

# Workshop information

## e-Infrastructures workshop

Het West-Indisch Huis  
Herenmarkt 99, Amsterdam

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## Plenary speakers

### ***Dr. Xue-Bin Chi***

Dr. Xue-Bin Chi works for the Computer Network Information Center of the Chinese Academy of Sciences. CNIC was established in 1995 to provide among others network facilities, supercomputing and infrastructure for scientific databases for Chinese science.

### ***Dr. Aad van der Steen***

Dr. Aad van der Steen studied mathematics at the Delft University of Technology while providing computational support at the Interuniversity Reactor Institute in Delft. After a short stay as a mathematical modeller at the Environmental Ministry he started working for the Computing Centre of the Utrecht University and as an advisor to NCF for High Performance Computing. He obtained his PhD. from the Computational Physics Department of the Utrecht University on the subject of benchmarking High Performance computers. He currently heads the High Performance Computing Group at Utrecht University in The Netherlands. Since 1990 he is responsible for the benchmarking of the computer systems for the Dutch scientific community via NCF, the computer branch of the Dutch Science foundation NWO.

Aad van der Steen is well known for his "Overview of recent supercomputers", which has been published since 1992 and is currently in its 15th edition. He has a long record in benchmarking of High Performance computers. He is author and editor of the online EuroBen Benchmark.

### ***Latif Ladid***

Latif Ladid holds an ESCAE (France), and did post-graduate work in business and administration in the UK. He is currently the President of IPv6 Forum, and serves as a Trustee of the Internet Society (ISOC). With support from the IETF IPv6 Working Group and the IPv6 Deployment Initiative, Latif founded the IPv6 Forum in May 1999. Additionally he is Chair of the European IPv6 Task Force and Vice Chair of the North American IPv6 Task Force).

As he researcher he is involved with multiple European Commission Next Generation Technologies IST Projects including 6INIT ([www.6init.org](http://www.6init.org)), 6WINIT ([www.6winit.org](http://www.6winit.org)), Euro6IX: [www.euro6ix.org](http://www.euro6ix.org), Eurov6 ([www.eurov6.org](http://www.eurov6.org)), and NGNi, <http://www.ngni.org> ). He is also a project initiator of the first IPv6 Security & Privacy project called Security Expert Initiative ([www.seinit.org](http://www.seinit.org)). He is also a member of a number of other organisations and committees, such as 3GPP2 PCG ([www.3gpp2.org](http://www.3gpp2.org)), IEC Executive Committee, the United Nations ICT TF Policy WG and the ITU-T Informal Forum Summit.

He has worked in various managerial and marketing positions at Nixdorf Computers in Germany, and Hewlett-Packard in the Middle East, as International Sales Manager at ComputerLand Europe in Luxembourg, and as Managing Director of ComputerLand Switzerland. From 1992 to 1998, he was with the Canadian Internet and internetworking specialist, DEVELCON, where he served as Vice President of Sales and Business Development. In 1998, Latif joined Telebit Communications A/S as Vice President, Sales EMEA (In June 1999, Ericsson acquired a major share in Telebit, creating Ericsson Telebit A/S). He served, from 1996 to 1998, as chairman of Global-ISDN.

# Accounting

## *Session chairs:*

**John Gordon, CCLRC**  
**Kors Bos (NIKHEF)**

### **John Gordon**

John Gordon is the Deputy Director of CCLRC's e-Science Centre. He is currently the Deputy Project Leader of GridPP, the UK's largest Grid project which is building a production grid for particle physics in the UK and leads the UK part of the Operations and Support SA1 in EGEE, the largest FP6 Grid Infrastructure project.

Until late 2004 John was the Director of the UK's Grid Support Centre which provided support for all the UK's e-science projects. Other current work includes The Large Hadron Collider Computing Grid where he represents the UK on the Grid deployment Board and other panels.

The CCLRC e-Science Centre has a mission to gridify the large-scale facilities at CCLRC, including ISIS, a high power Neutron scattering source, SRS, the existing synchrotron radiation source and its successor Diamond which opens in 2007, roughly the same time as the LHC. eSC is also involved in e-science projects from most of the UK Research Councils, the UK's Digital Curation Centre, and leads the work on building and running the UK's National Grid Service.

