TerraFLOPS
Service for earth-system-research
Newsletter
Deutsches Klimarechenzentrum
Modelle & Daten

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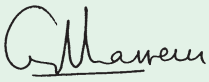
TerraFLOPS
Service für die Erdsystemforschung

Note of Thanks

(by Guy Brasseur) The new super computer and data system, now in their operational phase at DKRZ, have been financed by BMBF, the Federal Ministry of Education and Research. On behalf of the scientific community involved in Earth System Modelling, we would like to thank BMBF, and specifically Staatssekretär Dr. U. Thomas, who has committed up to 60 Millions Euros to support a climate computing facility in the next 10 years. We also thank Dr. N. Binder at BMBF and the Max-Planck-Society in Munich for facilitating the implementation of the project. The operational costs associated with the DKRZ facility will be covered by the four shareholders: MPG, University of Hamburg, GKSS and AWI.



In this issue

Official Inauguration of the HLRE

On September 10th the official inauguration ceremony for HLRE took place. The event started with a lively press conference. Journalists from press agencies, newspaper and journals as well as from radio and TV-stations took the opportunity to get statements from the directors of DKRZ, Guy Brasseur and Wolfgang Sell, from NEC's marketing manager Jörg Stadler and from two renown scientists which have been both users and consultants of DKRZ for many years: Mojib Latif and Hans von Storch. Dozens of articles and features, covering the new scientific opportunities and substantially improved working conditions for climate research provided by DKRZ, appeared in regional and national media.

Tadao Kondo, the Associate Senior Vice President of NEC Solutions donated a granite plate displaying the name "Deutsches Klimarechenzentrum GmbH" in

（有）ドイツ気候計算センター

Japanese letters (as shown above) to DKRZ.

Keynote speaker of the public session was Staatssekretär Dr.-Ing. E.h. Uwe Thomas, from BMBF, the

Staatssekretär Dr.-Ing. E.h. Uwe Thomas, from the Federal Ministry of Education and Research, here listening to Prof. Guy Brasseur was special guest and keynote speaker of the cere-

Service

How to get CPU-time for YOUR application

The DKRZ is open to all interested research groups working on climate and earth system modelling. The centre's scientific steering committee (WLA) selects admissible projects. Scientific quality and the need for high performance computing and data archiving resources are the principal selection criteria.

International groups can be accepted if they contain a significant German contribution or provide services in compensation to German groups. A positive review of the project by German funding agencies such as German Science Foundation (DFG) or Federal Ministry for Research and Education (BMBF) or by the European Commission is an advantage, but not necessary.

Applications for the allocation of resources should be submitted online at

http://www.dkrz.de/Antrag

Federal Ministry of Education and Research who talked about the necessity of sustainable development to obtain a maximum of global welfare. This talk was followed by addresses from representatives of the shareholders of DKRZ and its scientific steering committee. All speakers emphasized the importance of earth system modelling and the importance of a facility like HLRE for the modelling community.

In a scientific session, Tadashi Watanabe from NEC, Walter Zwieflhofer from ECMWF and John Mitchell from the Hadley Centre gave an overview on requirements, technical challenges and scientific challenges for a high performance computing centre dedicated to earth system modelling. Some of the slides can be found at

http://www.dkrz.de/Einweihung.html

Figures (top left to bottom right): Mr. Kondo (NEC Solutions, Associate Senior Vice President) presenting the granite plate. - The directors of DKRZ talking to Staatssekretär Thomas and to Mr. Kondo. - The audience (in the front row Prof. K. Mehlhorn, vice-president of MPG). - W. Sell, G. Brasseur and U. Thomas.- The german-japanese event ended with beer and sushi.

HLRE Phase 2 Configuration

On October 7th we started Phase 2 of the HLRE by providing four additional SX-6 nodes to our users. Another four nodes are up and running and will be made available to our users at the end of this year. Currently they are used for evaluation purposes. For example the new version of the Network queuing system (NQS) is installed and tested on these nodes before bringing it into production.

The tape archive has been upgraded with some new tape drives. A forth silo has been mounted and will soon be integrated.

