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Updated program for the 2nd DEISA Symposium, May 4-5, 2006

The annual DEISA Symposium will take place in Palazzo Re Enzo, in Bologna, Italy, on May 4 - 5, 2006. In the scientific part of the program six "grand challenge" Extreme Computing projects currently in operation on the DEISA platform will be presented. The topics planned for the strategic part of the program are: eInfrastructures in Europe; and HPC trends and overview of new supercomputing architectures. The online registration for this Symposium is open at www.deisa.org/symposium until April 23, 2006.

The following computational scientists are confirmed speakers for this Symposium:

- Prof. P. Coveney, University College London (UK): *Large scale computation for materials and life sciences using DEISA*
- Prof. H. A. Dijkstra, Utrecht University (The Netherlands): *Use of ensemble climate simulations to detect variations in extreme event statistics*
- Prof. W. Hillebrandt, Max Planck Institute for Astrophysics (Germany): *Chasing the flames: The challenge of modeling thermonuclear supernova in 3D*
- Dr. K. Jansen, NIC/DESY Zeuthen (Germany): *The quest for solving QCD: Light quarks with twisted mass fermions*
- Prof. F. Pasian, Osservatorio Astronomico di Trieste (Italy): *End-to-end simulations of the Planck-LFI space mission*



The 2nd DEISA Symposium will be held in Palazzo Re Enzo, Bologna Italy. The event will begin on Thursday May 4, at 13.30 and end on Friday May 5, at 13.00.

- Prof. J. Jiménez Sendín, Universidad Politécnica de Madrid (Spain): *Computing wall turbulence at experimental Reynolds numbers*

Confirmed speakers for the strategic and technical part of the Symposium are:

- K. Baxevanidis, European Commission
- N. Geddes, EGEE project
- W. Brooks, National Aeronautics and Space Administration, US
- M. Levine, Pittsburgh Supercomputing Centre, US
- K. Wolkersdorfer, Forschungszentrum Jülich

Online registration open at www.deisa.org/symposium

Second DECI call in preparation

The DEISA Extreme Computing Initiative (DECI) consists of the identification, the enabling, the deployment and operation of a number of "flagship" applications in selected areas of science and technology. These leading, ground breaking applications must deal with complex, demanding, innovative simulations that would not be possible without the DEISA infrastructure, and which would

benefit - if accepted - from the exceptional resources from the Consortium.

From the first and very successful call for proposals in spring 2005 29 projects have been retained. These projects are currently carried out in DEISA. A second call is already in preparation and is expected to be launched soon.

Channel 2000: Computing wall turbulence at experimental Reynolds numbers

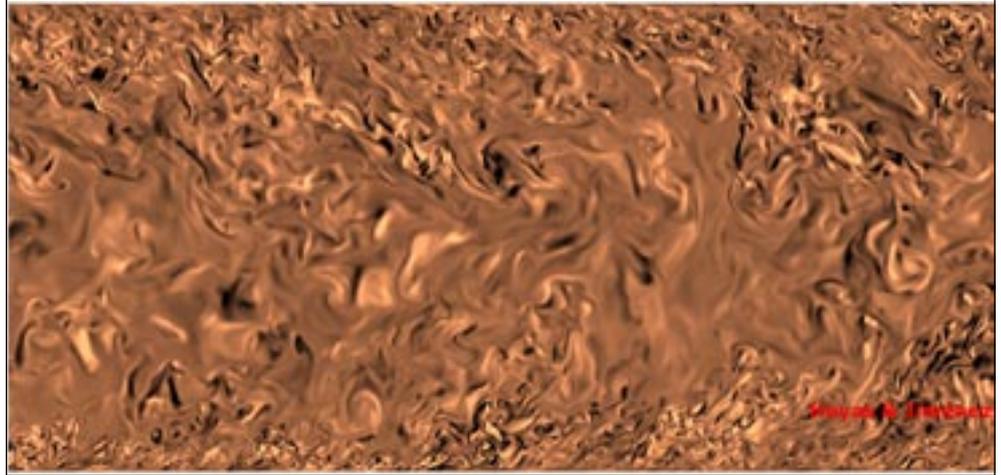
Sergio Hoyas¹ and Javier Jiménez², School of Aeronautics, Universidad Politécnica. 28040 Madrid, Spain

Using direct numerical simulation (DNS) of turbulent channels at a higher Reynolds number ($Re_\tau=2000$) and in larger computational domains than those available up to now, we study the dynamics of the turbulent logarithmic layer, and the interaction between the large scales of wall turbulence away from the wall, and the small scales near it.

