## FP7-INFRASTRUCTURES-2010-2

# **HP-SEE**

High-Performance Computing Infrastructure for South East Europe's Research Communities





Deliverable 2.2

National HPC task-force modeling and organizational guidelines

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**Abstract:** Deliverable D2.2 defines the guidelines for set-up of national HPC task forces and their organisational model. It identifies and addresses all topics that have to be considered, collects and analyzes experiences from several European and SEE countries, and use them to provide guidelines to the countries from the region in setting up national HPC initiatives.

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## Preface

Core European eInfrastructure for large-scale eScience research consists of the backbone GÉANT network; distributed storage & computing infrastructure - European Grid Initiative (EGI); and the PRACE initiative providing tier-0 High Performance Computing (HPC) infrastructure. South-East European eInfrastructure initiatives aim for equal participation of the less-resourced countries of the region in the European trends. SEEREN initiative established a regional network and the SEE-GRID initiative the regional Grid, with majority of countries now equal partners in GÉANT and EGI. BSI project established the GÉANT link to the Caucasus, active until mid-2010. However, HPC involvement of the region is limited. Only few HPC installations are available, not open to cross-border research; while the less-resourced countries have no mechanism established for interfacing to the pan-European HPC initiatives.

HP-SEE focuses on a number of strategic actions. First, it will link the existing and upcoming HPC facilities in the region in a common infrastructure, and provide operational solutions for it. As a complementary action, the project will establish and maintain the GÉANT link for Caucasus. Second, it will open this HPC infrastructure to a wide range of new user communities, including those of less-resourced countries, fostering collaboration and providing advanced capabilities to researchers, with an emphasis on strategic groups in computational physics, chemistry and life sciences. Finally, it will ensure establishment of national HPC initiatives, and act as a SEE bridge for PRACE. In this context, HP-SEE will aim to attract the local political & financial support for long-term sustainable eInfrastructure.

HP-SEE aspires to contribute to the stabilisation and development of South-East Europe, by overcoming fragmentation in Europe and stimulating eInfrastructure development and adoption by new virtual research communities, thus enabling collaborative high-quality research across a spectrum of scientific fields.

The main objectives of the HP-SEE project are:

- 1. Empowering multi-disciplinary virtual research communities. HP-SEE will involve and address specific needs of a number of new multi-disciplinary international scientific communities (computational physics, computational chemistry, life sciences, etc.) and thus stimulate the use and expansion of the emerging new regional HPC infrastructure and its services.
- 2. Deploying integrated infrastructure for virtual research communities. HP-SEE will provide and operate the integrated South-East European eInfrastructure and specifically the HPC eInfrastructure for the region. In the project context this focuses on operating the HPC infrastructure and specific end-user services for the benefit of new user communities, and establishing the continuation of the GEANT link to Caucasus.
- 3. Policy development and stimulating regional inclusion in pan-European HPC trends. The inclusion of the new Virtual Research Communities and the setting up of the infrastructure, together with a set of coordinated actions aimed at setting up HPC initiatives in the region, aims to contribute to regional development and ensure that countries in this outermost European region will join the pan-European HPC trends.
- 4. Strengthening the regional and national human network. The project will capitalize on the existing human network and underlying research infrastructure to further strengthen scientific collaboration and boost more effective high-quality research and cooperation among participating SEE communities.

The expected results of the project are:

- 1. Project management information system established
- 2. Promotional package available
- 3. National HPC initiatives in core countries established
- 4. HPC related Memorandum of Understanding on the regional level
- 5. Set of inter-disciplinary applications running on regional infrastructure

- 6. Regional HPC resources available to target virtual research communities
- 7. Realization of Network Connections and deployment of relevant management and monitoring tools
- 8. Application software environment deployed
- 9. Establishment of a relevant for the region HPC technology watch

The HP-SEE project kicked-off in September 2010 and is planned to be completed by August 2012. It is coordinated by GRNET with 13 contractors participating in the project: major lead institutes in the region for computing aspects of eInfrastructures in Bulgaria, Romania, Turkey, Hungary, Serbia, Albania, Bosnia-Herzegovina, FYR of Macedonia, Montenegro, Moldova (Republic of), Armenia, Georgia, Azerbaijan. The total budget is 3.885.196 €. The project is funded by the European Commission's Seventh Framework Programme for Capacities-Research Infrastructures.

The project plans to issue the following deliverables:

Del. no.	Deliverable name	Nature	Security	Planned Delivery
D1.1	Project management information system and "grant agreement" relationships	R	СО	M01
D2.1	Procurement guidelines analysis	R	PU	M04
D2.2	National HPC task-force modeling and organizational guidelines	R	PU	M09
D2.3	HPC centre setup cookbook	R	PU	M14
D2.4	Regional collaboration modalities and European integration feasibility	R	PU	M16
D2.5	Final report on international collaboration	R	PU	M24
D3.1	Internal and external web site, docs repository and mailing lists	R	PU	M02
D3.2	Promotional package	R	PU	M03
D3.3	HPC training and dissemination plan	R	PU	M03
D3.4	Regional & national training and dissemination events report	R	PU	M12
D3.5	Promotional package	R	PU	M13
D3.6	Regional & national training and dissemination events report	R	PU	M24
D3.7	Final plan for the use and dissemination of foreground	R	PU	M24
D4.1	Target applications analysis	R	PU	M05
D4.2	Report on application deployment and support	R	PU	M12
D4.3	HPC programming techniques guidelines	R	PU	M20
D4.4	User community engagement and applications assessment	R	PU	M24
D5.1	Infrastructure, Network and Management Deployment Plan	R	PU	M05
D5.2	Infrastructure overview and assessment	R	PU	M12
D5.3	Infrastructure deployment plan	R	PU	M14

Infrastructure overview and assessment	R	PU	M23
Tender evaluation results 1	R	PU	M02
Tender evaluation results 2	R	PU	M03
Network Implementation and equipments configuration	R	PU	M04
Deployment of essential network services and management tools	R	PU	M09
CSIRT/NOC Cooperation Report and Harmonization of Efforts among South Caucasus NRENs	R	PU	M15
Software scalability analysis and interoperability issues assessment	R	PU	M06
Design of interoperability and scalability solutions	R	PU	M12
Permanent technology watch report	R	PU	M20
Assessment of interoperability and scalability solutions	R	PU	M22
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Legend: R = Report, O = Other, PU = Public, CO = Confidential (only for members of the consortium incl. EC).

