Number 1 : 2007

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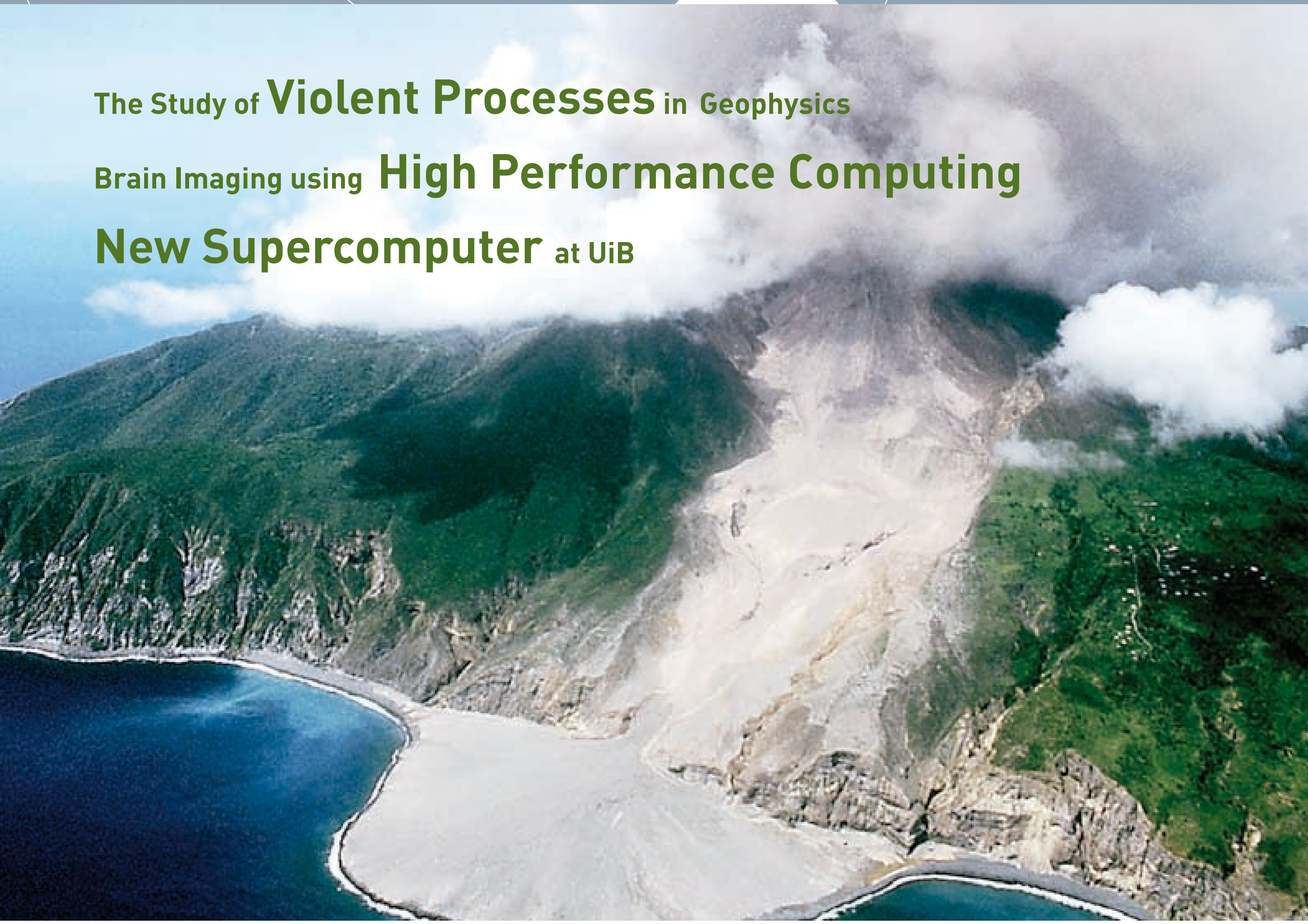

The Study of **Violent Processes** in Geophysics

Brain Imaging using **High Performance Computing**

New Supercomputer at UiB

notur The Norwegian metacenter for computational science

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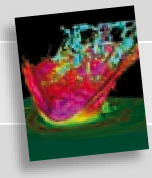
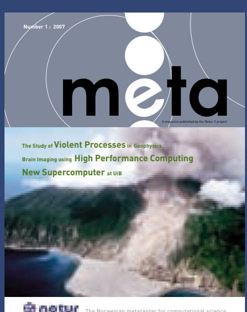


Cover picture: The Soufriere Hills volcano on the Caribbean Island Montserrat



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EDITORIAL

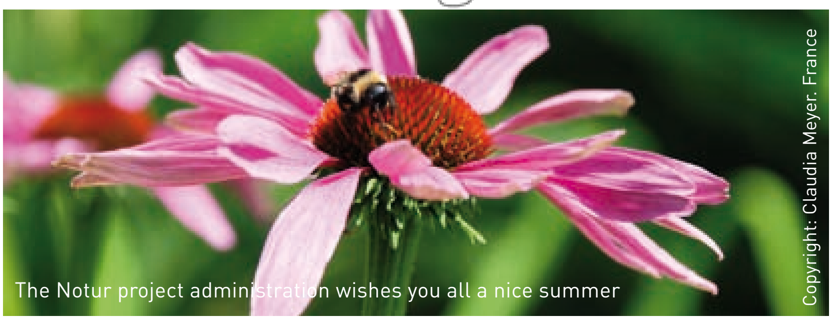
A number of exciting events have taken place since the last issue of META.
Early this year, the eVITA programme on e-Science and e-Infrastructure from the Research Council of Norway approved the establishment of the NorGrid project that will connect several computing and storage resources in Norway with grid middlewares. The project will represent Norway as part of international grid projects. It will also take care of the Norwegian commitments towards CERN for the analysis and storage of large amounts of data that will be generated by CERN's Large Hadron Collider later in 2007.

In April, the eVITA programme approved considerable extra funding for new investments in the national infrastructure for computational science. The extra funds enable the Notur project to establish new large computational resources in 2007. The University of Oslo is currently expanding its compute cluster (titan) by adding seven new racks with more than 200 nodes. The University of Bergen recently concluded an open procurement process and will install a large Cray XT4 system before the end of this year. The new facilities will be made available to all groups involved in education and research at Norwegian universities, colleges and research institutes through the Notur project. The new resources will represent a dramatic boost in the computational power that is provided to the Norwegian research community.

Another focus area is storage of scientific data. A new project will be established with the objective to establish and operate an infrastructure that provides non-trivial services to scientific disciplines for which storage and publication of digital data is crucial. The infrastructure will provide transparent access to distributed storage resources, provide large aggregate capacities for storage and data transfer, and optimize the utilization of the overall resource capacity. The storage infrastructure will however be an integrated part in the national e-Infrastructure and will be connected to the compute systems, networks, and other data storage systems that are located at several major centers in Norway.

Norway also joined the Partnership for Advanced Computing in Europe (PACE). PACE brings together the supercomputing centres of fifteen European countries, with the goal to strengthen European research, engineering and science by the establishment of so-called Petaflop (1000 Teraflops) systems from 2010. Petaflop systems are more than fifteen times larger (in peak performance) than the largest supercomputer that is currently in operation in Europe and are indispensable to secure Europe a competitive role in pioneering research.

In this issue of META and issues later this year, more information will be given about these new activities and resources.



The Notur project administration wishes you all a nice summer

FEATURES

PACE Initiative secures Europe's supercomputing

As of 2010, European researchers will have access to a European High Performance Computing ecosystem that includes some of the world's leading supercomputers, thanks to the new 'Partnership for Advanced Computing in Europe' (PACE).

AUTHOR

Jacko Koster
Managing Director,
UNINETT Sigma

In 2006, the European Strategy Forum for Research Infrastructures (ESFRI) identified High Performance Computing as a strategic priority for Europe. Scientists and engineers must be provided with access to capability computers of leadership-class to remain competitive internationally and to maintain or regain leadership. Supercomputers are an indispensable tool to solve the most challenging problems through simulations and enable researchers to create and improve knowledge about complicated problems in a way that is not possible with the help of traditional research methods as development of theory and physical experiments in laboratories. In addition, the need for more compute resources and therefore bigger computers is rapidly increasing within many scientific fields, and there exist important, but complicated scientific problems which only can be solved with the help of compute resources that are too costly to be financed by one single country alone. Many scientists within Chemistry, Physics,

Representatives from the different countries which signed the Memorandum of Understanding for the new PACE-Initiative.

future

Geoscience and Medicine are already today totally dependent on compute intensive simulations to advance their research.