### **Kors Bos**

Kors Bos (1947) is a senior scientist working at NIKHEF in Amsterdam and CERN in Geneva. He is a member of the e-IRG since its inception in 2003, and a founding member of Gridforum Netherlands. He is the chair of the Grid Deployment Board for the LHC Computing Grid Project (LCG) at CERN.

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## ***Accounting - Introduction***

In the Rome eIRG meeting it was decided that accounting for the grid is technologically immature and related policies should be deferred to future presidencies. The first part of that statement is still true; there has been progress but it has been slow.

## **Progress**

In the Den Haag white paper the following pilots and studies were recommended:

- Gathering accounting best practices from existing consortia and computing centres and transferring them to solutions based on open standards
- Detailed exploration of accounting use cases
- Grid market pilots to identify bottlenecks and practical challenges in the economic models
- Pilots for utilisation of banking systems with grid resource billing
- Studies on legislation issues concerning resource trading
- Development of common vocabulary for accounting terminology
- Intensifying international collaboration in defining common accounting standards and interoperability between existing and future solutions

My personal knowledge of progress is limited so I don't want to list a restricted set of work and exclude anyone so I propose the discussion session should gather information on progress in each of these areas for the white paper. I believe that six months since the last workshop is insufficient time for pilots to have been launched and completed so we are probably limited to work that was already underway or deviations in bigger projects.

## Updates From Specific Projects/Pilots

- EGEE has deployed APEL, an RUS, on its production service and the wider LCG.
- DGAS has been deployed in production on INFNGrid in Italy in anticipation of wider deployment in EGEE and on a prototype of the EGEE gLite middleware.
- SGAS has been deployed on SweGrid since before the last eIRG.
- the NextGRID project [www.nextgrid.org](http://www.nextgrid.org) has started work on the contract and ontology aspects of accounting.
- MCS has been benchmarked on the UK National Grid Service and has a prototype working with PayPal.

## Standards

- The GGF UR-WG usage record was incorrectly described in the last white paper. It has now been adopted by a number of grid projects (EGEE, TeraGrid, NGS, OSG, SweGrid, NextGrid, LCG, NorduGrid, GridIT) and appears to be approaching a de facto standard. It will be interesting to compare their implementations for interoperability, comparison of extensions, subsets etc..
  - GESA-WG has been in hibernation for some time and no progress has been made since November.
  - RUS-WG has recently had a renewal of activity. The revised spec is on track for submission to the GGF editor in the near future.
  - The relevant GGF work on negotiation is taking place in the GRAAP Working Group.
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## Summary Prior to Workshop

There are a variety of existing projects implementing technical architectures for usage recording and access control in a closed community. There are possibilities here to work on interoperability and data exchange. There are fewer attempting to explore the much larger phase space of economic models in the truly open market. This is where there is obvious scope for new projects and the inclusion of experiences from existing projects who are only just getting round to an accounting phase. There is also scope for increasing the community to learn from the experiences of telcos and others with similar markets.

The Authorisation strand of AAA is more mature than accounting and there is scope for some of its work to be applied to accounting implementations to address issue of privacy, authorisation, and security.

## Roadmap

- We should not be prescriptive about the economic model used between users and owners of resources but we should allow an infrastructure that is flexible in these negotiations. A truly open and flexible system may be some way off though, so the roadmap may wish to consider a phase of support for restricted methods of working.
- There is a gap in the infrastructure for reliable, trusted third parties, which the roadmap should address.
- Security and privacy standards should be addressed
- Internationalisation: there are already Grids that stretch beyond Europe so the engagement of other political-economic areas at an early stage will be important.

# Legal issues in e-Infrastructures

## *Session chair: Prof. Kees Stuurman (UvT)*

Kees Stuurman (1956) is professor of information technology regulation at the Tilburg Institute for Law, Technology and Society (TILT) since 2001. Next to his academic work he is partner of Van Doorne attorneys and civil law notaries in Amsterdam, and practice group leader of Van Doorne's IP/IT group.

He holds masters degrees in physics and in law from the Vrije Universiteit Amsterdam. From 1985 until 2000 he was (senior) research associate at the Computer/Law Institute of the Vrije Universiteit Amsterdam. In 1995 he obtained his doctorate in law based on a study of the legal significance of technical standards in the field of information technology and telecommunications.

