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Next months deadline for articles is: 29th May 2006

## EGEE Grid Attacks Avian Flu

The National e-Science Centre (NeSC) is a partner in a Europe-wide initiative to develop computer software that will speed up the development of drugs to treat avian flu and malaria. The large-scale international project which is using the EGEE (Enabling Grids for E-science) and associated computing Grid infrastructures to help medical scientists find cures up to a hundred times faster than they would using conventional laboratory techniques.

One of the targets of existing drugs today on the market is viral neuraminidase, an enzyme that helps the virus to proliferate and infect more cells. As this protein is known to evolve into variants if it comes under drug stress, drug resistance becomes a potential concern in case of an influenza pandemic.

Scientists have been able to screen thousands of potential cures online in only a few weeks - instead of many months using existing trial and error methods. The software, developed for the EGEE initiative, allows scientists to sift through whole libraries of chemical compounds and see very quickly which might be effective. Last month alone, EGEE supercomputers simulated the reactions of 300,000 chemical compounds in the quest to combat avian flu.

In April staff from the National e-Science Centre at the Advanced Computing Facility at the University of Edinburgh provided resources to run jobs screening for Avian Flu. The UK has provided large resources for these tests with 11 GridPP sites in the UK.

The challenge of the in silico drug discovery application is to identify those molecules which can dock on the active sites of the virus in order to inhibit its action. With the results from in silico screening, researchers can predict which compounds and chemical fragments are most effective for blocking the active neuraminidases in case of mutations.

For the docking of 300,000 compounds against 8 different target structures of Influenza A

neuraminidases, 2000 computers were used during 4 weeks in April – the equivalent of 100 years on a single computer. More than 60 000 output files with a data volume of 600 Gigabytes were created and stored in a relational database. Potential drug compounds against avian flu are now being identified and ranked according to the binding energies of the docked models.

This drug discovery application against the avian flu virus was jointly deployed by the Genomics Research Center, Academia Sinica, Taiwan; Academia Sinica Grid Computing Team, Taiwan; Corpuscular Physics Laboratory of Clermont-Ferrand, CNRS/IN2P3, France; Institute for Biomedical Technologies, CNR, Italy, in collaboration with the EGEE project, the AuverGrid regional grid in Auvergne, and the TWGrid. This work took place in collaboration with the EMBRACE network of excellence and the BioInfoGrid project. The majority of computing is conducted on the WISDOM platform; in addition, a light-weight application framework called DIANE was also adopted in this challenge and used to perform a sizeable fraction of the total activity to enable efficient computing resource integration and usage. The UK particle physics Grid is part of the EGEE project.

"With these results, the Grid demonstrates that it is a powerful and reliable resource for scientists, opening up new research possibilities and improving existing methods," said Viviane Reding, European Commissioner responsible for Information Society and Media.

For more information on the drug discovery application against the avian flu virus email [ywu@gate.sinica.edu.tw](mailto:ywu@gate.sinica.edu.tw)

For more information about EGEE please see <http://www.eu-egee.org/>



## NeSC Training Outreach and Education

The NESC Training Outreach and Education Team is running a 2 day induction to the National Grid Service on 12/13 June at the University of Westminster. This gives a practical-oriented introduction to the data and computational services of the NGS. <http://agenda.cern.ch/fullAgenda.php?ida=a062302>

This is followed by a 1-day course on using the P-GRADE portal with the NGS. The P-GRADE Grid Portal enables the creation, execution and monitoring of data-driven computational workflows in distributed Grid environments by high-level intuitive graphical interfaces.

<http://agenda.cern.ch/fullAgenda.php?ida=a062303>

## Second International Conference on e-Social Science 28-30 June 2006, Manchester, UK

Registration is now open for the above event with "early bird" registration available until the 21st of May and reduced rates for students.