Top: *Currently the HLRE Computer server consists of 16 SX-6 nodes with 64 GFlops peak performance and 64 GByte of memory each. The picture shows all 16 compute nodes set up in two rows and, in the foreground two of five cabinets containing the IXS crossbar switch which connect each of the currently 128 vector CPUs which each other CPU.* ***Left:*** *The archive is build from 3 storage tek silos equipped with a total of 50 tape drives. The total capacity is 6 PetaBytes.*

Model Support

The group ‚Modelle & Daten' (M&D), attached administratively to the Max-Planck Institute of Meteorology, is supporting the German climate research community in all aspects related to the application of numerical climate models and associated diagnostic software. This includes the adaptation of models to new computing platforms (optimization, parallelization), configuring the models for new experiments (domains, resolutions, boundary conditions), upgrading models with new physical parameterizations, as well as running and supervising experiments.

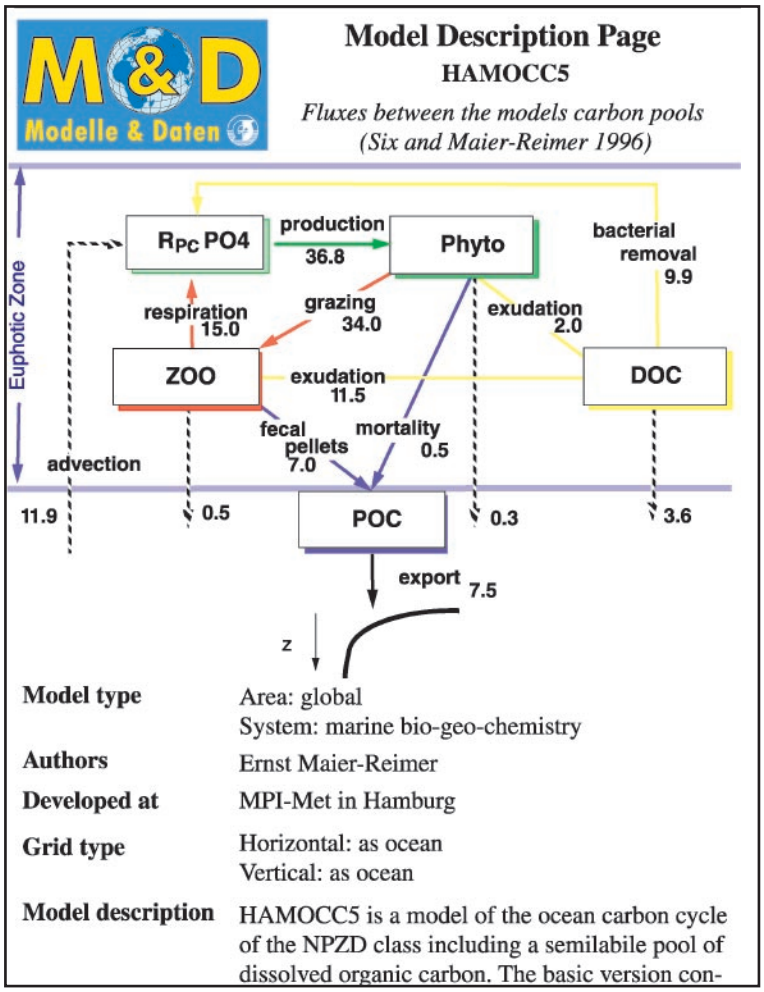
The growing number of scientists and projects, and also the growing-together of the European scientific communities, requires the development and maintenance of a climate modelling infrastructure, which promotes efficient climate research and cooperation, national and European wide. This necessitates the specification of community models which will be supported by M&D and quality criteria these models must meet. The scientific steering committee of M&D, the WLA (see TerraFlops 1, page 3), is involved in this process which is still going on.

Meanwhile, M&D has set up a documentation of models it is supporting, which includes not only candidates for community models, but also models which have been supported so far, in order to offer a continuation of support of ongoing research activities for the German climate research community. The documentation is on the internet, accessible for the whole Earth Science research community. It also includes tables of experiments, which have been run with the participation of M&D

http://www.mad.zmaw.de

The model pages include a short description of the model, the setup supported by M&D (domain, resolution etc.), resource requirements, contact persons, links to other documentation, and the level of support given by M&D.

