NSC News
2006:1
National Supercomputer Centre at Linköpings universitet

Mozart: new half terabyte SMP system at NSC

A new computer system with Sweden's largest shared memory has now been installed at NSC.

The hardware in the new system consists of an SGI Altix 3700 Bx2 with 64 Intel Itanium 2 processors, 512 GB of memory and with SGI's NUMAflex global shared-memory architecture. The system has been funded by the Swedish Research Council via the Swedish National Infrastructure for Computing (SNIC).

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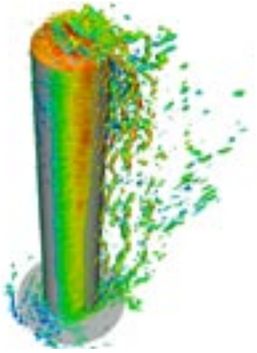
Air flow calculations on Monolith



Associate professor Siniša Krajnović at Chalmers discusses how to use the Monolith cluster to calculate the air flow around a Volkswagen Golf and other objects.

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Computing in the environment's service

A new cluster at the Swedish Institute for Meteorology and Hydrology will be used in emergiencies to predict the spread of airborne pollutants like poisonous chemicals and radioactive fall-out.

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Long term support and quick decisions

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The newsletter of the National Supercomputer Centre, NSC News, now appears in a new format with the language changed into English. The aim of the newsletter remains, however, the same, to spread information about NSC and our activities to users of our resources, partners and to people with a general interest in high performance computing. We hope that you will enjoy reading it also in the future!

Sometimes new opportunities appear with short notice and it is important to act quickly but still with a focus on quality. During the last months we have had a number of such challenges. In late October 2005 NSC was granted support from the Swedish National Infrastructure for Computing (SNIC) for a shared memory (SMP) resource. Since the only large SMP resource, the SGI Origin 3800 at NSC, had to be taken out of service early in 2006 we had to put all our effort into finding a replacement for this resource already before the end of 2005. We managed, and the new national SMP resource, an Altix 3700 Bx2 system from SGI, is now in operation. An article describing the new system is presented in this issue of NSC News.

Late in November, we were approached by the Swedish Radiation Protection Authority, SSI. They were interested in improving the national capability in performing simulations for predicting atmospheric transport of air pollutants. This resulted in the design of new hardware, which for financial reasons had to be purchased before the end of 2005. In close collaboration with SSI and SMHI we were able to finish the whole process in less than a month. The new system was delivered by Advanced Computer Technology (ACT) and is now in full production. Niclas Andersson at NSC, who was the project leader for this system, describes the hardware below.

When the Swedish Government took the decision to participate in the European UCAV (Unmanned Combat Aerial Vehicle) demonstrator program, Neuron, we knew this would affect also NSC. In order to catch up with the somewhat delayed project plans, Saab asked us to deliver a new HPC system within a period of less than two months. Right now we are working hard to put the system in operation and to deliver it to Saab in time for their first simulations on Neuron.

We are really proud that we were able to act according to the demands of our partners in all the cases described above. It is important, however, to bear in mind that the ability to make quick and accurate decisions is based on experience and a continuous build-up of technical skills over many years. This is made possible by long-term support of basic skills of design and operations of HPC systems. The pay-off of such support is not always directly visible to users and partners but nevertheless is critical for successful operations of any HPC center.

Strengthened resources for environmental protection

NSC has expanded the computing resources at the Swedish Institute for Meteorology and Hydrology (SMHI) with an HPC cluster. The cluster is used for simulations for predicting atmospheric transport of air pollutants. In emergencies it can be used for predicting the spread of air carried infections, poisonous chemicals and radioactive fall-out.

The cluster consists of 26 nodes, each equipped with 2 Xeon processors (3.2 GHz) and 2 Gigabyte of primary memory. The cluster has 4 Terabyte secondary storage and shares its Infiniband interconnect with SMHI's existing HPC production resources for weather forecasting, which are also operated and maintained by NSC.

The resource is financed by the Swedish Emergency Management Agency (KBM), the Swedish Radiation Protection Authority (SSI), and SMHI.

The hardware was delivered by Advanced Computer Technology AB just before christmas 2005.

