DEISA Newsletter

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS

Vol. 2, 2007

3rd DEISA Symposium: Towards Petascale Computing in Europe

The DEISA Symposium will take place May 21-22, 2007 at the Bavarian Academy of Sciences and Humanities, Munich, Germany. This year, the DEISA Symposium will focus on the initiatives and strategies being deployed to enhance the outreach of high performance computing in Europe.

The DEISA Symposium is traditionally held once a year during the spring. In previous years, the Symposium focused on the scientific and technological issues related to the operation of the DEISA infrastructure.

The meeting will start on Monday, May 21 at 13:30 h and will end on Tuesday, May 22 at 12:30 h. The Participation is free of charge but subject to on-line registration at http://www.deisa.org/symposium. The registration will close on May 7.

Monday 21, afternoon:

- Opening of the Symposium, T. Goppel, Bavarian State Minister of Sciences, Research and the Arts
- HPC strategies in Europe, M. Campolargo, EU
- HPC strategies in the US, C. Catlett, Argonne, US
- The Japanese Petascale project, K. Miura, NAREGI – Tokyo, Japan
- Existing HPC focused infrastructures: TeraGrid, J. Boissereau, Texas, USA
- Existing HPC focused infrastructures: The role of DEISA, V. Alessandrini, CNRS, France
- New HPC initiatives in Europe (eHPC), A. Bachem, Jülich, Germany

Tuesday 22, morning:

- Technology trends for petascale computing, A. Bode, Munich, Germany
- Scientific cases for petascale computing in Europe:

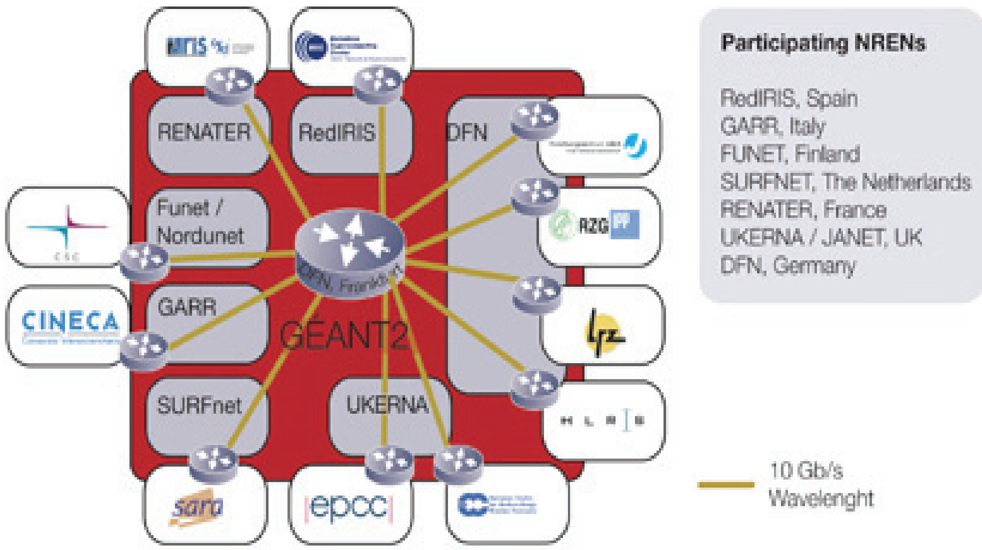
- Climate modelling, J. Marotzke, Hamburg, Germany
- Petascale requirements of ITER, K. Lackner, Garching, Germany
- Europhysiome initiative, N. Smith, Oxford, UK
- Astrophysics, G. Yepes, Madrid, Spain
- Nanosciences, S. Bluegel , Jülich, Germany.

Titles of talks are provisional.

Registration open at www.deisa.org/symposium.

DEISA 10 Gb/s network infrastructure in production

DEISA has passed its 10 Gb/s network "proof of concept phase" and is now in production since February 2007. In autumn last year DEISA started to upgrade the 1 Gb/s network infrastructure that has delivered a stable service for three years. Since DEISA relies on high bandwidth interconnects across computing platforms to deploy and operate its innovative infrastructure for High Performance Computing in Europe, a future upgrade was planned just in the beginning of the project. The DEISA network team designed the new infrastructure in close collaboration with their associated NRENs and GÉANT2 and produced detailed specifications for the future network layout in mid of 2005 already. A new wavelength based infrastructure across Europe was designed. Finally at the end of 2006 most of the NRENs and GÈANT2 had upgraded their networks and were able to offer such Lambda services. So the prerequisites for the implementation of the private DEISA European wide high speed WAN had been available. In January 2007 the first sites could be connected via the dedicated wavelengths and first interoperability tests could be started. After extended



Final DEISA 10 Gb/s production network (mid of 2007)

testing in the "proof of concept phase" the network could go into production without noticeable interruptions.

The current infrastructure connects the seven sites BSC (Spain), IDRIS (France), FZJ, HLRS, LRZ, RZG (all Germany) and SARA (The Netherlands) via 10 Gb/s wavelengths to a central switch at Frankfurt managed by DEISA. The remaining DEISA sites CINECA (Italy), CSC (Finland) and ECMWF (UK) are connected via the old 1 Gb/s network infrastructure to the new one. It hadn't been planned to have direct network connectivity to DEISA for the eleventh <*Continues on page 2*>

DEISA Training

30 May - 1 June 2007
CSC - Finnish IT center for science,
Espoo, Finland

Program and registration soon available at www.deisa.org/training

<Continued from page 1>
site, EPCC (UK), until now, but this will change in future allowing EPCC to participate in the DEISA infrastructure. It is expected to have the remaining sites connected to the 10 Gb/s infrastructure within the next 3 month, having a full DEISA site connectivity for all sites available. Currently spanning four European countries the final network will have connectivity to leading supercomputer sites in seven countries of Europe.

