Proc. Estonian Acad. Sci. Phys. Math., 2005, **54**, 2, 111–127

The first scientific results from the Estonian Grid

Andi Hektor[a], Lauri Anton[b], Mario Kadastik[a], Konstantin Skaburskas[c],
and Hardi Teder[b]

[a] National Institute of Chemical Physics and Biophysics, Rävala pst. 10, 10143 Tallinn, Estonia; andi.hektor@cern.ch
[b] Estonian Educational and Research Network, Raekoja plats 14, 51004 Tartu, Estonia
[c] Institute of Technology, University of Tartu, Vanemuise 21, 51014 Tartu, Estonia

Received 2 September 2004, in revised form 31 March 2005

Abstract. We present the first scientific results, technical details, and recent developments in the Estonian Grid (EG). Ideas and concepts behind Grid technology are described. We mention some most crucial parts of the Grid system, as well as some unique possibilities in the Estonian situation. Scientific applications currently running on the EG are listed and the first scientific computations and results of the EG are discussed. The computations show that the middleware is well chosen and the EG has remarkable stability and scalability. We present the collected results and experiences of the development of the EG and add some ideas of its near future.

Key words: radiation physics, Grid technology, scientific computations.

Abbreviations: API – Application Programming Interface, ARC – Advance Resource Connector, CA – Certification Authority, CE – Cluster Element, CERN – European Organization for Nuclear Research, CMS – Compact Muon Solenoid, CP/CPS – Certification Policy and Certification Practice Statement, CPU – Central Processing Unit, DNS – Domain Name System, DOUG – Domain decomposition On Unstructured Grids, EDG – European DataGrid, EENet – Estonian Educational and Research Network, EG – Estonian Grid, EU – European Union, EUGridPMA – European Policy Management Authority for Grid Authentication, GGF – Global Grid Forum, GIIS – Grid Index Information Service, GRIS – Grid Resource Information System, GSI – Grid Security Infrastructure, GT – Globus Toolkit, LCG – LHC Computing Grid, LDAP – Lightweight Directory Access Protocol, LHC – Large Hadron Collider, MC – Monte Carlo, MDS – Monitoring and Discovery System, MPI – Message Passing Interface, NICPB – National Institute of Chemical Physics and Biophysics, OGSA – Open Grid Services Architecture, PC – Personal Computer, PKI – Public Key Infrastructure, QDRL – Quasi Dynamic Resource Locator, RAM – Random Access Memory, RSL – Resource Specification Language, SC – Special Component, SE – Storage Element, UT – University of Tartu.

1. INTRODUCTION

Since the beginning of the computer age, supercomputers have been at the forefront of scientific computation due to high resource and computational needs. This approach has changed in the past years. As building a stable supercomputer is a very expensive task, more and more is invested in search for cheaper and more flexible alternatives [1]. On the other hand, many international scientific experiments will need a huge computational power in near future and it will be impossible in practice to cover these needs using any one supercomputer. Additionally, nowadays the communities and experimental facilities of international scientific experiments are distributed geographically. The Grid technology promises solution for the both sides [2]. It is an ideology of using low-cost personal computer clusters as the building blocks and the Internet to connect the blocks. By interconnecting them through the so-called Grid middleware we can put together a “virtual” supercomputer [3].

In modern terms, the Grid is a standardized layer of software between the cluster query systems, storage elements, users, and other Grid resources. The Grid middleware is the component that will bind all kinds of resources (different hardware architecture, different operating systems, etc.) into a uniform system with standardized tools. Its power lies in parallelization and massive execution of computational tasks, so-called Grid jobs. It enables scientists to create a computational job, split it into many independent sub-jobs and then send them to the Grid. Finally, after the jobs are calculated, the results are downloaded and analysed. That kind of parallelizable computation is most suited for massive scientific calculations like detector simulations and data analysis in high-energy and radiation physics, genetics, and bioinformatics, climate modelling and weather forecast, but it is also suited for many commercial purposes, for example rendering animations in movie industry, simulation of electronic systems, etc. A deeper overview of Grid ideology and technology is given in the books by Foster and Kesselman [3] and Berman et al. [4].

There are many projects under development, leading to a diversity of technological approaches, for example UNICORE, Globus, Legion, Gridbus. Some of them support only a minimal set of functionality (e.g. Globus), others try to develop a maximum set of tools and functions (e.g. UNICORE) [5].

Some international scientific collaborations will very soon need Grid technology: LHC at CERN [6], the Planck Mission for analysis of cosmological background radiation [7], analysis of the human genome at the Human Genome Project [8], etc. CERN is a leading developer and user of Grid technology due to the schedule of the LHC experiment (starting in 2007) [9].

It is important to mention that the Grid system does not cover the functionality of supercomputer one-by-one. On the one hand, the Grid has many additional possibilities of large-scale collaboration, but on the other hand it lacks several functionalities of a typical supercomputer. The strongest restriction is the inability to use shared or distributed memory parallel computing in the geographically distributed Grid environment. This restriction comes from the latency of Internet connection. Finally, the speed of light sets a natural limit for shared memory on the geographical scale.

In the present paper we propose a new method for modelling some spectra of the mobile small gamma spectrometer: we combine the MC method in radiation physics and distributed calculations on the Grid. Due to experimental complications and expenses, the numerical modelling is a suitable method to model gamma spectrometers. Unfortunately it needs much computational resources. In the Grid we can divide our MC simulation into hundreds of independent sub-simulations and send them to the Grid. This is a practical way for computations, but a good possibility of testing a Grid system as well. We used the statistics of the sub-jobs to estimate the stability and reliability of the system.

