TerraFLOPS
Service für die Erdsystemforschung

Newsletter • Deutsches Klimarechenzentrum --- Modelle & Daten • **Newsletter**

Editorial

(by Joachim Biercamp) The mission of DKRZ is to provide not only state-of-the-art supercomputing and data service but also associated services enabling the scientific community to conduct top of the line earth system and climate modelling. This goal which is also emphasized by the management structure of DKRZ (see box below) is highlighted by two articles in this issue of TerraFLOPS: The cover story describes a small project supported by DKRZ and M&D which introduces teachers and high school students to methods of climate simulation and the analysis of climate data. On pages 6 and 7 we give a short overview over the contributions of DKRZ and M&D to the adaptation of "Grid computing" - a new software technology which is expected by many people to soon become a valuable and enabling technology for the collaborative solution of complex problems - to the needs of climate research.

Changes in DKRZ management

In January, Guy Brasseur took over his new responsibilities as head of the Earth and Sun Systems Laboratory at NCAR in the US and ended his term as director of DKRZ.

Members of the new management board are Maximilian Prugger, who has been the managing director since January 2005, and two newly appointed directors: Prof. Jochem Marotzke, director at the Max Planck Institute for Meteorology, who took over from Guy Brasseur as scientific director and Stefan Heinzel, director of the Computer Center Garching, who is acting as technical director of DKRZ.

As a next step, the shareholders of DKRZ are planning to re-open, together with the University of Hamburg, the search for a university professor for scientific computing in the geosciences, who will hold a joint appointment as the new general manager of DKRZ.

A Cooperation Network between Schools and Research Facilities

"Climate Change and its impacts"
A project within the program „NaT-Working" of the BOSCH-Foundation

DKRZ and „Models & Data"(M&D) participate in a project aiming at an enhanced cooperation between schools and research facilities, advancing the interest of adolescents in natural sciences and particularly in climate research. Introductory school courses given by teachers cover the basics of the climate system and climate change. Teachers and pupils are supported through informative material, climate model data and advice by scientists. Furthermore, selected individual pupils may get more comprehensive support during an internship directly at the institutes. General project results and individual results of the participating schools and classes will be published on the web.

M&D and DKRZ introduce teachers and pupils to scientific methods used in climate research, specifically to the analysis and visualisation of simulation data. Teachers and pupils can also get advice with regard to

Figure 1: At a symposium - organized within the project "Climate change and its impacts" - scientists presented the latest results in climate research to pupils and teachers.

In this issue

specific questions or help with the selection of appropriate literature. The other project partners are the Institute for Coastal Research at GKSS Geesthacht (analysis of weather and climate data) and the University of Lüneburg (project administration and support for web publishing).

The project started in August 2005 and will run for three years. The Robert Bosch foundation provides funds for material, travel expenses and student assistants.

During the first year of the project three workshops were held, covering the planning of the project itself, scientific talks and the presentation of first results by selected pupils.

As an introduction to the state of the art in climate research a full day symposium with talks by scientists was organized (figure 1), in which more than 200 pupils and teachers participated.

During two half day training courses held by M&D and DKRZ, teachers and pupils could learn and practice the analysis of climate model data. The typical workflow demonstrated comprises the selection and download of data from the CERA data base [1], the processing of the data with the CDOs [2] and finally the data visualisation with GrADS [3]. Each of the courses had more than 20 participants.

Further support to enable the pupils to work locally in their schools with the data was given by a student assistant and by individual scientists.

Some schools have already started to work with the data and scientific literature.

More information is available at the project web page [4].

[M. Böttinger, D. Kasang]

[1] http://cera-www.dkrz.de/CERA/

[2] http://www.mpimet.mpg.de/~cdo

[3] http://www.iges.org/grads/

[4] http://www.hamburger-bildungsserver.de/index.phtml?site=themen.klima.bosch

Informatics year - Supercomputer Day

The Science Year 2006 is devoted to the field of informatics. It follows the Einstein Year 2005 and is the seventh in a series of Science Years launched by the Federal Ministry of Education and Research (BMBF).

Within the framework of the Informatics Year the CeBIT hosted the supercomputer day. The seven leading German supercomputer centres presented themselves and the scientific work enabled by these centres. The DKRZ was represented by Joachim Biercamp who talked about "Greenhouse or ice-age: Where are we heading?" (figure 2) and showed the DKRZ image video. An attentive audience and many questions demonstrated the great public interest in our work.