The support level ranges from 1 to 3. Level 1 indicates that the model is distributed by M&D, together with the available documentation (Server-version). A level 2 support means that the model is adapted to different computer platforms/architectures (PC, workstation, vector machine, parallel machine) and model domains or resolutions. With level 3, M&D is actively supporting the development of a model (interfaces, coupling, parallelism, optimization, inclusion of parameterizations...). At present, model pages are available for ECHAM4, HOPE-G, MOM3, ECHO-G, HAMOCC5, REMO, WAM_cy4, ERSEM, ECHOHAM1, OPA/ORCA2, and OPA/ORCA2-LIM.



Upper part of the Web page giving the support activities of M&D for the HAMOCC5 model of marine bio-geo-chemistry.

Climate research involves more and more the use of coupled numerical models. These are in many cases interactive models of the climate subsystems (atmosphere, ocean, chemistry, ...) which have been developed stand alone at different research sites. M&D has responded to this situation by providing interfaces to the OASIS coupling software for the models it is supporting. OASIS is a user friendly software for climate model coupling, developed at Cerfacs (Toulouse, France) and used worldwide. It has considerably facilitated the exchange of components and the cooperation between groups (EU project SINTEX).

Future evolution towards efficient and portable coupling environments is currently under way in the EU project PRISM. M&D is leading the work package "system installation, communication and networking" which is developing a web-based interface for model deployment and launching of experiments, and the work package "Model assemblage", that integrates the software developed within PRISM and climate component models. Therefore, M&D will continue to provide high-quality portable modelling tools in a user-friendly environment.

[Stephanie Legutke, M&D]

Mountain-wave induced polar stratospheric clouds

[Thomas Birner, Andreas Dörnbrack, DLR-Institute for Atmospheric Physics]

http:://www.op.dlr.de/ipa/

[Thomas Schoenemeyer, NEC-European Supercomputer Systems];

http://www.nec-ess.com/

The crucial role of polar stratospheric cloud (PSC) particles in driving the catalytic ozone destruction cycle is now widely recognized. These clouds form during polar winter if the stratospheric temperature falls below a certain threshold (usually far below 190 K). The Antarctic polar vortex remains mostly stable throughout the whole winter. Air inside the vortex cools therefore down to very low temperatures resulting in a synoptic-scale (order of 1000 km) coverage by PSCs. In spring, sunlight triggers the ozone destruction on these particles and leads to the yearly Antarctic ozone hole. On the other hand, the Arctic polar vortex is often too warm for the formation of synoptic-scale PSCs because of disturbances by transient planetary waves. However, cold areas on a mesoscale (order of 100 km) can be produced by adiabatic cooling of rising air parcels within stratospheric mountain-waves. These mountain-waves are excited by flow over topography such as Greenland or northern Scandinavia.

During the international field campaign SOLVE/THESEO 2000 [1, 2] such mountain-wave induced PSCs have been explored above northern Scandinavia by the DLR Ozone Lidar Experiment (OLEX) on board the DLR Falcon F-20 research aircraft (see also [3]). One particular PSC measurement is shown in Figure 1. Superimposed are simulated isentropes (lines of constant potential temperature - a conservative quantity under adiabatic motions) and contours of temperature below the frost point. The simulations were performed using the non-hydrostatic weather prediction model MM5 [4] in shared memory parallel mode (OpenMP) on 4 CPUs of the T-Systems Solutions for Research SX-5 system at DLR Braunschweig (1 node with 16 CPUs). A grid refinement scheme has been applied - an outer domain with 2 two-way nests in it: 24, 8, and 2.67 km horizontal resolution and 91x91, 121x121, and 181x181 grid points. In the vertical direction 65 levels were used with a resolution of about 500 m. Radiative and moist processes were switched off and the initial and boundary values of the model integration were prescribed by 6 hourly analyses of the ECMWF global model. The 16 hour integration used about 27 CPU-hours and 2.2 GByte memory. Each saved date occupied about 310 MByte disk space. The overall performance on the 4 CPUs of the SX-5 was about 4 GFLOPS.

