increase the risk for hemolysis as well as platelet activation and thrombus formation. It is also suggested that turbulence may be involved in the pathogenesis of atherosclerosis. The peak Reynolds number in the human aorta is about 10000 under normal resting conditions, and thus blood flow is in the transitional regime.

Experimental in-vitro studies of turbulent flows have been conducted in straight circular pipes with constrictions, representing idealized models of stenosed vessels since the 1980s. Reynolds numbers from 250 to 2000 were considered and only the axial velocity component was measured. Post-stenotic turbulence was found for a Reynolds number of 1000 or higher whereas for Re=250 and 500 the flow remained laminar, although periodic shear layer oscillations were detected in the latter case.

The first computational approaches to predict transitional pipe flows were presented fairly recently and to the present day a number of computational works have been published. Many of these employ Reynolds Averaged Navier-Stokes (RANS) turbulence models. These are solved directly for time averaged flow quantities, and thus are not capable of capturing the dynamics of the flow. Furthermore, a RANS model always contains coefficients calibrated using known, and relatively simplified, flow conditions implying that RANS models are not generally applicable to arbitrary flows. Several RANS models are available in the literature, all having their own set of advantages and disadvantages.

On the other end of the spectrum there is Direct Numerical Simulations (DNS) of the full Navier-Stokes equations which is the most accurate computational method available in order to simulate turbulent flows. In contrast to RANS modeling, DNS resolves all the turbulent motions in the flow. However, a DNS quickly becomes enormously costly in terms of computational resources when the Reynolds number is increased and the geometrical complexity of the model is also severely restricted due to the numerical methods used in DNS. Very few works employing DNS for constricted tube flow (with Reynolds numbers ranging from 200 to 1000) have been published.

Figure 1: Instantaneous axial-velocity for four different time steps reveals a fluctuating flow in a post-stenotic region.

Huge demand for HPC capacity

The demand for HPC capacity in the application round for Large Scale allocations from the Swedish National Allocations Committee, SNAC, was higher than ever this spring. A total of four million core hours per month was applied for on Neolith which was about four times what was available. Roughly one quarter of Neolith is available for Large Scale applications in each of the two yearly allocation rounds. The other half is for Medium Scale applications. The rapid increase in demand for time has also been seen in Medium Scale applications this spring. The increase is in both number of applications and in size.

Most other SNIC resources, at NSC and other sites, were also over-sought in the Large Scale application round. For example the system Akka at the High Performance Computing Center North, HPC2N, in Umeå was also very popular with more than three million core hours per month applied for.

PETER MÜNGER

Mechanics

Figure 2: The second invariant of the rate of strain tensor displays the complexity of the turbulent flow field with a highly disturbed flow, as expected, in the immediate post-stenotic region

Large Eddy Simulation (LES) is a computational method that combines the advantages of RANS models and DNS. The large, energy carrying turbulent eddies are resolved in time and space, while the small eddies are modeled. Although the computational cost is considerably higher for LES compared to RANS, the cost is much less in comparison to DNS. Still, most of the flow dynamics of interest is resolved in LES, and it commonly demonstrates a superior performance compared to RANS. Furthermore, transition to turbulence can be resolved with LES, and complex geometries are not a general limitation. Hence, LES seems to be a very promising method to employ when subject specific models are to be assessed for diagnoses, intervention planning or follow-ups.

In the present work LES is used to systematically investigate the sensitivity of the turbulent transition in stenosed pipes to outer disturbances. The Reynolds number ranges from 500 to 2000. The geometry consisted of a circular pipe with a cosine shaped stenosis with a 75% reduction of the cross-sectional area was prescribed at the stenosis. Upstream the stenosis the length of the pipe was 4 diameters (D) and the downstream length was 20D.

An incompressible, homogeneous, Newtonian fluid was assumed. At the inlet a fully developed Poiseuille flow was applied, and perturbations of various intensities were superimposed onto the velocity profile. No-slip was prescribed at the pipe surface and the walls were rigid. The simulations were performed on a fully structured mesh containing 6 Million Cells (MC), with reduced cell size in the stenotic and post-stenotic regions. In the vicinity of the pipe wall the cell size was also gradually reduced. The non-dimensional wall distance, y+, was less than 0.2 in the fully turbulent region for Re = 2000. ANSYS Gambit 2.4 (ANSYS, Inc., Pittsburgh, PA, USA) was used for the meshing.

The present work was carried out using the flow solver ANSYS Fluent 6.3 (ANSYS, Inc., Pittsburgh, PA, USA). This solver employs a cell-centered finite-volume method based on a multi-dimensional linear reconstruction scheme, permitting computational

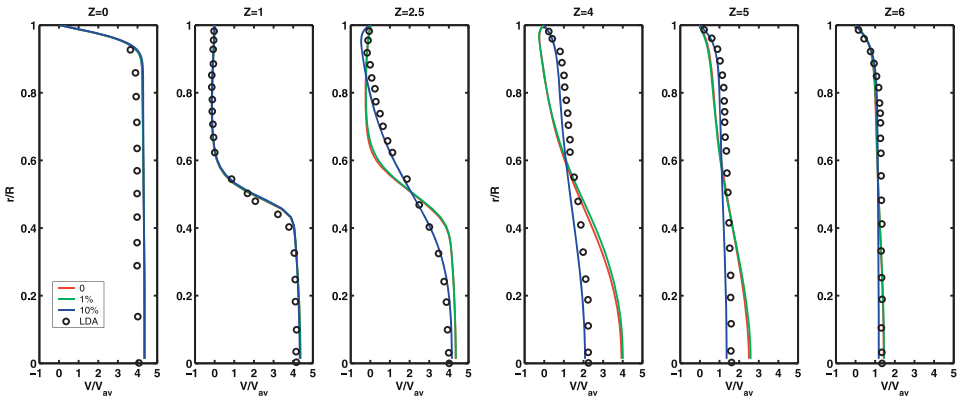


Figure 3: Large Eddy simulations compared to Laser Doppler Anemometry measurements.

