

DEISA Newsletter

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS



Vol. 1, 2007

DEISA Training: Positive Contribution to Research



The next DEISA training will take place at the Barcelona Supercomputing Center on March 7 - 9.

In mid-October 2006 the 2nd DEISA training session was held at Forschungszentrum Jülich, Germany. 30 scientists and experts in supercomputing gathered to discuss topics of HPC and Grid within the DEISA infrastructure. The event started with a general introduction to the DEISA infrastructure, such as the Common Production Environment (CPE) and UNICORE.

The special topic of this training session was "Performance and Portability", addressing issues for application developers on improving application performance while keeping optimal portability.

The discussions covered topics on code optimization for large shared-memory clusters, over communication and I/O design to performance analysis with different tools. Supporting the theoretical input from the HPC experts, the participants had the opportunity to experience the DEISA infrastructure first-hand in the "Access to DEISA" hands-on session, introduced with this event. Presentations of use cases for the DEISA infrastructure concluded the event, giving insight to recent success stories on improving the scalability of a climate modeling code as well as to visions for collaborative online-visualization utilizing the underlying DEISA infrastructure.

The collected feedback forms prove this training event to be an overall success, creating a positive contribution for the participants' research activities as well as in understanding how the DEISA infrastructure can aid them in achieving their goals. The next opportunity for scientists to participate in a DEISA training session will be on March 7-9, 2007 at the Barcelona Supercomputing Center in Spain. This session's special topic will be "Performance measurements and codes optimization".

Registration to the next training is open at www.deisa.org/training.

2nd Wave of Extreme Computing

The DEISA Extreme Computing Initiative (DECI) has been launched in 2005 to enhance DEISA's impact on science and technology. Every spring a European Call for Extreme Computing Proposals is published. The 2nd Call for Proposals from spring 2006 has resulted in over 40 proposals by scientific teams with members from twelve European countries. The scientific areas covered include Materials Science and Quantum Chemistry, Life Sciences, Astrophysics and Cosmology, Earth Sciences and Climate Research, Computational Fluid Dynamics, Plasma and Laser Physics. Requests for supercomputing resources exceeded available resources by a factor of three. A total of 23 projects were retained for operation in 2007, in line with the recommendations of the national evaluation committees. The enabling and preparational work for the new projects, started in autumn last year, is an ongoing effort. The first of these challenging projects, starting in January, include:

- DNS-BUMP: A French-led team of scientists from France, Germany, Italy, Sweden and UK is working on a better understanding of the mechanism of wall turbulence. They have started to perform numerical simulations of channel flows over curved surfaces at a high Reynolds number at the inlet.

- PROCORE: A Swiss-Hungarian team has started with simulations on the reactivity of pyrite (FeS_2) which strongly depends on its surface defects. The aim is to establish a direct link between theoretically predicted surface sites and experimental data retrieved from X-ray photoemission spectra (XPS).
- BBH: A German team has started black hole and gravitational wave simulations to push forward the connection of the fields of numerical relativity and gravitational wave data analysis. To produce complete waveforms, numerical simulations of the full nonlinear Einstein equations are required, which poses a challenging problem in physics, mathematics and high performance computing.
- SEISSOL: The interior structure of the earth and its geophysical properties have been mainly studied with seismological methods. Computer simulations of the propagation of seismic waves represent an invaluable tool for the understanding of the wave phenomena, their generation and their consequences. Aim of the project is the simulation of a complete, highly accurate wave field in realistic 3D media with complex geometry and geological rheologies, and thus provide simulations of realistic earthquake scenarios.

DEISA Symposium

Towards Petascale Computing
in Europe

21 - 22 May 2007
Munich, Germany

www.deisa.org/symposium

- COMSIMP: Knowledge of past climate variability is crucial for understanding current and future climate trends. For the first time sufficient computational resources are available to carry out millennial-scale simulations with a comprehensive Earth System Model. Climate history requires that these experiments are started in the year 800 and run until the year 2000. To discriminate between internal variability, natural external forcing (orbital, solar, volcanic), and the anthropogenic-induced greenhouse-gas forcing, it is necessary to carry out an ensemble of several 1200-year long integrations with a relatively high-resolution Earth System model using high-end HPC facilities. Innovative infrastructure and sophisticated environments, such as offered by DEISA, is necessary to perform and manage such a challenging project.

For more details about the described projects, www.deisa.org/applications/projects2006-2007.

Simulations of Turbulent, Active and Rotating Stars

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The STARS project aims at modelling in a self-consistent and three-dimensional way the complex, time dependent and nonlinear dynamics present in the Sun and stars. In particular we wish to understand stellar magnetic activity, that depending on the spectral type of the star considered can be cyclic (solar type stars) irregular (very low mass stars, with spectral type later than M3), or even for stars with stellar mass greater than 2 solar mass, without any activity or simply possessing a modulated signal (probably due to the presence of a fossil field in their stably stratified, radiative envelope). The mechanism thought to be at the origin of the magnetism seen in solar type stars or in low mass stars is likely to be linked to dynamo action in the upper convective layers of such stars. The simultaneous existence of convective turbulent motions (that could even possess helicity), of rotation and its associated differential rotation and shear layers in stars, favour the emergence of a small and/or large scale magnetic field through induction. For more massive stars, possessing a convective core, understanding the interaction between the dynamo generated magnetic field and the probable fossil magnetic field of their radiative envelope constitute a major challenge in stellar fluid dynamics.

To study in great details the interaction between convection, rotation and magnetic field in stars is the main scientific goal of this project.