His research activities cover a broad range of topics, varying from e-commerce law (contracting issues, electronic signature, consumer protection), computer contracts, legal aspects of certification and standardisation, to liability issues relating to information technology and telecommunications. He participated in a large number of national and international (European) research projects and acted as a reviewer for the European Commission and for the Dutch Science Foundation (NWO).

Currently, the main focus of his academic work lies in the field of regulatory aspects of information technology and other high technologies (e.g. biotechnology and nanotechnology) with a specific focus on self regulation (codes of conducts, standards, certification etc.).

His law practice focuses on legal aspects of IT and telecoms transactions, including contracting issues, public procurement, outsourcing and electronic commerce. He is amongst other things a member of the board of the Netherlands Association for Information Technology and Law, member of the legal expert committee of ECP.NL (ElectronicCommerce Platform Nederland), and member of the editorial board of The Computer Law and Security Report.

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## *Legal issues in e-Infrastructures*

### **Some questions to be addressed:**

1. Which legal issues could in general be identified in relation to GRID's?
2. What is the sense of urgency in identifying and debating the legal issues relating to GRID's?
3. Which GRID model or models could be used in structuring the discussion of legal issues relating to GRID's?
4. Which relevant GRID distinctions can be made in discussing the legal issues (e.g. closed/open, types of participants, geographical coverage, commercial/not for profit, .....).
5. Which legal issues could be linked to short term/medium term/long term developments in the field of GRID's?
6. Which approach should be followed to further identify and evaluate legal issues relating to GRID's?

# Generic versus disciplinary grids

## *Session chair: Prof. dr. Manuel Delfino*

Manuel Delfino is Professor of Physics at the Universitat Autònoma de Barcelona, Spain (UAB) and Adjoint Researcher at the Institut de Física d'Altes Energies (IFAE) in Barcelona. He is currently the Director of the Port d'Informació Científica (Scientific Information Port) in Barcelona and the Coordinating Principal Investigator of the LHC Computing Grid Project in Spain and of the Southwest Europe Federation in the EU Enabling Grid for E-science project. He was on leave during 1999-2002 serving as Leader of the Information Technology Division of CERN, the European Organization for Nuclear Research based in Geneva, Switzerland.

Prof. Delfino holds a B.S. in Applied Mathematics, Engineering and Physics, an M.S. in Physics and a Ph.D. in Physics with a minor in Computer Science, all from the University of Wisconsin in Madison, USA.

Prof. Delfino's research results in particle physics include the first direct evidence for weak neutral currents between electrons and positrons using the MAC detector at the Stanford Linear Accelerator Center and precision measurements of Z boson decays to leptons using the ALEPH detector at CERN. On the scientific instrument side, he participated in the development of the first large scale gas calorimeters in the 1980s and more recently in development of the ATLAS Scintillating Tile Calorimeter.

Prof. Delfino has devoted a large portion of his career working on integrating distributed computation into scientific activities. He led the ALEPH FALCON quasi-online data processing facility based on a farm of loosely coupled commercial processors and he was the spokesperson of the CERN RD-47 project which served as proof of concept for building large-scale processor farms using inexpensive Personal Computers. While at CERN, he helped to launch the EU DataGrid and the LHC Computing Grid projects.

Prof. Delfino proposed in 2001 the creation of the Port d'Informació Científica (PIC), an innovative center focused on providing Grid-enabled resources for data-intensive scientific computing. PIC was created in October 2002 and is currently funded through a collaboration agreement between CIEMAT (Ministry of Education and Science, Spain), DURSI (Department of Universities and Research, Catalonia), UAB and IFAE.

# International connectivity

## *Session chair: Prof. dr. Dany Vandromme*

Dany Vandromme is a member of the e-IRG on behalf of France. He has been director of GIP RENATER since July 1st, 1998. Vandromme was appointed professor in 1988 at the National Institute for Applied Sciences at Rouen. As a researcher, he is responsible of the Computational Fluid Dynamics Laboratory (LMFN), a component of CORIA, UMR 6614 of CNRS (National Center for Scientific Research). Research domain is the numerical modeling applied to supersonic and reactive flows with a special interest for turbulence physics.

Responsible for the regional network SYRHANO (Upper Normandy region) since its beginning in 1993, and chairman of the networking and computing Centre of Upper Normandy (CRIHAN) since its création (1992), Dany Vandromme has been a user of ARPANET in the early 80's, and later on, of INTERNET, as a post-doc and associate research fellow at NASA Ames Research Center from 1980 to 1990.