A task force for High Performance Computing for Europe developed in 2006 the fundamental concepts proposed by ESFRI to create a true pan-European Research Infrastructure named Partnership for Advanced Comuting in Europe or PACE for short. The PACE initiative brings together the supercomputing centres of 14 European countries. At a ceremony in Berlin on April 17, the partner countries signed a Memorandum of Understanding that defines the PACE partnership. The countries involved are Austria, Finland, France, Germany, Greece, Italy, Norway, Poland, Portugal, Spain, Sweden, Switzerland, the Netherlands and the UK. On the basis of the MoU, the PACE consortium submitted in May, a project proposal to Europe's Research Framework Programme 7.

By joining the PACE consortium, Norway is actively involved in international cooperation within supercomputing for research and education. The aim of the PACE collaboration is to provide scientists in Europe with optimal access to supercomputing and significantly boost the knowledge, development and availability of hardware and software technologies in this area. The PACE collaboration will contribute to a European High Performance Computing ecosystem by establishing a number of very powerful capability resources, so called Tier-0 systems, that have a computing power that is significantly larger than the largest supercomputer owned by any of the partner countries alone. Tier-0 resources are expected to be in the petaflop range and can perform more than 1.000.000.000.000.000 operations per second and as such provide at least ten times more computing power than today's biggest computers in Europe.

According to the terms of the Memorandum of Understanding, the partners will use the next two years to define and implement the process leading to establishment of the European HPC Tier-0 infrastructure. In this preparation phase, which will run up until 2010, the organisational framework will be created for the Tier-0 infrastructure. This includes the management structure, a legal basis for the cooperative relations and guidelines concerning the software developments and hardware technologies that are needed. The organization and management structure should become a strong umbrella to foster further pan-European infrastructure projects. As HPC technology requires continuous evaluation and development, the preparation also involves putting in place a market and technology awareness programme in order to define and evaluate prototypes and conceptual designs of the key hardware and software elements, with due consideration to developing the European potential in HPC. PACE will prepare the deployment of petaflop systems in 2009/2010 by procuring prototype systems that will be used for porting and benchmarking libraries and codes from major scientific user communities, as well as for evaluating technical requirements and procurement procedures. The preparatory phase will also establish collaborations with the European IT-industry to influence the development of new technologies and components that are promising for petaflop systems to be procured after 2010.

With the MoU, the partners also aim to promote the utilization of the envisaged infrastructure for scientific and industrial goals requiring HPC resources above those available in member states. The consortium will promote the development of grand challenge applications, while a scientific steering body and peer review process will ensure that the infrastructure will be used for excellence and competitiveness in science and engineering as well as optimal usage of the resources.

The best part of the costs of the project after 2010, estimated at around €400 million, is to be met by the participating countries. The national funds are supplemented by the European Union through Research Framework Programme 7.

Nordic Computational Grand Challenge Survey

In the autumn of 2006, the Nordic research community was invited to identify 'Grand Challenge' problems in science that are considered important to the research community and whose solutions require access to large scale computational or storage resources for an extended period of time. The goal was not to obtain a listing of already existing projects, but to encourage scientists to describe well-defined scientific problems that will be of significant importance in their fields of research in the coming years. The invitation offered scientists the possibility to describe research objectives independently of any limitations in nationally available resources.

The survey was commissioned by the Danish Agency for Science, Technology and Innovation, the Finnish IT center for Science CSC, the Research Council of Norway, and the Swedish Research Council.

A total of thirty-four Grand Challenge problems were received. The Grand Challenges come from a variety of disciplines, including earth sciences, biosciences, physics, fluid dynamics and chemistry. A considerable number of submissions were supported by research groups from three or four countries. The responses indicate that there is an interest within the Nordic research community for support of Nordic collaborations to tackle large computational and multi-disciplinary problems. Also increased collaboration between the projects and organizations that are responsible for providing the national infrastructures for computational science should be encouraged such that large aggregate resources can be provided to research communities that address large-scale problems.

The final report can be downloaded from www.notur.no/publications.

Brain Imaging and Computa
using High Performance an

Segmentation and quantification of brain tissue and brain anatomy from 3D magnetic resonance image (MRI) acquisitions is currently being applied worldwide in studies of the human brain and represents a clinically important and very competitive field of research.

AUTHORS

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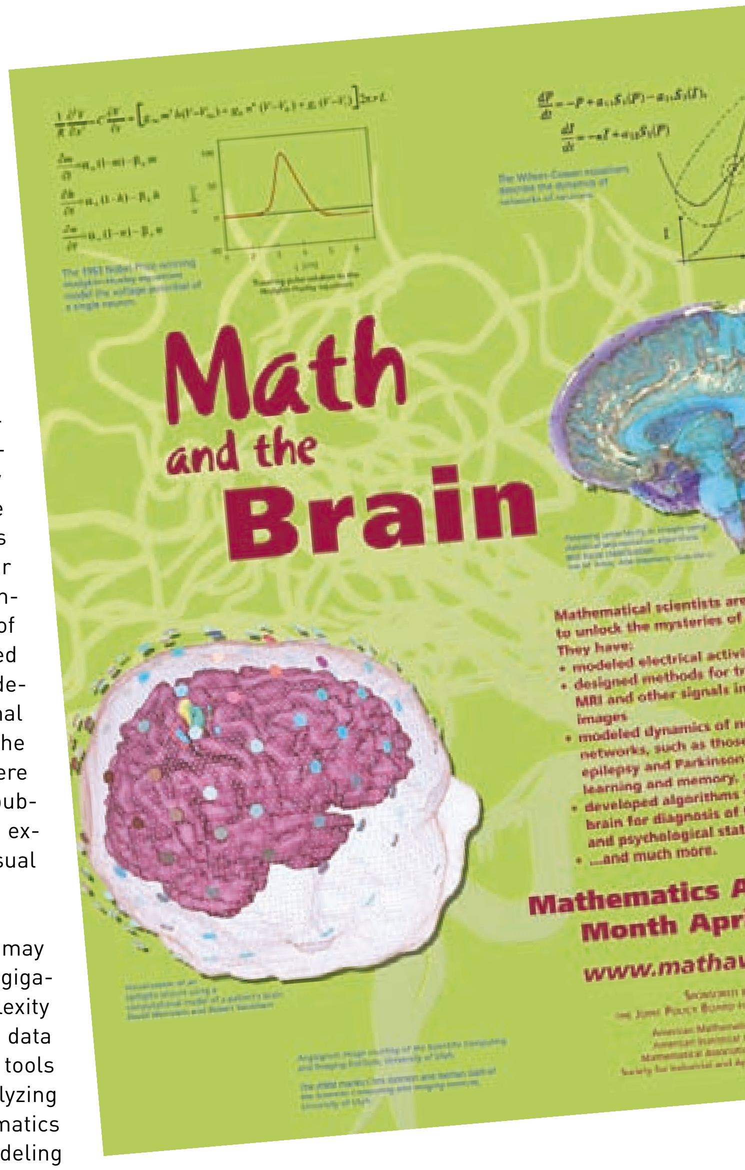
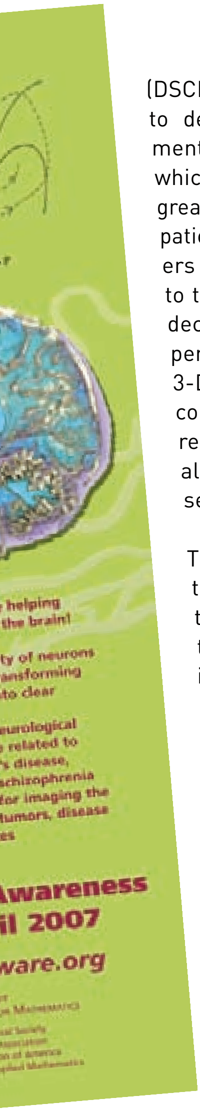
Recently, the American Statistical Association, the Mathematical Association of America, and the Society for Industrial and Applied Mathematics defined the theme for the Mathematics Awareness Month 2007 to be 'Mathematics and the Brain', with spcial emphasis on brain imaging. Imaging methods depend heavily on mathematics and computational tools, and image-based computational neuroanatomy has emerged over the last decade fueled by advances in differential geometry and statistics [14, 15]. One of the main directions in mathematical imaging during the last decade, with numerous applications in brain imaging, is the use of partial differential equations (PDEs) and level-set methods [3, 6], where also the Bergen Image Processing Group, BBG has made contributions [19,21]. While each imaging modality uses different mathematical methods, the challenge is to combine and process raw sensor data to form coherent and meaningful images and local tissue information. Many new imaging methods are used to study properties of the brain. A spectacular imaging modality for non-invasive assessment of brain function, is so-called blood oxygenation level dependent contrast functional MRI (BOLD fMRI), where the Bergen fMRI-group were pioneers in Scandinavia publishing their first fMRI experiment on primary visual processing in 1995 [18].