[J. Biercamp]

http://www.informatikjahr.de/

Figure 2: The DKRZ presentation was given in the future talk area of the CeBIT. Two large LCD screens on both sides of the scene displayed a "climate mood video" compiled by Michael Böttinger attracting quite a number of listeners.

Science Night

On October 29th, 2005, DKRZ participated in the Science Night („Nacht des Wissens") in Hamburg and presented its supercomputer system HLRE and some of the results of the climate and earth system simulations (figure 3) to the interested public. More than 10.000 people used the opportunity to visit DKRZ and/or the 27 other participating institutions. Since the event was so successful the 2nd Science Night is planned for 2007.

Figure 3: Virtual reality visualisation of the aerosol-climate model ECHAM-HAM

M&D Internet presence

The Models and Data Group (M&D) relaunched its web presence at:
http://www.mad.zmaw.de
in December 2005 with completely restructured and reorganized websites in a clear new layout. The new websites are based on the free Open Source Content Management System TYPO3, which offers full flexibility and extendability while featuring an accomplished set of modules and extensions. The latest news from M&D are available via the RSS feed:
http://www.mad.zmaw.de/news/rss.xml

[K. Fennig]

New CERA Web-Interface

The new CERA user interface is available for general use. This interface is based on Java Servlets and JSPs (Java Server Pages) and therefore doesn't require any extra client-side software installation or special firewall configuration. Additionally, the interface has been enhanced by the inclusion of NetCDF support, several format-conversion and processing functions (e.g. regional selection) and metadata printing/xml-export. For further information please visit the CERA portal page at:
http://cera.wdc-climate.de

[M. Kurtz]

CERA: Record database at World Data Centre for Climate

The World Data Centre for Climate (WDCC) and DKRZ run CERA - the largest scientific database in the world (figure 4). This was confirmed in the international ranking list of the world's largest databases published by the Winter Corporation in September 2005:
http://www.wintercorp.com/VLDB/2005_TopTen_Survey/2005TopTenWinners.pdf
CERA stores 220 Terabytes which is about twice as much as the database of a well known search engine.
The WDCC database contains the latest research data on the state of the climate and anticipated climate changes. 115 TeraBytes of storage are exclusively dedicated to IPCC simulation data for the next IPCC report AR4. Other parts are dedicated to a huge variety of projects including observational and satellite data. Please contact *data@dkrz.de* if you are interested in storing your data within WDCC. The system is implemented in an Oracle relational database coupled to the HSM system at DKRZ. A unique approach allows the cost-effective operation of the database on a reduced set of disks.
All data is available online for download at:
http://cera-www.dkrz.de
In 2005 more than 600.000 downloads were carried out by the WDCC users.

[H. Thiemann]

Data Management Concept

As announced in the last TerraFLOPS (No 6, page 7) a new data management concept has been proposed by DKRZ, M&D and the usergroup. Being strongly supported by the WLA at its last meeting on the 20th of January 2006, the data management concept in its first phase is implemented for new projects. Further information is published at the webpage of DKRZ:

http://www.dkrz.de/dkrz/services/docs/Archivkonzept_Stand-Jan2006-V08

Figure 4: The grand prize for CERA as the largest scientific database in the world awarded by the Winter Cooperation

Press Review

DKRZ has introduced a press review on its website. At
http://www.dkrz.de/dkrz/about/pressespiegel
newspaper articles and reports about DKRZ are listed and, if available, linked.

[J. Meyer]

Criteria for Consortium Runs

At its meeting on the 20th of January 2006 the WLA approved the criteria for consortium runs which were proposed by the usergroup. These criteria (only in German) can be found at the M&D website at:
http://www.mad.zmaw.de/service-support/consortium-model-runs/

[J. Meyer]

# *Barotropic free oscillations of a global ocean model including the full self-attraction and loading effect*

[Malte Müller, Institute of Oceanography at the University of Hamburg]

http://www.ifm.uni-hamburg.de

The elevations of the sea surface and those of the ocean bottom determine the variability of the vertical expansion of the water column. The associated mass redistribution influences the earth's gravity field and additionally deforms the sea bottom due to the mass loading when taking the elasticity of the earth into account. Together, these secondary effects of ocean dynamics are named self-attraction and loading effect (LSA) and are interesting both for the physics of the ocean and for the solid earth.