Fig. 2: Photograph of the polar stratospheric c

Regions of temperatures below the frost point correspond very well with the measured PSC. It is evident that the mountain waves downstream of the Scandinavian mountain range (visible in the isentropes) caused the low tem-

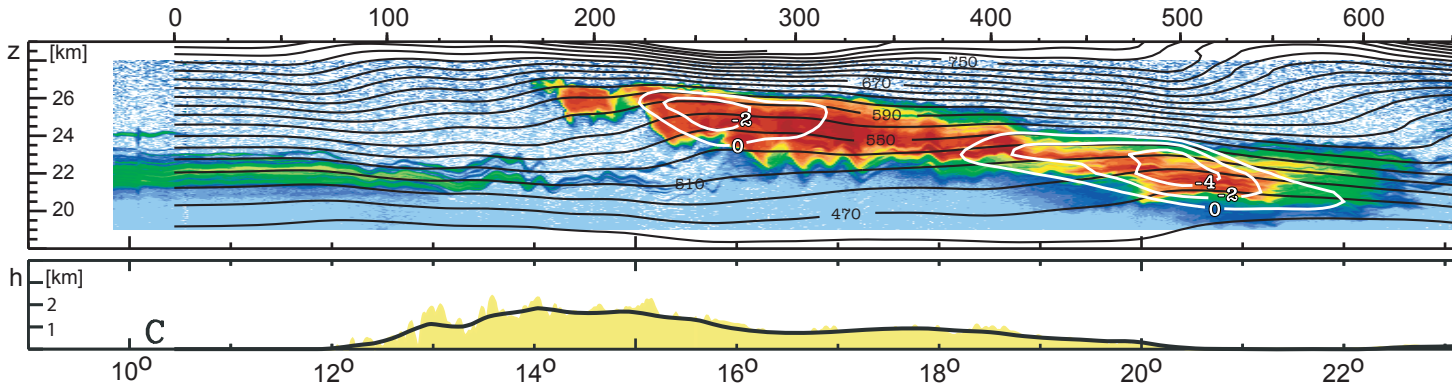
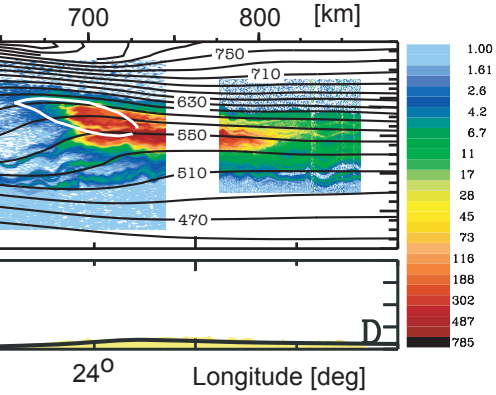


Figure 1: Back scatter ratio at 1064 nm along a cross-mountain flight leg (at about 65° N latitude) of the DLR Falcon on 26 Janu are MM5 potential temperature (black lines) and temperature below the frost point (white contours, assuming a volume mixing rati the second model domain. Bottom panel: elevation of the topography below the flight leg (gray shading: digital topography in 1 km h from the second model domain).

cloud shown in Fig .1, taken during the flight

peratures. However, the measured smaller scale wavy PSC structures cannot be resolved by this MM5 simulation. Therefore, up-to-date applications of MM5 by our group rather need grid points up to 300x300 horizontally and more than 200 vertical levels. Additional physical options are needed for particular applications. Using those settings, one reaches the limits of the current SX-5 system at DLR.



uary 2000 (colour shading). Superimposed o of 5 ppm) along the flight leg taken from horizontal resolution, black line: topography

The exact life cycle of PSC particles is still not fully understood. Mountain-wave induced PSCs are an ideal natural laboratory to observe this life cycle. In the darkness of the polar night, it is essential to predict the most likely positions of the PSCs in order to guide aircraft or balloons. Therefore, our group supports those campaigns by two sets of stratospheric forecasts (synoptic-scale and mesoscale). The synoptic-scale set includes animations of the past (last 15 days) as well as future (next 84 hours) vortex development and forecasts of the tropospheric and stratospheric flow around northern Scandinavia. This set is based on analyses and forecasts of the T511/L60-ECMWF global scale model.

