NeSC III Annual Report 2007

Dave Berry, National e-Science Centre

1 October 2007

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The project has had a successful first year. A particular highlight was OGF20, which was held in Manchester with the support of the University of Manchester; NeSC took the lead in bringing this event to the UK and organised both the programme and the sponsorship arrangements. The project has also provided infrastructure support to the e-Science All-Hands Meeting 2007.

On the infrastructure front, both Edinburgh and Glasgow have taken delivery of new SRIF-funded resources and these are being integrated with the activities of NeSC. Both sites have contributed to the ETF and are working towards NGS partnership.

UK e-Science Technical Report Series

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Annual Report 2007

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1 Abstract

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2 Background

The National e-Science Centre has been hosted by the Universities of Edinburgh and Glasgow since 2001. It embodies a very wide range of activities which have provided a focus for UK e-Science. These activities enable and promote e-Science within the UK, as well as represent UK programme internationally.

NeSC III is a two-year project, running from 1st August 2006, which continues core activities of this work. It aims to provide a central focus for leadership, coordination and promotion of the UK e-Science programme and to foster excellence in interdisciplinary research.

The *NeSC III* project is one of a number of projects that provide national support to the UK e-Science programme. Others include *Gridnet2*, which supports standardisation activity; *E-STORM*, which funds the annual e-Science All-Hands Meeting; the *UK e-Science Envoy*; and *E-SciNet*, which provides travel and networking facilities to support the uptake of e-Science technologies. In addition, of course, the UK e-Science programmes funds regional e-Science centres and institutes such as the e-Science Institute, OMII-UK and the Digital Curation Centre.

3 Project Structure

3.1 Overview And Goals

The NeSC project is a small part of the work actually undertaken at the National e-Science Centre. This section describes the goals of the project as set out in the proposal to EPSRC, which includes funded and unfunded work. Later sections concentrate on the operation of the funded activities.

Goal	To be achieved through
Provide National leadership and coordination, and international representation of UK e-Science.	▪ Continued participation by NeSC members in a range of high impact national and international activities ▪ Provision of an authoritative published knowledge base (based upon the website) to be an authoritative source for all UK and international e-Scientists. ▪ A set of high quality key e-Science events to be run on behalf of the community each year ▪ Hosting other e-Science events on a cost recovery basis for a wide range of communities and strategic partners. ▪ Hosting of, and participation in, international delegations. ▪ Developing an advisory role for e-Infrastructure for the JISC ▪ Continuing support of the AHM in 2006 and 2007 ▪ Acting as a home for the GridNet and eStorm national enablement projects.
Promote research excellence based upon existing and newly developing areas of strength	▪ Continuing to lead research in our existing areas of technical strength. ▪ Establishing projects in two new areas. ▪ Further strengthening our links with major research groups regionally, nationally and globally.
Inform and contribute to development of the national e-Infrastructure and international standards	▪ Participation in the ETF, GOSC, NGS, STF, ATF and their successors ▪ Participation in the OGF and other standards bodies ▪ Leading the development of regional e-Science infrastructure and extending this to become the Scottish element of the NGS ▪ Provision of Access Grid facilities
Enable e-Science outreach and uptake in the Regional community	▪ Organising events aimed specifically at regional institutions to promote e-Science understanding and engagement ▪ Fostering grant proposals from the regional community. ▪ Running an annual outreach event for Scottish Industry.
Stimulate e-Science education	▪ Leverage our MSc courses, and our leadership of the ICEAGE project ▪ Run an annual UK education event.
Optimise benefit to the UK community through synergy with other activities.	▪ Synergy from our co-location with e-Science Institute, EPCC, the training activity, the DCC and our role in projects such as EGEE. ▪ Leading UK and European training and staff development activities. ▪ Interaction with industry and the IECnet knowledge transfer network.

3.2 ACTIVITIES

The NeSC III project is structured into several activities. Each activity has defined goals and milestones and is led by a nominated member of staff. Section 4 of this document gives a detailed report of the work of each activity over the past year.

The overall status of the activities is as follows:

- Community Events – on track
- AHM Support – on track
- Regional Outreach – on track
- Web Site Redesign – behind schedule
- Knowledge Base – behind schedule
- E-Infrastructure – on track
- IT Support – behind schedule
- Stimulating e-Science Education – on track
- National Leadership – on track

In addition, the NeSC III project has indirectly enabled a wide range of research activities in both universities (Edinburgh and Glasgow). It has also enabled engagement with standards development work via the OGF and OGC.

3.3 COMMUNITY REQUIREMENTS

The NeSC III project serves the UK e-science community. Therefore the project staff must discover and collect the requirements of that community. The project must be seen to meet community requirements.

Often it will make sense to collect requirements for all activities together. In such cases they shall collect requirements for as many activities as possible. Activity leaders may follow up particular issues as appropriate.