Discovering the flow around a Golf

During the 1970s, the Volkswagen Corporation developed Golf I, which was a starting point for one of the most successful classes of passenger vehicles ever built.

The main feature of this car was its distinct slanted back. The original model had a steep back-end angle of 45 degrees with respect to the plane of the vehicle's roof. The drag coefficient of this car was 0.4, which was not bad for that time (the author's relatively new car has a drag coefficient of 0.3.).

It is well known that streamlined bodies produce a smaller wake, which is beneficial in terms of reducing air resistance. Thus, engineers gave the Golf a more streamlined shape by decreasing the angle of the rear slanted surface to 30 degrees. When the new design was tested in the wind tunnel it was found that the drag increased by some 10% – thus the exact opposite of what was expected. After this surprising result, tests were conducted for all other angles and it was found that something unusual takes place with the drag coefficient when this angle is between 28 and 32 degrees. By looking at the air flow it was found that the separation (i.e. when the air stream is no longer attached to the surface) could occur either at the top or at the bottom of the inclined rear end (rear window).

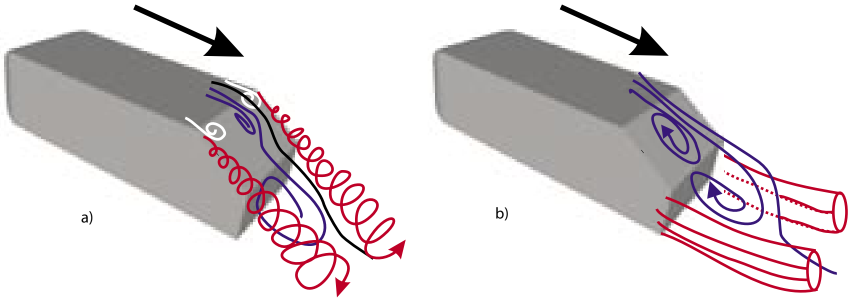


Figure 1. Schematic representation of the time-averaged flow around a Golf-like car with the rear window at an angle of a) 25 degrees, b) 35 degrees.

Vehicle drag

To explain the implication of this flow behavior for our readers, we need some concepts on vehicle drag. The force of air resistance, called drag in the case of cars, is caused to some 80–90% by low pressure on its rear-end surface, caused when the air flow surrounding the car separates at the rear and forms a region of recirculating flow (called wake) behind the car. When the car travels through the air, friction retards the movement of the surrounding air. Once the flow separates at the rear end, the friction forces disappear and the air stream accelerates, causing a decrease in pressure. The low pressure results in a force that draws the car backwards, i.e. drag. The sooner the flow separates, the larger the region of low pressure becomes and the drag increases. If we apply this concept to our Golf, we realize that the drag could be both low and high when the angle of the rear end was between 28 and 32 degrees depending on whether the separation was on the lower edge or the upper edge of the rear window. At the same time another car was developed at Volkswagen, namely Polo I, and similar flow behavior was observed in the wind tunnel test.

Airflow

At the beginning of 1980s, engineers made a generic model of a Golf car (shown in Fig.1) to study this flow phenomenon. The main feature of this simplified Golf-like car is that the angle of the rear window could be varied between 0 and 90 degrees. This model, called the Ahmed body after its creator, produced the same change of the drag with the angle of the rear window as that observed on detailed cars. During the past two dec-

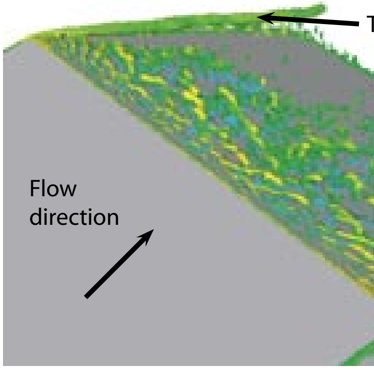


Figure 2. Instantaneous vortices on the rear window of t
vortices are traveling upstream and downstream, respe

Mozart, the new half terabyte SMP system at NSC

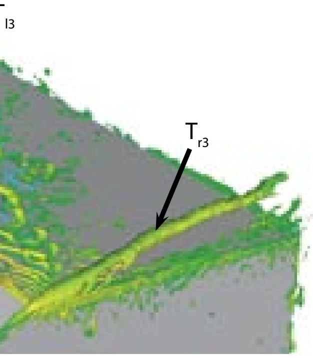
NSC has during the past year been in discussions with SNIC concerning replacement of the SGI Origin 3800 system that we have operated since 2001.