The mesoscale set of MM5 forecasts is launched whenever the ECMWF model predicts favourable conditions for mountain-wave induced cold temperatures above northern Scandinavia. In the winter 2001/2002, those MM5 forecasts were produced on SX-5 using a single domain with 121x121 grid points (18.2 km horizontal resolution) and 60 vertical levels (500 m resolution). The initial and boundary values were prescribed by the ECMWF forecast. All results were finally presented on our web page, [5]. For the next field campaign in winter 2002/2003 (VINTERSOL, [6]) the MM5 forecasts will be produced using the new HRLE-System at DKRZ in Hamburg (based on the SX-6 system). For this purpose the source code of MM5 has been slightly modified by DKRZ and system analysts of NEC-ESS. Due to optimization in the planetary boundary scheme as well as in the radiation scheme and the solver routines a higher degree of vectorization and increased vector length could be achieved. Together with improvements in the Fortran90-compiler, the performance of MM5 increased to more than 10.4 GFLOPS on 4 CPUs of the SX-6 with OpenMP parallelization. An 48 hour forecast can be provided this way for two domains simultaneously (an outer domain: 109x109 grid points (21 km horizontal resolution), an inner domain: 244x244 grid points (7 km horizontal resolution), and 60 vertical levels) within about 4 hours real-time. The ratio of elapsed time of the simulation to predicted time is thus about 1:12 on 4 CPUs. This demonstrates the high effective performance of vector systems even with a small number of CPUs. Compared to the winter 2001/2002 we are now able to produce forecasts with more than double horizontal resolution.

Since the DKRZ SX-6 system includes several nodes, each having 8 CPUs, our group will be able to achieve needs for MM5 runs like the above specified and beyond, benefiting additionally from multi-node parallel options like MPI for MM5.

REFERENCES

[1] ***http://cloud1.arc.nasa.gov/solve/***

[2] ***http://www.nilu.no/projects/theseo2000/***

[3] Dörnbrack, A., T. Birner, A. Fix, H. Flentje, A. Meister, H. Schmid, E. V. Browell, and M. J. Mahoney, Evidence for inertia gravity waves forming polar stratospheric clouds over Scandinavia, J. Geophys. Res., 107, 10.1029/2001JD000452, 2002.

[4] ***http://www.mmm.ucar.edu/mm5/mm5-home.html***

[5] ***http://www.pa.op.dlr.de/arctic***

[6] ***http://www.ozone-sec.ch.cam.ac.uk/***

The Data Challenge of Earth System Modeling

A very important aspect of the new HLRE System besides its sheer compute power is its data storage capacity and the balance between Compute-Server, Data-Server and network. Significant progress has been made since February 2002 with the installation and start of operation of the HLRE. The transition from the old system to the HLRE phase 1 went smoothly without any major disturbance of the data handling activities of the DKRZ customers. The new system is heavily used. The amount of data exchanged at the network interface of the Data Server increased from about 500 GByte per day in the beginning of 2002 up to a maximum of about 3 TByte per day in August 2002. Despite this significant increase in the transfer rate there is still enough capacity available in the system configuration for further increase which we expect during phase 2 operations.

Scheduled for operational use in December 2002 a Global Filesystem (GFS) connected to the Compute- and Data-Server will allow transparent access to the archived data from the Compute-Server and speed up this access significantly. The GFS currently in use only connects the nodes of the Compute Server "hurrikan".

Unitree on the HLRE Data Server

After signing the HLRE contract the Data-Server configuration was improved in the long term. Starting in December 2002 the Data-Server will be a homogeneous system of IA64 based Linux computers manufactured by NEC for the Hierarchical Storage Management (HSM) services. Until then the HSM is run on two Fire 4800 systems from Sun Microsystem. Since Ocober 1st, 2002 these are complemented by an IA64 based NEC AzusA system with hostname "ds1" which is partially integrated in the HSM production service. Porting of relevant portions of the HSM-software and testing of all software components is carried out jointly by DKRZ, M&D, NEC and Legato. For a full integration further program porting and testing is needed, especially for the integration of Unitree and the heterogenous GFS coupling of Compute- and Data Server.

Oracle on the HLRE Data Server

Another challenge accompanying the introduction of the HLRE is the data management. Accustomed methods for data storage and retrieval will fail very soon when large consortia simulations will be made including many groups in the design and evaluation of such runs. Data management based on file names is no longer feasible as reliable means for data processing. Therefore M&D and DKRZ with the support of external groups will develop semantic data management further to become a vital tool for data analysis in the future. The Oracle DBMS is an important part to provide semantic data handling. Since the Oracle software is not yet provided in the server environment for Linux operating systems there is still a need to run Oracle for the time being on Sun Microsystems platform as it is done in DKRZ since several years.

