



Proceedings of the UK e-Science All Hands Meeting 2004

Nottingham, UK

31st August – 3rd September

Editor

Simon J Cox

© EPSRC Sept 2004

ISBN 1-904425-21-6

Sponsored by

JISC, BAE SYSTEMS, IBM®, Intel®, Microsoft®,

Sun microsystems®

JISC

BAE SYSTEMS



Microsoft®



We make the net work.

Welcome and Introduction

Tony Hey, Director of the UK e-Science Core Programme

Dear Colleagues

We are now some three years into the ambitious UK initiative set out by John Taylor under the banner of e-Science. It is important to recognize that e-Science is about both the invention and the exploitation of new IT techniques and systems. Its goal is to enable real research – not ‘virtual research’ - and allow scientists to do ‘faster, better or different’ research. Thus the e-Science programme is inherently multidisciplinary – challenging computer scientists to discover new techniques and technologies to meet the needs of the researchers, challenging the pioneering scientists prepared to try to exploit these new research tools to aid their research agenda, and challenging the computer systems builders and university IT and library services to build systems that will support such experiments. It is clearly another huge challenge to keep all parties happy and engaged with this agenda. The All Hands Meetings are one mechanism to support the interchange of ideas and problems of the different communities.

At this stage of the programme, it is worthwhile reminding ourselves that the essential idea for this endeavour can be traced right back to the 1960’s and the birth of the Internet. Such an e-Science infrastructure as we now envisage is in fact very close to the vision that the psychologist J.C.R.Licklider (‘Lick’) took with him to ARPA when he initiated the research projects that led to the ARPANET. Larry Roberts, one of his successors at ARPA and principal architect of the ARPANET, describes this vision as follows:

“Lick had this concept of the intergalactic network which he believed was everybody could use computers anywhere and get at data anywhere in the world. He didn’t envision the number of computers we have today by any means, but he had the same concept – all of the stuff linked together throughout the world, that you can use a remote computer, get data from a remote computer, or use lots of computers in your job. The vision was really Lick’s originally.”

The ARPANET of course led to the present day Internet - but the killer applications have so far been email and the Web rather than the distributed computing vision described above. In the early 1960’s, Licklider only envisaged needing to connect a small number of scarce, expensive computers at relatively few sites. Over the past thirty years Moore’s Law – Gordon Moore’s prediction that the number of transistors on a chip would double about every 18 months so that the price-performance is halved at the same time – has led to an explosion in the number of supercomputers, mainframes, workstations, personal computers and PDAs that are now connected to the Internet. Although Moore’s Law – at least if the IT industry continues to be based on silicon technology - must come to an end when feature sizes of transistors begin to approach atomic dimensions, the IT revolution still has perhaps a decade or more to run. Already

we are beginning to see intelligent sensors and RFIDs – intelligent tagging devices - being connected to the network. In addition, new high-throughput experimental devices are now being deployed in fields as diverse as astronomy and biology and this will lead to a veritable deluge of scientific data over the next 5 years or so.

Scientific collaborations have long been connected by the high speed national research networks that constitute the underlying fabric of the academic Internet. Under the banner of 'e-Science', scientists and computer scientists around the world are now collaborating to construct a set of software tools and services to be deployed on top of these physical networks. Since this software layer sits between the network and the application level software it is often referred to as 'middleware'. The ambitious goal is the creation of a core set of middleware services for scientists that will provide them with the capability to routinely set up secure, controlled environments for collaborative sharing of distributed resources for their research. Collectively, these middleware services and the global high-speed research networks will constitute the new 'e-Infrastructure' (in Europe) or 'Cyberinfrastructure' (in the USA) for collaborative scientific research. In the UK we refer to this middleware as 'Grid Middleware' although we are conscious of the fact that the present Grid middleware components only offer a small part of the functionality we require.

We are now at a critical stage in the development of the middleware layer of this e-Infrastructure. The good news is that with the recent Web Services Resource Framework proposal, Grids are now explicitly recognized as being a sub-set of the more general Web Services world that is being enthusiastically supported by the entire IT industry. The bad news is that Web Services themselves are still 'work in progress' so we must adopt conservative strategies to safeguard our UK investment and ensure that we converge on the eventual standards that emerge from GGF and OASIS. However, on the positive side, as I am sure you will see at this year's All Hands Meeting, there are now some encouraging signs of scientists deriving real benefit from the e-Science infrastructure.