Using the Grid was very promising. The Grid middleware employed was sufficiently stable for this type of computations. The results of the MC modelling are realistic and give some needed hints for the experimental set-up in the future.

2. ARCHITECTURE OF THE GRID

To ensure unified standards, the GGF sets the specifications and agreements for Grid systems: OGSA, RSL, etc. [10]. As mentioned, not all Grid projects follow the specifications precisely and there are some freedom and uncovered areas in the specifications and agreements.

Figure 1 presents the layered architecture of a typical Grid system [2]. For a fully functional Grid one needs the following components (named by the GGF [10] and NorduGrid project [11]):

- CE – an actual node/farm/cluster/supercomputer on which Grid jobs are executed. Typically, in a Grid environment this is a Linux farm with some

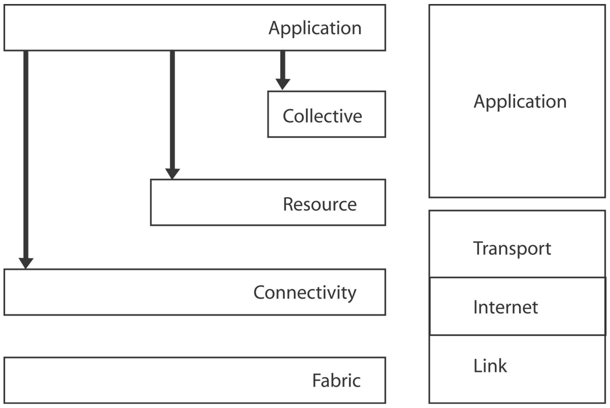

Fig. 1. The logical layers of the Grid connected to the layers of the Internet.

job scheduling system. The frontend of the farm is connected to the Grid, where it accepts Grid jobs and submits them as local jobs. Once the jobs are finished, it will return the results as specified.

- SE – a node that has some data storage resources attached to it and is available for Grid usage. As the Grid is a decentralized system, there is a need of storing input and result files in a common place for easier management. Special storage elements were designed for this purpose, allowing storage and retrieval of files through the Grid.
- QDRL, also known as the GIIS – is responsible for information propagation of Grid resources through the entire network. The CE and SE register their resource information to the local GRIS, which is typically located in the CE or SE itself. The GRIS registers its address in the nearest QDRL, which then propagates the GRIS location up its chain.
- User Interface – a command line or graphical interface allowing user to submit new Grid jobs, monitor existing ones, retrieve results, kill running jobs, etc.
- Special Component or Device – a special facility connected directly to the Grid, for example a particle detector, an environmental sensor, etc.

A typical Grid middleware toolkit, the GT, is produced by the Globus project [12]. The GT is in itself not a fully functional Grid middleware, but a Grid middleware toolkit/API. It is popular: many middleware packages have been built upon the GT and rely upon its functions for the basic functionality like the GSI, MDS (QDRL is based on the MDS, which is a modified LDAP system), Globus-IO (for file transfers), etc. The Globus project itself is a collaboration connecting many scientific institutions, sponsored by many organizations like NASA, IBM, Cisco, Microsoft, etc. [12].

2.1. Security of the Grid

A very important aspect of the Grid is the ability to submit and download jobs in a secure way from anywhere in the world. Most Grids under development around the world use PKI as a method for the authentication of the actors of the Grid [13]. Following PKI, every user and resource element in the Grid has to have a certificate signed by CA. Employing PKI gives a unique possibility in Estonia. It is possible to use the local electronic ID-card (SmartCard) infrastructure in Estonia based on PKI for the potential Grid users [14]. It means that an Estonian inhabitant with a valid electronic ID-card can use that for the Grid. Thus, there is a possibility of saving resources using this ready PKI structure. The electronic PKI-based ID-card infrastructure is available only in some countries in Europe: Belgium, Estonia, Finland, and Sweden (T. Martens, pers. comm. 2004).

3. DEVELOPMENT OF THE ESTONIAN GRID

It is impossible to mark the exact moment of the birth of the Estonian Grid (EG). Therefore, the authors give a list of the memorable dates:

- **January–December 2003.** Some coordinative meetings at the EENet, NICPB, UT, and Tallinn University of Technology.
- **January 2004.** The first components of the EG: EG CA, β-level GIIS, the first computer in the EG established at the NICPB. Technical meeting of NorduGrid at the NICPB in Tallinn, the first public seminar of the EG.
- **February 2004.** The establishing of the Centre of High Energy Physics and Computational Science at the NICPB with the purpose of supporting the development of the local Grid applications for high-energy and radiation physics and material science.
- **February–March 2004.** The first multiprocessor clusters in the EG at the EENet and UT. The public Web page of the EG [15].
- **April 2004.** The first draft of the CP/CPS document for the EG CA. The first regular seminars of Grid technology at the NICPB and UT.
- **May 2004.** The collaboration protocol between CERN, LHC LCG, and the Republic of Estonia was signed. The first scientific software ported to the EG from the authors [16]. The establishing of the Grid Laboratory at the Institute of Technology of the UT.
- **June 2004.** The establishing of the EG technical coordination and supporting group [17]. The first massive tests on the EG.
- **July 2004.** The first massive scientific calculations on the EG.

The authors have participated and made presentations in various international meetings and conferences: the NorduGrid meetings in Lund, Tallinn, and Helsinki and the CACG Florence Meeting in Florence in 2004.