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## References

- [1] Project HP-SEE 261499 Annex I Description of Work
- [2] European Grid Initiative (EGI) official web site http://www.egi.eu/
- [3] HP-SEE official web site http://www.hp-see.eu/
- [4] PRACE project official web site http://www.prace-project.eu/
- [5] Swiss National Supercomputing Centre (CSCS) official web site http://www.cscs.ch/
- [6] Eidgenössische Technische Hochschule (ETH) official web site <u>http://www.ethz.ch/</u>
- [7] École Polytechnique Fédérale de Lausanne (EPFL) official web site <u>http://www.epfl.ch/</u>
- [8] Paul Scherrer Institute (PSI) official web site http://www.psi.ch/
- [9] Swiss Federal Laboratories for Materials Science and Technology (EMPA) official web site http://www.empa.ch/
- [10] Swiss Centre for Applied Ecotoxicology (EAWAG) official web site http://www.eawag.ch/
- [11] Swiss Federal Institute for Forest, Snow and Landscape Research (WSL) official web site http://www.wsl.ch/
- [12] Institut du Développement et des Ressources en Informatique Scientifique (IDRIS) official web site <u>http://www.idris.fr/</u>
- [13] Centre de Calcul pour la Recherche et la Technologie (CCRT) official web site <u>http://www-ccrt.cea.fr/</u>
- [14] Centre Informatique National de l'Enseignement Supérieur (CINES) official web site <u>http://www-ccrt.cea.fr/</u>
- [15] Grand Equipement National de Calcul Intensif (GENCI) official web site <u>http://www.genci.fr/</u>
- [16] Institut National de Recherche en Informatique et en Automatique (INRIA) official web site http://www.inria.fr/
- [17] General Secretariat of Research and Development (GSRT) official web site <u>http://www.gsrt.gr/</u>
- [18] Greek Ministry of Education Lifelong Learning and Religious Affairs official web site <u>http://www.minedu.gov.gr/</u>
- [19] Greek Research and Technology Network (GRNET) official web site http://www.grnet.gr/
- [20] HellasHPC project official web site http://www.hellashpc.gr/

- [21] Romanian National Authority for Scientific Research (ANCS) official web site http://www.ancs.ro/
- [22] Romanian Ministry of Communications and Information Society (MCSI) official web site http://www.mcsi.ro/
- [23] Romanian Ministry of Education, Research, Youth and Sports official web site <a href="http://www.edu.ro/">http://www.edu.ro/</a>
- [24] Fakulteti i Teknologjisë së Informacionit (FTI) official web site <u>http://www.fti.edu.al/</u>
- [25] Department of Physics of Faculty of Natural Sciences of University of Tirana official web site http://www.fshn.edu.al/
- [26] Ss. Cyril and Methodius University in Skopje official web site http://www.ukim.edu.mk/
- [27] Georgian Research and Educational Networking Association (GRENA) official web site <u>http://www.grena.ge/</u>
- [28] Georgian Shota Rustaveli National Science Foundation official web site <u>http://www.rustaveli.org.ge/</u>
- [29] Hungarian National Information Infrastructure Development (NIIF) official web site <u>http://www.niif.hu/</u>
- [30] Hungarian HBONE+ program official web site http://www.hboneplus.hu/
- [31] University of Lugano official web site http://www.usi.ch/
- [32] Centre of Excellence on Supercomputer Applications official web site <u>http://parallel.bas.bg/CE\_SuperCA/</u>
- [33] Institute of Information and Communication Technologies (IICT-BAS) official web site http://www.iict.bas.bg/
- [34] National Institute for Geophysics, Geodesy and Geography (NIGGG-BAS) official web site http://www.geophys.bas.bg/
- [35] Bulgarian Institute of Mechanics (IM-BAS) official web site http://www.mech.bas.bg/
- [36] Sofia University (SU) http://www.uni-sofia.bg/
- [37] Technical University Sofia (TUoS) official web site <u>http://www.tu-sofia.bg/</u>
- [38] Medical University Sofia (MUoS) http://mu-sofia.bg/
- [39] Large Hadron Collider (LHC) experiment official web site http://lhc.web.cern.ch/
- [40] European Organization for Nuclear Research (CERN) official web site http://www.cern.ch/
- [41] Extreme Light Infrastructure Nuclear Physics (ELI-NP) official web site <u>http://www.eli-np.ro/</u>

- [42] Facility for Antiproton and Ion Research (FAIR-GSI) official web site <u>http://www.gsi.de/</u>
- [43] International Thermonuclear Experimental Reactor (ITER/EURATOM) official web site http://www.iter.org/
- [44] Hungarian Academy of Sciences official web site http://mta.hu/
- [45] Hungarnet official web site http://www.hungarnet.hu/
- [46] Hungarian Grid Competence Center (MGKK) official web site https://www.mgkk.hu/
- [47] Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH) official web site http://www.nipne.ro/
- [48] Polytechnic University of Bucharest (PUB) official web site <u>http://www.pub.ro/</u>
- [49] West University of Timişoara (UVT) official web site <u>http://www.uvt.ro/</u>
- [50] Swiss Platform for High-Performance and High-Productivity Computing (HP2C) official web site http://www.hp2c.org/
- [51] Committee for IT Infrastructure (KfR) official web site http://www.dfg.de/dfg\_profil/gremien/hauptausschuss/it\_infrastruktur/index.html
- [52] German Research Foundation (DFG) official web site <u>http://www.dfg.de/</u>
- [53] Distributed European Infrastructure for Supercomputing Applications (DEISA) official web site <u>http://www.deisa.eu/</u>
- [54] PRACE assessment process http://www.prace-ri.eu/Assessment-process
- [55] HPC-EUROPA project official web site http://www.hpc-europa.org/
- [56] HPC-WORLD project official web site http://www.hpcworld.eu/
- [57] Italian Interuniversity Consortium High Performance Systems (CINECA) official web site http://www.cineca.it/
- [58] Montenegro Research and Education Network (MREN) official web site <u>http://www.mren.ac.me/</u>
- [59] Open Source Cluster Application Resources (OSCAR) http://oscar.openclustergroup.org/
- [60] Rocks open-source Linux cluster distribution http://www.rocksclusters.org/
- [61] Perceus installation and configuration tool http://www.perceus.org/
- [62] Extreme Cluster Administration Toolkit (xCAT) http://xcat.sourceforge.net/

- [63] Cfengine IT operations http://www.cfengine.com/
- [64] Parallel Distributed Shell (Pdsh) http://sourceforge.net/projects/pdsh/
- [65] Nagios industry-standard in IT infrastructure monitoring http://www.nagios.org/
- [66] Ganglia Monitoring System http://ganglia.sourceforge.net/
- [67] Romanian NCIT Cluster Homepage http://cluster.grid.pub.ro/
- [68] Official Gaussian web site http://www.gaussian.com/
- [69] Official Matlab web site http://www.mathworks.com/
- [70] SCOPUS International database of publications http://www.scopus.com/
- [71] HP-SEE Project, Deliverable 4.1 "Target applications analysis"
- [72] TeraGrid official web site https://www.teragrid.org/
- [73] HP-SEE Project, Deliverable 5.1 "Infrastructure, Network and Management Deployment Plan"
- [74] HP-SEE Project, Deliverable 8.1 "Software scalability analysis and interoperability issues assessment"
- [75] HP-SEE Project Wiki page http://wiki.hp-see.eu/
- [76] PRACE-PP Project, Deliverable 2.2.1 "Report on Analysis of Adequate Governance Structure"
- [77] PRACE-PP Project, Deliverable 2.2.2 "First Draft of Governance Document"
- [78] PRACE-PP Project, Deliverable 2.2.3 "Governance Document"
- [79] PRACE-PP Project, Deliverable 2.4.1 "Initial Report on the Peer Review Process"
- [80] PRACE-PP Project, Deliverable 2.4.2 "Final Report on the Peer Review Process"