Actions to solicit community requirements have included the following:

- Soliciting input from the E-Science Directors' Forum.
- Supporting the UK e-Science envoy. The e-Science envoy has requested support in the form of particular events, hosting international delegations, and similar activities.
- Supporting the Director of the ICT and e-Science Programme in EPSRC.
- Soliciting input from the Research Councils and JISC.

3.4 PROJECT DELIVERABLES

The only deliverable required by this project is the annual report, i.e. this document.

3.5 STAFF

All staff originally assigned to the project remain in place. Gill Maddy has returned from maternity leave.

4 Project Activities

This section of the report describes the funded activities of the NeSC III project. For each activity, we describe the work done over the period of the report, compare this progress against the original project plan, and then discuss plans for the second year of the project.

4.1 Community Events

Leader: Dave Berry

This activity supports the UK e-Science community by providing infrastructure and a venue for community events.

OGF20/EGEE User Forum: The NeSC III project successfully led the effort to bring OGF20 and the 2nd EGEE User Forum to the UK in May 2007. This event was very successful, being the largest meeting of the GGF/OGF to date (the previous largest being GGF5 in Edinburgh).

This was a major undertaking which took a significant effort. Initial planning began in the summer of 2006, arranging visits to possible venues. This process selected Manchester International Convention Centre. The University of Manchester and the National Centre for e-Social Science agreed to organise the local arrangements, for which we are very grateful. Dave Berry of NeSC was chair of the OGF20 programme committee; in his other role, as technical lead on the *Grid Computing Now!* Knowledge Transfer Network, he also organised the *Grids Mean Business* industry track. Mark Parsons, commercial director of NeSC, led the OGF20/EGEE sponsorship committee. NeSC also contributed to the arrangements of the exhibition.

UK e-Science was well represented at OGF20. Several workshops had UK organisers and/or a strong UK contribution. These included:

- The 2nd International Workshop on Campus and Community Grids
- Computational Steering on the Grid
- E-Science Technologies and Methodologies in Arts and Humanities Research
- OGC/OGF Collaboration Workshop
- The Astronomical Virtual Observatory – Building Operational Services on Pervasive Grids: Standards in Use

The *Gridnet2* project paid for four stands in the exhibition and these featured a range of UK projects and organisations. The *Grid Computing Now!* KTN also paid for a stand.

Other NeSC events: OGF20 and the EGEE User Forum took much of the project's effort in this year and also served as the site for some UK workshops. Nevertheless, NeSC continued to host other workshops and events throughout the year. We solicited input and suggestions via the e-Science Directors' Forum and the E-SciNet network.

The following table shows the events hosted by NeSC. These include events of general community interest and also meetings of particular projects or committees. It does not include meetings at NeSC organised by the e-Science Institute, Grid Computing Now!, or the NeSC training team. It also excludes meetings of local projects, unless these meetings were open to the national community.

The NeSC III grant includes funding to cover running costs for a limited set of 6 key community events per annum. These costs typically cover catering and the table shows which events received such funding. Other events were hosted on a cost recovery basis, in which NeSC provided the venue and registration services.

Title	Date	Type
UCLP Workshop	29-30 Aug	Unfunded, Open
GridPP 17	1-2 Nov	Unfunded, Open
EGEE User Information Group Meeting	30 Nov-1 Dec	Unfunded, Closed
OMII-UK Operations F2F Meeting	13 Dec	Unfunded, Closed
OMII-UK Management and Operations Meeting	14-15 Dec	Unfunded, Closed
LHCb Upgrade workshop	11-12 Jan	Unfunded, Open
Study of Users' Priorities for E-infrastructure for Research (SUPER)	16 Feb	Funded, Open
Agents and Grids: Towards the Intelligent Grid	19-20 Feb	Funded, Open
Models for a sustainable National Grid Service	22-23 Feb	Unfunded, Open
Database Preservation Workshop	23 Mar	Unfunded, Open
Lighting the Blue Touchpaper for UK e-Science – Closing Conference of the ESLEA Project	26-28 Mar	Unfunded, Open
Managing Scientific Workflows with OMII-BPEL	24-25 April	Unfunded, Open
Grid Computing and e-Science - Developing Links between China and the UK	11 Jun	Funded, Closed
Support for e-Research: Filling the Library Skills Gap	14-15 Jun	Unfunded, Open
Joint OSGC and ISSeG meeting	19-20 Jun	Unfunded, Closed
e-Science Directors' Forum	4 Jul	Funded, Closed

Progress against plans: As the table shows, in this year we contributed funds to fewer than the 6 events allowed in the project grant. This is primarily due to the time spent organising OGF20. Given the success of OGF20, including workshops that might otherwise have been supported at NeSC, we consider this to have been a good decision.

Plans for 2007-2008: Next year we intend to host 6 funded events as per the grant proposal and to continue to host other events on a cost-recovery basis. We will continue to solicit ideas for events from the e-Science Directors' Forum and other community contacts.