Media costs

The sheer amount of storage media for the data produced in simulations and postprocessing generates a problem: Since the expected media cost exceed the budget of DKRZ for these items in case that the storage attitude of DKRZ customers remains unchanged it is likely that besides CPU time also tape storage capacity will be a limited resource. Storage requirements in excess of these limits will be charged separately.

[Wolfgang Sell, DKRZ]

Using the data-server

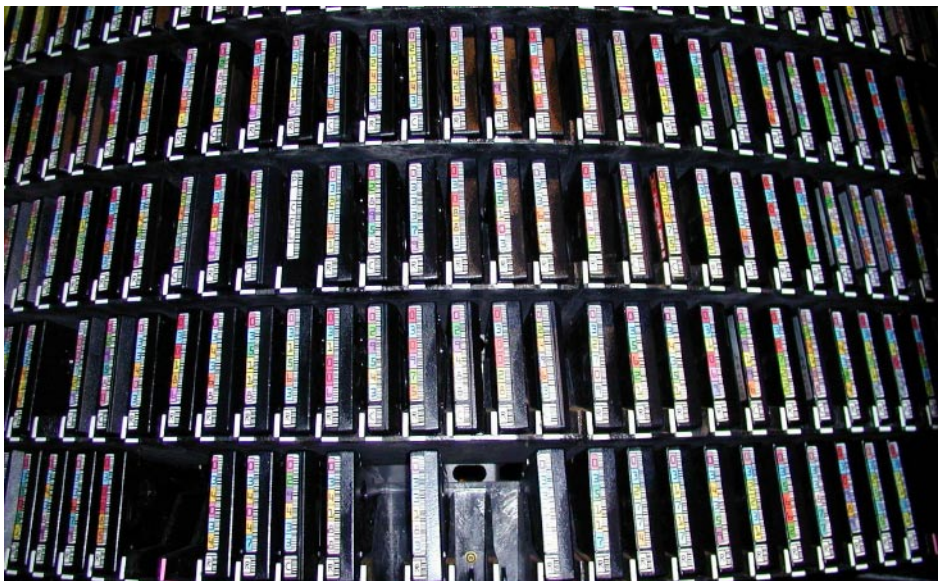
Every user having access to the DKRZ compute server "hurrikan" can permanently store his own data in our Unitree archive. Currently the archive can only be accessed via ftp to our data-server with hostname "schauer":

>ftp schauer.dkrz.de
>login: <hurrikan-username>
>password: <hurrikan-passw>

Climate data (such as results from model simulations and observations) provided by M&D data can be browsed and retrieved from the Oracle data base using the cera gateway located at

http://mad.dkrz.de/java/CeraStart.html

(See also TerraFlops Issue 1, May 2002). For further information contact ***data@dkrz.de***



View into one of the data silos containing hundreds of cartridges with coloured bar codes

Vorstellung des DKRZ User-Group-Committes

[Bernadette Fritsch (Sprecherin); Alfred-Wegner-Institute for Polar Research]
http://www.awi-bremerhaven.de/

Mit der Installation des neuen Rechners NEC SX-6 verfügt das DKRZ über einen leistungsfähigen Supercomputer. Er wird jeweils 50% von den Wissenschaftlern der Gesellschafter des DKRZ (MPG, Uni-HH, GKSS, AWI) genutzt. Die andere Hälfte steht Wissenschaftlern anderer Institutionen zur Verfügung, die Projekte über den wissenschaftlichen Lenkungsausschuss (WLA) beantragen können.

Damit ergibt sich ein relativ breites und auch inhomogenes Nutzerprofil. Auf der ersten allgemeinen Nutzerversammlung am 27. 03. 02 wurde daher vom wissenschaftlichen Geschäftsführer des DKRZ, Prof. G. Brasseur vorgeschlagen, ein Nutzerkomitee zu bilden. Vertreter aus 10 Einrichtungen trafen sich am 13.05.02 zu einer konstituierenden Sitzung des Komitees. Dabei wurden Wünsche und Anforderungen der einzelnen Wissenschaftlergruppen an das DKRZ formuliert. Ein Protokoll dieser Sitzung, wie auch der zweiten Sitzung des Komitees, welche im Anschluss an die Nutzerversammlung am 10 September stattfand, findet man unter

http://www.dkrz.de/DUG.html

Das Komitee versteht sich als Interessenvertreter aller Nutzer. Daher ist es offen für die Mitarbeit weiterer Vertreter aus Einrichtungen, die bisher noch nicht vertreten sind.

