



ESSENCE: A large model ensemble simulation

Scientists have long agreed that climate change could have a profound impact on the planet, from melting ice sheets and withering rainforests, to flash floods, droughts, loss of arable land, famines and mass migrations. Policymakers are still debating instead of taking mitigating action to limit greenhouse gases generated from human activities, the likely cause of recent climate change.

Climate experts however, began ranking the most fragile and vulnerable regions on the planet, evaluating the danger of sudden and catastrophic collapse in the 21st century. Although scientists cannot be sure precisely when each region will reach the point of no return, their assessment warns it may already be too late to save Arctic sea ice and the Greenland ice sheet, which they regard as most immediately in peril. By some estimates, there will not be any sea ice in the summer months by the middle of this century and some models predict this could happen as early as 2030 or even earlier.

To determine the causal chain between the increase in radiative forcing and observed climate change, climate simulation models are essential. In the past just one or a few transient coupled climate simulations were performed for a given emission scenario due to the high computational demand of a simulation.

To distinguish trends caused by natural climate variability from those induced by increased radiative forcing, a large ensemble of climate simulations is necessary. By averaging over all ensemble members the signal-to-noise ratio is enhanced. The natural climate variability cancels between the members, leaving only the forced signal.

The Ensemble SimulationS of Extreme weather events under Nonlinear Climate change (ESSENCE) project was set up, under the DEISA Extreme Computing Initiative (DECI), to study climate trends. "The main aim of the ESSENCE project was to compute an adequate estimate of the statistics of natural climate variability and hence be able to obtain a good signal-to-noise ratio for the forced signal due to the increase of greenhouse gases", says Dr. **Andreas Sterl**.

In the ESSENCE project, a 17-member ensemble simulation of climate was carried out using the ECHAM5/MPI-OM coupled climate model of the Max-Planck-Institute for Meteorology in Hamburg. All computer simulation runs, were driven by the A1b scenario of 21st century greenhouse gas concentrations, from the IPCC Special Report on Emission Scenarios (SRES). The A1b scenario assumes a growth of CO₂ that leads to a concentration of about 650 to 700 ppm by year 2100. Besides a basic ensemble of 17 runs three experimental ensembles were also performed. The baseline experimental period is 1950-2100. For the historical part of this period (1950-2000) the concentrations of greenhouse gases (GHG) and tropospheric sulfate aerosols are specified from observations, while for the future part (2001-2100) they follow the SRES-A1b scenario. Stratospheric aerosols from volcanic eruptions are not taken into account, and the solar constant is fixed.

The runs are initialized from a long run in which historical GHG concentrations have been used until 1950. By disturbing the initial state of the atmosphere different ensemble members are generated. Gaussian noise with amplitude of 0.1 K is added to the initial temperature field. The initial ocean state is not perturbed.

Model Used

All simulations were conducted with the ECHAM5/ MPI-OM coupled climate model. ECHAM5 was run at a horizontal resolution of T63 and 31 vertical hybrid levels with the top level at 10hPa. The ocean model MPI-OM is a primitive equation z-coordinate model. It employs a bipolar orthogonal spherical coordi-

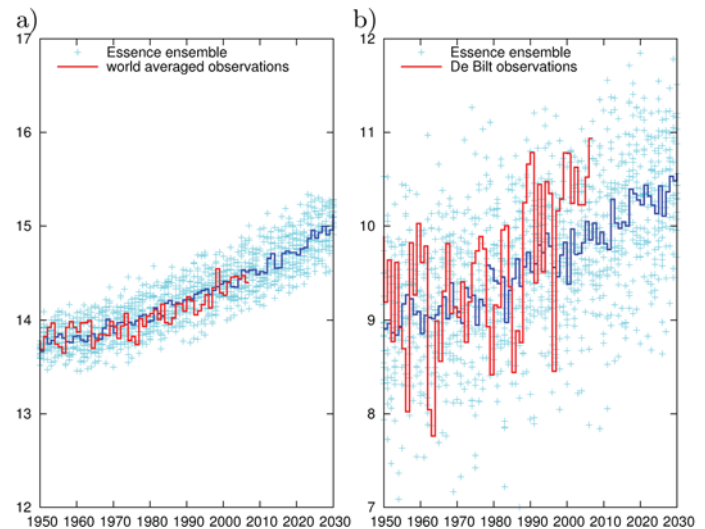


Fig. 1. Annual-mean surface temperature for the 17 ensemble members (light blue crosses), their mean (blue line) and observations (red line) for (a) the global average and (b) station De Bilt (the Netherlands).

nate system in which the north and south poles are placed over Greenland and West Antarctica respectively, to avoid the singularities at the poles. The resolution is at its highest, O(20-40km), in the deep water formation regions of the Labrador Sea, Greenland Sea, and Weddell Sea. Along the equator the meridional resolution is about 0.5°. There are 40 vertical layers with a thickness ranging from 10m near the surface to 600m near the bottom of the sea.