A typical fMRI experiment may collect as much as one gigabyte per hour. The complexity and sheer volume of the data require new mathematical tools for processing and analyzing the information. Mathematics plays a central role in modeling activation of various regions of the brain and the interaction among these regions. Another modality, assessing the blood flow and blood volume in the brain, voxel-by-voxel, is perfusion MRI. An important computational topic in first pass dynamic susceptibility perfusion imaging



The theme for Mathematics Awareness Month 2007 was 'Mathematics and the Brain' (www.mathaware.org), with special emphasis on brain imaging.

tional Neuroanatomy
d GRID Computing



(DSCMRI) is deconvolution, necessary to derive quantitative flow measurements from the image time series, which together with diffusion MRI has great diagnostic and prognostic value in patients with acute stroke. Researchers in Bergen have contributed also to this field, introducing novel (blind) deconvolution approaches to improve perfusion estimates [16], and a novel 3-D tracer kinetic model based on conservation of mass [20]. Magnetic resonance imaging techniques also allow for the measurement of water self diffusion in the brain.

This modality is denoted diffusion tensor MRI (DT-MRI) and has attracted a lot of attention both in the neuroscience community and in the applied mathematics community. In DT-MRI each voxel is assigned a tensor, where the tensor is used to non-invasively analyze the microstructure of white matter in the brain and to perform fiber tracking from the computed 3D vector field of principal diffusion directions. The Bergen Image Processing Group has been working with processing of recorded DT-MRI data for some years, including noise filtering and multi-tensor estimation and tracking [5, 17], and a natural next step is to include HPC in this research, e.g. [4, 8].

The aging brain

Our project on aging deals with data and research problems from a larger study related to cognitive aging, brain function and genetic markers. Another upcoming application (that we will not deal with any further in this short review) is related to local brain volume changes due to electroconvulsive therapy (ETC) in severely depressed patients. The effects of aging on the brain are widespread and have multiple etiologies. Genetics, neurotransmitters, hormones, and experience all have a part to play in brain aging. Aging has its effects on molecules, cells, vasculature, gross morphology, and cognition. As we age, our brains shrink nonuniformly, particularly in the frontal cortex and in several subcortical structures [22]. It has been reported that the volume of the brain and/or its weight declines with age at a rate of around 5% per decade after the age of 40. The shrinking of the grey matter is frequently reported to stem from neuronal cell death but whether this is solely responsible or even the primary finding is not entirely clear. As our vasculature ages and our blood pressure rises the possibility of stroke and ischemia increases and our white matter develops lesions. Memory decline also occurs with aging and brain activation becomes more bilateral for memory tasks. This may be the brain's attempt to compensate and recruit additional networks, or because specific areas are no longer easily accessed. It has been

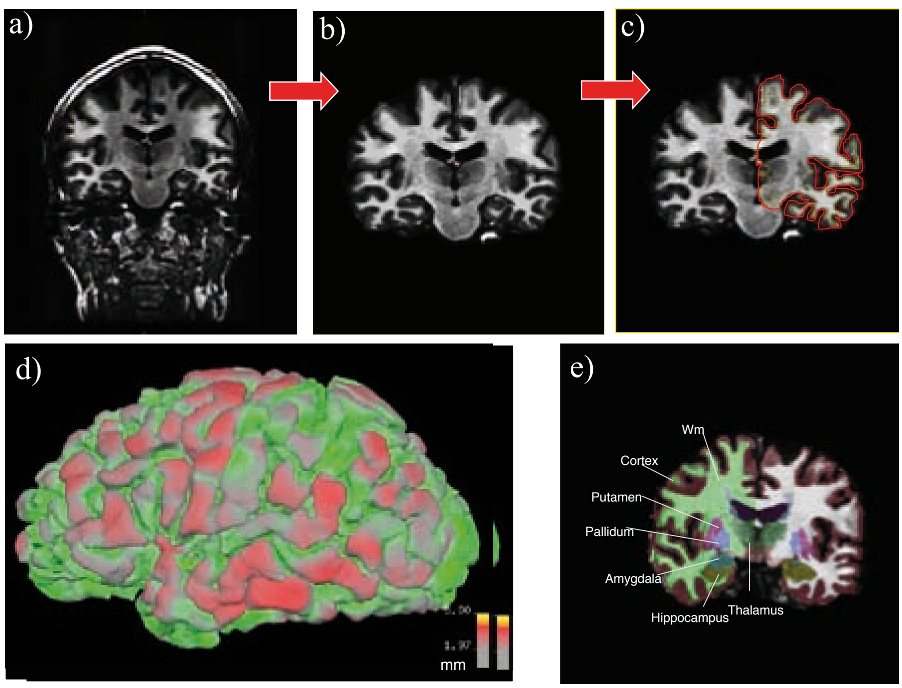


Figure 1: FreeSurfer workflow.
a) Original volume.
b) Skull stripped & normalized volume.
c) Grey matter (GM) / white matter (WM) boundary (green); pial boundary (red).
d) Cortical thickness map, representing the local distance between the two surfaces derived from the GM/WM boundary and the pial boundary.
e) Subcortical segmentation showing important subcortical grey matter nuclei.

shown that there is a relationship between cortical thickness and cognitive function in higher age [13]. While a close relationship between cognitive function and cortical thickness was found, only very small effects were observed for socalled executive functions. Findings indicate that both cortical preservation and, to some extent, thickening may be necessary to ensure optimal cognitive aging. Both processes are detectable by morphometric methods using a tool like FreeSurfer.

Data recorded in Bergen and Oslo

The brain image acquisitions being used in the present project were partly acquired on a 1.5 Tesla GE Signa Echospeed MR scanner at Haraldsplass Deaconess University Hospital in Bergen, with a standard 8-channel head coil. Up to now, we have successfully processed dual-volume SAG T1 3D FSPGR IR prepared sagittal acquisitions (TR/TE/TI/FA=9.5/2.2/450/7o with voxel-size 0.94×0.94×1.4 mm3) from 93 subjects. These MRI data are also an essential component in the French- Norwegian AURORA project, 'Brain tissue segmentation and morphometry from dual volume 3D magnetic resonance images - comparison of methods', where the objective is to test new methods and compare state-of-the-art software for brain tissue segmentation and brain morphometry. In addition, we have brain MRI data (dual volume MP-RAGE, segmented with the same software tools) acquired in Oslo, from more than 80 subjects [9, 10].

Open access datasets

Similar MRI brain data sets are now publicly available at the Open Access Series of Imaging Studies, OASIS under a liberal Data Use Agreement provided by Dr. Randy Buckner at the Howard Hughes Medical Institute at Harvard University, the Neuroinformatics Research Group at Washington University School of Medicine, and the Biomedical Informatics Research Network, BIRN.

Thus, the international brain imaging community are partly adopting the Open Data philosophy and practice (http://en.wikipedia.org/wiki/Open Data). BIRN is a geographicaly distributed virtual community of shared resources offering tremendous potential to advance the diagnosis and treatment of disease, and is changing how biomedical scientists and clinical researchers make discoveries by enhancing communication and collaboration across research disciplines. The BIRN initiative was among the winners of the annual Readers and Editors' Choice Awards at the IDG GridWorld Washington DC conference in September last year. One of the larger datasets in OASIS (16 GB) consists of a cross-sectional collection of 416 subjects aged 18 to 96. For each subject, 3 or 4 individual T1-weighted MRI scans obtained in single scan sessions are included. The subjects are all right-handed and include both men and women. One hundred of the included subjects over the age of 60 have been clinically diagnosed with very mild to moderate Alzheimers disease (AD). Additionally, a reliability data set is included containing 20 non-demented subjects imaged on a subsequent visit within 90 days of their initial session. Such data collections in the public domain allow research groups with competence in image processing and data analysis, but without direct access to medical MRI-scanners, to contribute to the development of quantitative neuroimaging methods.