A survey among Swedish HPC users, carried out in April 2005, confirmed the need of such a system to run several quantum chemistry program packages including Gaussian, and some user developed codes. Also VASP, used by the solid state physics community, needs a large memory for studies of large systems. Based on the results from this user survey, we performed benchmark tests with the codes mentioned above on a number of different SMP systems. In some cases, in particular VASP, we could also see a large speed-up for MPI executions on some of the tested SMP systems as compared to available clusters.

In order to avoid problems for the users of the SGI3K systems we had to make sure that the system would be available by the end of March 2006. Considering that the financing was granted

car with the Monolith cluster

ades many researchers have studied the flow around this model using both experimental and numerical techniques, focusing mosty on window angles of 25 and 35 degrees. The most recent experimental study, reported 2003, was very extensive and illustrated a clear difference between the flows around cars with these two angles of the rear window. The results of this study can be summarized as follows. The rear end at 35 degrees produces a flow that separates at the sharp edge between the roof and the rear window and forms a large wake bubble (blue curves in Fig. 1b). In contrast, when the rear window is at 25 degrees, the flow reattaches (i.e. the flow stream drops onto the surface) on the rear window of the car (see Fig. 1a). Unlike the steady (constant in time) flow around the 35-degree model, here the flow is very time dependent and changes at every instant. In addition, new flow structures in the form of cone-like vortices are formed close to the sharp side edges of the rear window (red curves in Fig. 1b). The flow around the body with the rear angle of 35 degrees was relatively well understood but the 25 degree body flow has puzzled researchers for many years. The experimental techniques were inadequate to study this complex and high frequent flow and the numerical methods used by previous researcher used mainly stationary equations (due to inadequate computer resources) that cannot deal with very unsteady flows. There were also few attempts to make time-dependent simulations, which failed for technical reasons concerning the method and which we will not discuss here.



he simplified Golf-like car. Red and blue
ctively.

> *The 25 degree body flow has puzzled researchers for many years.*

Monolith computations

With the introduction of the cluster Monolith at NSC, the author has found a tool that is capable of simulating this flow by solving complete time-dependent Navier-Stokes equations with a technique called Large-Eddy Simulation (LES). With LES we compute all turbulent vortices that are larger than the size of our computational cells, and only the influences of the smallest ones are approximated with some turbulence model. In practice we compute around 80–90% of all turbulence in the flow with this technique. It should be mentioned that computing so much of the turbulent structures requires very fine computational grids and short time steps (i.e. a large number of numerical time steps for simulating physical time that is required for study of the flow). In the case of our Golf-like car, 17.5 million computational cells and more than one hundred and fifty thousand time steps were used to achieve the necessary resolution of the turbulent structures. For this purpose a finite volume code using block decomposition and the MPI message passing system was run on Monolith on 32 CPUs at a time. The total computational time was around three and a half months (wall time). In addition, two simulations with smaller grids were run to establish numerical accuracy. These simulations resulted in a large amount of time-dependent data that were analyzed by the author and used to explore this flow in detail. For the first time we were able to follow this complex flow and answer questions that have waited for an answer for more than twenty years.

Results and conclusions

Here we shall present only a very small portion of the results of this study and the interested reader is referred to a large number of publications that have resulted from this work. One of the most important questions that this work has provided an answer to is the reason for the highly unsteady flow on the rear window of our Golf-like

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late in October 2005, the whole process of benchmarking, discussions with vendors, internal discussions, delivery, etc., had to be executed in an efficient manner.

The present SNAC users of the SGI Origin 3800 system have been informed about the procedure for transfer to the new system, which will occur during the first week of April.

Looking back at the process I would say that we can be really proud of what we achieved. We would also like to thank SGI for their quick delivery and helpful support.