This conference examines the impact of e-science or cyberinfrastructure on social science research and the social implications of this new technology. Topics to be discussed at the conference include:

- Case studies of e-Social Science research methods and applications.
- Enabling new sources and forms of sociological data through e-Social Science
- Infrastructure and tools for e-Social Science
- Middleware for data collection, sharing and integration
- Standards for metadata, ontologies, annotation, curation, etc.,
- Usability issues in the design of research tools and middleware
- Case studies of (e-)Research and (e-) Social Science research practices
- The benefits and challenges of large scale collaborative research
- Interdisciplinary research and e-Social Science
- International collaborations in e-Social Science
- Socio-technical issues in the development of e-Research and the Grid
- Ethical issues and challenges in the collection, integration, sharing and analysis of sociological and other personal data

Full details can be found at: <http://www.ncess.ac.uk/events/conference/>

Please subscribe to our monthly newsletter (<http://www.ncess.ac.uk/newsletter/>) or RSS feed for your blog to keep up to date with conference news.

National Centre for e-Social Science

## JISC Capital Programme: Call for Proposals

The Joint Information Systems Committee (JISC) invites institutions to submit funding proposals for projects in the following areas: e- learning, repositories and preservation, and e-infrastructure.

Funding is available for projects starting in September/October 2006 and running for a duration of ten months to two and a half years, depending on the area of work.

The deadline for receipt of proposals in response to this call is 12 noon on Thursday 22 June. A town meeting will be held in Birmingham on Wednesday 10 May 2006 to provide a forum for discussion of the call and its subject matter. Institutions will need to register to attend this free event, using the form available at:

[http://www.jisc.ac.uk/event\\_capitalprog\\_0506.html](http://www.jisc.ac.uk/event_capitalprog_0506.html)

Proposals may be submitted by HE institutions funded via HEFCE and HEFCW, and by FE institutions in England which teach higher education to more than 400 full-time equivalent students. Due to the funding streams available for this programme, other institutions are not eligible to bid, but may be involved as partners in projects

For further information see:

[http://www.jisc.ac.uk/funding\\_circular03\\_06.html](http://www.jisc.ac.uk/funding_circular03_06.html)

## The Institution of Engineering and Technology John Pinkerton Lecture and Dinner 2006 "e-Science and Cyberinfrastructure"

Lecture by Professor Tony Hey, VP Scientific Computing, Microsoft, USA Savoy Place, London, UK: Tuesday, 13 June 2006 at 6.00 pm (registration from 5.30 pm)  
<http://www.iee.org/events/pinkerton.cfm>

Don't miss this exciting opportunity to hear Professor Tony Hey, VP Scientific Computing, Microsoft, USA, speak at Savoy Place on 13 June.

As corporate vice president for technical computing, Tony Hey coordinates efforts across Microsoft Corporation to collaborate with the global scientific community. The talk will discuss the vision of "e-Science" innovation provided by multi-disciplinary and collaborative research. It will describe how the scientists and engineers are collaborating with computer scientists and the IT industry to create a new e-Infrastructure. When mature, it is clear that such an infrastructure will support the creation of dynamic 'Virtual Organisations' and collaborative environments for many types of application in both academia and industry.

You also have the opportunity to attend a networking dinner after the lecture, giving you the chance to further discuss the arising issues and network with your peers.

If you require any additional information, please contact the organisers:

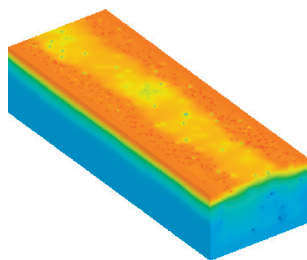
Email: [Eventsa1@theiet.org](mailto:Eventsa1@theiet.org) Tel: +44 (0) 1438 765648

## UK consortium to use e-Science and Grid technology to tackle nano-CMOS design challenges

The UK Engineering and Physical Sciences Research Council (EPSRC) in collaboration with leading design houses, chip manufacturers and ECAD vendors is funding a £5.3M (\$9.1M) project which will apply e-Science and Grid technology to tackle some of the fundamental challenges facing nano-CMOS design.