Software and data analysis

For the project on aging we are currently applying semi-automated state of the art methods as implemented in the FreeSurfer software package [7, 11, 12], developed at Athinoula A. Martinos Center for Biomedical Imaging, Harvard Medical School / MIT and freely available for downloading (http://surfer.nmr.mgh.harvard.edu) to segment different morphological and functional areas of the brain. This information, including volumes of specific brain regions such as the hippocampus, regional cortical thickness, and total gray matter and white matter, is then correlated to genetic markers (APOE [alleles: e2 e3 e4], CHRNA4 [T C], and BDNF [val met]) and results from extensive neuropsychological testing,

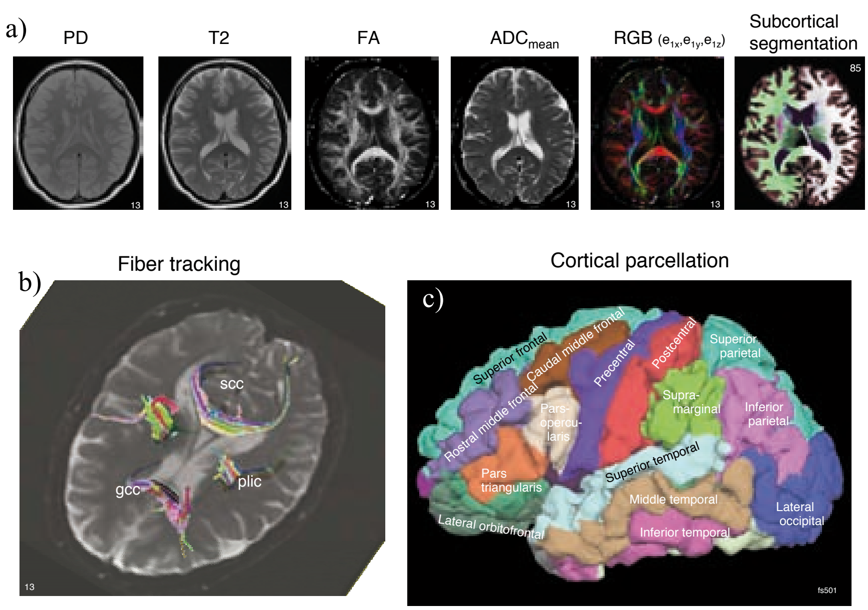


Figure 2: Segmentation and visualization of multispectral MRI acquisitions (dual volume structural 3D MRI and DT-MRI). a) Coregistered multispectral images from axial slice #13. b) Reconstructed fiber tracts from the DT-MRI recordings (scc = splenium corpus callosum; gcc = genu corpus callosum; plic = posterior limb of internal capsule). c) Color-coded cortical parcellation obtained automatically from FreeSurfer processing.
(Modified from [1])

e.g. WASI (IQ), CVLT (verbal memory), and PASAT (attention), obtained from the subjects participating in the aging study. Apart from non-trivial statistical analysis, a limiting factor in this research is computational resources. This is because the FreeSurfer processing chain of a single 3D dataset consumes about 22-26 hours on a hig-hend Linux workstation - and there are more than 200 datasets to be analyzed. Storage of data from one subject, including original image data and results generated during the work-flow, consumes about 300 MB. A particular challenge for a high-throughput, or a high performance processing chain is to make temporary results available to the end user for inspection and possible correction of segmentation failures before the next series of iterative algorithms are put into execution. Basically, for sequential processing of subjects with FreeSurfer on a single workstation, there should be a pause in the processing chain after about 30 min for the end user to check the quality of the Talairach transform and the skull stripping (Fig.1b). Then, a second break after about 14-16 hours, for checking the white and pial surfaces (Fig.1c), and then, a final inspection after about 5-8 hours with automated topology fixing and surface reconstruction (Figs. 1d and 2c). When manual corrections are needed, a whole segment of the processing chain has to be re-executed, extending the total processing time substantially. If the project is successful, the quantitative segmentation results together with the neuropsychological test data and the genotyping will provide important information about the human brain during normal and abnormal aging.

Current status of the project is reported in [1,2], and further processing will now take place at the HPC facility at Parallab in Bergen with advanced user support from NOTUR II. A GRID portal for FreeSurfer processing is also under construction [2]. Such technology might facilitate routine use of advanced quantitative imaging procedures, leading to better clinical diagnosis, prognosis and follow up in broad range of patients with brain pathology or neuropsychiatric disease.

RELEVANT LINKS

- Mathematics Awareness Month 2007: http://www.mathaware.org
- Bergen Image Processing Group, BBG: http://math.uib.no/BBG
- Bergen fMRI-group: http://fmri.uib.no
- Research related to cognitive aging, brain function and genetic markers: http://www.braingenetics.org
- The French-Norwegian AURORA project: http://www.isima.fr/aurorawiki
- The Open Access Series of Imaging Studies, OASIS: http://www.oasis-brains.org
- Neuroinformatics Research Group at Washington University School of Medicine: http://nrg.wustl.edu
- Biomedical Informatics Research Network, BIRN: http://www.nbirn.net

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Violent Processes in Geophysics

There is a book on my shelf with a title that now seems odd: ***Tsunami: The Underrated Hazard*** by Ed Bryant, published in 2001. After the tragic event of December 26, 2004, no one underrates the tsunami hazard. That day, a massive earthquake along the Andaman-Sumatra fault west of Indonesia triggered a tsunami that killed over 200,000 people in a region almost wholly unprepared for such an event. Bryant's book was intended to awaken a complacent public to this danger, but it took one of the deadliest natural disasters in human history to accomplish that.

AUTHOR

Galen Gisler
Researcher at the Centre for Physics of Geological Processes, University of Oslo

Simulation of tsunamis

I began studying tsunamis in the winter of 2002. My group at Los Alamos National Laboratory had just developed a powerful new computational tool, the adaptive-grid Eulerian hydrocode SAGE, for use in geophysics, astrophysics, and dynamic experimentation. The developers of the code needed an application of public interest to test it on and to showcase its capabilities. A workshop on tsunamis was being held that May in Hawaii, and that seemed an appropriate target to aim for.

Knowing little about the subject, we (with my Los Alamos colleagues Bob Weaver and Mike Gittings) began a series of calculations in two- and three-dimensions to simulate tsunamis that would be produced by the impact of asteroids into the ocean. Not surprisingly, we found that such an impact would produce an enormous splash, sending water (and particularly water vapour) to considerable heights in the stratosphere (Figure 1). On the other hand, the tsunami that resulted after the initial splash subsides turned out to be weaker in our computations than had been anticipated. The very violence of the process consumes and dissipates energy, and the waves produced by an impact decay much more quickly than seismically-induced tsunamis (Figure 2). Nearby coasts would be endangered by such an impact, of course, but unless the asteroid were very large indeed, the ocean basin would not suffer a catastrophic tsunami comparable to the Indian Ocean event of Boxing Day 2004.

Our result was by no means universally accepted. Five years later, at a recent conference in Washington DC about defending the earth against asteroids, tsunamis were still being regarded as the most serious danger from impacts. My talk at that conference apparently only injected momentary uncertainty ("more study is needed") into the dialogue.

That was my initial foray into geophysics — I was trained as an astrophysicist. But I was intrigued, and continued studying tsunamis and other violent geophysical events. This relatively new interest of mine led me to join the Centre for the Physics of Geological Processes (PGP) at the University of Oslo in April 2006.

The study of violent processes

There are few places on Earth that are untouched by signs of previous violence. Indeed all of our present landscape is formed in crucibles of varying intensity and duration. A profound and perhaps disturbing aspect of our aesthetic psychology is this: The more beautiful the landscape, the more violent the processes that caused it to come into being (Figure 3).

How do we study the violent processes that have shaped Earth's crust? As a species, we have witnessed a mere sample of them: volcanic eruptions that have obliterated whole islands (Santorini, Krakatau) and destroyed cities (Vesuvius, Soufriere Hills — see Figure 4), and others that have created new islands (Surtsey). Landslides, earthquakes, tsunamis, and floods have changed the topographies of places we have known. The enormous forces at play in Nature's realm are beyond the reach of laboratory physics. Even the greatest explosions produced by mankind in megaton-scale nuclear weapons are dwarfed by the energies of modest volcanic eruptions or earthquakes.