4. TECHNICAL DETAILS AND PROBLEMS

4.1. Choice of middleware and compatibility

The first problem facing a potential developer of a Grid system is finding a functional middleware. As mentioned before, there are many different possibilities, but most middleware packages are in a testing state with poor support for the users. We followed the tendency of CERN [9] and our neighbouring countries [11] and decided to use the middleware based on the GT. One of the well-supported and functional middlewares based on the GT, the ARC middleware, is developed by the NorduGrid project [11]. That is the first and foremost reason why this middleware is used for the EG.

The strongest alternatives of the ARC software were the EDG package (based on the GT) [18] and UNICORE [19]. The problem of EDG was insufficient user support. The problem of UNICORE is that it is not supported by CERN and some other international projects.

All the middleware packages are compatible on the level of OGSA. However, there are many non-compatible sub- or additional components in different Grid systems, e.g. the schema of the information system, management of storage elements, etc. Hopefully, these non-compatibilities will soon be resolved.

4.2. Grid Public Key Infrastructure

Traditionally each country has at least one CA for the Grid. (There are some exceptions, e.g. the NorduGrid project [11].) The CA of the EG follows the X.509 rules [20]. The CP/CPS document for the CA has been composed. It is presented online on the web page of the EG [21]. The CP/CPS document follows all rules of the EUGridPMA, it is synchronized with the EUGridPMA organization [22] and the local CA is trusted by the EUGridPMA members. In the near future, we will support the Estonian electronic PKI-based ID-card infrastructure [14] for the EG.

4.3. Information system and Web-based monitoring

The information system of the EG is based on the NorduGrid LDAP schema [23]. It is decentralized and follows a structure that is similar to the Internet DNS. There are typically three levels of information servers or QDRLs: the top-level QDRLs (so-called α-level), the second- (or country-) level QDRLs (so-called β-level), and the third- (or unit-) level QDRLs (so-called γ-level). The tree of QDRLs can be continued with an additional lower-level QDRL if needed.

The information coming directly from LDAP is not really human readable. Therefore, the Web-based monitoring interface is developed by the NorduGrid project. There are many online monitors available, for example the NorduGrid Monitor [24], EG Monitor [25], etc.

4.4. Present state of the Estonian Grid

Figure 2 gives a technical view of the development of the EG. It shows some important parameters of the EG: the total number of CPUs and total RAM connected to the EG. Currently, the EG has 7 CEs with a total of 62 CPUs. Most CPUs are from Intel (between 2.4 and 3.06 GHz) and the average RAM is between 512 MB and 1 GB. Two test SEs with 160 GB storage in total are available in the EG. The exact numbers and current situation of the resources are presented by the EG Monitor [25]. A typical link between the PCs of a CE is 1 Gbps. The fast Myrinet (2 Gbps) link is used at the NICPB cluster and the fast Scali link is used at the EENet cluster. The links between the CEs are limited by the typical Internet connection in Estonia (below 1 Gbps).

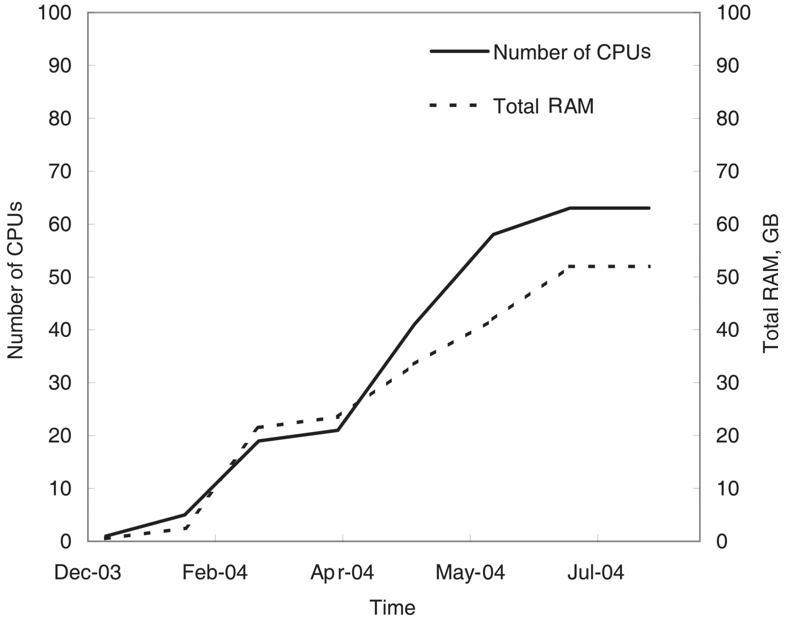

Fig. 2. The number of CPUs and RAM in the EG. Some new clusters are coming in the autumn of 2004.

4.5. General problems

Two kinds of problems were encountered during the building up of the EG: organizational and technical problems. Organizational problems are caused by the fact that the Grid is a distributed system. A similarity exists between the beginning of the Internet and Grid [2]. Special decisions are needed for resource sharing and local and general responsibilities. These can be reached by special contracts between resource owners and/or personal agreements between technical persons. At the moment all the problems have been solved on the level of technical and personal agreements. However, in the near future the EG will need some official agreements between resource owners.

Technical problems arise from the fact that Grid middleware is developing very rapidly. Generally, our choice, the NorduGrid ARC package has shown surprisingly good stability. Much more problems are connected to the management of the hard- and software of the clusters than to the middleware.