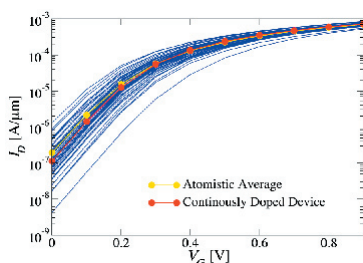
Progressive scaling of CMOS transistors, as tracked by the International Technology Roadmap for Semiconductors (ITRS) and captured in Moore's law, has driven the phenomenal success of the semiconductor industry, delivering larger, faster and, cheaper circuits. Silicon technology has now entered the nano-CMOS era with 40 nm MOSFETs already in mass production and sub-10 nm transistors scheduled for production by 2018. However the years of 'happy scaling' are over and the fundamental challenges that the semiconductor industry faces, at both technology and device level, will impinge deeply upon the design of future integrated circuits and systems.

It is widely recognised that variability in device characteristics and the need to introduce novel device architectures both represent major challenges to scaling and integration for present and next generation nano-CMOS transistors and circuits. The rapid increase in intrinsic parameter fluctuations stemming from the fundamental discreteness of charge and matter and their statistical impact on device behaviour is a major source of device variability. The intrinsic parameter fluctuations are fundamental, truly stochastic and cannot be eliminated by tighter process control.



Random discrete dopants and line edge roughness in a 35 nm MOSFET representative for the transistors that are in mass production now.

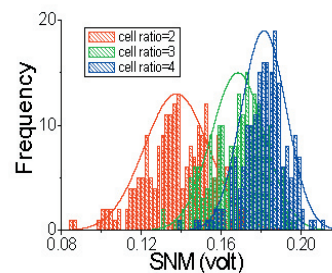
Random discrete dopants and line edge roughness in a 35 nm MOSFET representative for the transistors that are in mass production now. Corresponding variations in the current-voltage characteristics of 200 transistors with different dopant distributions. Corresponding distribution of the static noise margins in 6T SRAM cells.



Corresponding variations in the current-voltage characteristics of 200 transistors with different dopant distributions

The increasing device variability demands revolutionary changes in the way that future integrated circuits and systems are designed. Strong links must be established between circuit design, system design and fundamental device technology to allow circuits and systems to accommodate the individual behaviour of every transistor on a chip. Design paradigms must change to accommodate the increasing variability. Adjusting for new device architectures and device variability

will add significant complexity to the design process, requiring the orchestration of a broad spectrum of design tools by geographically distributed teams of device experts, circuit and system designers. This can only be achieved by embedding e-Science technology and know-how across the whole nano-CMOS electronics design process and revolutionising the way in which these disparate groups currently work.



Corresponding distribution of the static noise margins in 6T SRAM cells.

The University partners in this project include the Device Modelling and the Microsystems Technology groups at the University of Glasgow, the Advanced Processor Technologies group at the University of Manchester, the Electronic Systems Design Group at the University of Southampton, the Intelligent Systems group at the University of York and the Mixed-Mode Design Group at the University of Edinburgh. The e-Science and Grid technology will be provided by the National e-Science Centre run jointly by Glasgow and Edinburgh Universities and the e-Science North-West Centre at Manchester University. The industrial partners include ARM and Wolfson Microelectronics (two of the largest UK fabless chip design companies), Synopsys (the world leader in design software) and Freescale, National Semiconductors and Fujitsu (leading semiconductor chip manufacturers). The project also received the support of the National Microelectronics Institute, the Trade Association for UK microelectronics.

"This project brings together leading semiconductor device, circuit and system experts from academia and industry and e-Scientists with strong grid expertise. Only by working in close collaboration, connected and resourced using state-of-the-art e-Science and Grid technology, can we understand and tackle the design complexity of nano-CMOS electronics, securing a competitive advantage for the UK electronics industry". Said the Principal Investigator Professor Asen Asenov from the University of Glasgow.

### ESLEA's online guide 'Connecting to UKLight'

The guide builds upon the considerable experience and expertise built up within ESLEA of integrating applications with UKLight. It has a 'modular' structure which means that people of varying technical knowledge and competence can pick and choose the resources that apply to them. For example, the introduction contains material which helps non-technical managers understand some of the issues that their engineering, network and research staff might need to address. However, most of the resource is targeted at engineers and network support staff who will be responsible for implementation of the high speed connections. Not least, the value of the resource resides in the provision of ESLEA contacts who are willing to support others who need help connecting to UKLight/SJ5.