Last, but not least, the name of the system. Since the power was switched on January 27, exactly 200 years after the birth of Wolfgang Amadeus Mozart, we felt that the name of the great musician and composer was very well suited to use as the name for a high productivity (and short lived) resource.

SVEN STAFSTRÖM

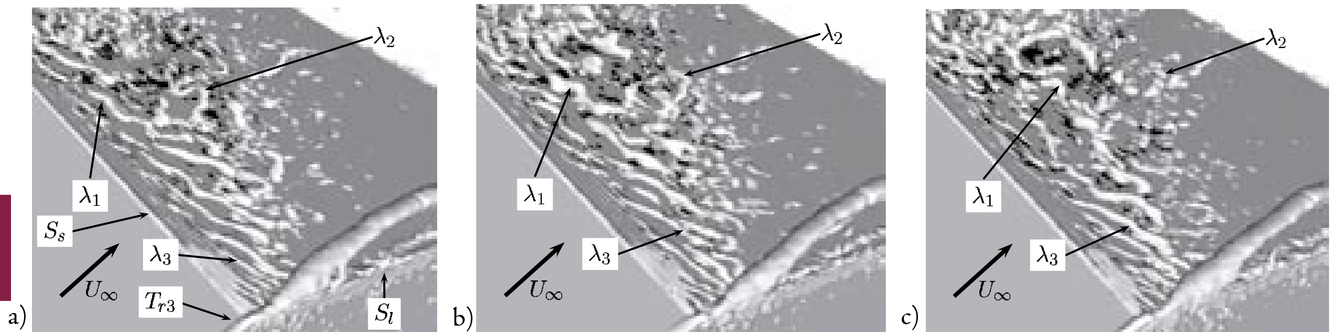

Figure 3. Three consecutive instantaneous pictures of the flow on the rear window. Flow is from left to right. The sharp edges between the roof and the rear window is denoted S_s and the slanted side edge is denoted by S_l.

car. Figure 2 shows vortices on the rear window of our car model. Two large cone-like vortices are formed above the sharp side edges of the rear window (note that only cores of these two vortices are shown in this figure). The left and the right vortices rotate clockwise and counterclockwise, respectively, and are similar to the vortices often seen on the wing tips of airplanes.

Besides the two pairs of vortices found in the experiments we discovered another, third, pair of these cone-like vortices that were very thin and close to the surface and could not be observed with the experimental equipment.

To understand the reasons for the unsteady flow on the rear window, let us consider the flow that was discovered in our simulations. The air flow separates at the sharp edge (S_s in Fig. 3a) between the roof surface and the rear window of the car. Elongated vortices that extend in the direction of this edge form as a result of this separation. The axes of these vortices are parallel with the edge close to the symmetry plane of the car. The vortices that are born close to the end of the edge (such as λ_3 in Fig. 3) are tilted so that they travel toward the center of the rear window. This behavior is caused by the cone-like shape of vortex T_{r3}). As it propagates downstream, it grows in diameter, pushing the λ vortices away from the slanted side edge of the rear window. The resulting orientation of the λ vortices closest to the T_{r3} is toward the center of the rear window. When the vortices formed along the middle part of the edge move downstream, they merge with each other to form slightly larger vortices such as λ_1 in Fig. 3a. The next step in their development is further merging and becoming larger, such as λ_1 in Fig. 3b, before their tip is lifted from the surface and forms hairpin-like vortices (see λ_1 in Fig. 3c). Their life as hairpin vortices with both legs attached to the slanted surface (such as λ_2 in Fig. 3a) is short. One of their legs separates from the surface or is simply broken, such as in λ_2 in Fig. 3b. Finally, around the half length of the rear window, the other leg of the vortex is destroyed (see λ_2 in Fig. 3c).