The first investigations of the influence of this effect on ocean dynamics were made in the context of modelling tides [1,4]. It turned out that the main structure of the tidal patterns is preserved but that the computed tide is generally delayed, when taking the LSA effect into account. Recent analysis in a barotropic ocean model driven by tidal forces, wind stress and atmospheric pressure was made in
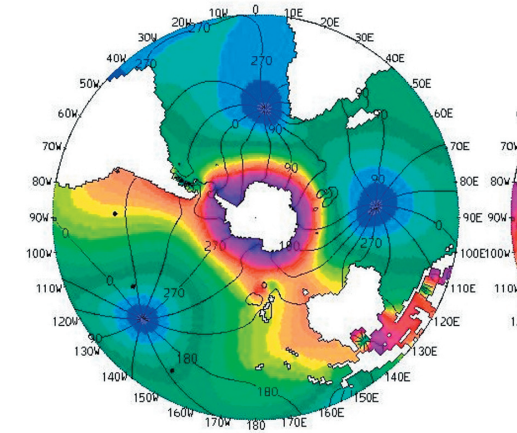
(a) Period: 32.64 h
Decay Time: 53.57 h

Figure 5: Examples for gravity modes: (a) Fi[...] around Antarctica. (Color contoured normali[...]

order to quantify the magnitude of the LSA term in the hydrodynamical equations, primarily to develop a simplified representation of the LSA term. The results showed that there are significant variations in magnitude, especially correlated with the time scale of the oceanic response.

For the understanding of the response of the oceanic water masses to external forcing the knowledge of the free oscillations of the global ocean is substantial. These oscillations consist of gravity and vorticity modes, primarily governed by the gravity of the Earth and by the Coriolis force, respectively (Figures 5, 6). They determine the response of the ocean to tidal forces (Figure 7) and are furthermore forced by wind stress and atmospheric pressure. First solutions of free oscillations of an ocean model with a realistic topography and a 4-5 degree resolution were obtained by Platzman et al. [3]. In the last 20 years no further endeavors have
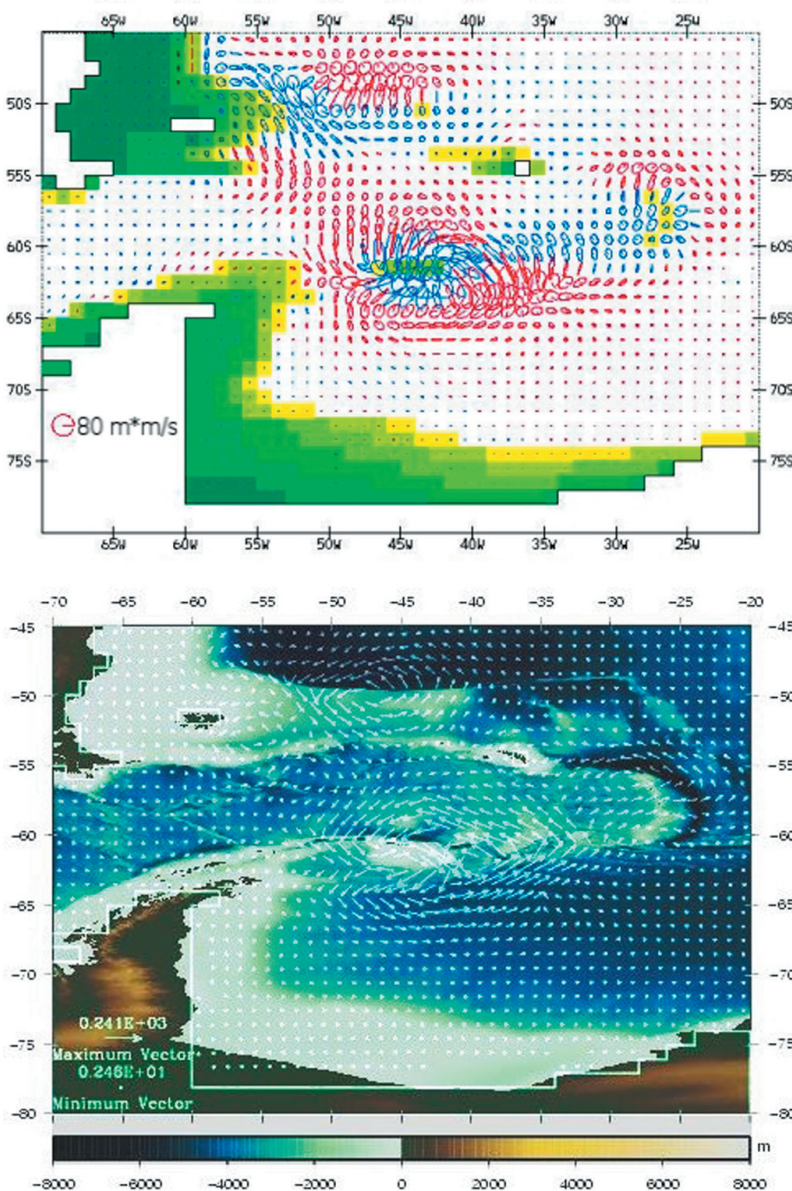