# Glossary

ANCS	National Authority for Scientific Research
ARC	National Authority for Scientific Research Application Review Committee
ARCAS	Advanced Computational Methods in Scientific Research
CCRT	Centre de calcul pour la recherche et la technologie
CERN	Organisation Européenne pour la Recherche Nucléaire
CINECA	Consorzio Interuniversitario del Nord est Italiano Per il Calcolo Automatico
CINES	Centre Informatique National de l'Enseignement Supérieur
CSCI	Comité Stratégique du Calcul Intensif
CSCS	Swiss National Supercomputing Centre
CUDA	Compute Unified Device Architecture
DEISA	Distributed European Infrastructure for Supercomputing Applications
DFG	German Research Foundation
EAWAG	Swiss Centre for Applied Ecotoxicology
EC	European Commission
EGI	European Grid Initiative
ELI	Extreme Light Infrastructure
EMPA	Swiss Federal Laboratories for Materials Science and Technology
EPFL	École Polytechnique Fédérale de Lausanne
ERC	European Research Council
ESFRI	European Strategy Forum on Research Infrastructures
ETH	Eidgenössische Technische Hochschule, Zurich
FAIR	Facility for Antiproton and Ion Research
GENCI	Grand Equipement National de Calcul Intensif
GPU GRENA	Graphics Processing Unit Georgian Research and Educational Networking Association
GRNET	Greek Research and Technology Network
GSRT	General Secretariat of Research and Development
HPC	High Performance Computing
HPSC	High Performance Scientific Computing
IBM	International Business Machines
ICT	Information and Communication Technologies
IDRIS	Institut du développement et des ressources en informatique Scientifique
INRIA	Institut National de Recherche en Informatique et en Automatique
ITER	International Thermonuclear Experimental Reactor
LHC	Large Hadron Collider
MCSI	Ministry of Communications and Information Society
MoU	Memorandum Of Understanding
MPI	Message Passing Interface
MREN	Montenegro Research and Education Network
NGI	National Grid Initiative
NIIF	Nemzeti Információs Infrastruktúra Fejlesztési
NSC OpenMB	National Supercomputing Centre Open Multi-Processing
OpenMP OSCAR	Open Source Cluster Application Resources
PRACE	Partnership for Advanced Computing in Europe
PSI	Paul Scherrer Institute
PUB	Polytechnic University of Bucharest
SEE	South East(ern) Europe
SLA	Service Level Agreement
TGCC	Très Grand Centre de Calcul
VRC	Virtual Research Communities
WSL	Swiss Federal Institute for Forest, Snow and Landscape Research
XCAT	Extreme Cluster Administration Toolkit

## Executive Summary

#### What is the focus of this Deliverable?

This deliverable focuses on providing guidelines for organization of national HPC initiatives in the SEE region. It offers detailed analysis and information on various aspects of the establishment and operation of national HPC centers, from the governance models and structures, coordination and funding, organization of the scientific assessment of HPC access proposals, to coordination of the HPC center, including the technical, user support, training and dissemination activities.

#### What is next in the process to deliver the HP-SEE results?

The contents of this deliverable will form a basis for the other work packages, most notably they will be useful for the work packages and deliverables from: WP2- National and Regional HPC initiatives and international liaison, WP3-Dissemination and Training, and WP4 – Virtual Research Communities support.

The complete deliverable and workflow progress is described in the project Annex-I - Description of Work [1].

#### What are the deliverable contents?

The deliverable presents details on the analysis of organization of national HPC initiatives and gives guidelines to SEE countries and partners, based on the inputs from several PRACE countries, as well as the inputs collected from HP-SEE project partners. The analysis presented in the deliverable addresses the following issues:

- Governance models for HPC initiatives: coordination of national HPC activities, MoU, national-level projects and funding issues.
- Peer review and scientific assessment for HPC access proposals.
- Coordination of HPC centers, including technical support, system management, training and dissemination activities, European coordination and interoperability, and user support.

#### Conclusions and recommendations

The analysis presented in this deliverable was based on the inputs from several PRACE countries, representing the experiences of the well-developed HPC initiatives, and on experiences, inputs and plans from the core HP-SEE countries (Greece, Bulgaria, Romania, Hungary, Serbia), as well as other general partners in the project.

First,, this deliverable has investigated possible governance structures for HPC initiatives, and identified several models, which include MoU-based entities, initiatives coordinated by the designated research institute or university, centers of excellence, consortia, and legal entities with mixed ownership. In particular, the following key guidelines for the governance of national HPC initiatives are identified:

- Coordination: managed by a council (board) and by a director/chair of the initiative (if established as a legal entity), or otherwise by a supervisory board and a coordinator appointed by a consortium or coordinating institution for the initiative. Depending on the organizational model of the HPC initiative, technical coordination is done by a technical director or appointed technical coordinator, assisted by a technical coordination board, with representatives from all national HPC centres.
- Scientific steering committee to be established to carry out the peer review of proposal for access to national HPC resources.

• User advisory/representation body to be formed as a responsible to give recommendations and feedback regarding all aspects of the operation of HPC infrastructure.

Second, the deliverable also gives exhaustive analysis on peer review scientific assessment of proposals for the use of HPC resources. Various assessment models are presented, which can be adopted by SEE countries. At present, peer review in the region is done by the NA4 activity of HP-SEE project. Experiences of PRACE countries from national calls, as well as from the PRACE access calls are therefore valuable inputs, and were presented here together with the inputs from HP-SEE partners. Analyzing the collected inputs, Chapter 3 identifies the most important principles to be followed by peer review process, as well as typical steps in the organization of the application assessment. The key guidelines identified:

- Scientific steering committee should be appointed, consisting of HPC experts with the background from various scientific fields, representing fairly all major user communities in the country. The committee opens calls for access to national HPC resources, defines procedures, creates the appropriate questionnaires and forms for the calls, and makes decisions on the priorities/quotas assigned to each scientific field.
- Prior to the scientific peer review of research proposal, each project has to successfully pass a technical review, done by the operational personnel at the HPC centre where resources are requested.
- Scientific steering committee should carefully follow up the results of the projects that are granted access to national HPC resources, and take necessary measures if the applied approach and the quality of the obtained results is not deemed satisfactory.

Third, the deliverable considers HPC centre coordination regarding various aspects. Here we summarize the key guidelines identified. Regarding the organization of the HPC centre, the deliverable identifies the following conclusions:

- Technical support/hardware management HPC centre system management at the fabric/hardware level, as well as at the base OS services level, is done by the technical support team. It coordinates its work with the operational and user support teams.
- Operational support
   Management and monitoring of HPC services as well as a support for resolving of
   issues and problems identified by end users is performed by the operational
   support team, which can be organized jointly with the technical support team.
- User support
   User communities and researchers whose proposals are granted access to HPC
   centres, local HPC centre users, as well as those preparing, porting and
   developing their HPC applications, are served by a user support team.