He was in charge of the networking and computing activities at the Engineering Sciences Department of CNRS from 1993 to 1998. As such, he was also supervising the CNRS laboratories depending from the section #10 of the "Comité National de la Recherche Scientifique".

As director of RENATER, Dany Vandromme works on evolutions of the public Internet in France, on technical aspects as well as on economy models, suited to the specific requirements of the research and education community.

Dany Vandromme represents RENATER in the European NREN consortium in charge of GEANT ([www.geant.net](http://www.geant.net)). Since January 2001, he served as member of the DANTE ([www.dante.org.uk](http://www.dante.org.uk)) Board of Director. Since January 2003, he is the Chairman of the DANTE Board.

He participates to the works of ICANN, through the non-commercial constituency (NCDNHC) of the Domain Name Supporting Organisation (DNSO).

He is one of the two French representatives in the European Strategy Forum for Research infrastructures (ESFRI). Dany Vandromme awarded as "Chevalier de l'Ordre National du Mérite" on January 31st, 2002.

## ***Session chair: Dr. Hans Döbbling***

Hans Döbbling joined DANTE as General Manager in August 2004. He studied physics, and obtained his PhD from the University of Heidelberg in 1981. He worked for twelve years as an experimental physicist in medium-energy nuclear physics at MPI für Kernphysik Heidelberg, at CERN in Geneva, at KEK in Tsukuba, and at PSI in Villigen.

In the early nineties, he became an IT services manager. He was head of the Analysis Software Development group at GSI in Darmstadt, and later in charge of the IT services of the European Molecular Biology Laboratory (EMBL) in Heidelberg.

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*“I believe that it is very important and worth while to define the borderline between networks and grids extremely well. It will help us to do the network job as good as possible.*

*In general I have cultivated a relatively critical view of the usefulness of universal grid applications for research. I tend to believe that dedicated developments will be more likely to be successful, but really have not enough insight into existing tool to argue this in depth.”*

# Advanced Computing Facilities

## *Session chair: Prof. dr. Victor Alessandrini*

Dr. Victor Alessandrini has been director of IDRIS since 1993. He holds a Ph D in Theoretical Physics. He was visiting scientist at Lawrence Berkeley Laboratory, USA and CERN Theory Division in the late 60's and early 70's. He is an Associate Member at the International Center for Theoretical Physics (1972-1976). In 1976 he was appointed Professor of Theoretical Physics at Paris XI (Orsay). He is scientific manager of EUROGRID (for the CNRS partner).

### **Competences in Physics :**

- Quantum Field Theory,
- Statistical Mechanics,
- Algorithms in Computational Physics.

### **Competences in Computer Science :**

- Computer architectures,
- Performance engineering, object oriented software development (C++, Java),
- Distributed Objects (CORBA) and distributed applications,
- Shared memory multithreading programming,
- Training in C++ and Threads.

## *Session chair: Kees Neggers*

Kees Neggers is Managing Director of SURFnet bv, and has been so since its establishment in 1988. SURFnet's mission is to develop and operate an advanced networking infrastructure for the research and higher education community in the Netherlands.

He was involved as an initiator and Board member in several International network related organizations such as RARE, TERENA, Ebone, Internet Society and RIPE NCC. Currently he is active in the set up of GLIF, the Global Lambda Integrated Facility. Present positions held in Internetrelated international activities include:

- Chairman of the RIPE NCC Executive Board
- European Co-Chair of the CCIRN
- Chairperson of the Global Lambda Integrated Facility (GLIF)
- Member of the Board of the IEEAF

# Network developments & grid requirements

## ***Session chair: Gigi Karmous-Edwards***

Gigi Karmous-Edwards is a research scientist at MCNC Research and Development Institute, a non-profit research organization in NC. She has twenty years of engineering experience, mainly in the network management of data communications. She helped initiate the IETF ADSL working group to help define ADSL management. In the last few years she has been looking at advanced optical networking technologies. She is chair of the Control Plane and Grid Integration Middleware Working Group of the Global Lambda Integrated Facility (GLIF). GLIF is a world-scale Lambda-based Laboratory for application and middleware development on emerging LambdaGrids, where applications rely on dynamically configured networks based on optical wavelengths.