Figure 6: Topographic vorticity mode around the Falkland Plateau and the South Orkney Islands with a period of 63.32 hours and an energy decay time of 12.23 hours. (a) Volume transport ellipses. Red contours indicatie anticyclonic rotation, blue ones cyclonic rotation; the circular volume transport given at the bottom left has a magnitude of 80 m^2/s.
(b) Color contoured bathymetry. Energy flux vectors: squaring the magnitudes given yields these quantities in $J/(sm)$.
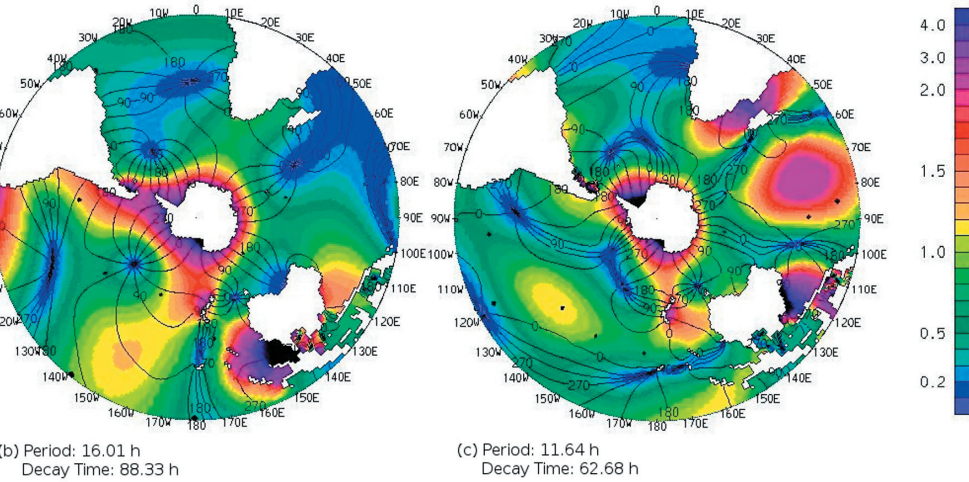
(b) Period: 16.01 h
Decay Time: 88.33 h

(c) Period: 11.64 h
Decay Time: 62.68 h

rst, (b) second and (c) third order Kelvin Wave travelling in a counterclockwise direction
zed amplitudes of sea-surface elevation and solid lines of equal phases)

cal libraries for computing the eigen-vectors and the associated complex eigenvalues. Thus a working memory of more than 500 GB is required and the matrix has to be distributed on at least 12 nodes of the HLRE. To solve the eigenvalue problem, a QR based

> ### *More than 600 out of 750 possible GFlops on 12 nodes*

method is used and the time consuming solving of a linear equation system within each step of this iterative method is done by a solver included in the ScaLAPACK package. Thanks to the help of the DKRZ and NEC, it is now possible to run the resulting program on 12 or 16 nodes and the overall performance is up to 609 or 632 sustained GFlops, respectively. Thus we can compute in a very efficient way a large spectrum of free oscillations of a linear barotropic ocean model including the full LSA effect.