Regarding the organization of activities and workflows of the HPC centre, the deliverable identifies the following guidelines:

- Planning of support teams While technical and operational support teams should be sized according to the amount of available hardware, the size of the user support team should critically depend on the size of active user communities, as well as the number and necessary effort to support them.
- Technical assessment of applications User support team, in collaboration with the operational support, should be responsible for technical assessment of applications.
- Support system (helpdesk) For each of the support teams, on-line troubleshooting tracking system should be deployed (helpdesk), such that end users and members of the support teams

could easily access it, and that the trouble tickets can be easily exchanged between different units.

- Training coordination HPC centre should organize regular training activities for its users and support personnel. For this reason, a dedicated person should be appointed as a training coordinator, and be responsible for organization of local training events, as well as collaboration with other HPC centres at the national, regional and EU-level on training activities.
- Dissemination coordination HPC centre should also appoint a person responsible for dissemination of information on centre's activities, as well as scientific dissemination.
- National and European coordination and interoperability Coordination of activities of the centre with other centres from the country, region or from EU-wide infrastructures (PRACE) is an important element for the successful operation of a national HPC centre. Technical manager/coordination of HPC centre should be responsible for this task overall.

# 1. Introduction

In this deliverable we provide guidelines for SEE countries in setting up national HPC task forces and initiatives. After a successful establishing of national Grid initiatives in the region and their integration into the European Grid Initiative [2], (via the SEE-GRID series of projects) several user communities were activated and involved in the application development, deployment and production use. Following this development, a number of research groups in the region have significantly advanced in the use of distributed and high performance computing resources. Their requirements for computing resources have grown over time, as the level of research has increased. Aiming to address relevant scientific topics and challenges, the availability of significant HPC resources now becomes an important issue, and HP-SEE [3] project is tasked with establishing regional HPC interoperable infrastructure, supporting identified user communities from computational physics, computational chemistry and life sciences, and develop and provide user and operational tools for HPC production use and monitoring.

An important aspect in providing these services and support to user communities is establishing of national HPC initiatives. Several countries from the region (Greece, Bulgaria, Serbia, Turkey; Hungary is about to join) are already members of PRACE, and together with Romania are actively working on procuring large HPC installations. The planning of these procurements and technical and support organization of national HPC centers is therefore one of their important activities, which is coordinated by the HP-SEE WP2 activity. Experiences from other European countries, especially the PRACE [4] partners, is seen as one of the very important elements to be considered in the planning process in the SEE region. In this regard, the deliverable will be highly beneficial not only to the core partners of the project (Greece, Bulgaria, Hungary, Romania, Serbia), but also to all other partners as they progress with the development and establishing of their national HPC programmes and initiatives.

The deliverable covers several important topics. From the policy point of view, we will examine possible governance models, coordinating bodies for HPC initiatives, nationallevel MoUs and projects, as well as longer-term funding possibilities. Another important topic is peer review/scientific assessment of proposals for the use of national or regional HPC resources. We also cover in depth HPC centre coordination and organization, through various aspects, including technical support, system management, and technical application assessment. The deliverable collects experiences and organization of the training and dissemination activities. European coordination and interoperability, as well as user support (operational and application) are extensively covered.

## 2. Governance

In this chapter we will analyze existing and planned governance structure of HPC initiatives in SEE countries, funding and HPC coordination bodies and their mandates, as well as their legal forms. We will also examine strategy/policy documents regarding HPC activities, existence and organization of committees that control access to the systems and resource allocation (scientific committees, access committees, operational committees). From the policy point of view, we will also examine the existence of national-level MoUs regarding the organization of HPC activities and their memberships, national-level projects on HPC infrastructure, technology, applications etc.

Since the experiences in this regard in the SEE region are still limited, we also include a short analysis of two PRACE countries, Switzerland and France, which are presented below.

#### Switzerland:

The Swiss National Supercomputing Centre [5] is part of ETH [6] Zurich, one of the two federal Swiss technical universities. ETH Zurich is the official legal entity and is part of the so-called ETH Domain, which summarizes the two Swiss federal technical universities ETH Zurich and EPFL [7] as well as four federal research institutes (PSI [8], EMPA [9], EAWAG [10], and WSL [11]). The ETH Domain is led by ETH Board, which reports to the Federal State Secretary for Education and Research. The State Secretary reports to Minister of the Interior. Furthermore, CSCS has an advisory board of international HPC experts.

#### France:

The three national HPC centres (CNRS/IDRIS [12], CEA/CCRT [13] and CINES [14]) operate the national resources for research applications. This part of their activities is coordinated by GENCI [15], from funding for equipment investment to resources allocation.

GENCI, Grand Equipement National de Calcul Intensif, is a legal entity taking the form of a "société civile" under French law, owned 49% by the French State represented by the Ministry for Higher Education and Research, 20% by CEA, 20% by CNRS, 10% by the Universities and 1% by INRIA [16].

Created in 2007, GENCI has the following missions:

- Implement and ensure the coordination of the major equipments of the national HPC centres, by providing funding and by assuming ownership.
- Promote the organization of an European HPC area and participate to its achievements; GENCI is the French representative in PRACE.
- Set up R&D collaborations in order to optimize HPC facilities and to anticipate novel technologies.
- Promote simulation and high performance computing in both fundamental and industrial research.

CEA also operates the French Tier-0 system for PRACE, curie, funded by GENCI as part of its commitment to the Hosting Member statute of France, in its Très Grand Centre de Calcul (TGCC) facility.

#### SEE region

While in the SEE region formal HPC initiatives are not common, where they are established mostly the Swiss model is used, where one research institute or university is tasked with the coordination of HPC activities, through the board, which includes representatives from various stakeholders from the country. However, more streamlined organization model, like the French one, could also be adopted in countries with several

prominent institutions in the HPC arena. The direct participation of the government in the HPC initiative is less likely in the SEE region, however, and the state is usually represented indirectly, by funding of the initiative through research institutes, universities and national research and infrastructure projects.

In the following we present short summary of HPC initiatives and governance structures from HP-SEE core countries (GR, BG, RO, HU, RS), as well as from a number of other countries participating in the project.

#### Greece:

HPC activities in Greece are coordinated on the funding level from the General Secretariat of Research and Development [17] (GSRT), which is supervised by the Ministry of Education Lifelong Learning and Religious Affairs [18]. In the frame of the PRACE Research infrastructure implementation GSRT has given its mandate to the Greek Research and Technology Network [19] (GRNET S.A.) to coordinate the HPC related activities in Greece. GRNET is a state-owned company, operating under the auspices of GSRT. Its mission is to provide high-quality eInfrastructure services to the academic, research and educational community of Greece and to disseminate ICT to the general public.

GRNET S.A. is a member of the PRACE-RI, since it was established (May 2010) and participates in the series of PRACE projects (PRACE Preparatory and Implementation Phase projects). The HellasHPC [20] project kicked-off on June 2010 and ended in January 2011, in the context of a call from the General Secretariat of Research and Technology concerning the establishment of national research networks in the areas concerning the research infrastructures included in the ESFRI roadmap [R XX]. In particular, HellasHPC focused on the High-Performance Computing service deployed by the PRACE (Partnership for Advance Computing in Europe) pan-European organization and the role of Greece in the implementation phases of the respective projects (PRACE-1IP, PRACE-2IP etc.).