Main Results

This DEISA-DECI project has been extremely fruitful in terms of understanding the complex interplay between turbulent convection and magnetism and to appreciate how difficult it is to compute a highly nonlinear and turbulent 3-D MHD solar dynamo model at low magnetic Prandtl number. It is the first time that dynamo action in a turbulent convective sphere at low magnetic Prandtl number is achieved in the solar context.

We can already say that the level at which dynamo action is successful against Ohmic decay is higher than in the corresponding case with high Pm number published in Brun et al. 2004. We have computed several models in order to reach the dynamo threshold while keeping a solar-like differential rotation profile. The first model had a magnetic Reynolds number around 300 (resolution $N_r=256$, $N_\theta=512$ and $N_\phi=1024$), the threshold determined by our previous

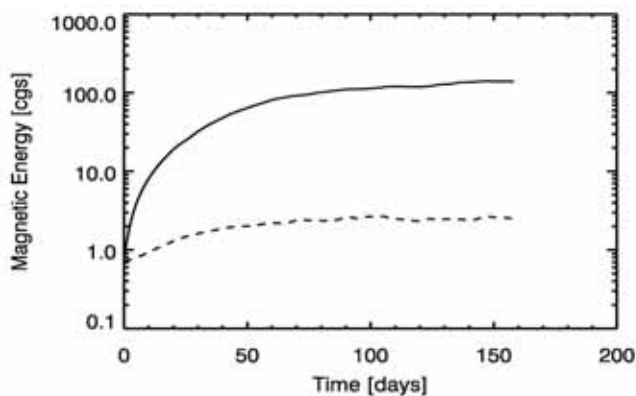


Figure 1: Temporal evolution over the 160 days of simulated time of the total and mean (dashed line) magnetic energy in a turbulent DEISA-DECI simulation of the solar convection at a Prandtl number Pm of 0.8.

study (see Brun et al. 2004). This model did not succeed and the seed magnetic finally decayed away. We then progressively increased the level of turbulence while keeping $Pm=0.8$ and we had to reach about $Rm=400$ (and a resolution of $256 \times 784 \times 1568$) to get a successful dynamo. This seems to indicate an increase of about 30% of the dynamo threshold with respect to the high Pm cases, and confirms that turbulence is actually making it harder to get a successful dynamo rather than easier (see for example Ponty et al. 2005).

We display on figure 1 the temporal evolution of the total (solid line) and mean (dashed line) magnetic energies of our latest successful DEISA DECI run. We can notice the linear phase (exponential growth) of the magnetic energy and then its nonlinear saturation via

the feed back of the Lorentz forces on the flow in particular in region of high vorticity through Maxwell stresses. The mean (axisymmetric) magnetic energy is found to be small ($\sim 1\%$) confirming that turbulent magnetized convection generates mostly non axisymmetric and highly intermittent fields, characteristic of a small scale dynamo process. To illustrate the richness of the simulations, we show on figure 2 a snapshot of the convective radial velocity, of the log10 of the enstrophy (square of the vorticity) and the associated dynamo toroidal magnetic field

in the bulk of the modelled convection zone. We see how turbulent the convective patterns are and how small scale and intricate the magnetic field can be. This indicates that the magnetic fields generated by dynamo processes in stellar plasma are likely to be disorganized (independently of the magnetic Prandtl number considered or possible inverse cascade processes), and that in order to get a large-scale organized field (mostly toroidal in nature), one needs to include an omega effect not only in the convection zone (as it is already the case in this simulation) but also in a sheared stable layer like the tachocline. A preliminary low resolution study seems to indicate that it is indeed the case, i.e a tachocline of shear is efficient at making stronger axisymmetric fields (Browning, Miesch, Brun et al. 2006).

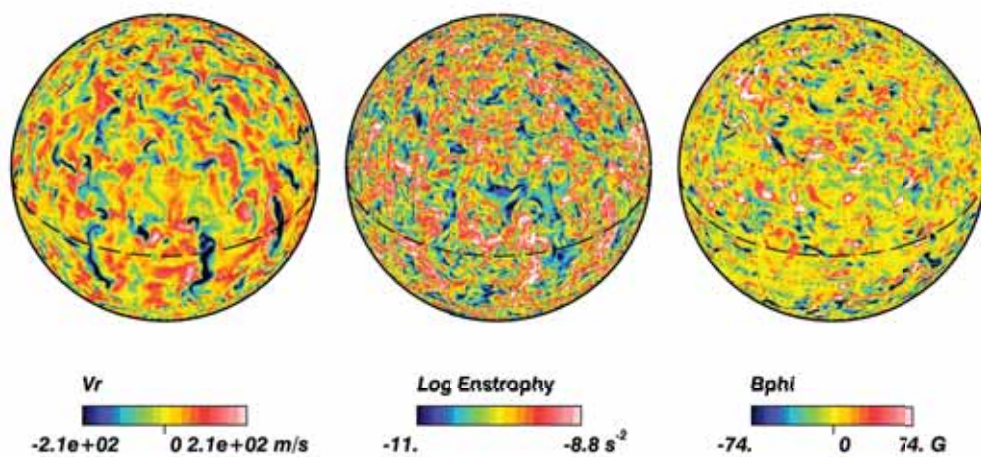


Figure 2: Snapshot of the radial velocity, log of enstrophy and toroidal magnetic field in the bulk of the highly turbulent convection zone of the DEISA DECI run. Highly intermittent convection and magnetic fields are observed in this first low Pm simulation of the solar convective envelope. We note the high degree of vorticity present in the downflows.