"The relatively large size of the ensemble enables us to clearly distinguish the forced signal from natural climate variability. We compared observed and modelled near-surface temperature trends and determined the statistical robustness of projected future trends of some important surface variables. We showed that in large parts of the world observed and modelled warming trends are statistically indistinguishable. We are therefore confident that the model captures the most important driving forces of the climate well, especially the radiative forcing due to increasing greenhouse gas concentrations. Over large parts of Eurasia and Africa the warming signal will be distinguishable from the noise within the next 10 years", says Dr. Sterl.

A great advantage of a large ensemble is the large noise reduction that can be achieved by averaging over all ensemble members. From the above simulations they were able to determine the year in which the forced signal (i.e., the trend) in the atmospheric (2 meter) temperature emerges from the noise. (Fig.3). A student t-test, in which the trend over a particular period is compared with the standard deviation of the noise, was used for this study.

The earliest detection times are found off the equator in the western parts of the tropical oceans, where the signal emerges as early as year 2000 (and for some regions even earlier), from the noise. In these regions the natural

climate variability is extremely low while the trend is only modest.

A second region with an early detection is the Arctic, where the trend is very large due to decrease of the sea-ice. The longest detection times are found along the equatorial Pacific where, due to El Niño, the variability is very high, as well as in the Southern Ocean and the North Atlantic, where the trend is very low.

By using a large ensemble under this DECI project the climate change trend studied above delivered invaluable results making it possible for policymakers to initiate informed mitigation actions.



Fig. 2. Dr. Andreas Sterl (right) discussing results from the ESSENCE project with his colleague Dr. Frank Selten (left) in front of a Tiled Panel Display (TPD) from SARA.

6th DEISA training session



Fig. 1. Hands On Session on DEISA training session in Stuttgart.

The 6th DEISA training session was organized at High Performance Computing Center Stuttgart (HLRS), Germany on March 5 - 7, 2008. In total 21 scientists and 9 experts in HPC and grid computing from 8 European countries participated to the event.

The purpose of the training was to enable fast development of user skills and know-how needed for the efficient utilisation of the DEISA infrastructure. The first part of the training gave a global description and introduction to the usage of the DEISA infrastructure. The second part of training introduced new ways to access to the DEISA infrastructure. On the third day of the training Use Cases were presented.

The overall assessment of the 6th training session was 'very good' 4.1 (evaluation criteria) from 1-5).



Fig. 2. Professor **Olaf Kolditz** explains the potential of GeoSys/Rockflow software at DEISA training session in Stuttgart.

Training sessions much appreciated

In total six DEISA training sessions have been organized in the period of July 2006 to March 2008. 133 scientists from 17 European countries have learned to exploit the European supercomputing environment as a result of participating to the DEISA training sessions. In addition, 20 scientific speakers and some 45 experts in HPC and grid computing have benefited from the event.

The collected feedback proves the training sessions have been very much appreciated by the participants. The overall assessment of the training sessions was 'very good' 4 (evaluation criteria from 1-5). 99.99% of the respondents said 'yes' to the question, whether the training helped them to achieve their objectives. Concerning the DEISA training session's contribution in support to participants' research activities, 64% of the respondents said that the training had either exceeded or achieved expectations, and 36% of the respondents said that the training had had positive contribution to their research activity. 112 participants have answered to the feedback questionnaire.

DEISA Symposium Advancing Extreme Computing in Europe

28 - 29 April '08, Edinburgh, UK



Talks from prominent DEISA users:

- **Structure Simulations in Vaccine Research** (Life Science), *Xavier Daura*, U. Barcelona, Spain
- **Molecular Switches at Metal Surfaces** (Materials Science), *Karsten Reuter*, FHI-MPG, Germany
- **Plasma turbulence and flows at conditions of transport transients** (Plasma Physics), *Jukka Heikkinen*, U. Helsinki, Finland
- **Simulating the Photodissociation of Triiodide** (Materials Science), *Lucas Visscher*, U. Amsterdam, The Netherlands
- **Gravitational Wave Signals from Black Hole Coalescence** (Astrophysics), *Sascha Husa*, MPG, Germany
- **Protein-Surface-Interactions mediated by Water** (Nanobioscience), *Stefano Corni*, INFN-CNR, Italy

The registration will close on on April 21.

www.deisa.eu/symposium

Nano-composites and bio-inorganic composites

Peter V. Coveney, James Suter, Mary-Ann Thyveetil, Shunzhou Wan, and Stefan Zasada, University College London, UK
Chris Greenwell and Rick Anderson, Bangor University, Gwynedd, UK

Our study shows that large-scale molecular dynamics simulations of layered silicate nano-composites and bio-inorganic composites involving full intermolecular interactions are now possible at realistic sizes using today's large-scale supercomputing facilities, such as those made available through the DEISA initiative. From the simulations in our study, we determined emergent properties, such as silicate (clay) sheet undulations, which are necessary for the calculation of material properties; and is the first step in constructing a multi-scale model of silicate nano-composites.