been made to improve these results, although in those days, due to the limited computer resources important features of the hydrodynamical equations were neglected and a relatively coarse resolution was used. For the first time, Zahel und Müller [5] computed barotropic free oscillations of a global one-degree ocean model including the Arctic Ocean and with explicit consideration of dissipative terms and parameterized LSA. They obtained altogether 61 free oscillations by means of inverse iteration (Wielandt method) with periods between 7.8 and 133.1 hours. To generalize this model the full LSA effect has also been included. The hydrodynamical differential equations thereby turn into integro-differential equations. Discretization of these equations using a finite difference model with a spatial resolution of 1 degree yields a set of linear equations with approximately 120.000 unknowns, represented by a full matrix. Although the entries of the matrix are generally non-zero, symmetries in the arrangement of the entries can be utilized to reduce the working memory of the model to less than 1 GB. Taking advantage of this memory reduction three single free oscillations were computed with a special modification of the Wielandt method [5] and four with the standard Wielandt method [2]. In the first case the model was time optimized with respect to the me-

thod itself, whereas in the latter case it was distributed with OpenMP on 8 CPUs and optimized for the HLRE with the help of DKRZ and NEC, reaching a performance of more than 20 GFlops on a single node of the SX-6. No more benefiting from the symmetries of the matrix and storing it in a general form was necessary to enable the use of routines of mathemati-
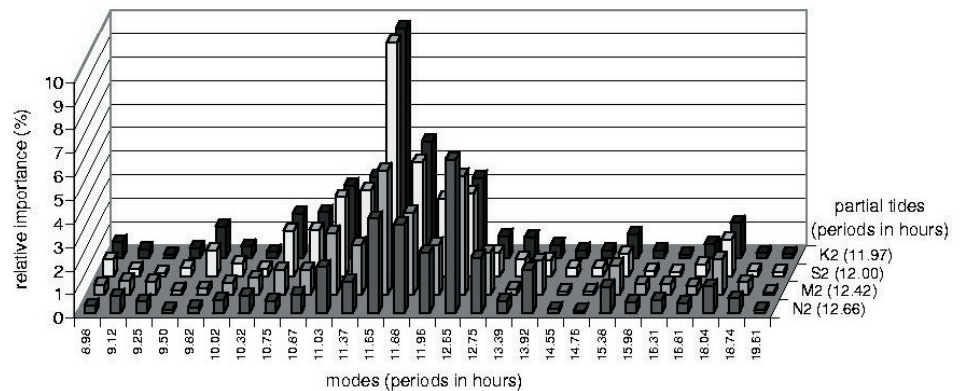

Figure 7: 1° World Ocean model of free oscillations with parametrized LSA: Relative importance of individual free oscillations when representing the realistic sea surface elevation of the main semi-diurnal constituents (N2, M2, S2 and K2) by superposing the fields of elevation of the free oscillations.

References

[1] Accad Y, Pekeris CL (1978) Solution of the tidal equations for the M2 and S2 tides in the world ocean from the knowledge of the tidal potential alone. Philosophical Transactions of the Royal Society of London A290: 235-266

[2] Müller, M (2003) Barotrope Eigenschwingungen im globalen Ozean unter Berücksichtigung des vollen Selbstanziehungs- und Auflasteffektes. Diplomarbeit. Inst Meereskd Univ Hamburg. 1-67

[3] Platzman GW, Curtis GA, Hansen KS, Slater RD (1981) Normal Modes of the World Ocean. Part II: Description of Modes in the Period Range 8 to 80 Hours. J. Phys Oceanogr 11: 579-603

[4] Zahel, W (1978) The influence of solid Earth deformations on semidiurnal and diurnal ocean tides. In P.Brosche and J.Sündermann: Tidal friction and the Earth's rotation.Springer-Verlag: 98-124

[5] Zahel W, Müller M (2005) The computation of the barotropic free oscillations of a global ocean model including friction and loading effects. Ocean Dynamics 55: 136-161
http://www.springerlink.com/openurl.asp?genre=article&id=doi:10.1007/s10236-005-0029-y

Grid technology projects at DKRZ

Grid computing is one of the latest approaches of high performance computing and collaborative data management. It is increasingly promoted as a solution for computing-, data- and community intense problems in science and business [1, 2]. In principal, a **computing grid** is a distributed shared network of standard computers. Yet, a powerful scheduling and management infrastructure enables the effective and consistent usage of the combined computing power of this multitude of CPUs. **Data grids** concentrate on the aspect of finding, accessing, exchanging data and their potential replicas securely and efficiently in virtual collaborations. All grid infrastructures are based on an elaborate security infrastructure for user authentication and authorization, using e.g. special *grid certificates*.

The DKRZ is currently involved in two different grid computing projects: the EU funded project "EGEE" (Enabling Grids for E-SciencE, [3]) and the German "C3 Grid" project (Collaborative Climate Community Data and Processing Grid [4]) within the German E-Science initiative (D-Grid [5]). The **EGEE** project aims at improving and broadening the use of the largest existing computer grid production infrastructure.