### ***Session chair: Dr. Anwar Osseyran***

Anwar Osseyran was appointed Managing Director of SARA in Amsterdam in 2001. Prior to that he held various senior management assignments in High-Tech companies. Anwar clearly has a strong industry background, which probably explains his keen interest in trying to understand the business value in HPC as opposed to compiling compute power... He's always looking for the ROI concept for within his projects.

His tenure at SARA has been marked by a focus on the benefits that the Academic and Research community can obtain from emerging technologies (Grid, Linux, Virtual Reality), a focus on less conventional, but fast growing, application areas (Bioinformatics) and on enhancing the networking infrastructure to allow collaboration and a broader and more effective use of the Supercomputing resources. SARA is now a key hub in the Northern European Grid (NEG) and in the European project called DEISA (Distributed European Infrastructure for Supercomputing Applications).

# User support

## *Session chairs:*

*Frank Harris (CERN)*

*Torsten Antoni (FZK)*

### ***Frank Harris***

Frank Harris obtained his D.Phil. at Oxford in 1970 and continued at Oxford in research in computing for particle physics, and also applied image processing and pattern recognition techniques in other application areas such as medicine and digital cartography. He was chairman of the inter-disciplinary Sub-Faculty of Computing at Oxford 1979-1980. He had major project responsibilities in the LEP/DELPHI experiment from 1986-1996, and following that in the LHC/LHCb experiment, including being the coordinator of grid activities. He was leader of the HEP workpackage in Datagrid 2002-4, and coordinated the HEP activity at the beginning of the EGEE project. He is currently based at CERN, and is deputy coordinator of the overall applications activity in EGEE, taking a special interest in the successful deployment and operation of all applications. He has been a principal author of many papers dating from 1970, and been active in graduate student supervision both at Oxford and CERN.

### ***Dr. Torsten Antoni***

Dr. Torsten Antoni attended University Karlsruhe, Germany. He studied physics specializing in astroparticle physics and graduating with a diploma thesis on experimental cosmic ray physics. After his graduation he did his PhD with a thesis on muons in cosmic ray air showers at the University Heidelberg, Germany, earning his degree in 2003.

Since 2004 he is working at Forschungszentrum Karlsruhe (FZK), Germany in the field of user support in the grid environment in the framework of the LCG and EGEE projects. He is Head of the Global Grid User Support (GGUS) group at FZK and member of two EGEE user support working groups (ESC, UIG).

# User support in EGEE – experience and issues

(an overview to be presented as an introduction to discussion on ‘user support’)

*Torsten Antoni, Frank Harris*

The EGEE project brings together experts from over 27 countries with the common aim of building on recent advances in technology and developing a service grid infrastructure which is available to scientists 24 hours per day. The project aims to provide researchers in academia and industry with access to major computing resources, independently of their geographic location. The EGEE project focuses on attracting a wide range of new users to the grid, and concentrates on three core areas:

- To build a consistent, robust and secure grid network that attracts additional computing resources.
- To continuously improve and maintain the middleware in order to deliver a reliable service to users.
- To attract new users from industry as well as science and ensure they receive the high standard of training and support they need.

The EGEE infrastructure is built on the EU Research Network GÉANT and exploits grid expertise generated by many EU, national and international grid projects to date.

Due to the strong connections between the different types of support needed in a grid environment (e.g. user support, operations’ support) in the EGEE project it was decided to handle all support matters with one coherent model. **This model is based on "regional support with central coordination"**.

Users are viewed as existing within Virtual Organisations (VOs), which are geographically independent groups of collaborating scientists. Users can make a support request (via a web form or email) at a central helpdesk provided by GGUS (Global Grid User Support), or via their Regional Operations' Centre (ROC) or VO. Within the GGUS helpdesk there is an internal support structure for all support requests. The ROCs and VOs and the other project wide groups such as the Core Infrastructure Centre (CIC), middleware groups (JRA), network groups (NA), service groups (SA) will be connected via a central integration platform provided by GGUS. The process of integrating all of these organisations will take place during 2005 and is expected to be complete in 2006.

The central helpdesk keeps track of all service requests and assigns them to the appropriate support groups. In this way, formal communication between all support groups is possible. To enable this, each group has to build only one interface between its internal support structure and the central GGUS application. Alternatively the support units can use the GGUS system directly as their helpdesk.