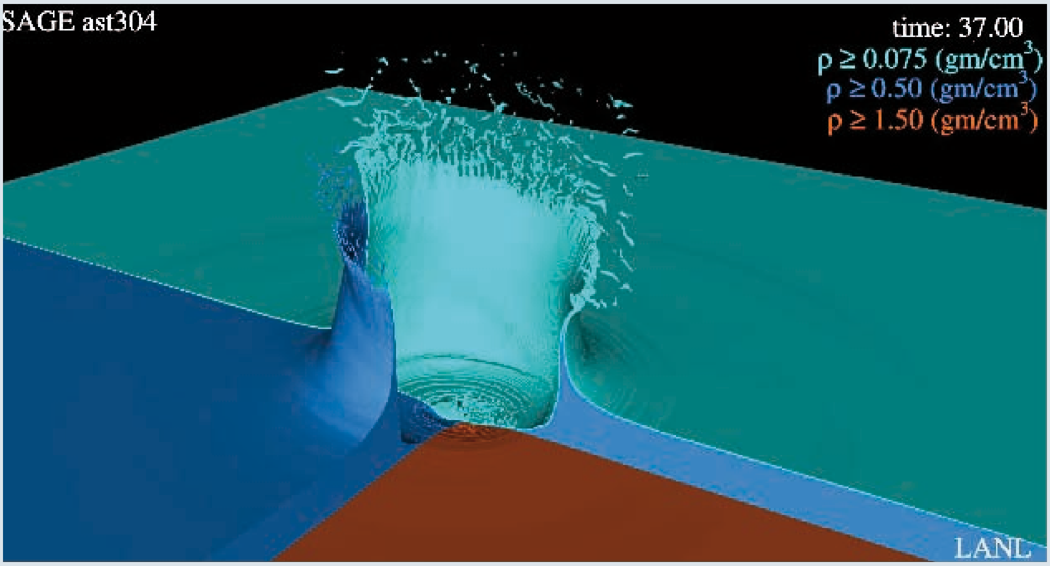


Figure 1. The splash resulting from the impact of a large asteroid into a 5-km deep ocean reaches high into the stratosphere. The impact was at a 45-degree angle, from the right, yet the transient water crater is very nearly symmetric. The ocean floor in this threedimensional calculation is slightly dimpled. The calculation was done with the Los Alamos adaptive grid Eulerian code SAGE, using four materials: air, water, basalt for the ocean floor, and iron for the asteroid, 1 km in diameter. A significant quantity of water was vaporized in the initial impact event. In this and figure 2, we display three isosurfaces chosen to show the basalt floor, the bulk water, and the air/water mixed cells.

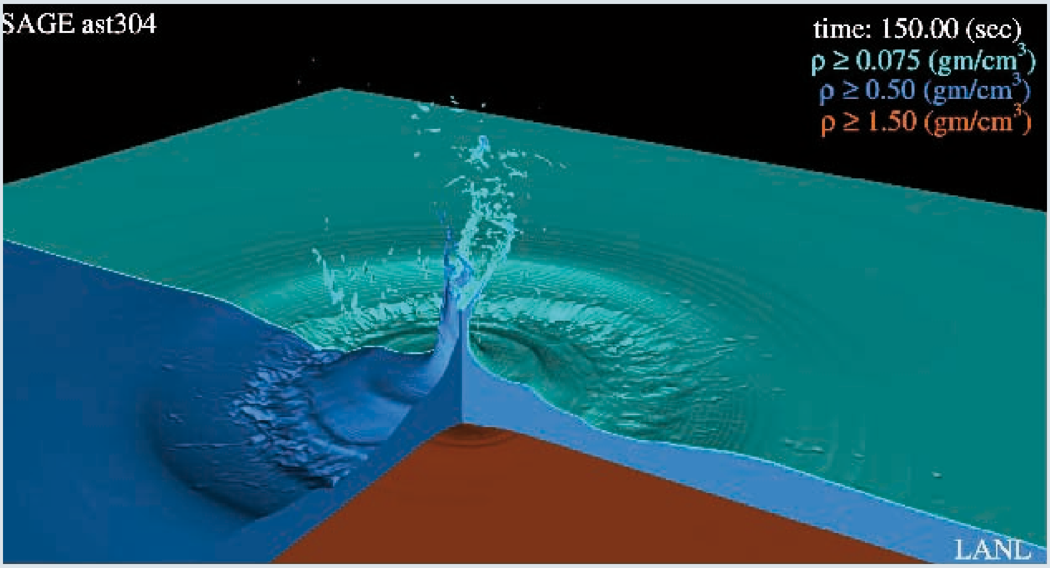


Figure 2. After the transient crater collapses and the splash subsides, a strong wave propagates toward distant shores but with wavelength much shorter than for tsunamis of seismic origin. The short wavelength implies less efficient long-distance propagation, and greater dissipation by interaction with the violently disturbed atmosphere. Asteroids of less than 500 m diameter would not pose a significant danger to shores more than 1000 km away, according to our calculations.

Figure 3. Crater Lake, Oregon, was produced by the violent collapse of a volcano nearly 8000 years ago. The cone called Wizard Island was formed several hundred years later in a smaller eruption. Hydrothermal activity continues to this day at the bottom of the lake.

Figure 4. The eruptions of the Soufriere Hills volcano on the Caribbean island of Montserrat during 1995-1997 forced the evacuation of the southern half of the island and caused the destruction of the former capital, Plymouth in the southwestern part of the island. Because of careful monitoring and planning, the vast majority of the affected population were able to escape. This photograph was taken as the International Space Station flew north of the island on 9 July 2001 (digital photograph number ISS002-E-9309, from NASA).

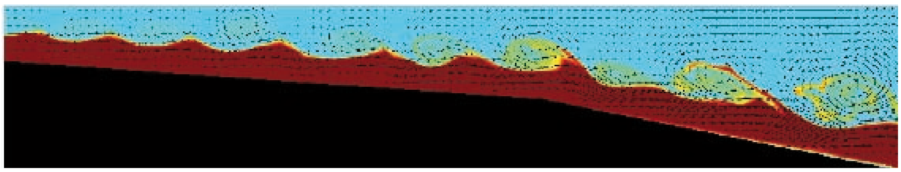


Figure 5. This portion of a frame from an underwater landslide simulation shows the early development of turbidity currents as slide material (red) mixes with water (blue). The turbidity currents are driven by an instability that depends on the inertia and viscosity of the two fluids. The wavelength of turbidite deposits left behind on the seafloor may be a diagnostic of the slide rheology.

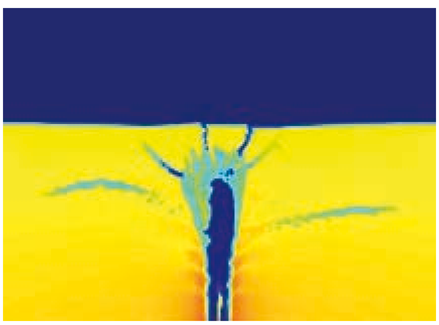


Figure 6. A sudden injection of hydrothermal energy, in the form of hot water, at the base of a weak column of material in Martian basalt, would produce a network of fractures that propagates up to the surface and releases volatiles to the atmosphere. Hydrothermal vent complexes may be easier to form on Mars than on Earth because of the lower surface gravity, so finding them could be an important diagnostic of the history of water on the planet.

We do study scaled-down examples of these violent events in experiments conducted in laboratories or in suitable outdoor settings with explosives and guns, and these help us to understand the physics and material properties that are involved. Scaling our understanding from the laboratory up to the sorts of events that shape Earth's crust requires the use of computational physics. The hydrocode SAGE, developed by a partnership of the Los Alamos National Laboratory and Science Applications International, is proving to be a highly useful tool in this area. It is a multi-material fluid code, which means that the fluid equations of motion are solved for a mixture of different materials. Each material is distinguished by its own equation of state, specifying what its density, elasticity, and rigidity are at given temperature and pressure. Materials start out in separate regions of the calculation, having different initial temperatures, pressures, and velocities. As the calculation evolves, they mix and exchange energy and momentum. SAGE is a finite difference code, with the equations solved on an Eulerian grid, but the grid is allowed to adapt according to gradients in material properties, focusing the computational power on places within the calculation where it is most needed for physical fidelity.