HEPiX Spring 2009 in Umeå

HEPiX is a conference for systems administrators working with computers for high energy physics, with a special focus on the LHC Compute Grid (LCG). It is held twice a year, and this spring it was at the HPC2N supercomputer centre in Umeå. There were approximately 100 participants, and 55 talks over the five days.

The talks covered such topics as LCG sites reporting on their status in preparation for the start of the LHC accelerator this autumn, how to build a new datacentre, systems administration tools, performance testing, and security. However, the most prominent topic was virtualisation. Almost a quarter of the talks were on this topic, and covered such things as the performance of different virtualisation techniques, how to manage virtual servers, and, not the least, security implications; there are thorns in the virtual rose garden as well...

As a whole, the conference was interesting, and provided a good opportunity to exchange experiences with colleagues.

The next HEPiX will be in October, at the Lawrence Berkeley National Laboratory in California, USA.

THOMAS BELLMAN

cells with an arbitrary polyhedral topology. A segregated solver with the fractional-step solution algorithm was used, and time control was obtained using a non-iterative time advancement scheme. The time step was set to get a Courant number less than 1. All simulations were run on the Linux cluster Neolith, at National Supercomputer Centre, Linköping University.

At Re=500 the flow was entirely laminar. These simulations were primarily used to validate the numerical set-up against experiments and DNS data. For Re=1000 the flow was highly transitional, and if no perturbations were applied, an intermittent behavior was detected with long periods of laminar and turbulent flows occurring. By introducing disturbances at the inlet a transition to turbulence was always observed, and increasing the disturbance level enforced an earlier transition and a shorter transitional region, thus indicating a strong sensitivity to outer disturbances as expected.

LES simulations at Re=2000 are, to our knowledge, the first scale resolving simulations performed for a non-pulsating flow in a circular, stenosed pipe, at a Reynolds number greater than 1000, Figure 1 and 2. For Re=2000 a distinct transition to a fully turbulent flow was always observed in the post-stenotic region of the pipe. The sensitivity to outer disturbances was less pronounced compared to Re=1000, still, a dependency on the magnitude of the disturbances was observed. Excellent agreement with experimental data was found with a medium-sized perturbation, Figure 3.

This works clearly demonstrates the capability of LES to correctly capture the flow dynamics in non-pulsating stenosed pipe flows and indicates the necessity to move from traditional RANS methods readily utilized in computational biofluid mechanics towards scale resolving simulations.

MATTS KARLSSON

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Vernissage in the computer hall

On the 28 April 2009, NSC inaugurated our first piece of artwork in the computer hall. It is the system Bore/Gimle performing calculations for SMHI, that now is artistically decorated with a painting, nicely contrasting to the traditionally computer grey, adding a new flavour to our computer hall. The artist is Kristin Winander, who besides painting also works with a wide variety of materials, including metals and textiles. She has had several exhibitions in Linköping, Norrköping, and Stockholm. The new painting at NSC symbolises air, land and water as the primary elements included in the calculations of weather forecasts.

NSC and SMHI staff at the inaugural ceremony with the artist Kristin Winander in the middle

UPCOMING EVENTS

ISC'09: International Supercomputing Conference
June 23 – 26, 2009, Hamburg, Germany.
http://www.isc09.org

IEEE NAS-09; IEEE International Conference on Networking, Architecture and Storage
July 9 – 11, 2009, Zhang Jia Jie, China.
http://www.eece.maine.edu/nas

Euro-Par 2009; European Conference on Parallel Computing
August 25 – 28, 2009, Delft, The Netherlands.
http://europar2009.ewi.tudelft.nl

IEEE Cluster 2009
August 31 – Sept. 4, 2009, New Orleans, Louisiana, USA.
http://www.cluster2009.org

ParCo2009; International Conference on Parallel Computing
September 1 – 4, 2009, Lyon, France.
http://www.ens-lyon.fr/LIP/ParCo09-3

PACT2009; The 18th International Conference on Parallel Architectures and Compilation Techniques
September 12 – 16, 2009, Raleigh, North Carolina, USA.
http://www.pactconf.org

ICPP-2009; 38th International Conference on Parallel Processssssing
September 22 – 25, 2009, Vienna, Austria.
http://www.cse.ohio-state.edu/~icpp2009

NSC'09 Conference with PRACE Code Porting Workshop and SNIC Interaction
October 13 – 15, 2009, Linköping, Sweden.

Topics:

- presentation of PRACE prototype systems
- examples of PRACE systems usage
- demonstrations of code porting issues
- user presentations
- 20 years of Swedish HPC

http://www.nsc.liu.se/nsc09

SC09; International Conference for High Performance Computing, Networking, Storage and Analysis
November 14 – 20, 2009, Portland, Oregon, USA.
http://sc09.supercomputing.org

HiPC 2009; 16th IEEE International Conference on High Performance Computing
December 16 – 19, 2009, Kochi, India.
http://www.hipc.org

CCGrid10; 10th IEEE International Symposium on Cluster Computing and the Grid
May 2010, Melbourne, Australia.
http://www.gridbus.org/~raj/ccgrid

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