In contrast, the C3Grid is an application driven approach, which aims at developing an infrastructure for the access and use of the existing large datasets in the German climate community.

Currently, the EGEE infrastructure consists of more than 20.000 CPUs and offers over 5 Peta-Byte of storage capacity. The DKRZ is part of the EGEE Earth Sciences Community, helping to identify suitable applications and support users to make use of this grid infrastructure.

Originally, the EGEE *middleware* effort was driven by the high energy physics community at CERN in order to store and process the amounts of data produced by the three large particle-collider experiments. The grid infrastructure provides the basis on which this data is processed, shared and analysed by the entire community of international institutions.

We observe the development of a similar research structure in climate and earth system science. TeraBytes of data are produced by a few increasingly detailed and

Figure 8: Grid is the ability to gain access to applicatio capacity or other computing resources over a network (us Grand Challenge problems such as climate and earth sys

comprehensive earth component models or coupled earth system models. The vast majority of data produced in numerical climate and earth system science experiments is stored in local file systems or in centralized databases (like DWD and the world data centres WDC Climate, WDC RSAT and WDC Mare) and archive systems (like the DKRZ archive). Thus, a seamless and fast access to the data is restricted to users of the local resources at present. But the produced data is interesting for a larger community, especially in the case of coupling experiments and consortium runs (e.g. IPCC simulations). For international and interdisciplinary collaboration the definition of restricted shared areas with secure and common data access can be very beneficial. The EGEE infrastructure provides a potentially ideal framework for data sharing and collaborative analysis. The existence of such an internationally shared data and modelling
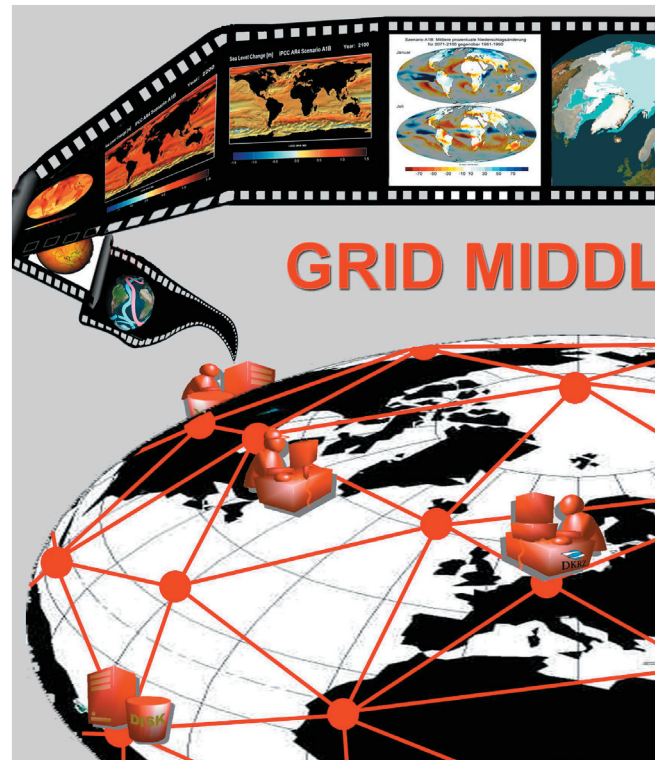

Grid terminology

Grid middleware denotes the infrastructure that translates and distributes the user requests transparently to the actual grid resources (e.g. computers, storage nodes)

Grid enabled resources or applications provide an interface to "communicate" with the grid middleware

Grid certificates are used to uniquely define identity and rights of users, services and resources. They are based on X.509 certificates, extended by the possibility to delegate rights in order to authorize components to act on the behalf of a certified user (or machine)

ns and data, processing power and storage ually the internet). Grids offer a way to solve tem modeling.

haven. The grid middleware components intelligently schedule data and computation jobs to the available resources, striving for optimal performance. The common infrastructure developed in the project will provide an opportunity to all major German earth science institutions to use grid technology in their scientific work. It will be built up in various phases, starting with the implementation of typical climate data analysis workflows. As prototypes for the use of grid technology, three standard climate workflows were identified: deriving time series of climate variables on surface level from ECHAM model data as raw data, or as processed data (like in CERA database; MPI and IFM-GEOMAR), diagnosis of different parameters, i.e. storm tracks (University of Cologne and Free University of Berlin), and chemical weather predictions utilizing ECMWF data (DLR). Central tools therein are collections of climate data operators (cdo [6]), and of diagnosis tools. The implementation of these workflows and