At the time of writing, the following funded events are already being planned:

- Planning for implementation of the SUPER recommendations
- High-throughput computing
- SRM2.2 Deployment Workshop
- Grids and Virtualisation

4.2 AHM SUPPORT

Leader: Susan McCafferty

This activity supports the UK e-Science All-Hands Meeting through web-based paper submission and registration as well as review processing and subsequent proceedings production. The event itself is run from the E-STORM project.

AHM2007: The new AHM website went live in January 2007. We received and processed 125 submissions to this year's conference, which were reviewed using our online system in May 2007. The PC meeting was fully supported, decisions were uploaded and NeSC informed the authors of their papers outcomes.

The programme has been developed and managed online. This year, the website has been enhanced; it is now driven by the database which has meant we have been able to make the provisional programme available online earlier than in previous years. All camera ready papers have now been submitted online and the proceedings document is being compiled.

We have successfully managed to get the proceedings of last years conference accepted to ISI proceedings. This will mean that this year's proceedings will be automatically included once we send the printed version.

Progress against plans: This activity is proceeding according to schedule.

AHM2008: We are already preparing for next years conference and will launch the 2008 AHM website in December after feedback from this year's conference. We would expect to start accepting papers from January 2008 onwards.

4.3 REGIONAL OUTREACH

Leader: Richard Sinnott

Outreach Events: We have made considerable efforts with regard to the transfer of e-Research know-how to the wider Scottish communities. These have included the following presentations and outreach events:

- M. Mineter, *Introduction to the Grid*, invited talk at the Scottish Crop Research Institute workshop, August 2006
- D. Fergusson, *EGEE, ICEAGE, WISDOM and Grids*, seminar, University of Abertay, September 2006
- R.O. Sinnott, *Grid Challenges and Opportunities*, seminar, University of Stirling, October 2006
- NeSC Training Team, *Grid Computing and the National Grid Service – Induction*, training course, University of Edinburgh (EUCS), October 2006
- R.O. Sinnott, *Life Science Grids*, seminar, University of Aberdeen, November 2006.
- R.O. Sinnott, *Grid Challenges and Opportunities*, seminar, University of Aberdeen, January 2007.
- M. Mineter, *e-Science in the UK*, seminar, University of Edinburgh (EDINA), February 2007.
- R.O. Sinnott, *Glasgow e-Research Support for the Life Sciences*, seminar, University of Glasgow (IBLS), February 2007.
- R.O. Sinnott, *Getting Data on and off the Grid at Glasgow*, e-Science Workshop, University of Glasgow, March 2007.
- R.O. Sinnott, *e-Biological Research*, seminar, Pharmacology Research Centre, University of Strathclyde for Scottish Bioinformatics Forum, April 2007.
- R.O. Sinnott, *e-Clinical Research at Glasgow*, seminar, University of Glasgow (Beatson Institute, Garscube), August 2007.

These have included presentations and demonstrations at Glasgow (three), Edinburgh (two), Aberdeen (two), SCRI, Abertay, Stirling, and Strathclyde. Presentations have also been made to Scottish wide efforts such as the Scottish Bioinformatics Research Network and to the Scottish Bioinformatics Forum. We are also directly supporting these projects through, for example, grid enabled software developed for biochemical pathway simulation (developed as part of the DTI

Beacon project) and through the development of a Drug Discovery Portal in collaboration with the University of Strathclyde.

In addition, our leadership of the proposal for a Scottish Grid Service, as described under the Infrastructure activity, has strengthened links with the other Scottish universities.

Progress against plans: We proposed to hold three outreach events each year. In practice, we have found shorter seminars at other institutions a more valuable way of conducting outreach, rather than workshops per se. We have established good contacts with four other Scottish universities via these outreach activities.

Plans for 2007-2008: For the future we will continue to engage with the wider Scottish research communities on exploiting e-Research possibilities. This will be through proactive engagement and targeted workshops to university research needs and specific areas of interest. In particular, we plan to engage some of the Scottish research pooling initiatives, such as SINAPSE, SULSA, SICSA, ScotChem and SUPA.

The proposed Scottish Grid Service, if funded, will include funds for continuing this regional outreach and backing it up with regionally-focused e-Science training and support for application-specific user interfaces.

4.4 Web Site Redesign

Leader: Anna Kenway

Our present web site has grown organically since the establishment of NeSC and it has become apparent that it is in need of a redesign. This process will result in both a better-structured presentation of more information and new technical features to provide enhanced functionality.

Requirements Gathering: The redesign has proceeded in the following stages:

- A preliminary stage involving discussion with interested parties and with members of JISC staff who recently carried out a successful redesign of their own web site.
- A mock-up design of the top level page. This provided a structured presentation of all UK e-Science activities and institutes.
- A requirements gathering process, which included an online questionnaire linked from the top level NeSC website, and focus group sessions which included discussion of the mock-up design.
- A second version of the design, substantially changed from the mock-up, including a new top level page for NeSC, and new pages for the e-Science Institute, Training Outreach and Education, Regional Research and Community Services.

