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DEISA: Extreme Computing in an Advanced Supercomputing Environment

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DEISA (Distributed European Infrastructure for Supercomputing Applications) is a consortium of leading national supercomputing centres in Europe. Starting in 2004 it deploys and operates a persistent, production quality, distributed infrastructure for supercomputing applications. It connects eleven European supercomputing centres in seven different countries via a dedicated high bandwidth network, enabling seamless and transparent access to a Europe-wide shared global file system. The coordinated operation of this environment is tailored to enable new, ground breaking applications in computational sciences. Scientists from all over Europe have successfully used this platform for extreme computing endeavours with concrete scientific impact, benefiting from the DEISA Extreme Computing Initiative DECI.

This Mini-Symposium highlights the scientific impacts achieved so far with the DEISA infrastructure, while also giving a forum for the extensive enabling work done for applications running in the DECI and encouraging discussion of current limitations of distributed computing as well as future developments.

Mini-Symposium Contributions

For a better overview of the key areas involved, the Mini-Symposium was thematically grouped into three sessions related to the topics infrastructure, applications, and scientific projects.

In the first session, the key note presentation by Victor Alessandrini from IDRIS-CNRS, the coordinator of DEISA, on *Enabling Cooperative Extreme Computing in Europe*, outlines the objectives and design principles of DEISA: To act as a vector of integration of High Performance Computing (HPC) resources at continental scale in Europe, and to enable seamless access to, and high performance cooperative operation of leading supercomputing platforms in Europe. Through the DEISA services, deployed on top of a dedicated high speed network infrastructure connecting computing platforms, and by using selected middleware, capability computing across remote computing platforms and data repositories is enabled. By reviewing the existing services for the DEISA Infrastructure which allow the execution of challenging computational science projects within the

DEISA Extreme Computing Initiative, it is demonstrated how DEISA has been paving the way to the deployment of a coherent HPC environment in Europe. Persistency of the services is regarded mandatory to support and cooperate with new initiatives like PRACE in the area of HPC, to advance towards the efficient operation of a future European HPC ecosystem.

In his presentation about *Effective Methods for Accessing Resources in a Distributed HPC Production System*, Andrea Vanni from CINECA presents the different options for different user needs how to best access the distributed DEISA infrastructure.

Details about the design and specific features of the global file system GPFS, being used at continental scale both by DEISA and by TeraGrid, are given in the talk by Klaus Gottschalk from IBM about *GPFS: a Cluster Filesystem*.

In his contribution *Submission Scripts for Scientific Simulations on DEISA*, Gavin Pringle from EPCC presents how DEISA users can also manage their batch jobs and data via the DEISA Services for the Heterogeneous management Layer, or DESHL, which is both a command line tool and an application programming interface to support workflow simulations, automatic code resubmission, and DEISA usage as a multi-site Task Farm.

In the application related session, Alice Koniges from Lawrence Livermore National Laboratory reports about *Development Strategies for Modern Predictive Simulation Codes*. The work describes the process of designing modern simulation codes, based on a set of development tools, libraries and frameworks suitable to reduce the time to solution, assuring, at the same time, portability and modularity.

Hermann Lederer from RZG et al. presents in the talk *Application Enabling in DEISA: Hyperscaling of Plasma Turbulence Codes* an example of application enabling for plasma turbulence simulation codes with high relevance for the European fusion community. It is shown how, in a joint effort of application specialists from DEISA and theoretical plasma physicists two important European simulation codes have been adapted for extreme scalability and for portable usage within the heterogeneous DEISA infrastructure.

In the third session related to scientific projects, Frank Jenko et al from IPP report in *First Principles Simulations of Plasma Turbulence within DEISA* about the DECI project GYROKINETICS. Magnetic confinement fusion, aiming at providing an energy resource free of CO_2 emissions, depends on a large degree on the value of the so-called energy confinement time. Two of the most advanced tools describing the underlying physical processes, codes ORB5 and GENE, have been used in DEISA to address some of the outstanding issues in fusion research.

Alessandra S. Lanotte et al, from CNR in Italy, in her talk *Heavy Particle Transport in Turbulent Flows* shows the results of the DECI Project HEAVY: State of the art Direct Numerical Simulation (DNS) of heavy particles in an homogeneous and isotropic stationary forced turbulence flow at Reynolds number $Re_\lambda \simeq 400$ The simulation was the most accurately resolved numerical simulation of Lagrangian turbulence done worldwide.

Marc Baaden from CNRS presents *Membranes Under Tension: Atomistic Modelling of the Membrane-Embedded Synaptic Fusion Complex*, studied in DECI project SNARE. Simulations allow to better understand the guiding principles of membrane fusion, a target for studying several pathologies such as botulism and tetanus.

The mini-symposium and the selected presentations document the transition from an initial test environment to a now mature production-oriented infrastructure, and thus the role and global importance of DEISA for a future European HPC ecosystem.