In pursuit of this goal HellasHPC carried out a number of activities with the purpose to investigate the current status of HPC in Greece, to identify user requirements, and to provide a proposal for the role of Greece in PRACE, presenting in parallel a national strategy for the development of HPC infrastructures in Greece. The basic activities that the project conducted were the following:

- 1. A compilation of a national survey involving the country's largest academic and research centers.
- 2. The authoring of an HPC technologies state of the art document.
- 3. The organization of two workshops, one in the Aristotle University of Thessaloniki and one in the National Hellenic Research Foundation.
- 4. A National HPC Strategy proposal compiled in the context of the project's WP3 activity.
- 5. The signature of an MoU from all 35 participating institutes that participated to the HellasHPC project.

The above results of the project have been communicated to the finding body and its respective ministry.

#### **Bulgaria**:

The importance of development of HPC infrastructure for Bulgarian science is recognized in the National Roadmap for Scientific Infrastructure, approved on 21 September 2010 by the Council of Ministers, where the 5th complex out of 7 is defined as "Bulgarian Supercomputer Center" with scientific and technical coordinator defined as the Center of Excellence "Supercomputer Applications" [32]. This consortium corresponds to the national project with the same name "Centre of Excellence Supercomputer Applications" funded by National Science Found (NSF), coordinated by IICT-BAS.

#### Romania:

The main components of the public Romanian HPC infrastructure are: a) the resource centres of the research institutes and universities, which are financed by the National Authority for Scientific Research [21] (ANCS), and b) the National Supercomputing Centre (NSC), which was established in 2010 and is financed by the Ministry of Communications and Information Society [22] (MCSI).

ANCS is the government's specialized body with the mission to define, apply, coordinate, monitor and evaluate research, development and innovation policies, in accordance with the Government Strategy and Programmes. In this respect, it fulfills the responsibilities and undertakes the attributes of the Ministry of Education, Research, Youth and Sports [23] in the fields of scientific research, technological development and innovation.

The current strategy of ANCS is based on the *National Strategy for R&D and Innovation for 2007-2013*, and the *National Plan for R&D and Innovation for 2007-2013*. In this framework, ANCS supports the research in the following ITC directions:

- computer science
- advanced informatic systems for e-services
- communication technologies, systems and infrastructures
- artificial intelligence, advanced robotics and autonomous systems
- security and accessibility of information systems

The HPC infrastructure for research and education was created through the funding by ANCS of various independent R&D projects, or by making use of the EU structural funds under the Sectorial Operational Programme for Increasing the Economic Competitiveness. Today, the main contribution to this infrastructure comes from 10 parallel computing systems (one BlueGene/P supercomputer and 9 HPC clusters with more than 200 cores each), which are hosted by 3 R&D institutes and 5 universities. These main HPC centres totals more than 7700 cores and approx. 50 Tflops Rpeak, and are interconnected through the large bandwidth NREN RoEduNet.

Regarding the NSC, this has been provided in a first stage by MCSI with medium-size computing capacities (896 cores), which should ensure support for e-Governing, cyber security, and, on a lesser extent, research in targeted areas.

#### Hungary:

In Hungary there is no separate HPC program as all HPC-related efforts are merged into the National Information Infrastructure Development [29] (NIIF) Program. This program is responsible for any infrastructure related development and operations efforts, such as the academic data network, scientific trust federations, and collaboration infrastructures. The Program is regulated by Hungarian Government Regulation 5/2011 (II.3.) that replaced the former Regulation 95/1999. (VI.23.). The Regulation appoints the National Information Infrastructure Development Institute (NIIFI) that belongs the Ministry of Development to be the executor of the Program and assigns yearly budget to the Program accordingly. NIIFI also receives funding from the EC Structural Funds to augment its already-existing scientific infrastructure. Currently an infrastructure development program called HBONE+ [30] (a merger of TIOP1.3.2 and KMOP4.2.1.A initiatives) had been approved and is being executed. Within the frameworks of this program approximately 4mEURO has been established to support the development of 4 HPC sites representing a total of 50Tflops computational capacity and 1.5Pbytes of storage in Hungary.

#### Serbia:

The research sector in Serbia for a long time is expressing its need for HPC resources. The main already active user communities are from the fields of mathematical and physical sciences (high energy physics, condensed matter physics, astronomy and astrophysics, meteorology), computational chemistry, computer science, as well as from electrical and mechanical engineering. Further interest is expressed from climate change community, and from researchers working on constructions integrity estimates.

In the past the need for HPC resources was partially fulfilled through the establishment of Academic and Educational Grid Initiative of Serbia (AEGIS), and participation of Serbian research institutes and universities in regional and pan-European Grid infrastructures. However, for a number of user communities the resources provided by Linux-cluster-based Grid infrastructures are not suitable due to one or more of the technical and performance reasons, and HPC resources become necessary.

Taking into account this and growing HPC needs of Serbian research communities, Ministry of Science and Technological Development of the Republic of Serbia has designated the Institute of Physics Belgrade (IPB) as a coordinating institution for all HPC activities. Serbia joined the PRACE initiative in December 2008, dully represented by IPB. As of 2010, IPB is a partner in HP-SEE and PRACE-1IP projects, and it will also represent Serbia in PRACE-2IP.

On the national level, IPB has focused HPC activities on establishment of the Blue Danube National Supercomputing and Data Storage Facility, in collaboration with the Ministry of Science and Technological Development of the Republic of Serbia until the beginning of 2011, and after the government was restructured, with the newly formed Ministry of Education and Science of the Republic of Serbia. The Blue Danube facility will be part of the IPB, located in a new building that will be designed and built specifically for this facility. This facility will be integrated into PRACE infrastructure as a Tier-1 center during the PRACE-2IP project.

During 2010, the government of the Republic of Serbia adopted National Strategy of Scientific and Technological Development 2010-2015, which identifies HPC and supercomputing as one of priorities for Serbia, and affirms the plan to establish national HPC center.

Until then, IPB team coordinates HPC activities in Serbia in collaboration with all interested partners, based on the national level MoU which covers both HPC and Grid computing.

#### Albania:

HPC initiative is not formalized in government level. Several research institutions are in collaboration, formal and/or informal, shaping a bottom-up HPC initiative. Actual interinstitutional activities are limited in framework of HP-SEE project where FTI [24] is in collaboration with a team from Department of Physics of Faculty of Natural Sciences of University of Tirana [25], and some informal contacts with Department of Mathematics and Informatics of Faculty of Economy of University of Tirana.

#### FYR of Macedonia:

There is no National HPC initiative yet. As far as the infrastructure is concerned, the Ministry of education and science finances the upcoming HPC lab. The Ministry is the owner of the equipment and the Computer science and engineering faculty at UKIM [26] will operate it. The establishment and the format of the National HPC Initiative are discussed at the academic and governmental level.

There are no special strategic documents concerning HPC. The management of the HPC resources is not yet covered by any formal documents. Assess, usage and review policies will be produced, but their format and organization is still not defined.