The following aspects of the technical implementation of the new website have so far been addressed:

- Implementing tools that we expect to incorporate in the new NeSC website, including iCal functionality and a dynamic event calendar.
- Researching various content management systems: we now have a good idea of what is available.
- Analysing the website structure and developing early design specifications.

We are currently developing further and liaising with stakeholders to improve and finalise the design.

Progress against plans: The redesign process has been more involved than we expected. We believe that the end result is a better design than would otherwise have been the case, with more input from our stakeholders. The process was complicated early on by plans for a wider UK

e-Science web site; these plans have now been put on hold due to lack of funding. This effort has included a six month appointment of an additional web site developer, using funds from other sources.

In addition, we want to complete the move of the web site to new hardware before deploying the new design. This move has been severely delayed, as described in the section on IT infrastructure, which has had a knock-on effect on the content activity.

Plans for 2007-2008: Clearly the most important task is to implement the new design, as this will allow us to provide an extended knowledge base with enhanced functionality. This work is progressing well. We have identified a source of funds to extend the employment of our second web site developer for 6 months, which will greatly support this activity. We will begin the implementation on a development server and port it to the new outsourced server when complete.

4.5 KNOWLEDGE BASE

Leader: Iain Coleman

Knowledge base: NeSC has committed to maintaining its provision of a high quality knowledge base founded on the web site. This includes news and information about UK e-Science and NeSC activities, links to e-Science resources in the UK and worldwide, an index of information on current e-Science projects that involve UK researchers, and a repository of papers and technical reports. The website also hosts information on events and research themes at the e-Science Institute, the All-Hands Meeting and the NeSC Training, Outreach and Education web pages (which include information about EGEE training courses throughout Europe).

This information resource has been enhanced during the reporting year by:

- Improved management and presentation of technical papers and reports. There is now consistent presentation of technical reports on the web site, with professional editorial oversight.
- A programme to systematically gather project information. This is an ongoing, labour-intensive activity to amass material for the new version of the web site discussed below.
- A proactive effort to acquire material from UK e-Science researchers. Technical reports and other research documentation have been actively solicited, including a request for reports from the UK Grid Engineering Task Force that provided three of the ten new reports in the UK e-Science Technical Reports Series.

The production of content for the knowledge base has benefited from the collocation of the NeSC/eSI science writer, the *Grid Computing Now!* technical journalist and EGEE outreach personnel.

One of the first tasks that we undertook was to update the index of UK projects and staff engaged in e-Science. We made good progress on this at first but it has proven to be a significant undertaking that would require more staff than we have available. Staff at other centres are also too busy to update the central database. As noted in the discussion of the Web Site Redesign activity, there were some initial plans for a UK e-Science web site, but these are on hold due to lack of funds.

NeSC newsletter: We have continued to produce a regular monthly newsletter. This year, we have redesigned and extended the newsletter to include articles by the NeSC/eSI science writer and editorials by the UK e-Science Envoy. We have solicited input from other e-science centres and have seen an increase in such contributions. We have also liaised with the EPSRC/JISC and GridPP press officers, sharing relevant information and announcements. The feedback we have received suggests that the community has appreciated these improvements. Each month, the newsletter is typically among the top 20 downloads from our web site, with a readership between 2,000 and 3,000.

UK e-Science reports: The following technical reports were published in the UK e-Science series during the period covered by this report:

UKeS-2007-04 *Exludus Evaluation for ETF*, Christopher Mountford, published Jul 07

UKeS-2007-03 *Report on Lightweight SRM Evaluation - UK Grid Engineering Task Force*, David McBride, Steven Young, Tim Parkinson and David Wallom, published Jul 07

UKeS-2007-02 *An Evaluation of the CROWN Middleware for the Engineering Task Force*, Tim Parkinson, Mark Hewitt and David McBride, published May 07

UKeS-2007-01 *Study of User Priorities for e-Infrastructure for e-Research (SUPER)*, Steven Newhouse, Jennifer M Schopf, Andrew Richards and Malcolm Atkinson, published Apr 07

UKeS-2006-07 *Report of the User Requirements and Web Based Access for eResearch Workshop*, edited by Jennifer M. Schopf, Iain Coleman, Rob Procter, and Alex Voss, published Nov 06

UKeS-2006-06 *Review of Network Provision for Research Needs*, John Duke and Andy Jordan, published Oct 06

UKeS-2006-05 *A Visualization Service for the National Grid Service: A Workshop to derive User Needs*, R.S. Kalawsky, published Oct 06

UKeS-2006-04 *Information Services for Smart Decision Making: An eSI Event Theme Prototype - Final Evaluation*, Jennifer M Schopf, published Oct 06

UKeS-2006-03 *Report of the e-Frameworks Meets e-Science Workshop*, Edited by Jennifer M Schopf and Iain Coleman, published Sep 06

UKeS-2006-02 *Large-scale data sharing in the life sciences: Data standards, incentives, barriers and funding models (The "Joint Data Standards Study")*, Phillip Lord, Alison MacDonald, Richard Sinnott, Denise Ecklund, Martin Westhead, Andy Jones, published Aug 06

Progress against plans: The newsletter and UK e-Science reports are progressing according to plan. As noted above, we discovered that the task of keeping UK-wide information up to date required more staff time than we had available.