This resource can be viewed at:  
[www.eslea.uklight.ac.uk/cnctg\\_uklight\\_intro.html](http://www.eslea.uklight.ac.uk/cnctg_uklight_intro.html)

## Grid Computing Now! Nationwide Grid Computing Competition

The Grid Computing Now! competition in partnership with the British Computer Society (BCS). is open to students and young professionals to develop solutions to 21st century challenges using the capabilities of grid computing technologies. The competition has the backing of the National e-Science Centre, Intel, Microsoft and includes judges from the fields of science, technology, design and government.

The winner will be eligible for a six week paid Grid Computing Now! project Internship hosted by Intellect, the UK hi-tech association in Summer 2007. The winner will also be eligible to attend the Microsoft European Research and Innovation day held in Brussels, enjoy a year's free membership of the British Computer Society and receive an Xbox 360, with the offer of Microsoft Windows Server 2003 Standard 10 CALs and Microsoft Compute Cluster Server for the prize winner's employer/university. There will also be prizes for the runners up.

The entrant will have to develop a submission of up to 500 words describing the problem and their approach to a solution using grid computing technologies. The submissions will be reviewed by the organising committee and selected candidates will be invited to submit a more complete entry.

The deadline for initial entries is 30 June 2006 and up to 10 shortlisted entrants will be invited to present their entries to the judges at the competition final on 28 September at the BCS offices in Southampton Street. If you would like to enter the competition or would like more details please visit:

[www.gridcomputingnow.org](http://www.gridcomputingnow.org)

The International Conference on the Preservation of Digital Objects (iPRES 2006) will be held October 8-10, 2006 at Cornell University, Ithaca, NY U.S.A.

The theme of this year's iPRES is Words to Deeds: Collaboration in the Realm of Digital Preservation. Following on the successful iPRES 2005 held September 14-16 in Goettingen, Germany, iPRES 2006 Plenary Sessions will explore topics in Preserving Multimedia Objects, e-Journal Preservation, Certification, and National Efforts in Digital Preservation. Concurrent sessions on Tools of the Trade; Selection, Workflow, and Accession; eScience and Digital Preservation; Metadata; Business and organizational issues; and Repositories are tentatively planned.

We invite contributions in these areas by sending a brief abstract to [ipres2006@cornell.edu](mailto:ipres2006@cornell.edu). Deadline for contributed papers is August 15, 2006. The deadline for early registration is September 1, 2006.

For details about the iPRES 2006 agenda and to register, please visit our web site: <http://ipres.library.cornell.edu/>

## UK e-Science at SC2006: Call for proposals

The UK e-Science programme will show its success across a range of application areas at SC06: <http://sc06.supercomputing.org>, the premier international conference for High-Performance and Grid Computing.

As in previous years [<http://www.nesc.ac.uk/events/sc2005/>], our exhibition stand will provide space for 12 continuous demonstrations and a mini-auditorium space for presentations and panel discussions. Last year about 1200 visitors registered their names at our stand, which illustrates the potential for dissemination of UK e-Science projects at this event.

Proposals will soon be invited for demonstration systems, auditorium events and videos. We are eager to present applications across a wide range of subjects, including social sciences, medicine, the arts and humanities as well as the more established areas of e-science. We are also keen to show applications that leverage collaboration with e-Science infrastructure such as the NGS, EGEE and OMII-UK, or with researchers across multiple organizations.

The conference will run from 11-17 November at the Tampa Convention Centre in Florida. The exhibition that is the subject of this call will run from the evening of Monday 13th until the afternoon of Thursday 16th. Auditorium events & videos will be scheduled throughout.

You will soon be able to submit applications using a form on the NESC website. Proposals are requested by 31st May. Successful candidates will be informed by 14th June. Enquiries should be addressed to:  
Dave Berry [[daveb@nesc.ac.uk](mailto:daveb@nesc.ac.uk)].

## CALL FOR PARTICIPATION - CLADE 2006

Challenges of Large Applications in Distributed Environments  
Paris, France, June 19, 2006, <http://www.mcs.anl.gov/~bair/CLADE2006/>

In conjunction with the 15th International Symposium on High Performance Distributed Computing (HPDC-15)

This workshop focuses on the complex issues that arise in large-scale applications of distributed computation, and promotes the development of innovative applications that effectively use distributed resources, e.g., to adapt to heterogeneity and dynamics in space and time.