5. SCIENTIFIC APPLICATIONS PORTED TO THE ESTONIAN GRID

5.1. Modelling and analysis software for the international Compact Muon Solenoid experiment

The CMS experiment [26] involves one of the biggest high-energy particle detectors at the LHC at CERN scheduled to begin operation in the year 2007. The LHC will collide 7 TeV proton beams head on. It can also collide beams of heavy ions such as lead with total collision energy in excess of 1250 TeV. The main objective of the CMS and LHC is to explain the origin of particle mass, flavour and possible unification of fundamental interactions at high-energy scales. In the Standard Model of particle interactions all the charged fermions acquire masses due to the spontaneous breaking of gauge symmetry via the Higgs mechanism, predicting the existence of a physical neutral scalar particle, the Higgs boson.

The CMS collaboration involves about 1990 scientists from 150 institutions of 31 countries. The scientists of the NICPB have been engaged in that project since 1996. One of our tasks is to study and port the CMS software to simulate, digitize, and analyse event creation in the CMS detector. The software consists of the following three parts:

- CMKIN [27] – an MC physics generation application written to simplify the use of different MC generators like PYTHIA [28], HERWIG, TAUOLE, TopRex, etc. It is used to generate ideal proton-proton collisions and the produced particles, and its output is taken as input to OSCAR.
- OSCAR [27] – simulates particle passage through the CMS detector and simulates hits in different parts of detectors. It uses the Geant4 software package that is described in the next subsection.
- ORCA [27] – the actual tool that will be used also when the real detector goes online. It is currently used for data reconstruction from simulated runs and also for later analysis.

One event in the above software means one proton-proton collision within the CMS detector. The collisions will happen approximately 10^8 times per second when the LHC will go online. It means that the data production of the detectors of the LHC will be huge, about 10 000 TB data per year. The analysis of this data needs computational power that is equal to about 100 000 fast modern PCs. Fortunately, the events can be looked at as separate entities as they do not depend on other events and the Grid can be the solution for the data analysis.

The current tests that have been performed on the EG have been the creation of data sets from CMKIN particle generation to ORCA reconstruction and also some preliminary analysis. The code has worked remarkably well and we have managed to produce many events for later more detailed analysis.

5.2. Parallel solver for linear systems of equations

DOUG is a black box parallel iterative solver for finite element systems arising from elliptic partial differential equations [29]. Employed in conjunction with a finite element discretization code, DOUG will solve the resulting linear systems using an iterative method and provide a range of powerful domain decomposition preconditioners.

The code is designed to run effectively in parallel on virtually any machine that supports MPI. The matrix-vector operations arising in the iterative method are parallelized using the graph partitioning software, and additive Schwarz preconditioners can be constructed automatically by DOUG using only minimal input. A full additive Schwarz preconditioner with an automatically generated coarse grid is provided in 2D and 3D. DOUG makes no assumptions whatsoever about the finite element mesh which the problem arises from; it may be as unstructured as necessary and only the basic output from the mesh generator and the finite element discretization are required as inputs to DOUG.

Currently, DOUG is mainly used in solution of matrices having block structure, which arise from discretization of coupled systems of different differential equations (like the Navier–Stokes flow equations), and in assessment of the stability of nuclear power station cooling systems. This research is carried out in collaboration with scientists from Bath University and AEA Technology in the UK.

DOUG has a graphical user interface implemented as a Web-interface [30]. The Grid-awareness is added to the Web-interface for DOUG and it is available for the EG users. During the development of the Grid-enabled Web-interface the problem of action on the Grid by the interface on behalf of the user and necessity of managing users' credentials – Grid-proxies – had arisen. Those issues were successfully solved by using MyProxy (Online Credentials Repository [31]) and appropriate developing and coding of the interface. We have two MyProxy servers installed on the EG.

5.3. Radiation and particle physics

Geant4 is a software toolkit for the MC simulation of the passage of particles through matter [32]. Its application areas include high-energy physics and nuclear experiments, medical, accelerator, and space physics studies. Geant4 covers the energy scale from 250 eV to some TeV for most of the known particles and interaction processes.

Geant4 is used like an external library for many software packages: the OSCAR software mentioned above, medical software for radiotherapy for cancer treatment, etc. The Geant4 software was developed by the RD44 group [33], as a result of world-wide collaboration of about 190 scientists participating in more than 10 experiments and 20 institutions in Europe, India, Japan, Canada, and the United States.

Three collaboration projects use Geant4 in environmental physics, medicine, and particle/radiation detectors in Estonia. Therefore we are interested in supporting and using the Geant4 software at the EG. The first scientific calculations on the EG have been done using the Geant4 software.

5.4. Coming scientific and nonscientific applications

There is one group (headed by M. Karelson) using and developing the UNICORE middleware for the Open Computing Grid for Molecular Science and Engineering (OpenMolGRID) project in Estonia [34]. Additionally, many other work groups in Estonian science and technology (analysis of gene information, climate modelling, material science, etc.) are interested in Grid technology and the EG. The interest is arising in the commercial sphere as well. Some companies need computational power in different topics: material engineering, nuclear safety, computer animations, military applications, etc.

6. THE FIRST SCIENTIFIC CHALLENGE OF THE ESTONIAN GRID

6.1. Monte Carlo simulations in radiation physics

For the first massive test of the EG we made some intensive scientific computations using the Geant4 software package. In our study the MC method is used to model the operation of a scintillation detector installed in a prototype radiation surveillance unit on a small unmanned airplane, the so-called Ranger. Planned measurements by Ranger are complicated and dangerous for humans (e.g. radioactive cloud, etc.), thus, the detection capability has to be estimated by calculative means. Most importantly the limits of the detector have to be estimated [35].