We also investigated the structure and stability of linear and plasmid DNA at realistic sizes, intercalated between sheets of layered double hydroxides, which is important for understanding its use in gene therapy and drug delivery, and also has direct relevance to origins of life studies. On a technical level, we were able to demonstrate and effectively use the interoperability between NGS, TeraGrid, and DEISA using the Application Hosting Environment.

Mesoscopic phenomena occur only in large systems

Our goal in this study is to be able to simulate "life sized" clay platelets that are not constrained by periodic boundary conditions, and thus can reproduce previously unexplored behaviours, such as clay sheet undulations. This allows the calculation of material properties that are hard to obtain experimentally due to the disordered nature of the platelets.

The size of the simulation we will undertake is more akin to a "mesoscopic" scale simulation but with the increased detail of full interatomic interactions. This is vitally important for nano-composites, such as clay-based filler composites, where one dimension of the filler is in the nanometre range. Without the detail of atomistic simulation, important features will not be included, such as clay-polymer interactions that may be "smeared" out. However, large simulation sizes are required to capture the "mesoscopic" phenomena, such as undulations of the clay sheets, which occur over length scales of tens of nanometres.

As yet, no simulation has been large enough and accurate enough to capture the motions and interactions of a clay sheet over such long and short length scales to capture all the features of a layered silicate nanocomposite.

Two types of clay simulated

We have used the state-of-the-art molecular dynamics code LAMMPS. LAMMPS possesses almost linear scaling with the number of processors and system size. We used several efficient classical molecular dynamics algorithms that reduce wall clock time, which are required for the large-scale simulations.

We also used the Application Hosting Environment (AHE), a lightweight hosting environment for running unmodified applications on grid infrastructures, to integrate DEISA resources with the US TeraGrid at the 2007 Supercomputing Conference and TeraGrid 2007 Conference.

We focused on two different types of clay: montmorillonite, cationic clay commonly used as filler in clay-polymer nanocomposites, and layered double hydroxides (LDHs), an anionic clay which can accommodate polar organic compounds between its layers and forms a variety of intercalated compounds.

Properties of systems extracted

We simulated several models: montmorillonite hydrated and surrounded by long chain poly(ethylene) glycol molecules, Layered Double Hydroxide hydrated and with linear and plasmid 480 base pair DNA intercalated between the layers.

From the simulations, we extracted the materials properties of clay platelets, which are required in the calculation of the elastic properties of clay-polymer nanocomposites. These new types of composites have recently received much attention due to their enhanced materials properties with the addition of a small filler weight.

We also addressed the intercalation of DNA into layered double hydroxides (LDHs), which has various applications including drug delivery for gene therapy and origins of life studies. The large size of the simulation allows the DNA to be simulated in three forms: double-stranded, linear and plasmid up to 480 base pairs. From these simulations, we identified the structural changes the DNA undergoes when in contact with the LDH surface and suggested reasons for the enhanced stability at high temperatures and pressure.

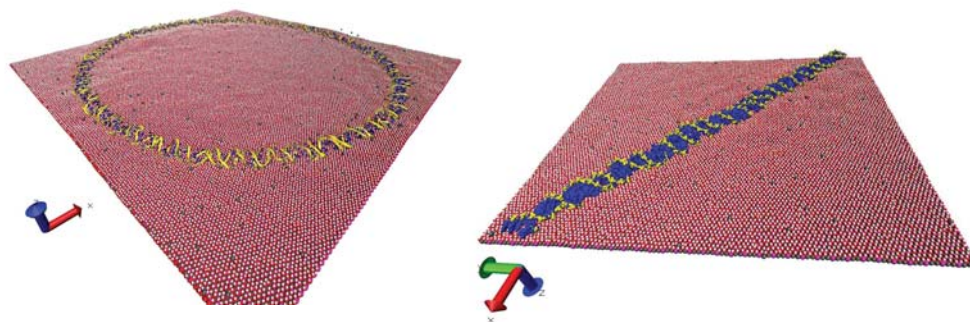


Fig. 1. and Fig. 2. 480 base-pair plasmid DNA (left) and single stranded DNA (right) on a sheet of layered double hydroxide clay. Water molecules are not displayed.