Wall-bounded turbulence has been studied for a long time, but it is only recently, in fact only with this experiment, that we are beginning to be able to represent the logarithmic layer linking the near-wall and outer flow regions. This is the location of the self-similar energy and momentum cascades which are the essence of turbulent flows.

The problem is not just of scientific interest. Wall-bounded turbulence is the interface between the ambient fluid, water, or air, and moving vehicles, and between flows and pipes and channels. The large scales, for example, play an important role in the dispersion of chemical agents in the atmosphere, and more than half of the friction drag in vehicles resides in the near-wall and intermediate layers. The hopes of controlling and alleviating all these phenomena pass through the understanding of their dynamics

The main objective of the simulation was to run enough time to get statistically converged properties of the flow. From previous experience this requires about 10 washouts (250 h/ U in the present case, where h is the channel half-thickness and U the centreline velocity). The computation is carried out in a doubly periodic domain in the two wall-parallel



Spanwise component of vorticity. Visit <http://torroja.dmt.upm.es/~sergio> for this and other pictures.

directions, which is chosen large enough to minimize artefacts due to the spurious periodicity. From our experience with lower Reynolds numbers we have chosen a domain size of 25×10 channel half-thicknesses. This procedure, although both memory and CPU time demanding, allows us to compute any property of the flow with greater accuracy than that of experimental measurements in laboratory flows. In particular it allows us to access variables, such as time- and spaced-resolved velocity gradients and vorticity, which cannot be measured in the laboratory.

The code is based on previous versions developed by our group during the past fifteen years, and broadly follows the standard spectral code developed at the end of the 1980s by groups at Göttingen and at NASA Ames, although the wall-normal discretization uses compact finite differences. It is written in C

and Fortran, and is parallelized using MPI, with an excellent speed-up. This simulation uses a grid of $2 \cdot 10^{10}$ points, demanding 400GB or RAM memory.

This was a very costly initiative. It ran for about 5,000,000 CPU hours on 2048 processors during the pre-production phase of the MareNostrum supercomputer at the Barcelona Supercomputing Center. We obtain also 800,000 CPU hours, needed in order to run two washouts more and to complete our study, assigned through a DEISA project.

The simulation has generated approximately 25 TB of raw data, that we are now analyzing, most of them open to the community.

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1st DEISA training: highly scalable parallel applications

To enable fast development of user skills and know-how needed for the efficient utilisation of its infrastructure, DEISA will organize six training sessions between mid 2006 and mid 2008. These events will take place in Finland, France, Germany, Italy and Spain.

Each session will be composed of a common one-day-long introductory part and a second part dedicated to a specific topic. The introductory part will give a global description and introduction to the DEISA infrastructure and

will describe the general middleware services for data management, the usage of the Common Production Environment and the detailed utilisation of UNICORE. The second part will be composed by talks and tutorials on different selected subjects, like highly scalable parallel applications, data intensive computing, distributed computing and coupled applications, etc.

The number of participants will be limited to 30 persons per session. Scientists from all European countries or members of industrial

organizations involved in high performance computing are invited to attend. For each session, DEISA will take charge of the travel and living expenses of 15 participants from countries other than the host country where the training session takes place.

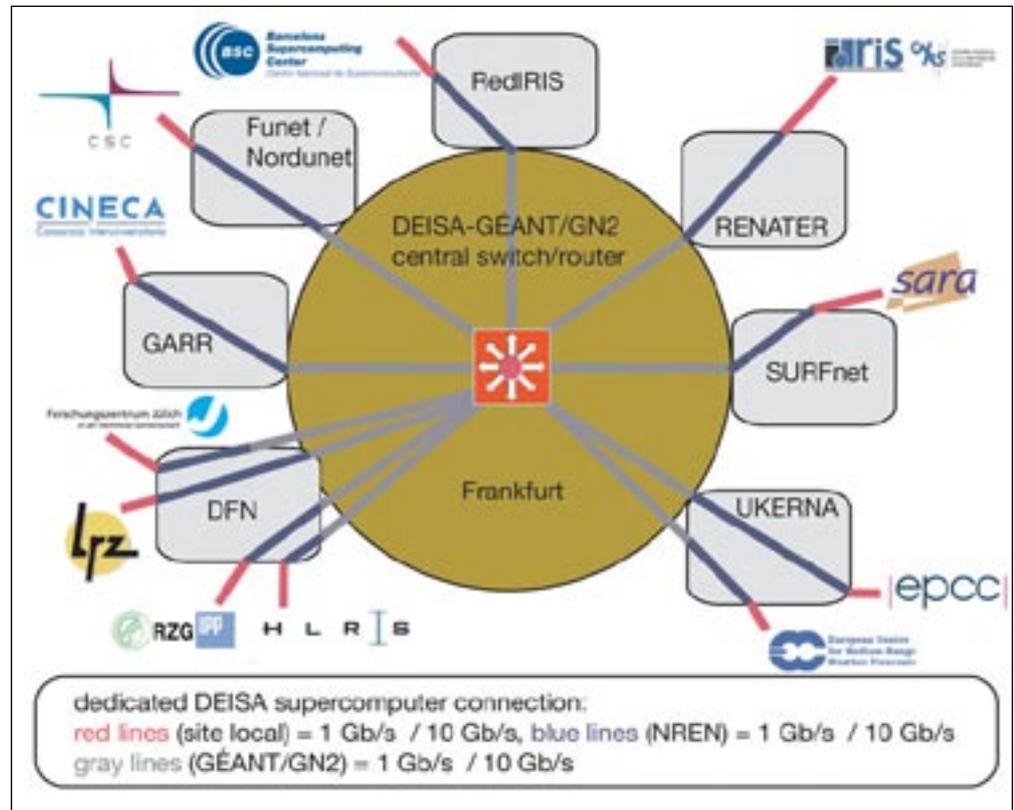
The first event will take place in Paris on July 3-5, and the dedicated part of this session will be devoted to the highly scalable parallel applications. The detailed agenda and the registration form will be available at www.deisa.org.