In this study we analyse the simplest case: an isotropic radioactive point source on the ground and the detector directly above the source at different heights. A very practical question for radiation surveillance is the difference of the spectra between different heights. We modelled the spectra at the heights of 150 and 100 m (Fig. 3).

We have to simulate billions of gamma events to get statistically good histograms. Therefore the calculations are very time-consuming. The number of registered gamma quants N follows the approximate equation

$$N \propto \frac{1}{r^2}\exp(-\mu r), \tag{1}$$

where r is the distance between the detector and the point source and μ is the attenuation coefficient of the environment between the source and the detector. Thus, the statistical uncertainty of N is

$$\mathrm{err}_N = \sqrt{N} \propto \frac{1}{r}\exp\left(\frac{-\mu r}{2}\right). \tag{2}$$

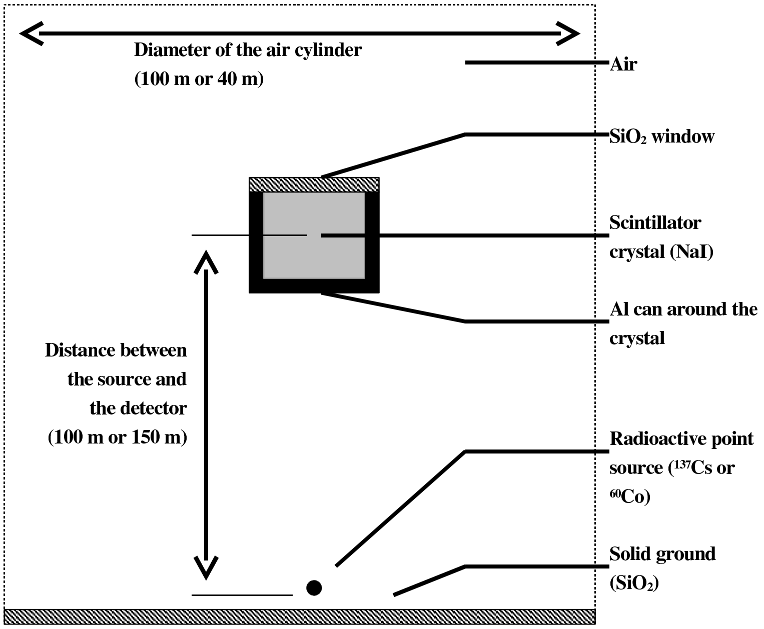

Fig. 3. The schematic cross-section of the simulated system. The detector crystal is a cylinder, about 15 cm in diameter and about 5 cm in height.

Luckily an intrinsic property of radioactive emission events (and the MC calculations as well) is that all events are independent and we can split the computations to smaller subtasks. So, this task is excellent for testing a Grid system. In an ongoing study we focus mostly on testing the EG using Geant4 simulations. An overview of the experiments, exact details of the calculations, and the results obtained will be published in a forthcoming paper.

We built up our model in Geant4 (release 5.2), and compiled and made some test runs locally on a Linux PC (2.8 GHz Intel Pentium4, 1 GB RAM, RedHat 9.0). Typical compilation time of the source code of the model was a few minutes. If the distance between the point source and the detector is between 100 and 150 m, then the calculation time is between 0.05 and 0.2 ms per a source event.

The second step was to send the computations to the EG. There are two possibilities of sending a Grid job to the Grid. First, we can send the source file of our code to the Grid and it compiles and runs on a Grid node (CE). It means that the external libraries (e.g. Geant4) have to be installed to the CE before sending the job. Second, we can compile our code locally and then send the compiled binary to run on a CE of the Grid. The drawback of the last case is that the CE has to have a suitable operation system, correct version of glib, etc. In addition, if the binary file is large, then much time is spent on uploading it. In the case of our Geant4 radionuclide detection simulation, the binary file is rather small (3.7 MB). It runs on most CEs in the EG and therefore we prefer the last variation.

We simulated all the possible combinations: two different radionuclides (^{137}Cs and ^{60}Co), two different detector positions (100 and 150 m), and additionally we changed a parameter of the system, the radius of the air cylinder around the system (we used two different radiuses, 40 and 100 m). In all, there are 8 different cases. For satisfactory statistics in each case 80 billion events were simulated. In total it means $8 \times 80 = 640$ billion events. We divided the total set of the simulations (640 billion) into sets of 1 billion events. The computation time of a set is reasonable (8–16 h) and in compliance with the recommended maximum cycle of the random number generator of Geant4 [32,36]. All 640 sets were submitted as Grid jobs to the EG.

Figure 4 shows the results of the simulations for ^{137}Cs and Fig. 5, for ^{60}Co. We present the spectra only for the radius of 40 m. There is only a very slight difference between the 40 and 100 m radiuses. It is very close to the error limit and therefore we do not present the curves of the 100 m radius in the figures. We can see a clear difference between two detector positions, 150 and 100 m. To estimate the concrete detection limit, we have to compare these curves with the local natural radioactivity background case-by-case. The line structure in the Compton continuum region needs additional study.