SAGE runs on a variety of platforms from laptop or desktop machines to clusters with thousands of cores. It has recently been ported to machines here in Norway for use by PGP scientists. I show here some simulations of violent geophysical events that I have done with this code.

Tsunamis caused by landslides are of concern in Norway because of events like the Tafjord landslide tsunami in 1934 and the great Storegga undersea slide 7000 years ago. Undersea landslides frequently leave remains on the sea floor known as turbidites, layered deposits from the turbidity currents in the mixed slurry that produced the slide. With our Los Alamos collaborators we have been investigating how the spacing of layers in turbidites may depend upon the constitutive properties of the slide material (Figure 5).

Some past episodes of climate change on Earth may have been triggered by rapid

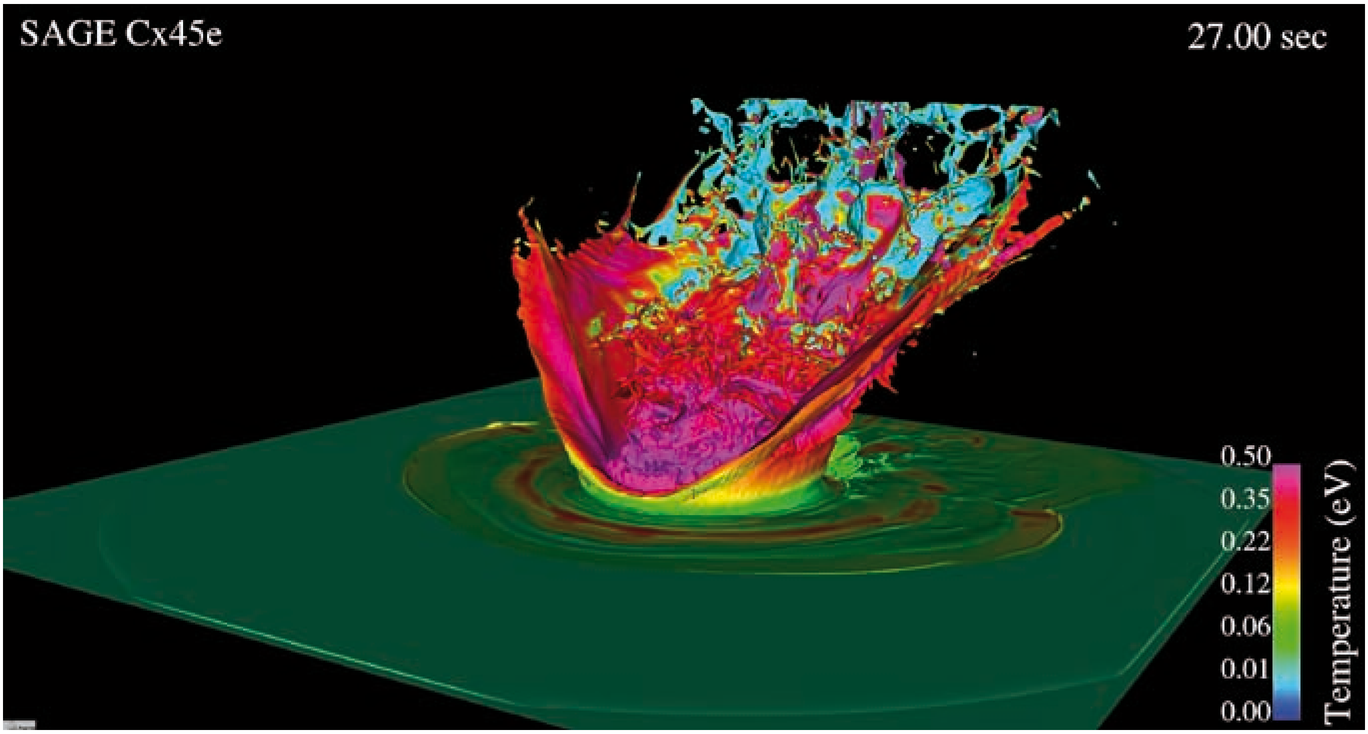


Figure 7. The impact of a large asteroid into a carbonate platform ejects trillions of tonnes of hot volatile material into the stratosphere. Here the impactor was a 10 km diameter asteroid coming in at an angle of 45 degrees from lower left. We are looking at an isosurface of density coloured by temperature in electron volts (one electron volt corresponds to a temperature of 11604 degrees Kelvin). The impact associated with the end of the Cretaceous period left a crater at Chicxulub, Mexico, in one of the most extensive carbonate platforms then in existence on Earth. The upper layers of the target are extremely volatile under the conditions of an energetic impact, and contained chemicals that contributed to a severe climate change and poisoning of the atmosphere.

releases of gases from hydrothermal vent complexes, related to large-scale volcanic activity, and linked to episodes of mass extinction. These complexes are actively being studied by scientists at PGP through fieldwork and modeling. We have recently undertaken modeling of these complexes to compare how such complexes might evolve differently depending on properties of the host rocks. One such study has prompted us to suggest that venting from such complexes might have been more common on Mars in the past if the planet had water to support them (Figure 6). Thus a search for signs of hydrothermal activity on Mars might lead to important new insights on the history of water on Mars and thus its potential for having supported life at one time.

One of the greatest mass extinction events in geological history occurred at the end of the Cretaceous period, when all of the dinosaurs, ammonites, and many other land and marine families became extinct. Over the last three decades, the impact of a large asteroid onto the carbonate platform of Mexico's Yucatan Peninsula has emerged as the prime culprit for that extinction event. Since early 2003 my Los Alamos colleagues and I have done three-dimensional simulations of that event in order to learn what the angle of impact and the energy of the projectile were (Figure 7). So far we have concluded that the angle had to be fairly steep in order to excavate the amount of material accounted for in the worldwide distribution of ejecta, and that the kinetic energy of the projectile had to be in excess of 100 million megatons.

The study of violent processes such as these helps us to interpret Earth's history as it is written in the rocks. A side benefit is an increase in our ability to exploit geological resources for societal needs. But perhaps most importantly this study helps us to understand the hazards that may befall Earth in the future and to protect lives and environments.

The new supercomputer will be located in The High Technology center at the University of Bergen.
Copyright: Jan Kåre Wilhelmsen, UiB.

A new 5
comput

About BCCS

The Bergen Center for Computational Science (BCCS) is a department of UNIFOB AS, affiliated with the University of Bergen. BCCS initiates and administrates externally financed research projects with special emphasis on computational science. BCCS conducts research in computational biology, computational mathematics and scientific computing. A main objective of BCCS is to exploit the synergies between its groups and boost cross-disciplinary activity. Parallab is the high performance computing unit in BCCS that operates and supports the supercomputer facilities hosted by the university. The University of Bergen is partner in the Notur project.
For more information:
http://www.bccs.uib.no/

1 Teraflops Cray XT4 Super-
er for Norwegian research

The University of Bergen and Cray Inc announced on June 18 that the university will acquire one of Europe's most powerful supercomputers.

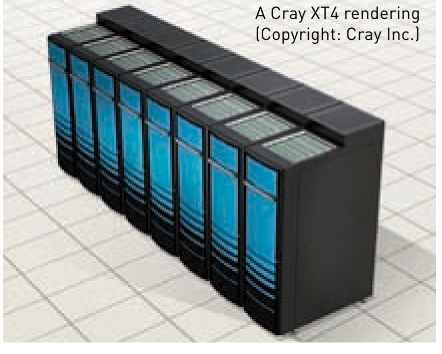
The contract calls for a Cray XT4 supercomputer system with peak performance of 51 teraflops (trillion floating point operations per second) to be installed later this year at the Bergen Center for Computational Science (BCCS). The supercomputer will be used for advanced research in fields including marine molecular biology, large scale simulation of ocean processes, climate research, computational chemistry, computational physics, computational biology, geosciences, and applied mathematics.

"The new Cray supercomputer will increase the computational power available to our broad community of Norwegian and international users by a factor of 100 and will enable them to run much larger and more complex problems," says Professor Petter E. Bjørstad, director of the Bergen Center for Computational Science (BCCS). "The University of Bergen has strategic research initiatives within marine sciences, climate and life sciences that will benefit enormously from this decision."The Cray XT4 will replace the three 32-way IBM p690 nodes (total 499 Gflops) that have been in operation at BCCS since January 2002.