#### Georgia:

There is no governance structure of the HPC initiative in Georgia and no dedicated funding for HPC activities. The only project related to HPC is HP-SEE project whose partner from Georgia is GRENA [27]. This is partly connected to the reorganization of science in Georgia, with which all research institutes became part of universities starting from 2011. The only mechanism to fund research in Georgia is via Shota Rustaveli Science Foundation [28] grants and there is yet no dedicated program for Grid and HPC activities. Regarding the HPC infrastructure, research groups are mainly using computer

resources available at their institutions or distributed infrastructures in which they participate (i.e. HP-SEE one).

## 2.1. Coordinating body

In this section we describe how coordination of HPC activities is organized in various countries. We start with the two PRACE countries, then we analyze the coordination in the core HP-SEE countries, and also give details on a number of other HP-SEE countries.

#### Switzerland:

HPC activities in Switzerland are coordinated by CSCS [5] and its National HPCN Steering Committee. The committee is led by the president of the ETH [6] Board. Other members are the president of ETH Zurich, the president of the cantonal university of Lugano [31] and a delegate of the State Secretary.

On the national level, the overarching goals as well as investment funds for supercomputers of CSCS [5] are defined in a national HPCN strategy. The current strategy covers the years 2009 to 2015. The operational aspects of CSCS are defined in a performance agreement between CSCS and ETH [6] Zurich management. The performance agreement has duration of 4 years.

#### France:

In France, HPC activities are coordinated by GENCI, Grand Equipement National de Calcul Intensif. It is a legal entity taking the form of a "société civile" under French law.

#### Greece:

The coordinating body of HPC activities in Greece as stated above is the Greek Research and Technology Network [19] (GRNET S.A.).

#### Bulgaria:

HPC activities in Bulgaria are coordinated by the "Bulgarian Supercomputer Center", as specified in the National Roadmap for Scientific Infrastructure, approved on 21 September 2010 by the Council of Ministers. Scientific and technical coordination is done by the Center of Excellence "Supercomputer Applications" [32]. The roadmap also recognizes the consortium for this complex, which consists currently of:

- Institute of Information and Communication Technologies [33] (IICT-BAS)
- National Institute for Geophysics, Geodesy and Geography [34] (NIGGG-BAS)
- Institute of Mechanics [35] (IM-BAS)
- Sofia University [36] (SU)
- Technical University Sofia [37] (TUoS)
- Medical University Sofia [38] (MUoS)

The roadmap defines the role of the Ministry of Transport, Information Technology and Communications as a financial manager of this complex. This consortium corresponds to the national project with the same name "Centre of Excellence Supercomputer Applications" funded by National Science Found (NSF), coordinated by IICT-BAS.

#### Romania:

Acting as main financier and official body that approves the R&D projects involving High Performance Scientific Computing (HPSC), ANCS [21] recently conducted a survey regarding the existing resources and the requirements of the scientific community. After analysing the responses received from various research groups of more than 30 institutions, a number of HPSC development objectives have been set, among which:

1. Development of the national network of HPSC centres and creation of new centres, in order to fulfill the growing needs of research;

2. Supporting the main directions of research in major scientific areas that require HPC for modeling and simulation, which are, according to the survey, Computational Physics, Computational Chemistry, Astronomy & Astrophysics, Life Sciences, Meteorology and Environmental Sciences;

3. Providing HPC support for large scale, long-term international collaborations to which Romania participates, such as the LHC [39] (Large Hadron Collider) – CERN [40] experiments, ELI-NP [41] (Extreme Light Infrastructure – Nuclear Physics), FAIR-GSI [42] (Facility for Antiproton and Ion Research), ITER/EURATOM [43] (International Thermonuclear Experimental Reactor), etc.;

4. Strengthening the role of the scientific research and education community in the coordination at the national level of the HPSC activity;

5. Organisation of a national competence network for the evaluation of the software applications and allocation of computing time, composed of researchers with HPSC experience;

6. Connecting to the European partnerships regarding the HPSC infrastructure, such as PRACE.

In order to reach the objectives 4 and 5 above, ANCS supports the foundation of a professional non for profit association for the promotion of the advanced computational methods in scientific research (ARCAS), as a legal body which will have an important role in the coordination of the national HPC activities

The adoption of a common HPC and cloud-computing strategy is currently discussed by ANCS together with MCSI [22] and other decision factors. In this framework it was established that ANCS will continue to coordinate the HPSC domain, while MCSI will mainly focus on the applications of cloud-computing in e-governing, on the IT support for the implementation of EU directives, and for the guidance of small and medium-sized enterprises development.

#### Hungary:

The NIIF Program that all HPC related efforts currently belong to has practically two coordinating bodies: the Program Board and the Technical Board. The former is responsible for high-level policy and budget coordination as it represents all the ministries as well as the Hungarian Academy of Sciences [44]. The Technical Board, on the other hand, deals with the mid-term (1 year – 3 years) technical strategy. There are two additional forums helping the work of the two boards above: the Hungarnet [45] Association representing the social background and the user base of the national infrastructures, and the Hungarian Grid Competence Center [46] (MGKK) that incorporates the 7 largest grid role-player organizations in the country.

#### Serbia:

Institute of Physics Belgrade (IPB) coordinates all HPC activities in Serbia, according to the decision of the Ministry of Science and Technological Development of the Republic of Serbia from 20 October 2008.

#### FYR of Macedonia:

The main point in the discussion about the establishment of the National HPC Initiative is whether it should be separate entity or joined with the National Grid Initiative. There are arguments for both of the proposals. Separate entity would provide better visibility and broader governmental support, since the NGI is formally supported by the Ministry of Information Society and the HPC equipment is owned by the Ministry of science and education. On the negative side of this proposal is the modest user community, which has to be split in two separate initiatives. If the HPC Initiative would be joined with the NGI, this would provide single and stronger initiative, with shared resources, but with lower visibility. The most credible outcome is to establish separate Initiative, formally supported by the Ministry of education and science, and sign a letter of collaboration with the NGI governing the sharing of the resources and other policies.

## 2.2. National-level MoU

While fully established national HPC initiatives may not be very common in the SEE region since they require endorsement and funding from the government, collaboration between research institutes and universities in the HPC area is quite common, and MoUs represent the usual form used to coordinate such collaboration.

#### Greece:

One of the objectives of the HellasHPC [20] project was the signature of the MoU between all the participating in the projects institutes. Since Greece had already a memorandum of understanding in the area of Grid computing (the HellasGrid MoU) it was decided that this MoU should be extended to cover also HPC as well as Cloud related activities and include also the new participating institutions with involvement in HPC activities and where not included in the Grid MoU. The main aim of this MoU is the definition of a collaboration framework among its partners for the provisioning of national services in the areas of Grid, HPC and cloud computing and the interoperation of those infrastructures with the corresponding European ones. At the time of writing this deliverable the MoU is given for signature to the 33 partners that participate in this.

#### **Bulgaria:**

National Roadmap for Scientific Infrastructure, approved on 21 September 2010 by the Council of Ministers specifies the main lines of HPC activities that have to be undertaken under complex 5: Bulgarian Supercomputer Center: High Performance Infrastructure for Computer Modelling, Simulations and Research with applications in industry, medicine, pharmaceutics, energy, transport, finances and ecology.