It is also very encouraging to welcome the Joint Information Systems Committee as a major sponsor of this year's meeting. Their involvement is very much to be welcomed since they well understand the need for a stable infrastructure to support the global 'virtual well-founded laboratory'. The new JISC-funded National Grid Service is also on display at this meeting and the benefits of a constructive synergy between Research Councils and the JISC is well illustrated by this and by the £6.5M JISC-funded UKLight 'lamda' network. This infrastructure investment will not only inform UKERNA's SuperJANET5 procurement but also enable the UK and UKERNA to play a leading role in collaborations with the international research networking community. What is particularly pleasing, however, is to note that EPSRC have recently approved three major research projects that will be using UKLight as a research testbed.

These are early days in the life of e-Science but it is encouraging that more and more countries around the world are now funding e-Science programmes along similar lines to the UK programme. We will also hear at this meeting about developments on the 'Cyberinfrastructure' initiative in the US and about the EC project 'EGEE', the major EU Research Infrastructure initiative in Framework 6. I hope that the announcement of

the 2004 Spending Review will enable the UK research community to build on its early successes in e-Science and deliver a truly useful and stable infrastructure for collaborative science.

I hope you all enjoy the meeting and find the formal presentations and workshops interesting and useful – but I also hope that you find the informal interactions with colleagues as or more useful!

Tony Hey

Director of the UK e-Science Core Programme

Welcome and Introduction

Ron Perrott, Chairman of the All Hands Steering Committee 2004

Dear Colleagues

This is the third All Hands e-Science Meeting to be held in the UK. Last year, a highly successful meeting was held at Nottingham under the title 'Delivering e-Science'. This year the location is Nottingham again and the theme of the Meeting is 'e-Science Broadening the Horizon'. This is an important conference for the UK's e-Science Initiative as it provides a forum for all e-Science researchers, developers and users, and those who are just curious to see the project results and what progress which has been made in the area.

The Meeting has been structured into an academic programme which comprises oral presentations, poster sessions, mini-workshops and "birds of a feather" sessions. In addition there is a major exhibition which provides a forum to demonstrate e-Science results and achievements. Each of the Regional e-Science Centres and the new Centres of Excellence and many other projects under the e-Science umbrella, have taken booths in the Exhibition Hall to demonstrate their work. Delegates are invited to spend time at the Exhibition talking to the experts involved in a wide range of projects.

The academic Programme includes four major Keynote Addresses, namely, we have Dr Sangtae Sang Kim, the Director of the NSF Cyberinfrastructure, Professor Mike Brady of Oxford University and principal investigator of the eDiamond Project, Dr Bob Jones of CERN who will talk about the EU EGEE project and Ian Foster of Argonne National Laboratory and one of the originators of Globus. In addition Tony Hey will give an address on the achievements and the future of the e-Science Programme. I would like to express our thanks and appreciation to all of the speakers for generously giving of their time to participate in the Meeting.

This year the organisation of the Meeting has expanded to meet the increasing needs of a larger and more comprehensive meeting. In particular special thanks are due to Programme Committee, Chaired by David Walker and Malcolm Atkinson and their 50 programme committee members who handled the refereeing of the large number of submitted papers, to Carol Becker and her colleagues at the EPSRC Secretariat for the smooth organisation of the event and to Anna Kenway and Susan Andrews of National e-Science Centre for the excellent management of the website and the paper submission activity.

Ultimately, however, the success of the conference will be judged by how well the delegates have participated, learnt, interacted and established contacts with other researchers in different fields. The Committees and the e-Science Directorate have provided the funding, the venue, and the environment to allow these objectives to be achieved. It is now up to all of us to ensure that the Meeting is an outstanding success.

I wish you a successful, stimulating and rewarding meeting and look forward to seeing you again at future All Hands Meetings.

Ron Perrott
Chairman
All Hands Steering Committee

All Hands Conference 2004 Steering Committee

Representatives:

Ron Perrott	Queen's University, Belfast (Chair)
Malcolm Atkinson	National e-Science Centre
Ken Brodrie	University of Leeds
John Brooke	University of Manchester
Charlotte Capener	BBSRC
Simon Cox	University of Southampton
Jim Fleming	EPSRC
Neil Geddes	CCLRC (PPARC)
Keith Haines	Reading e-Science Centre
Mark Hayes	University of Cambridge
Marina Jirotko	University of Oxford
Andy Keane	University of Southampton
Tom Kirkwood	University of Newcastle (MRC)
Marta Kwiatkowska	University of Birmingham
Bryan Lawrence	RAL (NERC)
Andrew Martin	University of Oxford
Diane McLaren	MRC
Tom Rodden	University of Nottingham (ESRC)
Rob Smith	University of Newcastle
Mike Sternberg	Imperial College (BBSRC)
David Walker	University of Cardiff

Officials:

Anne Trefethen	EPSRC/DTI
Audrey Canning	DTI
Carol Becker	EPSRC
Dolly Parkinson	EPSRC
Anna Kenway	National e-Science Centre
Susan Andrews	National e-Science Centre

Welcome and Introduction

David Walker, Chairman of the All Hands Programme Committee 2004

Dear Colleagues,

AHM 2004 received 250 submissions, which is an increase of over 45% compared with the previous year. This large number of submissions indicates a vibrant and expanding e-Science research community in the UK. The technical programme for AHM 2004 consists of:

- 3 tutorials.
- 6 Birds-of-a-Feather sessions.
- 5 mini-workshops featuring 30 presentations.
- 4 plenary sessions featuring 5 keynote talks.
- 24 regular sessions arranged in 4 parallel tracks with a total of 100 presentations.
- A poster session featuring about 60 posters.

All submissions to AHM 2004 were rigorously reviewed under the control of the Programme Committee. The acceptance rate for regular papers was 62%, and for mini-workshop papers it was 56%. The reviewing process was conducted to a tight schedule, and the Programme Committee and the other referees did a great job in ensuring that all reviewing was completed on time and to a high standard. Susan Andrews of NeSC also deserves special thanks for developing the online tools that made the reviewing and composition of the programme much easier. Finally, I am very grateful for the help, advice, and hard work of Prof Malcolm Atkinson who served as Vice-Chair of the Programme Committee.

I hope you find the AHM 2004 programme stimulating and enjoyable.

David Walker
Chairman
AHM 2004 Programme Committee

AHM 2004 Programme Committee

David Walker	University of Cardiff
Malcolm Atkinson	National e-Science Centre
Simon Cox	University of Southampton
Mario Antonioletti	EPCC
Jim Austin	University of York
Bob Bentley	University College London
Dave Berry	National e-Science Centre
John Brooke	University of Manchester
Geoff Coulson	Lancaster University
Jon Crowcroft	University of Cambridge
Peter Dew	University of Leeds

Paul Donachy	Queen's University Belfast
Alistair Dunlop	OMII
Glenn Gapper	BAE Systems
Neil Geddes	CCLRC
Ian Grimstead	Cardiff University
Keith Haines	University of Reading
Terry Harmer	Queen's University Belfast
Mark Hayes	University of Cambridge
David Hutchison	Lancaster University
Stephen Jarvis	University of Warwick
Marina Jirotko	University of Oxford
Andy Keane	University of Southampton
Steven Kenny	Loughborough University
Kerstin Kleese van Dam	CCRLC
Michael Kirton	QinetiQ
Bryan Lawrence	CCLRC (NERC)
Ian M Leslie	University of Cambridge
Bob Mann	University of Edinburgh
Andrew Martin	University of Oxford
Richard McClatchey	University of West England
Linda McCormick	University of Glasgow
Robin Middleton	CCLRC
Peter Murray-Rust	University of Cambridge
Dave Newbold	University of Bristol
Steven Newhouse	Imperial College
Ken Peach	CCLRC
Ron Perrott	Queen's University, Belfast
Omer Rana	Cardiff University
Tom Rodden	University of Nottingham (ESRC)
Lakshmi Sastry	CCLRC
Nigel Shadbolt	University of Southampton
Ian Sommerville	Lancaster University
Georgios Theodoropoulos	University of Birmingham
Nigel Thomas	University of Newcastle-upon-Tyne
Paul Watson	University of Newcastle-upon-Tyne
David Williams	CERN

Other AHM 2004 Reviewers

John Ainsworth	University of Manchester
Rashid Al-Ali	University of Cardiff
Harith Alani	University of Southampton
Peter Allan	CCLRC - Rutherford Appleton Lab
David Allsopp	QinetiQ
Ashok Argent-Katwala	Imperial College
David Bacigalupo	University of Warwick
Richard Baldock	University of Edinburgh
Lisa Blanshard	CCLRC - Daresbury Laboratory