Specific points for discussion centring on the EGEE support model are

- Practical experience so far with processing ‘user’ tickets
- Building of a knowledge base for problems and solutions
- Provision of a repository and portal for documentation, FAQs and news
- Problems of integrating all groups into central system
- Service level agreements and escalation mechanisms

We note that there are other essential activities within the EGEE project which provide ‘support’ to a broad spectrum of users. These include

- The provision of education to the wide variety of users
- The easy access to information on a broad range of topics of interest to users
- Support for the initial interfacing of applications to the grid, and ongoing support for applications as they move to production use

## *Session chair: Prof. dr. Harvey Butcher*

Harvey Butcher is Executive Director of ASTRON. He studied at the California Institute of Technology, receiving a B.Sc. in Astrophysics (Honors) in 1969. In addition to his studies he worked on the first survey of the sky at infrared wavelengths (the Two Micron Sky Survey project), both as an observer and in the development and use of infrared instrumentation. From 1970 to 1974 he held the position of research scholar at the Mt Stromlo and Siding Spring Observatory, receiving his PhD from the Australian National University in 1974. His dissertation research involved the construction of one of the first operational high resolution echelle spectrographs in astronomy. As Bart Bok Fellow at the Steward Observatory of the University of Arizona from 1974 to 1976 he worked on the development of a Cassegrain echelle spectrograph for the 90-inch telescope on Kitt Peak. From 1975 he worked with early CCD detectors, and during his tenure from 1976 to 1983 as Astronomer at the Kitt Peak National Observatory, Tucson, he worked to develop general purpose CCD systems for use both at Kitt Peak and at Cerro Tololo Inter-American Observatory in Chile. In 1983 he became Professor of Observational Astronomy at the University of Groningen and Director of the Kapteyn Observatory, Roden. In 1991 he was became Executive Director of ASTRON. He is currently working on the Lofar and Square Kilometer radio telescope (SKA).

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*"Our civilisation must understand the processes that influence the physical world and develop tools to manage our environment. Remote sensing and computational modelling have in recent years become important research activities toward these ends.*

*The next phase in the effort will be to sense and model the environment in real-time. The paradigm to be employed involves dynamic, non-linear, numerical simulations guided by real-time measurements from wide-area networks of in situ sensors and intermittent data from remote sensing satellites.*

*The wide-area nature of the problem leads to consideration of how one may add extensive sensor networks to the resources of the GRID. In many cases, one wishes to enable the real-time fusion of high volume data streams with ensembles of continuously evolving models, making use both of the data transport capabilities of the GRID and of its storage and computational resources. "*

# Requirements from the research field

## *Session chair: Prof. dr. Berend Smit*

Berend Smit (1962) obtained his PhD Chemistry in 1990 at Utrecht University. He is director of CECAM in Lyon since 2004. After starting his career at Shell Research in Amsterdam, he became a professor in 1997 at the University of Amsterdam. In 1998 he received the Gold medal of the Royal Dutch Chemical Society. He is Editor of the Journal of Computational Physics since 1999 and since 2002 has also been Editor of PCCP. He published more than 170 papers which have received a total of over 5500 citations

Berend Smit co-authored with Daan Frenkel the book *Understanding Molecular Simulations* (Academic Press, 2nd edit., 2002). Together with the first edition this book has been cited over 1500 times and is used as the text book on molecular simulations in many universities. A quotation of a review "... this book brilliantly lays down the scientific foundations of the simulational approach..." (Physics World, 1997). In 2003 a Chinese translation appeared. On the basis of this book the authors have organized the Amsterdam Molecular Simulation School which has attracted over last 5 years 300 (young) scientists from all over the world.

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Computational physics, more particularly computer simulation is playing an ever growing role in basic and "applied" sciences. Needless to say that this success is to a large extent based on the development of computers as computing and storing tools, not to mention the internet and the web. In the field of computational material science Europe is playing a leading role. Europe has two important research networks, the ESF programs Psi-k and SIMU that represent over 20 European countries and involve over 1000 research groups. The combined activities of these groups will become even more visible in connection with the planned European Super Computers, which would multiply in the next 5 years the present super computer power by a factor of 100-1000.

To keep Europe at the forefront of the field this infrastructure needs to include both *hardware* and *software* issues. These include both HPC and local clusters or workstations on which much outstanding research is done. The infrastructure must embrace both software management, at the level of links such as GRID, and software development concerning the performances of the actual codes used in the calculations. Both development and subsequent training must be included, for development is useless without the training in its use.