The Cray XT4 supercomputer will not only serve the high-end computational needs of scientists at the University of Bergen. Also research groups at other Norwegian universities and colleges as well as research institutions will get access to the facility. The new supercomputer will also be used for research and development by international organizations, European research groups and research projects, and cooperating scientists from international institutions. Later this year, researchers will be able to apply for access to the facility through the Notur project.

"We are honored that the University of Bergen chose Cray as their partner to provide very high-end computing capability to support the university's extended research community," says Peter Ungaro, Cray's president and CEO. "This decision strengthens our international presence and fortifies the Cray XT4 supercomputer's leadership in meeting the demanding needs of leading-edge scientific researchers for unrivaled performance and scalability." "The University of Bergen award is another major victory that increases Cray's presence in Europe," says Ulla Thiel, Cray Vice President Europe. "We are very excited about this win and look forward to a close collaboration with the University of Bergen to make this supercomputer installation a joint success of BCCS and Cray."

The project is funded by the University of Bergen in partnership with the Research Council of Norway through the Notur project, the Institute for Marine Research, and UNIFOB AS.


A Cray XT4 rendering (Copyright: Cray Inc.)

About the Cray XT4

Building on the success of the Cray XT3 system, the Cray XT4 is a massively parallel processor (MPP) supercomputer purpose-built to deliver exceptional sustained application performance for challenging scientific and engineering problems. Cray's SeaStar2 3D torus interconnect, advanced MPP operating system and high-speed global input/output make it possible for users to scale applications to thousands of processors without performance loss. The system's scalable processing element uses x86 64-bit AMD Opteron processors that employ HyperTransport technology for high bandwidth and reduced latency.
For more information:
www.cray.com/products/xt4/

The Cray XT4 installation at BCCS provides a total of 1388 quad-core compute nodes of which 128 nodes are equipped with 8 GByte memory, while the remaining nodes have 4 GByte memory. The system has a theoretical peak performance of 51.1 Tflops. For storage, a DDN (Data Direct Networks) solution with three double-controllers and a capacity of 288 TByte is used that provides a sustained bandwidth of 6 GByte/s for read/write. The system has an estimated power consumption of 270 kWh. More information about the Cray XT4 at BCCS will be provided in the next issue of META.

NorGrid
- The Norwegian Grid Infrastructure

NorGrid is a newly established project with the aim to develop and maintain a national grid infrastructure for computational science in Norway. The infrastructure will provide grid-based services that enhance the utilization of the existing compute and storage resources in the national infrastructure for computational science provided by Notur and will facilitate the transparent sharing of data between user groups.

Mission
A mature grid infrastructure that unites distributed resources for computation and storage is presently not in place in Norway. To enable the Norwegian research community to benefit from the advances in modern grid technologies and keep up with the developments abroad, it has by now become necessary to create a broad and nationally coordinated grid infrastructure project.

The long term vision of the project is that the resources in the national e-Infrastructure will be accessed through a grid interface. The grid infrastructure will as such connect resources that are located at several major research centers in Norway, including heterogeneous computing systems, data storage systems, networks, and possibly scientific instruments.

The purpose of the project is to:
* deploy and enable the development of new services that add value to the existing e-Infrastructure for computational science.
* enable grid-based calculation and data storage in a broad range of scientific and technological applications.
* help researchers to create and to participate in computational challenges of scope and size unreachable on single facilities alone.

An important task of NorGrid will be to enable scientific applications on the grid. In addition, the project aims to stimulate the adoption of grid technologies in the Norwegian research community, provide a platform that is attractive for grid research and development work in other research projects. The project also aims to reduce the management and organizational overhead of international cooperation around grid computing and related infrastructure projects.

Organization
The project consortium consists initially of NTNU, UiB, UiO, UiT, UNINETT, and UNINETT Sigma. The project consortium includes the major centres in Norway that operate large scale resources that are relevant for the national grid infrastructure and have a wide experience in providing user support, as well as centres that have a wide experience in software development. The diversity and strengths of the individual centres will be exploited as much as possible. UNINETT Sigma is coordinator of the project.

The national grid infrastructure will be built on the existing computational, storage, and network infrastructure.

Collaborations
A major objective of the project is to link the national infrastructure for computational science to relevant projects abroad. Internationally, grid infrastructure projects are being established, grid technologies are being developed and grid applications are being deployed at a rapidly increasing pace and scale. The developments in Europe are to a large extent driven by large collaborations such as EGEE and by the need to process and store the large amounts of data generated by the high-energy physics experiments at the Large Hadron Collider (LHC) at CERN. A worldwide hierarchical WLCG grid infrastructure is being developed for this purpose. The Nordic Data Grid Facility (NDGF) is a collaboration between the Nordic countries. The (distributed) Nordic Tier-1 in the WLCG collaboration is coordinated by NDGF and NorGrid provides the Norwegian contribution to this collaboration. The EU KnowARC project, coordinated by the University of Oslo, as well as NDGF aim to improve and extend the technology in the Advanced Resource Connector (ARC) grid middleware that is used within the Nordic countries, and which at the outset is the middleware chosen for the NorGrid project. Also collaborations on the national level will be pursued. These include for example the adoption of federated authentication, capitalizing on the authentication infrastructure deployed by the institutions under the Feide project.

The NorGrid project aims to link the national activity to these national and international developments and adopt the relevant technologies, enable Norway to participate in large pan-European scientific efforts, and provide modern grid services and a competitive infrastructure to the Norwegian research community.

A key step in the development of a full European Grid Initiative is to build on National Grid Initiatives (NGIs). The EGEE III project that is currently being defined (and should start in the first half of 2008) will implement a first step towards such federation of national initiatives. It is therefore important that a Norwegian grid infrastructure comes in place in 2007. NGIs have already been established in many countries. NorGrid aims to be the Norwegian NGI.

Advanced user support

The Notur project enables scientists to apply for advanced user support projects. Advanced user support aims at helping scientists to improve or extend the computational performance and capabilities of their applications. This can be in a number of ways, including code parallelization, porting, optimization, benchmarking, improving user-interfaces, and software development. Advanced user support is also for scientists that have a need for high-end resources but are unfamiliar with parallel computing architectures and parallel programming languages. A main aim is also to achieve a better utilization of the supercomputer facilities. Advanced user support is meant for scientists with compute- and data-intensive applications as well as scientists that start using the resources in the national infrastructure. Users can apply for advanced support by sending an application to the Notur project.

NOTUR ADVANCED USER SUPPORT IN 2007

In February 2007, there was a call for applications for advanced user support projects. A total of 7 applications were received. The applications were evaluated by the Resource Allocation Committee that decides on the distribution of compute resources to research projects.
The following projects were approved:

ARNE BRATAAS,
Institutt for fysikk, NTNU.
Quantum transport in ferromagnetic semiconductors

RITSKE S. HUISMANS,
Department of Earth Sciences, UiB.
Advanced Solution Methods for Geophysical Simulation of Plate Tectonics

SIGNE KJELSTRUP,
Kjemisk institutt, NTNU.
The implementation of a parallel algorithm for the evaluation of the Coulombic Long-Range interactions and electrical charge fluctuations

TORBJØRN ROGNES,
Institutt for informatikk, UiO.
Efficient large-scale biological sequence comparisons on cluster architectures

KENNETH RUUD,
Institutt for kjemi, UiT.
Analysis, optimization, parallelization and porting of the MRChem code

DAG SLAGSTAD,
SINTEF Fisheries and Aquaculture, Trondheim.
Improved parallel performance of a 3D coupled hydrodynamic-ecological model system

The next call 2007.2 for applications for advanced support has deadline August 30, 2007.

Expansion of compute cluster at the University of Oslo

The compute cluster titan at the University of Oslo will soon be expanded by 224 Sun Fire x2200 nodes. Each node will be equipped with two AMD Opteron 2.6 Ghz dual-core processors, 16 GB memory and two 250 GB SATA disks.

The dual-core processors will be replaced by quad-core processors late 2007. Also 160 nodes of the existing cluster will then be upgraded (from dual-core) to quad-core processors, 16 GB memory, and two 250 GB disks. The nodes will be connected by Qlogic (Silverstorm) Infiniband switches.

Overall, the cluster will be expanded by about 21 Tflops by the end of 2007. The upgraded cluster will be part of the Notur project and researchers from all Norwegian universities, colleges and research organizations will be able to apply for access to the facility later this year through the Notur project.

The next issue of the META magazine will contain more information about the titan cluster.