Chris Booth	QinetiQ
Jeremy Bradley	Imperial College
Frederic Brochu	University of Cambridge
Alan Bundy	University of Edinburgh
Wei Cai	Lancaster University
Kate Caldwell	Cambridge e-Science Centre
Stuart Charters	University of Durham
Neil Chue Hong	Edinburgh Parallel Computing Centre
Nathan Ching	University College London
Jeremy Cohen	Imperial College
Adrian Conlin	University of Newcastle
James Currall	University of Glasgow
Michael Dales	University of Cambridge
Rob Davis	University of York
Matthew Dovey	University of Oxford
David Dupplaw	University of Southampton
Denise Ecklund	National e-Science Centre
Donal Fellows	University of Manchester
David Fergusson	EGEE & National e-Science Centre
Magnus Ferrier	National e-Science Centre
Martyn Fletcher	University of York
R. F. Fowler	CCLRC - Rutherford Appleton Lab
Nathalie Furmento	Imperial College
David Gavaghan	University of Oxford
Jonathan Giddy	Welsh e-Science Centre
Rolly Gilmour	University of Glasgow
Cecilia Gomes	New University of Lisbon, Portugal
Daniel Goodman	University of Oxford
Paul Grace	Lancaster University
Murtaza Gulamali	Imperial College
Stephen Hall	Lancaster University
Steven Hand	University of Cambridge
Stephen Harris	University of Oxford
Martin Hendry	University of Glasgow
Pawel Herzyk	University of Glasgow
Mark Hewitt	University of Newcastle
Hugo Hiden	University of Newcastle
D Higgins	University of Glasgow
Chris Hinds	University of Oxford
Conrad Hughes	National e-Science Centre
Danny Hughes	Lancaster University
Alastair Hume	Edinburgh Parallel Computing Centre
Mike Jackson	Edinburgh Parallel Computing Centre
Tom Jackson	University of York
Mark Jessop	University of York
Liviu Joita	University of Cardiff
Bob Jones	CERN
Mike Jones	University of Manchester

Roy Kalawsky	Loughborough University
Noel Kelly	Queen's University Belfast
Ewan Klein	University of Edinburgh
Sylvia Knight	University of Oxford
Charles Kubicek	University of Newcastle
Erwin Laure	CERN
Andy Lawrence	University of Edinburgh
William Lee	Imperial College
Peter Li	University of Newcastle
Karen Loughran	Queen's University Belfast
Simone Ludwig	University of Cardiff
Ananta Manandhar	CCLRC - Daresbury Laboratory
Bruce Mason	University of Cardiff
Anthony Mayer	Imperial College
Julie McCabe	Queen's University Belfast
Gavin McCance	CERN
Mark McCoghlan	Queen's University Belfast
Mark McColgan	Queen's University Belfast
Steve McGough	Imperial College
Mark McKeown	University of Manchester
Mike Mineter	EGEE & National e-Science Centre
Isi Mitrani	University of Newcastle
Lee Momtahan	University of Oxford
Soraya Kouadri Mostefaoui	University of Fribourg, Switzerland
S Nagella	CCLRC - Rutherford Appleton Lab
Ieaun Nicholas	University of Cardiff
Werner Nutt	Heriot-Watt University
Mohammed Odeh	University of the West of England
Kevin O'Neill	CCLRC - Rutherford Appleton Lab
Clive Page	University of Leicester
Kevin Page	University of Southampton
A Pakhira	CCLRC - Rutherford Appleton Lab
Juri Papay	University of Southampton
Andrew Pasley	University of York
Terry Payne	University of Southampton
Mark Prentice	Queen's University Belfast
Rob Procter	University of Edinburgh
Mustafizur Rahman	University of Oxford
Russell Ross	University of Cambridge
Nigel Shadbolt	University of Southampton
Andrew Simpson	University of Oxford
David Simpson	Queen's University Belfast
Richard Sinnott	National e-Science Centre
Jim Smith	University of Newcastle
Rob Smith	University of Newcastle
Roger Smith	Loughborough University
Tony Solomonides	University of the West of England
Daniel Spooner	University of Warwick

Amos Storkey
Shoaib Sufi
G Swallowe
Aaron Turner
Michael Turner
R Tyer
Andrew Usher
Gareth Waller
Jie Xu
Wai Kit Yeung
Yi Zhang
Yong Zhang
Irfan Zakiuddin

University of Edinburgh
CCLRC - Daresbury Laboratory
Loughborough University
University of York
BAE Systems
CCLRC - Daresbury Laboratory
University of Cambridge
Queen's University Belfast
University of Leeds
Lancaster University
University of Birmingham
University of Cambridge
QinetiQ

Welcome and Introduction

Simon Cox, Editor of the All Hands Proceedings 2004

Welcome to the proceedings of the UK e-Science All Hands meeting 2004. On this CD you will find pdf versions of the papers which were presented in the regular sessions, workshops, and as posters at the conference.

Many thanks to:

- The All Hands Meeting 2004 programme committee for refereeing the papers
- Event Coordinators at EPSRC: Carol Becker and Dolly Parkinson.
- The team at the National e-Science Centre for their invaluable help: Gill Maddy, Dr Anna Kenway and Susan Andrews.
- Our sponsors for these proceedings.

Special thanks to Susan Andrews for her diligence, patience, and tireless efforts in bringing the proceedings together.

I hope that you will find this a useful resource.

Prof Simon Cox
University of Southampton