As we mentioned earlier, the mystery of this rear-window flow was in its unsteadiness. Several researchers had hypothesized that the unsteadiness of this flow is caused by oscillations of large cone-like vortices themselves. We found these vortices to be relatively steady (time independent), and this was confirmed just recently by an experimental study. What we discovered was that the interaction between λ vortices is the reason for the high levels of unsteadiness at the lower part of the rear window of the car model. As the λ vortices traveling in the streamwise direction (such as λ_1 and λ_2 in Fig. 3) approach the middle part of the rear window, they break up (as described above) and meet the λ vortices coming from the upstream corners (such as λ_3 in Fig. 3). These meetings result in a large number of collisions that together with the break-up of vortices described above make this region of the flow very unsteady. Thus we have discovered that the unsteady character of the flow in the lower part of the rear window is not a direct consequence of the cone-like vortices. It is rather the result of their indirect influence on the λ_3 vortices, making them change their paths (as previously mentioned) and interacting with vortices such as the λ_1 and λ_2 vortices.

Continuing work

This demonstrates only one of several discoveries we have made in our simulations. The breakthrough in this research was only possible by using a time-dependent numerical simulation and cost-efficient Linux cluster such as Monolith. This was the only parallel computer at that time that could offer the necessary computer performance over a long period of time. The author is today using Monolith to explore another complex flow, namely the flow around a finite cylinder such as a chimney. It is difficult to investigate this flow due to complex vortex interaction and unsteadiness. Our first LES simulation on Monolith has already discovered an extremely complex flow picture, shown on page 1.

The aim of this work is not only to understand the flow but also to make an extensive database that can be used by other researchers who are studying this flow. Normally such databases are produced with experimental tests in wind tunnels. One of the conclusions we drew in our work on the Golf-like car was that prediction of the flow from our simulation was in excellent agreement with the experimental data. Furthermore, much more data were obtained and we were able to explain this flow for the very first time. This has led to greater confidence in numerical simulations of flows around vehicles and other bluff bodies (such as cylinders).

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KALENDARIUM

HPC 2006: High Performance Computing Symposium: Grand Challenges in Computer Simulation – SCS Spring Simulation Multiconference.

2–6 April, Huntsville, AL.
http://www.caip.rutgers.edu/hpc2006/

IPDPS 2006: 20th IEEE International Parallel & Distributed Processing Symposium

25–29 April, 2006, Rhodes Island, Greece.
http://www.ipdps.org

GPC 2006: The First International Workshop on Grid and Pervasive Computing

3–5 May, 2006, Tunghai University, Taichung, Taiwan.
http://www.hpc.csie.thu.edu.tw/gpc2006/

NOTUR 2006: The 6th Annual Gathering on High Performance Computing in Norway

11–12 May, 2006, Bergen, Norway.
http://www.notur.no/notur2006/index.html

MSST2006: 14th NASA Goddard, 23rd IEEE Conference on Mass Storage Systems and Technologies

15–18 May, 2006, Maryland, USA.
http://storageconference.org/2006

CCGRID 2006: 6th IEEE International Symposium on Cluster Computing and the Grid

16–19 May, 2006, Singapore.
http://pdcc.ntu.edu.sg/ccgrid2006

SGIUG 2006; SGI Worldwide User Group 2006 Technical Conference and Tutorials

5–9 June, Las Vegas, USA.
http://www.sgiug.org

PARA'06; Workshop on state-of-the-art in Scientific and Parallel Computing

18–21 June, 2006, Umeå, Sweden.
http://www.hpc2n.umu.se/para06/

HPDC-15: The 15th IEEE International Symposium on High Performance Distributed Computing

19–23 June, 2006, Paris, France.
http://hpdc.lri.fr

CLADE 2006: Challenges of Large Applications in Distributed Environments

Held in conjunction with HPDC-15.
19–20 June, 2006, Paris, France.
http://www-unix.mcs.anl.gov/~bair/CLADE2006/

ISC 2006: International Supercomputer Conference

27–30 Juny, 2006, Dresden, Germany.
http://www.supercomp.de/

ICPADS 2006: 12th International Conference on Parallel and Distributed Systems

12–15 July, 2006, Minneapolis, Minnesota, USA.
http://www.icpads.umn.edu/

ICPP 2006: The 2006 International Conference on Parallel Processing

14–18 August, 2006, Columbus, Ohio, USA.
http://www.cse.ohio-state.edu/~icpp2006

Euro-Par 2006: European Conference on Parallel Computing

29 August–1 September, Dresden, Germany.
http://www.zhr.tu-dresden.de/Euro-Par2006/

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