Plans for 2007-2008: The production of content and editorship of the UK e-Science report series will continue in the established and successful fashion. We will continue to solicit contributions from the national community.

Alison McCall, who has edited the newsletter over the first year of the project (and earlier) will leave NeSC in September. Gillian Law will take over this role for the second year of the project.

We will reduce the scope of the content collection work. We will engage with the research councils in order to get information about their e-science programmes entered into our database. We will also visit some regional e-Science centres to generate articles for the newsletter, links with our other knowledge transfer and e-uptake activities, and to encourage them to update the information in the national knowledge base.

4.6 E-INFRASTRUCTURE

Leader: Richard Sinnott

This activity covers our contribution to UK-wide e-Infrastructure efforts such as the ETF, STF and Campus Grids SIG. It also includes our work in leading the development of regional e-infrastructure. Much of this activity is the result of staff funded from other sources; the principal exception being our “ETF engineer” at Glasgow, Christopher Bayliss, who is 50% funded to work on ETF and related NeSC activities.

Technical development: Staff at both Edinburgh and Glasgow have participated in technology evaluations for the ETF. We have been predominantly engaged with completing the GT4 and OMII evaluations, and the current SRB evaluation. We have also been involved in day to day ETF

activities, which include reading and commenting on draft reports, attending meetings and taking minutes when appropriate.

On the GT4 / OMII evaluation, NeSC Glasgow were involved with the GT4 side of the evaluation which included installing GT4 and developing patches for it to add functionality to match the NGS flavour of GT2. During this we discovered some incompatibilities with newer versions of GT4. We were also involved in writing the report of these experiences.

The SRB evaluation involved installing the SRB and experimenting with its configuration. NeSC Glasgow developed an automated tool for analysing upload performance and we are currently gathering an extensive set of results which will form the performance evaluation section of the report. Due to bandwidth problems discovered late in the evaluation NeSC Glasgow had to reinstall SRB on a new machine and rerun all tests.

Prior to these efforts we were involved in a range of activities including Condor, RAVE and security related evaluations amongst others.

We have also contributed to the Campus Grids SIG, sharing best practice of technologies such as resource brokers and Condor. Extra support for this SIG comes from the EPSRC E-SciNet network project, which is held at NeSC with UCL as co-investigators.

Local and Scottish infrastructure: NeSC is a key driving force behind the efforts to establish a Scottish Grid Service (SGS). This will build on the major new hardware resources at Scottish universities and will, if successful, underpin a range of research. It will particularly support the numerous cross-Scotland research pooling bids such as SICSA (Informatics & Computing Science), SINAPSE (Brain Imaging), SULSA (Life Sciences) and others. The development of the case for support included a major assessment of the requirements of an e-Infrastructure across multiple disciplines with over 80 completed detailed questionnaires from a range of end users and administrators from a range of disciplines. The completed case has been endorsed by eight major universities across Scotland with letters of support from their Vice Principals and has now been submitted for review. If funded, the SGS would provide considerable personnel covering areas, including systems support, grid operations management and the development of research environments (such as portals) for specific application domains.

At Glasgow, the NeSC activity is now fully integrated into Computer Services both administratively (with all NeSC staff now on open ended contracts working for Computing Services) and technically through campus wide projects such as GLASS. The roll-out and take up of Shibboleth based single sign-on across campus wide resources to provide secure access to student records; campus file storage; web mail and the Moodle virtual learning environment has involved close collaboration and co-operation between Computer Services, Management Information Services, the Registry/Human Resources and NeSC. NeSC also supports campus grid efforts through projects such as nanoCMOS, where we are now able to use a variety of heterogeneous resources across the university including the major new ScotGrid cluster; Condor pools and Sun Grid Engine resources in the department of electronics.

At Edinburgh, NeSC provides middleware support and requirements gathering for the university's research computing facility, working in close partnership with the university's Information Services (IS) division. IS supports research computing at the Advanced Computing Facility (ACF). IS and EPCC provide operations and platform development support with NeSC and EPCC providing middleware and applications support. IS is also responsible for the research network and UKLight connections. NeSC led the procurement of a new 512-core cluster for the Edinburgh Advanced Computing Facility, working closely with IS.

UK infrastructure: At Glasgow, we are in the final stages of making the (GridPP & SRIF) ScotGrid cluster available as part of the NGS (initially as an affiliate). We are also directly working with the NGS technical support teams at various levels. For example, through projects such as the JISC-funded VPman project, we have deployed a VOMS server and successfully shown how finer-grained VO-specific access to large scale clusters can be achieved through exploitation of

associated technologies such as LCMAPS and LCAS. Transferring this know-how to the NGS support teams is on-going.