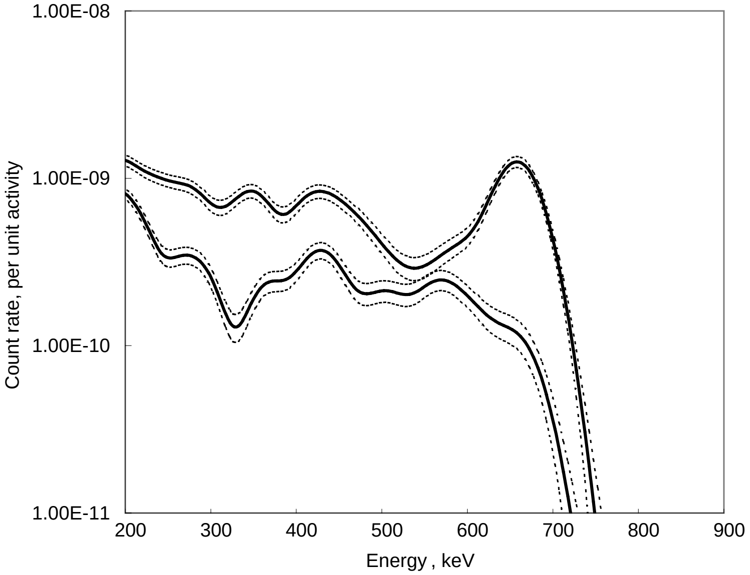

Fig. 4. Two sets of spectra of ^{137}Cs for the heights of 100 and 150 m in logarithmic scale. The upper solid curve represents the height of 150 m and the lower one that of 100 m. We can clearly see the energy peak on the upper curve at 662 keV. The Compton continuum region has the line structure. The reason for the line structure needs additional study.

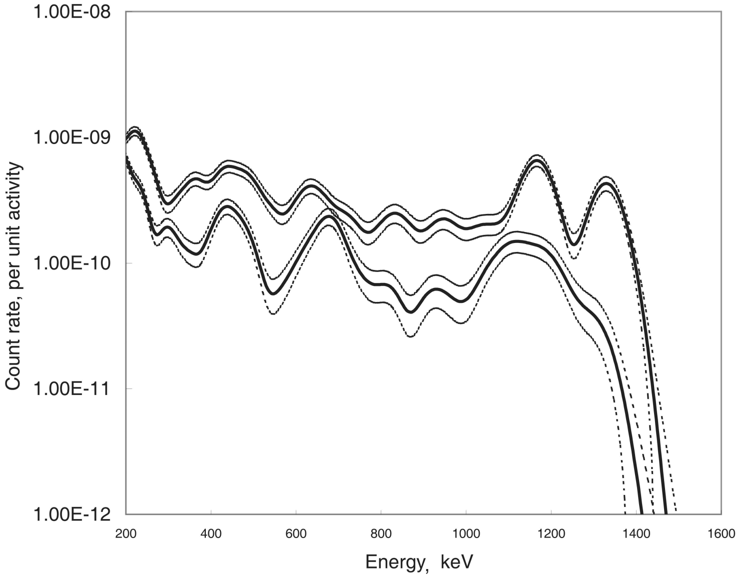

Fig. 5. Two sets of spectra of ^{60}Co for the heights of 100 and 150 m in logarithmic scale. The upper solid curve represents the height of 150 m and the lower one that of 100 m. We can clearly see the energy peaks on the upper curve at 1173.2 keV and 1332.5 keV. The Compton continuum region has a similar structure to the calculated spectra of ^{137}Cs (Fig. 4).

6.2. Reliability of the Estonian Grid

The speed of the CPUs used was between 2.4 and 3.06 GHz (Intel Pentium 4) and the available RAM per PC was between 512 MB and 1 GB. The total time of the computations was 417 CPU days.

The results were very promising. No jobs failed due to the Grid middleware. In total, 17 jobs (2.6%) failed during the computations, probably due to random hardware errors. These jobs were resubmitted to the EG and finished successfully. The instability of the hardware/software due to the external factors (blackouts of electric grid, overheating, etc.) caused 16 post-processing errors (2.5%).

However, we only tested some functionalities of the Grid. The stability of the data management and runtime environments need additional testing.

7. SUMMARY AND CONCLUSIONS

The first experiences and tests of the EG have been promising. The development of the EG has been impressive, especially if we compare the results and the resources spent. The installation of the middleware, management of the middleware, and management of the CA of the EG, certificates, QDRLs, EG Monitor, and some CEs/SEs are done mostly as volunteer work.

The first scientific calculations on the EG show that it is a very useful tool for the computational scientists, especially in the field of computational particle and radiation physics. If the authors compare the earlier experiences of the computations on the PC clusters [37,38], the use of the Grid simplifies the scientific computations substantially.

During the first year of the EG the authors have experienced many technical and organizational problems and bottle-necks, presented here in short.

- **Instability of the hardware of the CE.** It is a typical problem for the managers of PC farms and clusters and parallel computers. In our case it was mostly caused by electric blackouts or overheating. Using the Grid can mitigate the problem – the Grid job automatically finds a working CE using the information system of the Grid. Naturally, if a Grid job is already running on the CE, then a hardware error can be fatal for the job.
- **Software management on the Grid.** There is no good and general solution for that problem. It is possible to send an executable file together with the job to the Grid, but this is reasonable only if the executable file is small and does not have many external dependencies. Many international Grid projects are working in that field and hopefully some general solutions are coming soon. Additionally, some problems are connected to the commercial licensing politics.
- **Lack of the accounting and banking system of computing time.** The problem is very urgent and needs a quick solution. For example, one solution can be the so-called SGAS [39], developed by the SweGrid project [40].
- **Lack of the general job management tool for the users.** It is very complicated to manage many running Grid jobs at the same time: resubmitting filed or incorrect jobs, collecting data, etc. A solution can be the universal job manager software produced by H. T. Jensen and coworkers ([http://www.cs.aau.dk/∼htj/nordugrid/master_thesis.ps]).
- **Lack of the interface for the electronic ID-card (SmartCard).** The interface for the SmartCard/ID-card is under development by the authors.
- **The organizational structure of the EG.** The Grid is a distributed system and does not need to be highly centralized. However, at least some technical and political agreements are needed: the trust of the CA, exchange mechanisms and rates of the computational time, etc.