The CLADE 2006 keynote will be by Terry Harmer, Technical Director of the Belfast e-Science Centre, entitled "Gridcast - a Next Generation Broadcasting Infrastructure?"

Steven Newhouse, Deputy Director of OMII, will also be giving and invited talk entitled "Real Users – Real Requirements: 25 Conversations with UK eScience Projects."

### REGISTRATION

Registration for CLADE 2006 is in conjunction with HPDC-15. When you register for HPDC-15, please make sure that you also register for the CLADE workshop. Registration can be found at the website :

<http://hpdc.lri.fr/index.php?section=Info=registration>

## Awards for e-Science in the Arts and Humanities

A range of ground-breaking awards to develop the application of e-Science in the arts and humanities are announced by the Arts and Humanities Research Council (AHRC) and the UK e-Science Core Programme, through the Engineering and Physical Sciences Research Council (EPSRC).

The EPSRC and Core Programme are funding three ground-breaking e-Science demonstrator projects to show how e-Science technologies can be applied to advance the understanding of complex research issues in the arts and humanities. They are: Virtual vellum: online viewing environment for the grid and live audiences, University of Sheffield, A virtual workspace for the study of ancient documents, University of Oxford and Motion capture data services for multiple user categories, University of Newcastle.

AHRC is funding six e-Science workshops which will produce reports that explore issues and/or develop schemes relating to the applications of e-Science in the arts and humanities. They are: User requirements gathering for the humanities, University of Oxford, Geographical information system e-Science: developing a roadmap, Queen's University Belfast, Performativity/place/space: locating grid technologies, University of Bristol, The Access Grid in collaborative arts and humanities research, University of Sheffield, Building the Wireframe: e-Science for the arts infrastructure, University of Central England and ReACH: researching e-Science analysis of census holdings, University College London.

Together the demonstrators and workshops will cover the three main types of grid: the computational grid for the sharing of processing power, the data grid for the sharing of data resources, and the Access Grid for high-technology video-conferencing. The projects include a number of exciting collaborations between computer scientists and arts and humanities scholars, and cover a wide range of research both in humanities subjects and in the creative and performing arts. The types of data involved comprise not only of text, but also geographical data, sound, and images - 2- and 3-dimensional, still and moving, real and virtual. These projects will show that e-Science can be important for the arts and humanities as well as the natural sciences, medicine, engineering, and increasingly the social sciences.

The demonstrators and workshops will be supported by the new Arts and Humanities e-Science Support Centre (AHESSC) at King's College London, which is funded by the Joint Information Systems Committee (JISC), and is a part of the joint AHRC-JISC Arts and Humanities e-Science Initiative. As a further part of this initiative, a joint call for bids is expected in late Summer 2006 for research project awards (to a total value of at least £1.2 million) and six 4-year postgraduate studentships.

Further information about e-Science in the arts and humanities is available at <http://www.ahessc.ac.uk/>.

Judy Redfearn, EPSRC

## Building a heart model to probe disease

What causes heart disease - and how can it be prevented or cured? Experiments using heart tissue are unable to provide all the answers. Now, however, the Integrative Biology project is pioneering an alternative approach. It involves searching for clues in the most sophisticated computer models of the heart ever created.

The task is beyond the capabilities of even the largest supercomputer. So the project is harnessing the services of the UK National Grid Service (NGS) which pools the resources of many computers at many different sites, including the UK's two academic supercomputers. By building a suitable computing infrastructure, IB is enabling heart researchers to access this vast wealth of computing power as though it were held on their own PCs.

The project is led by Oxford professors David Gavaghan and Denis Noble, who described the first mathematical model of a heart cell for his PhD thesis in 1960. Much present heart modelling builds on this early work. Sharon Lloyd, also at Oxford, is leading the development of the computing infrastructure.