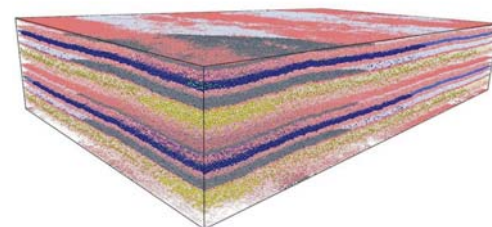


Fig. 3. Visualisation of a sodium montmorillonite clay system, containing approximately ten million atoms. The z direction has been expanded ten times to assist viewing. In large system sizes, the development of thermal undulations can be seen.

DEISA Materials Science Portal

Thomas Soddemann, Johannes Reetz, Andreas Schmidt, Hermann Lederer, RZG, Max Planck Society, Germany

Physical, chemical, and biological processes for many problems in computational physics, biology, and materials science span length and time scales of many orders of magnitude. For example, on the microscopic level, bond distances between atoms are typically in the order of Angstroms, and atoms vibrate at a frequency of approximately 10^{13} Hz. However, on the other hand, phenomena and applications of practical interest occur on a time scale of seconds, and system sizes can be microns or larger. A Grand Challenge in computational physics, biology, and materials science is to link these vastly different time and length scales.

Efficient and user-friendly usage of materials science simulation codes

Objectives of the JRA1 team are the support and deployment of important materials science simulation codes for efficient and user-friendly usage within the DEISA grid infrastructure. In close collaboration with leading computational scientists in Europe, important applications have been selected for special support and integration into the DEISA environment.

Seamless, straightforward access to applications and simple job support

The work has been focused on the development of a dedicated DEISA Materials Science Portal, on the optimization of important materials science applications, and their integration into the DEISA environment as well as the DEISA Materials Science Portal. The selection of codes was triggered by requirements from the DEISA Extreme Computing Initiative (DECI) and the work was carried out in close collaboration with authors of the respective codes and with the DEISA user Support Activity SA4.

The DEISA Materials Science Portal was developed and deployed, and seven materials science codes have been supported therein: NAMD, LAMMPS, GROMACS, CPMD, CP2K, PWScf, and Wien2K.

The DEISA Materials Science Portal provides simple, seamless, and straightforward access to these important off-the-shelf applications and offers simple job support as well as components tailored specifically for the targeted materials science applications.

The DEISA Materials Science Portal

The DEISA Materials Science Portal offers a straightforward access to DEISA resources, following a threefold strategy:

- A rich internet application based access independent of the location of the user
- DEISA Materials Science Portal Web Services, enabling integration into the user's own applications
- UNICORE Client with application-specific plug-ins

Rich Internet application

The DEISA Materials Science Portal offers a rich internet application based access independent of the location of the user. Accessing compute jobs and their data from anywhere anytime with just a web browser becomes more and more important for DEISA users. Portals leveraging Web 2.0 technologies provide the necessary means to allow users to create, submit, and manage jobs securely from any location with Internet access. The DEISA Materials Science Portal is based on the Portlet Specifications (JSR 168, 286, 303) and makes extensive use of AJAX in order to provide the best usability experience. Furthermore, all components are directly accessible and can hence be used in third party created content mesh-ups.

Access via UNICORE client

Many users are already familiar with the UNICORE 5 client. It is a rich client application used for assembling, submitting, and managing jobs in UNICORE based Grid infrastructures, such as DEISA. The UNICORE client offers the user a variety of plug-ins to enhance its basic functionality e.g. by supporting specific applications. The JRA1 team developed and enhanced UNICORE client plug-ins for CPMD and Wien2k which are available for download via the DMAS portal and from the UNICORE project's web site (only CPMD).



Fig. 1. DEISA Materials Science Portal: Snapshot of a molecule view with the help of the embedded Jmol applet.

SOAs with DEISA Materials Science Portal web services

As a side effect of the DEISA Materials Science Portal architecture, all functional components can be accessed utilizing Web Service interfaces. Hence, users can create own applications by making use of the versatile Web Service API. Therefore, composite applications in terms of Service Oriented Architectures (SOAs) can be created. Here, interoperation between different grid infrastructures has been established, as already shown for AHE (Application Hosting Environment) from UK's RealityGrid.

Supported applications

Currently, DEISA Materials Science Portal (DMAS) supports various applications at various levels of integration. The following table gives an overview of the status as of February 2008.

Field	Application	UNICORE Client	DMAS Portal	DMAS Web Service
Classical Molecular Dynamics	NAMD	*	Supported	Supported
	LAMMPS	*	Supported	Supported
	GROMACS	*	Planned*	Planned*
DFT MD	CPMD	Supported	Supported	Planned
	CP2K	*	Supported	Supported
	PWScf	*	Supported	Supported
	Wien2K	Supported	*	*

*Supported via Simple Job Submission

Table 1. Supported application specific functionalities include: Input file creation support, syntax validation and semantics verification, management of dependent files like molecule conformations, structure information and pseudo-potential descriptions.