As Grid technology is a new and innovative topic in computational science and engineering, more courses and schooling are needed at the universities and other institutions. Additionally, the Grid is an international system and some interstate agreements are needed.

ACKNOWLEDGEMENTS

The authors would like to thank the team of the NorduGrid project for many very helpful suggestions. Thanks are due to Arto Teräs and Juha Lento at the Centre of Scientific Computations in Helsinki for helping set up the first components of the EG and giving a nice seminar at the NICPB in Tallinn; and to Kristjan Kannike, Endel Lippmaa, and Aleksander Trummal for very useful comments on the paper. Sincere thanks go to Martti Raidal for helpful suggestions and discussions in high-energy and particle physics and Eero Vainikko for valuable suggestions and discussions in scientific computations.

The following organizations and institutions are gratefully acknowledged:

- the Estonian Information Technology Foundation for the support for the completion of the PC clusters at the University of Tartu,
- the Estonian Science Foundation for grants Nos. 5135, 5935, and 5316,
- the EU 6th Framework Programme for the grant EC MC MERG-CT-2003-503626,
- the Ministry of Education and Research of Estonia for the support for the technical meetings of the EG,
- the Research Council of Norway (Nordplus Neighbour Programme) for the support for the NorduGrid technical meetings,
- the Swedish Institute (Visby Programme) for the support for Estonian students to study Grid technology at Lund University.

REFERENCES

1. National Research Council. *Realizing the Information Future: The Internet and Beyond*. National Academy Press, 1994.
2. Foster, I., Kesselman, C. and Tuecke, S. The anatomy of the Grid – enabling scalable virtual organizations. *Int. J. Supercomputer Applications*, 2001, **15**, 3–23 [arXiv:cs/0103025].
3. Foster, I. and Kesselman, C. *The Grid 2: Blueprint for a New Computing Infrastructure*. Morgan Kaufmann, 2003.
4. Berman, F., Fox, G. and Hey, A. J. G. *Grid Computing: Making the Global Infrastructure a Reality*. John Wiley & Sons, 2003.
5. Asadzadeh, P., Buyya, R., Kei, C. L., Nayar, D. and Venugopal, S. Global Grids and software toolkits: a study of four Grid middleware technologies. In *High Performance Computing: Paradigm and Infrastructure* (Yang, L. and Minyi Guo, eds.). Wiley Publishers, 2005 (in press) [arXiv:cs/0407001].
6. European Organization for Nuclear Research. http://www.cern.ch/.
7. The Planck Mission, the European Space Agency. http://www.rssd.esa.int/index.php?project=PLANCK.
8. Human Genome Project. http://www.ornl.gov/sci/techresources/Human_Genome/home.shtml.
9. LHC Computing Grid Project, CERN. http://www.cern.ch.
10. Global Grid Forum. http://www.ggf.org/.
11. Ellert, M., Konstantinov, A., Kónya, B., Smirnova, O. and Wäänänen, A. The NorduGrid project: using Globus toolkit for building Grid infrastructure. *Nucl. Instrum. Methods Phys. Res. A*, 2003, **502**, 407–410. http://www.nordugrid.org/.
12. The Globus Alliance. http://www.globus.org/.
13. Ellison, M. C. The nature of a usable PKI. *Comp. Netw.*, 1999, **31**, 823–830.
14. The Estonian Electronic ID-card Project, 2003. http://www.id.ee/.