Three modules are defined, related to hardware and software provision and expansion of the HPC activities towards partners in science and industry and attracting investment from private enterprises. The National Roadmap has been extensively consulted with interested research institutions and industry and thus serves as the legal basis of the future HPC activities (until 2020). The consortium is governed by the consortium agreement and all other documents related to the project "SuperCA" [32] and "SuperCA++". In this way the legal base for the national HPC initiative is extensive and covers all directions.

#### Romania:

Until 2008-2009, there has been a lack of national implementation of the HPC concept in Romania, as well as a relatively low interest in highly scalable computational intensive applications.

Four institutions with HPC activities and significant resources (IFIN-HH [47], ISS, UPB [48], and UVT [49]) decided in October 2009 the creation of the *Joint Research Unit for High Performance Computing and Supercomputing* by signing the *MoU regarding the Development of the National Infrastructure for HPC and Supercomputing*.

This MoU, which is valid until 2014, expresses the commitment of the partners in coordinating their efforts for the strengthening of the national HPC community and their collaboration in order to participate to European projects. The consortium, which was recognized by ANCS [21] in 2010, is open for accession of new members.

It is expected that the creation of the national association for the promotion of the advanced computational methods in scientific research ARCAS will be accompanied by a

new and more comprehensive memorandum, which will encompass more recent aspects of the HPC development in Romania.

#### Hungary:

The Hungarian Grid Competence Center [46] (MGKK), an organization incorporating the 7 most-dominant grid-interested parties, has a formal MoU that regulates the cooperation among the member organizations with respect to distributed computing and data storage. The MoU is open for the accession of new members.

#### Serbia:

Research collaboration and HPC and Grid infrastructure development and management in Serbia is organized based on the MoU signed in September 2007 and valid for 5 years, until September 2012. It covers coordination efforts to further develop academic and educational high performance computing facilities and help to integrate them into the national infrastructure. It also states further objectives of the MoU through organization of dissemination and training activities, collaboration on developing and deploying applications that will benefit from the use of the national infrastructure. This MoU also covers coordination of fund-raising efforts for the development of the national HPC and Grid infrastructure, as well as collaboration on joint participation in national and international, especially Framework Programme, research and infrastructure projects. MoU is signed by a number of research institutes, university computer centers and faculties, with active user communities interested in HPC and Grid computing.

### 2.3. National-level projects and longer-term funding

The first step in establishing and formalizing HPC initiatives in many countries is involving the policy makers and government through funding of national-level projects which are in part devoted to HPC, or have a significant HPC elements. Ideally, such projects are formulated through the national programme devoted to research infrastructures, but most commonly they are distributed over a number of scientific disciplines (physics, chemistry, computer science, engineering), where part of the funding is allocated for HPC equipment, while technical and application support are not explicitly funded.

#### Switzerland:

The mandate for HPC activities in Switzerland described previously set the funding framework for CSCS for supercomputer investments (6 years) and for operations (4 years). Furthermore, CSCS operates a national HPC competence platform called HP2C [50], as mandate of the National HPCN Steering Committee.

#### Greece:

GRNET [19] is in discussion with GSRT [17] for the acquisition of a National Supercomputer that will serve as a Tier-1 system. This would be the one of the first national HPC projects that will include funding for hardware acquisition, building preparation, as well as the operations of the supercomputer fir 3-4 years. A decision is being awaited on the exact level of funding and the structure of the project.

#### Bulgaria:

The core funding for the HPC activities in Bulgaria is defined in the National Roadmap for Scientific Infrastructure, approved on 21 September 2010 by the Council of Ministers, where the financial management is given to Ministry of Transport, Information Technology and Communications. The Roadmap specifies the figures for the funding and their expected sources:

 2011-2012 – 5 million leva (approx 2.5 million euro) – structure funds and national co-financing

- 2014-2015 5 million leva national financing
- 2017-2018 5 million leva European financing and national co-financing

It is expected that public-private partnerships will be formed and will provide 2 million leva (approx. 1 million Euro) for the period 2015-2016 and 4 million leva for the period 2018-2020.

The first phase includes the currently ongoing project SuperCA++ [32] from the NSF, as well as a few related projects, coordinated by partners from the consortium.

#### Romania:

As stated above, the existing national HPC infrastructure for science and education was created in Romania through the funding by ANCS [21] of many independent projects without full national coverage or global coordination. Consequently, currently there is no ongoing project at national level or longer-term funding.

This situation is expected to change in the near future as a result of the current assessment of the global HPC requirements which is performed by ANCS and whose results will be published in the *White Book of the High Performance Scientific Computing in Romania*.

In this framework, the analysis of the existing HPC resources and the of the growing needs of advanced computing for scientific research will hopefully lead to a positive decision regarding the development of a national-level infrastructure project supported through a long-term funding programme.

#### Hungary:

In Hungary there is a generic scientific infrastructure and also several service development programs. HBONE+ [30] incorporating two regional projects TIOP1.3.2 and KMOP4.2.1.A is responsible for the improvement of the Hungarian scientific infrastructure. The topics covered in that project are as follows: creating country-span hybrid data network based on lambda-rails, establishing 4 HPC sites at three major national universities as well as at NIIFI [29], reengineering the former collaboration tools to facilitate virtual communication, i.e. videoconferencing, and creating scientific trust federations.

Based on the infrastructure created within HBONE+, there is a service development initiative called TAMOP 4.1.3 that has formally terminated at the end of 2010 and that corresponds exactly to the same areas as identified in HBONE+. Among its numerous objectives this project aims at developing cloud services, scientific application portals, storage management systems, CRM interfaces, certificate management and administration tools and SLCS services.

#### Serbia:

The funding of research at Serbian institutes and universities is done exclusively through national and international projects. At the national level, research infrastructures are not funded directly, and until now there were no specific and organized national programmes aimed at providing shared facilities to Serbian research communities. The funding for equipment and infrastructure was mostly done through ad hoc calls, most notably National Investment Plan in 2006, 2007 and 2008 was beneficial in this regard. However, majority of running operation and support costs have to be covered from the budget of national research projects from various scientific disciplines, users of HPC infrastructures. A number of projects from physical sciences, chemistry, engineering have collaborated and managed to jointly use existing resources, supporting each other in covering costs of operation. However, funding for application support was quite sparse, and it was mainly up to PhD students and young PhDs to share the knowledge between various research groups.

In 2010, Ministry of Science and Technological Development of the Republic of Serbia, now integrated with the Ministry of Education (as of March 2011) to Ministry of Education

and Science, together with the Cabinet of the Deputy Prime-Minister for European Integration, have launched an initiative for improving research infrastructure in Serbia. During the call for national research projects (which was carried out in 2010, and the selected projects have started in 2011), specific part of the call was devoted to research infrastructure requirements. In addition to the equipment which will be granted to particular projects, the establishment of shared facilities is also currently in progress. The funding for this is secured partly from the Serbian budget and partly from the load by the European Investment Bank. Funding for 2011 should be at the level of 60 million euros, and the overall available funding for research infrastructure in this program is 200 million from the loan of the European Investment Bank, which has to be matched by the same amount of funding from the Serbia budget. The establishment of the national center for nano-science and national HPC center are part of the 2011 budget, and HPC center should receive the funding at the level of 7 to 10 million euros.