Heart modelling groups throughout the world are joining in, drawn to the capabilities provided by the computer infrastructure IB is developing. This is enabling them to do far more than build static models of the heart. By having almost instantaneous access to data, computing and visualisation software held on the NGS, the IB project allows researchers to change conditions in the heart and see how the model reacts in almost real time – the nearest thing to experimenting with a live heart.

Dr Blanca Rodriguez at Oxford University has been using a computer model of the rabbit heart to investigate one particular problem: optimum current strength when applying an electric shock to kick start a heart. If the current is too high, fatal damage ensues; too low and the patient dies before an effective strength is reached. She's been comparing the effect of electric shock strength on normal heart tissue with tissue that has been deprived of oxygen after a heart attack.

The Oxford group is working towards developing a heart model which couples the electrical and mechanical properties of heart muscle cells to create a model of a contracting heart. Other groups are using different properties of other types of heart cell to build their models. The ultimate aim is to integrate all the models to produce an over-arching model that takes into account all types of heart cells and all their properties. "Individual researchers or small groups of researchers work on individual bits. The key is how you ultimately couple these together – for example, cell behaviour with tissue movement with blood flow with electrical activity. No one at present has coupled all these things. It is a huge task," comments Mrs Lloyd.

Judy Redfearn, EPSRC

Forthcoming Events			
May			
16-18	TDWG sub-group meeting Taxonomic Databases Working Group (TDWG)	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/687/">http://www.nesc.ac.uk/esi/events/687/</a>
16	Browsing Genes and Genomes with Ensembl	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/678/">http://www.nesc.ac.uk/esi/events/678/</a>
17	Browsing Genes and Genomes with Ensembl	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/677/">http://www.nesc.ac.uk/esi/events/677/</a>
17	DCC Associate Network Meeting	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/673/">http://www.nesc.ac.uk/esi/events/673/</a>
19	User Requirements and Web based Access for eResearch	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/685/">http://www.nesc.ac.uk/esi/events/685/</a>
27	Ontology Engineering & Automated Reasoning	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/668/">http://www.nesc.ac.uk/esi/events/668/</a>
June			
7-9	RDF, Ontologies and Meta-Data Workshop	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/683/">http://www.nesc.ac.uk/esi/events/683/</a>
10	TDWG/GBIF GUILD-2 workshop	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/682/">http://www.nesc.ac.uk/esi/events/682/</a>
July			
9-21	International Summer School on Grid Computing	Jolly Hotel Delle Terme, Ischia, Italy	<a href="http://www.dma.unina.it/~muri/ISSGC06/">http://www.dma.unina.it/~muri/ISSGC06/</a>
17-18	Portals and Portlets	e-Science Institute, Edinburgh	<a href="http://www.nesc.ac.uk/esi/events/686/">http://www.nesc.ac.uk/esi/events/686/</a>
September			
18-21	All Hands Meeting 2006	East Midlands Conference Centre	<a href="http://www.allhands.org.uk/index.html">http://www.allhands.org.uk/index.html</a>
October			
31-2 Nov	GridPP	e-Science Institute, Edinburgh	
November			
30	NeuroGrid Annual Workshop	e-Science Institute, Edinburgh	

### NeSC at WWW 2006

Don't forget to visit the NeSC stand at the WWW 2006 Conference at the Edinburgh International Convention Centre. The event runs from the 23rd – 26th May 2006. For more information on the event go to <http://www2006.org/>. There will be information on future events, projects and staff will be there to talk to from both NESC and IECnet.

### Vacancy for Senior Administrator (maternity cover)

Based at the e-Science Institute in Edinburgh, there is a vacancy to join the NeSC Team as a Senior Administrator. Further details at: <http://www.nesc.ac.uk/career/>

### This month NeSc would like to welcome....

Brendan Hamill who joins us as the new EGEE II Project manager.

Tony Pan who is a visitor at The e-Science Institute during May. He is working with the DGeMap team.

If you would like to hold an e-Science event at the e-Science Institute, please contact:

Conference Administrator, National e-Science Centre, 15 South College Street, Edinburgh, EH8 9AA  
Tel: 0131 650 9833 / Fax: 0131 650 9819 / Email: [events@nesc.ac.uk](mailto:events@nesc.ac.uk)