15. Estonian Grid Project. http://grid.eenet.ee/.
16. Kadastik, M. LHC Physics and Grid Computing for CMS. Unpublished bachelor thesis, Tallinn University of Technology, 2004.
17. Technical Coordination and Support Group of the Estonian Grid. http://grid.eenet.ee/.
18. Kunszt, P. European DataGrid project: status and plans. *Nucl. Instrum. Methods Phys. Res. A*, 2003, **502**, 376–382.
19. UNICORE (UNiform Interface to COmputing REsources) Project. http://www.unicore.org/.
20. Internet X.509 Public Key Infrastructure: Certificate and CRL Profile. http://www.ietf.org/rfc/rfc2459.txt.
21. Certification Authority of the Estonian Grid. http://grid.eenet.ee/.
22. The European Policy Management Authority for Grid Authentication in e-Science. http://www.eugridpma.org/.
23. The NorduGrid Information System. http://www.nordugrid.org/.
24. NorduGrid Monitor. http://www.nordugrid.org/monitor/.
25. Estonian Grid Monitor. http://giis.eenet.ee/monitor/.
26. Compact Muon Solenoid Experiment, CERN. http://cmsdoc.cern.ch.
27. CMS Object-Oriented Projects. http://cmsdoc.cern.ch/.
28. Sjöstrand, T., Edèn, P., Friberg, C., Lönnblad, L., Miu, G., Mrenna, S. and Norrbin, E. High-energy-physics event generation with PYTHIA 6.1. *Computer Phys. Commun.*, 2001, **135**, 238–256 [arXiv:hep-ph/0010017].
29. DOUG (Domain decomposition On Unstructured Grids) Software Project, Bath University.
30. Tehver, M., Vainikko, E., Skaburskas, K. and Vedru, J. Remote access and scheduling for parallel applications on distributed systems. In *Computational Science – ICCS 2002: International Conference, Amsterdam, The Netherlands, April 21–24, 2002. Proceedings, Part I* (Sloot, P. M. A., Kenneth Tan, C. J., Dongarra, J. J. and Hoekstra, A. G., eds.). *LNCS*, 2002, **2329**, 633–642.
31. MyProxy – Online Credential Repository. http://grid.ncsa.uiuc.edu/myproxy/.
32. Agostinelli, S., Allison, J., Amako, K., Apostolakis, J., Aranjo, H., Arce, P., Asai, M., Axen, D., Banerjee, S. and Barrand, G. GEANT4: a simulation toolkit. *Nucl. Instrum. Methods Phys. Res. A*, 2003, **506**, 250–303.
33. Geant4 Research and Development Project, CERN. http://www.cern.ch.
34. Open Computing Grid for Molecular Science and Engineering (OpenMolGRID). http://www.openmolgrid.org.
35. Hektor, A., Kurvinen, K., Pöllänen, R. and Smolander, P. Monte Carlo simulation for a scintillation detector to be used in a prototyperadiation surveillance unit of Ranger. Report for the Finnish Scientific Advisory Board for Defence (MATINE), available only in a special agreement with MATINE, 2003.
36. Class Library for High Energy Physics, CERN. http://www.cern.ch/.
37. Hektor, A., Kolbe, E., Langanke, K. and Toivanen, J. Neutrino-induced reaction rates for r-process nuclei. *Phys. Rev. C*, 2000, **61**, 055803–055813.
38. Hektor, A., Klintenberg, M. C., Aabloo, A. and Thomas, J. O. Molecular dynamics simulation of the effect of a side chain on the dynamics of the amorphous LiPF6PEO system, *J. Mater. Chem.*, 2003, **13**, 214–218.
39. SweGrid Accounting System Project. http://www.pdc.kth.se/grid/sgas/.
40. SweGrid Project. http://www.swegrid.se/.

Esimesed teaduslikud tulemused Eesti Griidist

Andi Hektor, Lauri Anton, Mario Kadastik, Konstantin Skaburskas
ja Hardi Teder

On avaldatud esimesed Eesti Griidis saavutatud teaduslikud tulemused, antud lühike kokkuvõte ideedest ja põhimõistetest ning kirjeldatud lühidalt mõningaid teaduslikke rakendusi. Põhiosas on keskendutud esimestele teaduslikele arvutustele ja testidele. Lihtsa ja mobiilse gammaspektromeetri modelleerimiseks tegid autorid kiirgusfüüsikas rea arvutusi, mille põhjal võib tõdeda, et Griidi tarkvara (nn vahevara) on stabiilne ja skaleerub antud mastaapides väga hästi.

Griid on süsteem, kus geograafiliselt eri kohtades paiknevad arvutid ja spetsiaalseadmed (andmehoidlad, sensorid jne) moodustavad ühtse ressursi nii, et süsteemi kasutaja ei pea mõistma, kus täpselt tema ülesandeid lahendatakse. Griidi definitsiooni annavad OGSA, GGF-i ja RSL-i standardid ning kokkulepped. Griidi peamine eesmärk on ühendada erinevaid arvuteid, andmehoidlaid ja spetsiaalseadmeid nii, et nende kasutamine oleks lihtne ja mugav ka ilma sügavate teadmisteta superarvutuste vallas.

Eesti Griid alustas tegevust 2004. aastal. Artiklis on antud selle protsessi mõned olulised daatumid ja kirjeldatud tulevikuväljavaateid. Autorid arendavad ja toetavad Eesti Griidi jaoks mitmesugust teadustarkvara: CMS-i tarkvara kõrge energia füüsikas, DOUG-i tarkvara lineaarsete diferentsiaalvõrrandite lahendamiseks ja Geant4 tarkvara Monte Carlo simulatsioonideks kiirgusfüüsikas.

Mobiilse gammaspektromeetri modelleerimiseks kasutati tarkvara Geant4. Antud süsteem on mõeldud kiirgusallikate õhuseireks piloodita väikese lennuki abil. Oluliseks küsimuseks on antud süsteemi optimaalne lennukõrgus. Suurte detektorite puhul on töövahemik tüüpiliselt paarsada kuni tuhat meetrit. Väiksema detektori tundlikkus on väiksem ja seega keskenduti kahele võimalikule lennukõrgusele: 100 ja 150 m. Arvutuste abil tuvastati, et signaalide erinevus on nendel kõrgustel kriitiline. Kui 100 m juures on energiamaksimumid signaalis eristatavad, siis 150 m juures on see võimatu. Seega on seiresüsteemi optimaalne lennukõrgus 100 m juures.

Kokku kulus arvutusteks 417 protsessoripäeva. 640 Griidi saadetud tööst katkes arvutuste jooksul 17 (2,6%). Tundub, et põhjuseks olid riistvaralised vead, sest uutel katsetel õnnestusid kõik tööd. Lisaks sellele katkes 16 tööd (2,5%) pärast arvutuste lõppemist. Põhjused olid erinevad: arvutuste ajal toimunud elektrikatkestused jms.

Eesti Griid on end arvutusmahukas teaduses tõestanud. Siiski vajavad lahendamist veel paljud olulised probleemid, millele on täpsemalt viidatud artikli lõpuosas: korralduslik pool, arvepidamine arvutusaja üle jne.