Deployment of the new 10 Gb/s DEISA network infrastructure started

DEISA relies on high bandwidth interconnects across computing platforms to deploy and operate an innovative infrastructure for High Performance Computing in Europe. The DEISA SA1 activity produced detailed specifications for the dedicated bandwidth network infrastructure needed for the operation of the DEISA supercomputing Grid in phase 1 and phase 2 of the DEISA project. The phase 1 network connected all DEISA sites via a 1 Gb/s dedicated network connection. Within phase 2 it had been planned to connect a number of sites (FZJ, IDRIS, LRZ, RZG and SARA) with a 10 Gb/s uplink. This phase 2 has been started within the last weeks. Contracts with the associated NRENs are just being signed. A first connection between these sites will be initiated within the next two months.

In the future all DEISA sites will be connected with 10 Gb/s wavelength links to a central switch located in Frankfurt. This new enhanced infrastructure will be one of the fastest and state-of-the-art production network infrastructures in Europe. It is planned to have this network up and running with most DEISA sites by the end of this year.

The execution plan of the service activity, concerning the deployment of the extended network infrastructure, is dependent on the availability of the network infrastructure within the involved NRENs. GÉANT2 has been operational since the beginning of 2006. The NRENs in Germany (DFN), France (RENATER) and The Netherlands (SURFnet) are prepared to provide point-2-point links between national sites and the GÉANT2 infrastructure. Spain (RedIRIS), Italy (GARR), UK (UKERNA) and Finland (FUNet, Nordunet) are on the way to new infrastructures. Most systems are expected to be



Logical view of the new DEISA network interconnection.

connected within the first few months from now. All DEISA sites will update/upgrade their supercomputer systems over time, so the network connectivity has to be renewed, too. A steady update of the DEISA network infrastructure will be necessary.

The DEISA sites which will not be connected with 10 Gb/s in the beginning of DEISA phase 2, will get an access to this new network infrastructure as soon as the appropriate NREN is able to provide a suitable connection to the new GÉANT2 infrastructure. Sites running with 1 Gb/s links will be connected via the phase 1

network to the new central switch in Frankfurt until they can be integrated into the new infrastructure with 10 Gb/s. The figure above describes the logical view of the future DEISA network infrastructure.

More information on the DEISA supercomputing grid infrastructure is available at www.deisa.org/grid/

DEISA to be present at ICCSA 2006, in Glasgow, Scotland

DEISA will have a display at the 2006 International Conference on Computational Science and its Applications (ICCSA 2006) that will held in Glasgow, Scotland from 8-11 May 2006. The focus of the Conference is on the realms of computational science in parallel and distributed environments, encompassing the facilitating theoretical foundations and the applications of such large-scale computations. The Conference of-

fers the opportunity to discuss problems and solutions in the area, to identify new issues, and to shape future directions for research, as well as to help industrial users apply techniques of large scale parallel and distributed computations.

Key note speakers include Professor Tetsuya Sato, Director General of The Earth Simulator Centre (Japan), Dr. Steve Ashby, Deputy Associate Director for Computing Applications and

Research at the Lawrence Livermore Laboratory (USA) and Professor Jack Dongarra from the Computer Science Department University of Tennessee (USA).

More detailed information is available on the event website www.iccsa.org