Cluster Computing and Grid Computing

Cluster computing is targeted at sets of efficiently connected nodes in one location. In contrast to this Grid computing addresses the transparent use of organizationally and geographically distributed resources (e.g. clusters, storage).

their tools into the new environment will reduce the large number of data identification, extraction, conversion and transfer steps which are commonly necessary before any scientific evaluation can take place. The use of computer time and storage resources at different locations will be optimized, also addressing the problem of authentication and authorization. The DKRZ, as the central resource provider for the German climate community, will coordinate the deployment of the C3Grid infrastructure.

[S. Kindermann, K. Ronneberger]

platform would also improve the comparability and thus objectivity and scientific soundness of models and model results.

However, currently the access and processing of climate data is hindered by missing *grid enabled* interfaces to the established data resources. Moreover, absent and inappropriate metadata - describing content and location of data files - hampers data discovery. These missing functionalities are currently being developed in **C3Grid** work packages with strong participation of DKRZ and M&D. The C3Grid project has been set up to enable an easier and more efficient resource management for the climate community, in order to improve the efficiency of scientific work both in terms of data storage and of computing. Based on a standardised metadata description, data will be uniformly searchable and accessible via a portal, developed at AWI Bremer-

[1] http://gridcafe.web.cern.ch

[2] "Parallel computing: Clusters, Grids & Co" (2006), CT 3 174ff

[3] EGEE project hompage: http://www.eu-egee.org

[4] C3Grid http://www.c3grid.de

[5] D-Grid http://www.d-grid.de

[6] http://www.mpimet.mpg.de/~cdo

Links related to Grids in Earth System Science

http://www.d-grid.de

http://www.eu-egee.org

https://cdp.ucar.edu/

http://www.c3grid.de

http://ndg.badc.rl.ac.uk

http://www.earthsystemgrid.org

Services for Earth-System-Research

TerraFLOPS
Service für die Erdsystemforschung

OUR SERVICES

- **COMPUTER TIME FOR EARTH SYSTEM MODELLING:**
  Top level computing ressources and archive capacity are available to all interested research groups working on climate and earth system modelling. DKRZs scientific steering committee (WLA) selects admissible projects.
  INFORMATION: *http://www.dkrz.de/projects*
  EMAIL: *projects@dkrz.de*
  CONTACT: *Joachim Biercamp (EXT -314)*

- **SUPPORT FOR USERS:**
  Support for porting models to DKRZ computers, support for model optimisation, visualisation services and general user support to all users.
  INFORMATION: *http://www.dkrz.de/support*
  EMAIL: *beratung@dkrz.de*
  CONTACT: *Help Desk (EXT -275)*

- **LATEST ONLINE INFORMATION:**
  Announcements and latest news regarding DKRZ facilities and services:
  *http://www.dkrz.de/news (*on *http://www.dkrz.de/news/ann* for registered users).

- **COMMUNITY CLIMATE MODELS:**
  M&D provides numerical models and diagnostic software as well as user support for their application and carries out comprehensive climate model runs.
  INFORMATION: *http://www.mad.zmaw.de/*
  EMAIL: *model@dkrz.de*
  CONTACT: *Stephanie Legutke (EXT -104)*

- **DATA SUPPORT:**
  Provision, maintenance and easy access of climate research relevant data of different research groups as well as post-processing tools and the support of users of the climate data base.
  INFORMATION: *http://www.wdc-climate.de*
  EMAIL: *data@dkrz.de*
  CONTACT: *Michael Lautenschlager (EXT -297)*

- **MAILINGLIST:**
  For news regarding M&D, such as announcements of workshops and conferences, new models and datasets, changes in accessing M&D etc. send "*subscribe mad_info*" to *majordomo@dkrz.de*.

DKRZ
Deutsches Klimarechen-
zentrum GmbH
Bundesstraße 55
D-20146 Hamburg
Germany

Phone: +49 40 41173-334
Email: sekretariat@dkrz.de
Web: http://www.dkrz.de

M&D Modelle & Daten
Gruppe Modelle & Daten
Max-Planck-Institut für
Meteorologie
Bundesstraße 55
D-20146 Hamburg
Germany

Phone: +49 40 41173-397
Email: mad_office@dkrz.de
Web: http://www.mad.zmaw.de

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