Auf der ersten Sitzung wurde ich zum Sprecher der Gruppe gewählt, Heinke Schlünzen von der Universität Hamburg zu meiner Stellvertreterin. Ich arbeite seit mehreren Jahren am Rechenzentrum des AWI. Neben Ozeanmodellierung bilden Parallelisierung und Numerik die Schwerpunkte meiner Arbeit. Meine Aufgabe im Nutzerkomitee sehe ich darin, die Interessen der unterschiedlichen Nutzer gegenüber dem DKRZ zu vertreten. Bei auftretenden Probleme stelle ich mir eine Art von Hierarchie für die Bearbeitung vor:

1) Zunächst einmal nimmt der einzelne Nutzer Kontakt mit der Beratung des DKRZ auf und stellt sein Problem dar. In den meisten Fällen wird sich in diesem Schritt sicher eine Lösung finden lassen.

2) Sollte das DKRZ auf diesen Kontakt nicht angemessen reagieren, so kann sich der Nutzer entweder an das Nutzerkomitee wenden (entweder den Vertreter aus der eigenen Einrichtung oder direkt an mich). Wir werden dann zu untersuchen haben, inwiefern das Problem allgemeinerer Natur ist und vielleicht noch mehr Nutzer davon betroffen sind. Diese Kategorie von Problemen oder auch Wünschen an das DKRZ können wir sammeln und zu den Sitzungen des WLA vorher schriftlich einreichen, damit dann dort darüber beraten werden kann. Damit wird dem Anliegen ein wesentlich stärkeres Gewicht verliehen, als es für den einzelnen Nutzer möglich wäre.

Ich wünsche mir, dass wir auf diesem Wege eine gute Zusammenarbeit zwischen dem DKRZ und allen Nutzergruppen finden werden. Vorschläge, wie wir unsere Arbeit verbessern können, und aktive Mitarbeit in Nutzerkomitee ist jederzeit willkommen.

News from WLA

On June 27, the Scientific Steering Committee (WLA) had its 5th meeting at PIK in Potsdam. The meeting focused mainly on the implementation of the new HLRE hardware and on the question how these powerful resources could be used in the most effective way by the scientists. Procedures were discussed for assigning resources to research groups which guarantee an efficient usage of these resources but do not hamper the scientific work.

The WLA also elected a new executive board for a period of two years. Prof. Hans von Storch is the new chairman and Prof. R. Klein is vice chair. The third member of the executive board is Prof. U. Schumann. The minutes of the WLA-meetings are available (in German) at :

http://www.dkrz.de/WLA.html

Events

Upcoming: On February 20/21 2003 the Second Workshop on the Community Climate Model will be held in Hamburg. Two years after the 1. Workshop in Bremerhaven, a survey on what progress has been made and what are the main difficulties should be done. For more information on both the 1. Workshop held in Jan. 2001 and the up coming 2. Workshop please refer to ***www.mad.zmaw.de/Aktuelles***

Past: On October 24, a workshop on current and planned usage of the HLRE was organized by WLA, DKRZ and M&D in Hamburg. The current top users of DKRZ presented their scientific projects benefiting from the resources that are provided by DKRZ and M&D. Please refer to the agenda of the workshop (in German) at

www.dkrz.de/WLA-WS.html

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The DKRZ provides expertise and consultancy in visualization and animation of simulation data. In cooperation with user groups we produce high end visualisation and videos in broadcast quality. Shown here is a snapshot of a simulation with the chemical transport model MOZART (Model of Ozone and Related Tracers) studying the photo chemical formation of ozone as a consequence of the Sydney fire (Dec. 01 / Jan. 02) Displayed are wind field and the ozone anomalies mapped to an isosurface of the CO anomaly. Data courtesy of Max-Planck-Institut für Meteorology (J. Hölzemann, M. Schultz). Visualisation DKRZ (M. Böttinger).