At Edinburgh, we already provide access to Blue Dwarf (an IBM p690) as an NGS Affiliate. We have recently moved the middleware that provides our NGS Affiliate status to a more reliable platform, in preparation of applying for NGS Partnership. We have developed a close working relationship with EDINA - a JISC funded National Datacentre also based at the University of Edinburgh. NeSC and EDINA staff meet regularly and are cooperating on projects working towards exposure of nationally significant datasets on the NGS. This is particularly true in the geospatial area, where, as part of the JISC SEE-GEO project (Secure Access to Geospatial Services), an EDINA software engineer has shared desk space with engineers at NeSC.

Progress against plans: We are clearly progressing well, contributing actively to ETF activities and the NGS while leading regional developments.

Plans for 2007-2008: We will continue to participate in the ETF and Campus Grids SIG. If the bid for a Scottish Grid Service is successful, we will contribute resources and staff to that activity.

In Edinburgh, the results of our requirements gathering point to a combination of duplication of effort and lack of resources for research groups. We intend to work with groups to pool these efforts in three areas:

- Providing the infrastructure for sharing common bio-science databases and making these databases available through web services so that workflows can be designed around them and shared across research groups.
- Working across schools in the university on high-performance file systems to enable researchers to share data across compute resources and reduce duplication of data.
- Promoting and enabling Condor use around the University, thus pooling disparate University-wide compute resources.

In Glasgow, the e-Infrastructure development plans revolve around several key resources including the ScotGrid cluster and numerous other HPC facilities including a second 128-processor cluster managed by Computer Services; a new 128 processor bioinformatics cluster (managed by the Dept. of Computing Science); and a further cluster based in the department of electronics. Currently these are being accessed and used through projects such as the Scottish Bioinformatics Research Network and the EPSRC pilot project nanoCMOS.

We recognise however that a great number of researchers at Glasgow do not need access to HPC compute facilities, but rather require e-Infrastructure that allows them to manage their research data. To this end, NeSC at Glasgow are developing a range of bespoke solutions for the researchers at Glasgow leveraging where feasible (due to security considerations for example) the campus SAN. These included establishment of biobanks incorporating clinical and bioinformatics data resources in a secure environment for breast cancer and prostate cancer researchers amongst numerous others. Such facilities are based upon the roll-out of results from a range of NeSC projects such as VOTES, GEMEPS and GHI and NeSC Glasgow's various security projects.

In addition, we will develop an NGS Affiliate capability at Glasgow and move our Edinburgh NGS resource from Affiliate to Partner status.

4.7 IT INFRASTRUCTURE

Leader: David McNicol

Web site hosting: We have investigated possibilities for outsourcing the hosting of the NeSC web site and the associated database. It seemed that a suitable facility would be provided by the University of Edinburgh's Management Information Services (MIS) division. They offered a mirrored web site for the database with load balancing between the two sites, which would give a

more robust deployment than our current system. Their servers would also be better protected in the event of power failures and have a better back-up facility.

In the project proposal we stated that we would buy a new web server. We decided to pursue the outsourcing option instead as it offers better reliability and would reduce the load on the NeSC IT team.

Negotiations with MIS were thrown into a hiatus when the university's IT provision was substantially reorganised following a review. This took longer then we were told would be the case. We have now resumed negotiations and are discussing detailed SLAs.

In the meantime, our existing web server has continued to provide good service to the community.

NeSCForge: NeSCForge has continued to provide a reliable and useful service to the community.

Progress against plans: We are substantially – almost a year – behind schedule with the deployment of a new web server and database server.

Plans for 2007-2008: We are urgently progressing negotiations with the University of Edinburgh's Information Systems division regarding the hosting of our web server and database. In addition, we are looking to some commercial hosting companies as a contingency plan in the case that further problems arise.

The current installation of NeSCForge is nearing the end of its useful life. We plan to upgrade the software to a more recent version, running on new hardware.

4.8 STIMULATE E-SCIENCE EDUCATION

Leader: David Fergusson

Although this work is not funded by the NeSC III grant, we manage it as a project activity. This activity leverages our existing work in e-Science education locally, nationally and at the EU level, to stimulate further development of e-Science education in the UK.

2006-2007: Most of our activity this year has been on building a network of contacts and resources. The main outcomes for the UK have been:

- To form and lead a UK network of trainers and educators. This built upon Birds-of-a-Feather sessions at the last two UK AHMs and continued with a workshop in January 2007 at The National Institute of Environmental e-Science in Cambridge.
- Achieving additional funding under the JISC project *Barriers to Uptake of e-Infrastructure Services* with our responsibilities including to identify and help address barriers in training and education
- Further development of the Digital Library, which was initially created for EGEE, was further extended for ICEAGE, and now also hosts collections for "UK e-science" among others.
- Exploration of challenges in establishing a sustained e-infrastructure for education. Of particular note is that GILDA is becoming a multi-middleware grid and thus a single framework for the educational goals of comparing and combining different grid technologies.
- Ad-hoc meetings and discussions in the context of NGS training – for example at the Universities of Plymouth and Brunel, related to their education

Progress against plans: The project proposal envisaged an annual education event for the UK. As noted, our activity has focussed more on establishing a community and resources for that community. We believe the end result is worthwhile and that we are now better placed to instigate an annual education event.