2007
The major part of 2007 will be used to define the project and design and establish the middleware infrastructure with focus on availability and reliability. Later in the year, the infrastructure shall be made available to the user community.

More information on the project and its services will be available on the NorGrid web pages: www.norgrid.no

Further Information

EGEE - Enabling Grids for E-sciencE: www.eu-egee.org
WLCG - Worldwide LHC Computing Grid : lcg.web.cern.ch
NDGF - Nordic DataGrid Facility: www.ndgf.org
Feide – Federated Electronic Identity: www.feide.no

Speaker's Corner

For every issue of META, someone is invited to express his or her views, opinions, enthusiasm, worries, etc. about the role and importance of e-Infrastructure in Norway as well as abroad. In this issue, the word is given to Morten Hjorth-Jensen.

High-performance computing and **basic education in computati**

Back in 1999-2000, together with several colleagues at the University of Oslo, we felt strongly the need to enhance the visibility of high-performance computing (HPC). This was not only due to the fact that financing of high-performing computing was perceived as inadequate (perhaps a general attitude when it comes to research funds). More importantly, we had a vague perception that the usage of national supercomputing resources did not reflect many of the emerging fields seen on the international scene, such as computational materials science, computational finance and computational biology, just to mention a few. At that time the national HPC users came from few fields, fields which had long traditions in supercomputing, such as computational astrophysics, chemistry and physics and meteorology and oceanography. The question we posed ourselves then was how one could increase the number of national users and the visibility of the various HPC needs, and thereby build a basis for a larger HPC community, a community which in turn could augment the pressure on funding agencies. Obviously, whether a field wishes to utilize HPC resources or not depends essentially on the given community. And since Norway is a small country, the various fields obviously cannot reflect all international HPC trends.

At that time, we chose to focus on developing a series of HPC courses, with an emphasis on parallelization tools and programming languages. These courses were given as intensive one week courses in the period 2000-2003. The eight courses we gave were attended by almost 800 participants, with background from industry, public and private research institutions, universities and regional colleges. Some of these courses are now offered as regular courses. However, although these courses were offered in a HPC context, they did not necessarily increase the HPC visibility. More important are the new developments which took place after 2003. These developments have now paved the way for a unique possibility to incorporate high-performance computing concepts and ideas at a very early stage in our educational ladder. In particular, we are now in a position where HPC concepts like parallel computing can be introduced in present bachelor programs in the next two to three years.

There are several new aspects which have led me to this radical point of view. An important aspect is the formation of several centers of excellence with a strong computational science orientation and with several cross-disciplinary programs. Several of the people involved in the development of the above HPC courses are also deeply involved as principal investigators in these centers.

Moreover, the introduction of the new educational reform from 2003 opened the possibility for a more coordinated action in building up bachelor programs. At the University of Oslo, students from five bachelor programs in the natural sciences have now almost identical first semesters, with a traditional calculus course, a mathematical algorithm course and a programming course. These three courses are integrated in such a way that mathematical concepts like the definition of a derivative is extended to the presentation of algorithms for computing derivatives and programming the algorithms for these derivatives in high-level languages. In this way, one enhances an algorithmic thinking at a very early stage. These three courses

Morten Hjorth-Jensen is Professor in Physics at the Department of Physics and Center of Mathematics for Applications, University of Oslo.

onal science

include many other topics, such as algorithms for solutions of differential equations and various algorithms for computing integrals. The first semester forms then the basis for incorporating numerical exercises in a seamless way in many other undergraduate courses, without spending too much time on programming technicalities during the lectures. The students are then in a situation where they can solve much more realistic cases. The bonus for us teachers is that we can bring our research into basic bachelor courses at a much earlier stage. Furthermore, with the present preparation in computational skills, there is a short way to the possibility to introduce HPC concepts such as parallel computing.

Actually, I believe firmly that parallelization libraries could be introduced in the first semester, perhaps in connection with simple examples such as numerical integration. Since Python is used as programming language (an ideal language for such purposes) and most computer labs are used as parallel clusters, this could easily be implemented. In the second semester, students could then parallelize the Jacobi method for eigenvalues in the linear algebra course, or parallelize the solution of differential equations in the mechanics course. With such a framework, parallelization would cease to be a computing paradigm and become an obvious way of thinking HPC from day one.

I teach computational physics, both at the bachelor level and at an advanced level. This fall, I will include the MPI library in my undergraduate course on computational physics (fifth semester course) and the hope is that similar parallelization tools can enter at an even earlier stage in the not too remote future! That will truly strengthen the visibility of HPC.

A Storage Infrastructure for Scientific Data

The eVITA programme of the Research Council of Norway recently established a new project called NorStore whose objective is to establish and operate a national infrastructure that provides non-trivial services to scientific disciplines with a variety of needs for storing digital data. The infrastructure will provide easy, secure and transparent access to distributed storage resources, provide large aggregate capacities for storage and data transfer, and optimize the utilization of the overall resource capacity.

The storage infrastructure will be an integrated part in the national e-Infrastructure that serves a variety of sciences that are within the responsibility of the eVITA programme. In a number of areas like earth and climate sciences, computational physics, and biosciences, there is a need to store large and complex data sets. The infrastructure will be connected to resources that are located at universities, colleges, research and IT-centers in Norway, including heterogeneous computing systems, networks, other data storage systems, and possibly scientific instruments.

The infrastructure is open to all research environments in Norway and will be developed in accordance with international standards and developments. The project will be a broad and nationally coordinated effort and will co-exist with other national projects like the HPC project Notur and the Norwegian grid project NorGrid that already provide services to projects that have large and complex storage needs.

Notur: http://www.notur.no
NorGrid: http://www.norgrid.no
NorStore: http://www.norstore.no
eVITA: http://www.rcn.no/evita

notur www.notur.no

Return address: UNINETT Sigma AS, 7465 Trondheim, NORWAY

New allocation period

A new allocation period started April 2, and the Notur II project received 68 applications for computing time on the national supercomputing facilities. Of these, 10 were considered as big applications that requested 100 000 allocations units or more. The requested amount of computing time was bigger than ever before, and the Resource Allocation Committee had to make serious adjustments to the requests for resources. There was asked for 2,65 times more computing time than is available. For the ongoing period which lasts until September 30, the following resources are available: Magnum, Njord, Snowstorm and Tre.

More information about the application procedures and the available resources can be found on the Notur web pages **www.notur.no**

Important dates for the Notur user community

August 30: Deadline for applications for advanced user support

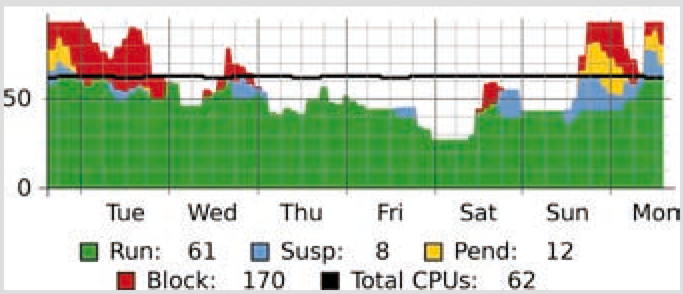
August 30: Deadline for applications for normal CPU-hour grants on the Notur facilities

More information can be found on **www.notur.no**

Machine status – a new service provided by the Notur project

The Notur web pages provide continuously updated load and queue statistics from the Notur supercomputer facilities. The aim of this service is to help users decide on which system to run their jobs in order to minimize job wait time and maximize resource utilization.

The statistics are visualized in a graph with four different classes: Number of processors in use by running jobs (green), number of processors requested by suspended jobs (blue), number of processors requested by queued jobs (yellow) and number of processors requested by ineligible jobs (red). The horizontal black line represents the total number of processors available for computation. There is one graphic illustration per installation.



The Notur II project provides the infrastructure for computational science in Norway. The infrastructure serves individuals and groups involved in education and research at Norwegian universities, colleges and research institutes, operational forecasting and research at the Meteorological Institute, and other groups who contribute to the funding of the project. Consortium partners are UNINETT Sigma AS, the Norwegian University of Science and Technology (NTNU), the University of Bergen (UiB), the University of Oslo (UiO), the University of Tromsø (UiT), and the Meteorological Institute (met.no). The project has a 10-year duration (2005-2014). The project is funded in part by the Research Council of Norway (through the eVITA programme) and in part by the consortium partners.