## **Discussion points**

- *Scientific software is an essential integral part of the European Cyber infrastructure* Computational methods have become so advanced it is not possible anymore that every scientist writes his own code. Groups rely on the availability of very sophisticated software for their research; this software needs to be maintained, ported to new machines, novel algorithms have to be implemented.
- *Development of novel algorithms is an integral part of the European Cyber infrastructure* Only if there is a direct link between state of the art research and those that maintain the codes, Europe will maintain a competing position.
- *The European Cyber Infrastructure should have instruments to secure academic software* At present academic software evaporates as soon as the thesis has been written, only in accidental cases the software is rescued.

*A follow up of this discussion will be at the workshop:*

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## **Workshop on a European Cyberinfrastructure**

12-13 July 2005

Accademia dei Lincei (Roma)

*Proposal for a European Cyberinfrastructure for Atomistic Simulations of Hard, Soft, and Biological Matter*

<http://abaddon.phys.uniroma1.it/index.php/Main/WorkshopLincei>

# Session on a "European Science Grid Organisation"

## *Session chair: dr. Lajos Balint*

Dr. Lajos Balint (Hungarnet Executive President, NIIFI Director of International Relations) has graduated and received his "doctor technicus" and Ph.D. degrees from the Technical University of Budapest, in 1969, 1976, and 1997, respectively. He is Executive President of Hungarnet, and Director of International Relations at the National Information Infrastructure Development Office (NIIFI) in Hungary. Earlier he has been affiliated at different research and development organisations in information technology, telecommunications, communication networks, human-computer interaction, and computer-aided design. He has been working on more than 40 grants/projects during the last 35 years. He is a part time Honorary Professor at the Technical University of Budapest. He has presented about 160 publications between 1969 and 2005. He has been a member/representative/officer at a number of national and international professional organisations, including TERENA, DANTE, GÉANT, ENPG, ISOC, etc.

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### Objective of the Session:

- Investigating necessity and possibility of establishing an organisation
- Answering questions
- Providing recommendations

The goal is to look for a constructive approach – which is a joint interest of

- ESFRI (the forum for Research Infrastructures in general)
- e-IRG (the group devoted especially to eInfrastructures)
- ENPG (the European Networking Policy Group)
- NRENs (the research communities operating the network)

### What organisation?

- Devoted to ..... (in a wide sense – but within boundaries)
- Enabling ..... (common, easy, secure, cost-effective use of resources)
- Supporting ..... (providers and users)
- Motivating ..... (innovative applications, improved resources and tools)

### What questions?

- Time-frame
- Grid(s) definition
- Extent of coverage (technical – organisational – financial + geographical)
- Involved resources / providers
- Involved users
- Involved applications
- Desired rigidity of rules and regulations

### What recommendations? (If any ...)

- Top-down or bottom-up
- Aims – goals – tasks
- Organisational framework (level, structure, fragmentation)
- Powers and responsibilities
- Financial background
- To-do-list

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A short presentation will introduce the issues. After that a discussion will investigate the related questions. Depending on the outcomes of the discussion, a proposal will be presented (offered for discussion). In case of agreement about it, the proposal will be amended by the comments coming out of the discussion. An open, constructive, positive discussion is hoped for.

## *Session chair: Dr. Patrick Aerts*

Dr. P.J.C. Aerts is currently chair of the e-IRG. He holds a PhD in Relativistic Quantum Chemistry from the University of Groningen. He is director and secretary of the board of the Netherlands National Computing Facilities Foundation (NCF) since the establishment of the foundation in 1990. The Netherlands National Computing Facilities foundation (NCF) is an independent organisation under the umbrella of the Netherlands Organisation for Scientific Research (NWO). NCF is responsible for the national high-end computing infrastructure and in charge of the Dutch academic supercomputing policy and infrastructure.

Patrick Aerts holds a number of additional functions, such as advisor to the board of 'ICT for Science' of the SURF Foundation, Chairman of the section of computer applications of the Royal Netherlands Chemical Society. Local coordinator for the establishment of Digital Academic Repositories (DARE-project). Theme-coordinator for the NWO-Theme Digitalisation and Informatisation. Dr. P.J.C. Aerts was recently a member of the ad hoc Evaluation Committees of national High Performance Computing Consortia in Norway and Sweden.