The JISC grant should secure our funding for this activity over the lifetime of the project.

Plans for 2007-8: In addition to continuing progress on the initiatives described above, we believe that they have done the groundwork that makes it timely to plan a workshop for e-science educators, as envisaged in the project proposal. These will be annual workshops, bringing together UK lecturers engaged in education related to e-science. The first is being planned for December 2007. This date will avoid collisions with major conferences in September/October and should be outside the semesters of most HEIs. The workshops will present progress in the above initiatives and will be a forum in which UK education can be discussed and advanced.

4.9 NATIONAL LEADERSHIP

Leader: Dave Berry

Staff at NeSC undertake a number of leadership tasks and activities beyond those funded by the project itself. These include organising visits from international delegations, the work of the UK e-Science Envoy, contributions to OGF, co-ordinating the UK e-Science presence at SC06, supporting the e-Science Directors' Forum, and participating in steering groups and JISC committees, among other work.

International delegations: During the period of this report, we were invited to visit the Swedish Research Council at request of the British Embassy in Sweden. We arranged this delegation, including directors of other UK e-Science Centres. We also attended and presented at the Malaysian Research & Education Network (MYREN) at the request of the British High Commission.

We co-ordinated the arrangements for the visit to the UK by representative of the Chinese Ministry of Science and Technology. Their visit included a day of meetings with senior staff at NeSC.

OGF: The NeSC contribution to the Open Grid Forum was particularly noticeable this year in that we led the organisation of OGF20, with local arrangements handled by the University of Manchester. This is described in more detail in the Community Events section of this report.

In addition, Malcolm Atkinson represents UK e-Science on the OGF board, thanks to the sponsorship of OGF provided by the Gridnet2 grant. This was a particular important year for OGF, as it saw the end of Mark Linesch's term at president and the selection of Craig Lee as his replacement. Craig Lee is already engaged with work at NeSC and eSI.

NeSC and EPCC also contribute to OGF working groups. Dave Berry is co-chair of the OGSA Data working group and Neil Chue Hong is co-chair of the OGSA ByteIO working group.

SC06, Tampa: NeSC co-ordinated the content of the UK e-Science stand at SC06. The stand was a showcase for UK e-Science, including demonstrations of projects funded by PPARC, MRC, ESRC, EPSRC and NERC, by groups from across the UK (including NeSC):

- Exploring the Universe
  - GridPP: Particle Physics on the Grid
  - AstroGrid: the UK's Virtual Observatory
- Exploring Our World
  - e-Social Science in action: a prototype geo-simulation portal
  - ClimatePrediction.net: Climate modelling through volunteer computing
  - IntBioSim: Biological Simulations
- Collaborative Software Infrastructures
  - OMII-UK: Software for the e-Scientist
  - E-Minerals: Making Grids Usable
- Collaborative Organisations
  - VOTES: Fine-grained security authorisation
  - GOLD: Virtual Organisations for the fine chemicals industry
  - Interactive Visualisation services

The stand had a programme with included ten presentations, including guest speakers from CERN and the University of Berkeley. The programme also included panel discussions about software licensing and about standards interoperability for job submission, and a showing of the BBC Horizon programme about the ClimatePrediction.net project. In addition, Malcolm Atkinson was invited to give a talk on the AIST stand.

UK e-Science Envoy: NeSC hosts the UK e-Science Envoy, who represents and co-ordinates the UK e-Science Core Programme. His activities for the year include, among others:

- Creating and leading the UK e-Science strategy group
- Representing the UK on the EU e-Infrastructure Reflection Group and initiating its Education and Training Task Force
- Attending quarterly meetings of bodies such as the e-Science Strategy Advice Team (which we hosted at NeSC in March 2007).
- Attending quarterly meetings of the Research Councils' e-Science Representatives.
- Contributing to JISC committees, including the Strategic e-Content Alliance, the Joint Committee for Support of Research and the JISC Board.
- Meetings with industry, such as a meeting with Sun Microsystems at NeSC in August 2006 and the official inauguration of SAP Research in Belfast.
- Giving the welcome speeches at AHM2006 and a keynote at Grid2006 in Barcelona.
- Attending other national and international conferences, such as the IEEE e-Science workshop in Amsterdam, the JISC conference and CompSci 2007.

Other activities: Peter Clarke is also a member of JISC committees, including the Joint Committee on Networking and the Joint Committee for Support of Research. He is a member of the e-Science SAT and chair of the STFC Strategic Computing Advisory Panel. He is also a member of the project management board of GridPP.

Richard Sinnott was on the international review panel for the Norwegian e-Science initiative (EVITA) and on the Singapore e-Science review panel.

Richard Sinnott was also directly involved in and co-author of the report outlining the roadmap for e-Science digital repositories across Europe. This was presented to the EU president in September 2007 and is to be used to shape future funding and research agendas dealing with large scale e-Science data sets across Europe.