The design of the DEISA network infrastructure was chosen to be a star topology, having one central point where all sites are connected to. The advantage of this design is the easy integration of additional sites by integrating one additional link for each additional site only. The network layout will allow to provide access to European projects as well as non-European projects (e.g. TeraGrid) without any major restructuring. So test scenarios can be established quite easily assumed trans-national connectivity is available.

The new enhanced infrastructure will be one of the fastest state-of-the art production network infrastructures in Europe. The future challenge will be to integrate all the shared European petascale systems becoming reality in the next few years with the already existing leading national supercomputing platforms, most of them integrated already today. Future developments in network technology (e.g. higher throughput, new enhanced technologies) will be integrated following the demands of the DEISA project and technology evolution.

The main mission of DEISA providing a basic vector of integration of HPC resources at a continental scope will remain the driving force for the DEISA network infrastructure.

QCD Simulations with Light Quark Flavors

Dr. Karl Jansen, John von Neumann Institute for Computing, Zeuthen, Germany

The project "QCD with twisted-mass fermions" (TMQCD) was conducted within the DEISA Extreme Computing Initiative (DECI). The framework of the project is non-perturbative computations for our theory of the strong interaction of the fundamental particles, the quarks and gluons. The theory describing this interaction is Quantum Chromodynamics (QCD). By discretizing space and time on a 4-dimensional space-time lattice it becomes possible to simulate QCD with numerical simulations which are, however, extremely demanding.

The aim of the project has been to explore the regime of small values of the pseudoscalar mass, $m_{PS} \approx 250$ MeV, which corresponds to a quark mass four times smaller than could be reached before. When started, this constituted a very challenging project since in the past it has been unthinkable that lattice QCD calculations could reach such small pseudo scalar masses and obtain precise results.

However, within this DECI project this ambitious goal could be fully accomplished. Although in total it has not only been the DEISA resources that led to these results, it is certainly so that the DEISA resources helped significantly to successfully complete the project. As an example for the outcome of the project, in figure 1 the dependence of the so-called pseudo scalar decay constant f_{PS} as a function of the quark mass is shown. In the plot, the numerical data are fitted against the prediction of chiral perturbation theory which is an analytical, effective low energy description of QCD. As can be seen, the fit is excellent and the very precise numerical simulation data allow determining a number of the low energy constants of chiral perturbation theory with a high, world record precision. The low energy constants in turn allow computing other physical quantities such as the scalar and the tensor scattering lengths of the pion, which can serve as a severe test of QCD as the theory of the strong interactions. The results of this DECI project establish the most precise constraints on these scattering lengths so far.

This DECI project has been one of the pilot projects within DEISA. It is thus not too surprising that the project encountered a number of difficulties in the beginning. However, many of these difficulties could be solved with the excellent help of the DEISA staff people at the supercomputer centers involved.

A very positive aspect of the project was the experience with the DEISA global file system GPFS-MC. In combination with the usage of UNICORE, it was very helpful and easy to define, submit and control the jobs and, in particular, the workflow, since the evaluation of physical observables on the raw data, the configurations, could be done on different machines of the DEISA infrastructure in a flexible and heterogeneous manner.

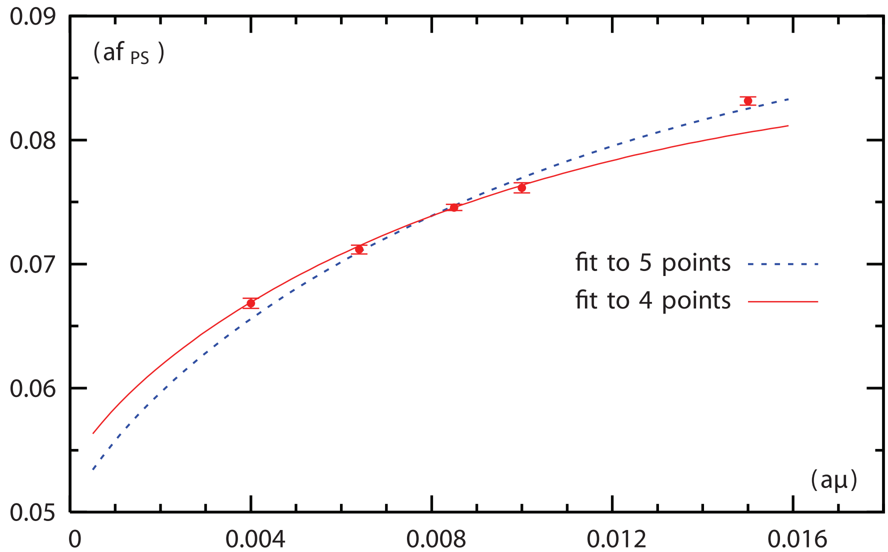


Figure 1: We show $a f_{PS}$ as a function of the quark mass $a\,\mu$ together with fits to chiral perturbation theory formulae. We present two fits, one taking all data and one leaving out the point at the largest value $a\,\mu = 0.015$.