Dave Berry is the technical lead of the *Grid Computing Now!* Knowledge Transfer Network, which encourages the uptake of e-Science technologies by UK industry. Dave has organised several webinars and other events that have brought together industry and academia.

5 Project Roles

5.1 Peter Clarke - Director and Principal Investigator

Professor Peter Clarke is Director of the National e-Science Centre and Professor of e-Science at Edinburgh. He was head of Particle Physics at University College London, and a Director and of the Network Centre of Excellence. He has worked at CERN for many years in the LEP and LHC programmes. He was a principal proponent leading to the UKLight R&D network for the UK, and now leads the ESLEA project to exploit optical networks for research applications. He has been on the PMB of the UK grid for particle physics (GridPP), the European Data Grid and the EGEE projects. He was a member of the Global Grid Forum Steering Committee and currently the JISC JCN and JCSR.

Project responsibilities include:

- Strategic decision making
- Liaison with ESI SAB
- Awareness raising and (human) networking activities

5.2 Richard Sinnott - Technical Director

Richard Sinnott holds a PhD from the University of Stirling. He was responsible for establishing an environment for e-Science at Glasgow. At Glasgow he lectures in Grid Computing and on the Modelling of Reactive Systems. He ran his own consultancy company based in Germany specialising in the area of formal technologies and their application to real time systems development, especially in the telecommunications domain. His current research is focused around Grid computing and its application to a broad spectrum of scientific areas especially the life science domain. He also maintains an interest in formal methods and their application to real time, distributed systems development.

Project responsibilities include:

- Leading the *Regional Outreach* activity and fostering projects across communities
- Leading the *e-Infrastructure* activity
- Managing the software engineer
- Interaction with Glasgow management on matters of facilities provision, sustainability of e-Science and strategic funding.
- NeSC III time commitments: 25%

5.3 Dave Berry – Project Manager

Dave Berry has a Ph.D. in Computer Science from the University of Edinburgh and over 10 years' experience of software development management in industry, with particular expertise in compilers, runtime environments and distributed systems. In the area of Grid computing he is primarily interested in Grid architecture. He is technical lead of the IECnet knowledge transfer network. He leads the OGSA Data working group of the GGF. He has also organized the programmes of many workshops at the e-Science Institute.

Project responsibilities include:

- Keep overview of the NeSC project plan, organise and execute the management plan described, ensure timely delivery on all promised elements, ensure regular documentation and reporting by deadlines,

- Convene the management committee
- Lead the *Community Events* activity
- Lead the *National Leadership* activity
- Manage promotion and representation at relevant events including AHM.
- NeSC III time commitment: 25%

5.4 SUSAN MCCAFFERTY – WEB AND DATABASE DEVELOPER

Project responsibilities include:

- Design and provide the implementation of the website in accordance with the content design.
- Advise on feasibility of content design.
- Provide technical support for related services including the AHM support and NeSC event hosting support.
- Susan is shared with the e-Science Institute, ensuring coherence between the two projects.

5.5 IAIN COLEMAN – SCIENCE WRITER

Project responsibilities include:

- Lead the *Web Site Content* activity.
- Design and maintain web site content.
- Ensure that the content is indexed in a clear and uniform way to maximise the opportunity for web-visitors to obtain contact points.
- Ensure that the content is kept constantly up to date, accurate and complete
- Ensure all direct NeSC-related activities are fully described
- Proactively seek information from other centres, projects, research councils and strategic partners such as JISC.
- Work closely with the JISC/EPSRC communications officer in Bristol.
- Manage the UK e-Science technical report series
- Iain is shared with the e-Science Institute, ensuring coherence between the two projects.

5.6 CHRISTOPHER BAYLISS - SOFTWARE ENGINEER

Project responsibilities include:

- Participate in ETF and STF work.
- Develop database services and file management services.
- NeSC III time commitments: 50%.

5.7 DAVID MCNICOL - SYSTEMS ADMINISTRATOR

Project responsibilities include:

- Lead the *IT infrastructure* activity
- Provision and maintenance of a reliable and resilient platform for the website
- Provision and maintenance of a reliable and resilient platform for NeSCForge
- Management of Access Grid maintenance, development and operations
- Management of basic computing support and network services
- NeSC III time commitments: 50%.

5.8 DAVID FERGUSSON - DEPUTY DIRECTOR, TRAINING OUTREACH & EDUCATION

Project responsibilities include:

- Lead the *Stimulate e-Science education* activity
- Manage the annual large education event

5.9 ANNA KENWAY - DEPUTY DIRECTOR, E-SCIENCE INSTITUTE

Project responsibilities include:

- Lead the *Wed Site Redesign* activity

5.10 EVENTS TEAM

Project responsibilities include:

- Logistics support (registration, accommodation, programme, front desk and delegate services during meeting)
- Technical support (computing infrastructure, demos and open guest network provision).Provide and develop the website.
- NeSC III time commitments: 1 FTE equivalent.