#### Albania:

Ministry of Innovation and IT has approved a project-proposal from Faculty of Information Technology [24] (FTI) of Polytechnic University of Tirana for creation of a small HPC node with a parallel system (based on Intel Xeon E5506, a total of 240 cores), to be funded by the Chinese government; implementation has not started yet. In framework of bottom-up initiatives in 2010 FTI did proposed a project (the second stage for ALBGRID – the grid and HPC initiative in Albania, to support both participation in HP-SEE [3] and EGI-InSPIRE [2]) in framework of the first call for the National Programme for R&D in IT 2010-2012, which was selected by the technical evaluation team but rejected by the board of the manager of the programme the Agency for Research Technology and Innovation.

# 2.4. Guidelines for the governance of national HPC initiatives

As can se be seen from the presented examples, the governance structure for a national HPC initiative can be setup in the form of a newly established legal body/organization (public entity, or enterprise owned by key stakeholder institutions), national agency or department of governmental research funding body, could be delegated to one of institutes, universities or HPC centres, or coordinated by a consortium of institutes, universities, and HPC centres. Each of these models has its benefits and limitations, and the appropriate model has to be chosen according to the specific environment and legal framework, as well as the funding model for research and development in the country.

However, whatever model is adopted, the following general functions are identified to be the most important, and should be implemented by all national HPC initiatives:

Coordination: management and technical coordination

The overall managerial coordination of the initiative is done by a council (board) and by a director/chair of the initiative (if established as a legal entity), or otherwise by a supervisory board and a coordinator appointed by a consortium or coordinating institution for the initiative. Depending on the organizational model of the HPC initiative, technical coordination is done by a technical director or appointed technical coordinator, assisted by a technical coordination board, with representatives from all national HPC centres.

Scientific steering committee
 Expert body which carries out the peer review of proposal for access to national
 HPC resources, defines the assessment criteria and procedures, oversees the
 implementation of access granted to research projects, and follows up the results
 and reports of such projects.

• User advisory/representation body

Representative body of the main user communities and member institutes and universities, which is responsible to give recommendations and feedback regarding all aspects of the operation of HPC infrastructure, in particular related to the operational support, user support, application porting, deployment of scientific libraries, as well as to assist HPC coordinators is capturing requirements for the future development of the infrastructure, procurements etc. In collaboration with the scientific steering committee and the coordinator, this body can suggest and work on application porting through newly formed working groups.

• Training and dissemination Training and dissemination activities should be also coordinated, preferably by an appointed coordinator and a team of experts from all member institutes.

## 3. Peer Review/Scientific Assessment

The scientific utility of the HPC resources, even difficult to quantify, can and must nevertheless be carefully estimated. Any decision-making scheme based on costs and benefits should consider the peer review procedure as an important tool that stimulates competition and significantly improves the scientific performance of the HPC infrastructure.

This section is dedicated to the analysis of the role played by peer reviewing in the framework of the scientific assessment that is performed in the HPC ecosystems. After discussing general aspects and various advanced European models, the HP-SEE [3] national case studies are presented and general guidelines are formulated.

At any scale (local, national or European), the judicious planning of HPC infrastructure development requires a preliminary survey of the computing needs of the beneficiary community. When this is a scientific community, the size of investment strongly depends, among other factors, on the estimated scientific output the infrastructure will provide. In this respect, peer reviewing remains the universally accepted method for estimating the quality and value of the scientific production. Therefore, once the HPC infrastructure is built, it is normal to measure the value of the applications it should support by using the same methods. Ranking the applications according to the results of the scientific evaluation by a group of experts is the most common procedure for improving the scientific efficiency of any HPC system.

An inspection of the existing examples shows that whenever the infrastructure investment is done from central financing sources (national or EC), the allocation of computing funds and compute time for scientific purposes is largely based on peer reviewing. The organization and the information flow can differ slightly from case to case, but the main components are always a scientific committee/commission (that performs/supervise the assessment of the candidate applications and ranks them in a panel according to the results of the peer evaluation), one or more allocation committees, and an efficient reporting system.

A representative example is offered by the Committee for IT Infrastructure [51] (KfR), which is funded by the German Research Foundation [52] (DFG). The members of KfR are scientific experts named by the DFG Senate; their task is to elaborate 5-year strategies, recommendations and reports regarding IT development in academia, and to evaluate major IT project proposals for funding. Also, the access to the public HPC centres of the proposed research projects is supervised by local scientific committees that allocate the computing time according to the results of the scientific assessment.

Similar procedures are implemented in other major national HPC infrastructures, e.g. in France and Switzerland (see the case studies below).

At the European level, PRACE [4] and, until recently, DEISA [53], provided models of access to the top-level HPC infrastructure, in which peer reviewing is playing a leading role.

PRACE assessment process [54] involves two separate review stages, performed by experts: 1) technical assessment; 2) scientific assessment. The review process is organized by the peer review Office, which is supervised by PRACE AISBL. The proposals which get positive technical and scientific assessments are ranked by the Prioritisation Panel, which is composed of scientific experts from all science fields.

According to the *Reports on the Peer Review Process* (D2.4.1-2), the peer review is defined as a process that must satisfy the following principles:

- Transparency assessment criteria and peer review procedure are known by applicants before submitting proposals;
- Expert Assessment assessment is performed by expert peer reviewers;

- Confidentiality the proposals and the identities of peer reviewers are confidential;
- Prioritisation by assessing the merit of each proposal against that of others;
- Right to Reply applicants can reply to assessments before the prioritisation;
- Managing Interests all participants declare interests in order to avoid conflicts;
- No Parallel Assessment for any proposal
- Ensure Fairness to the Science Proposed no applicant, institution or country will be favored

Beyond PRACE, the constant search for finding best practices for regulating the access to the HPC infrastructure at the global scale has led to the projects HPC-EUROPA [55] and HPC-WORLD [56], coordinated by CINECA [57]. The main objectives of the projects were the finding of an international peer-reviewing standard and models for the reviewing and selection of the applications which would be suitable for most HPC infrastructures.

Unlike the advanced HPC ecosistems presented above, the experience in this field of the SEE countries seems to be quite limited. The examples below show that in most of the cases there is currently no peer review system at the national level. This can be explained by the relatively low availability of centrally funded HPC infrastructure in these countries, which means the access to the computing resources is mainly locally controlled. Nevertheless, the access methods to the local centres involve in most of the cases the scientific evaluation procedures that respect the general principles presented above.

As the national HPC infrastructure and its funding system will evolve in the SEE states, the necessity of responsible use of the infrastructure and funds will naturally lead to the extensive application of the scientific assessment methods at the national scale. This is expected to happen very soon in countries which have long-term HPC development programmes, such as Bulgaria, Greece, Hungary, Serbia, etc.

In this respect, the current procedure of access to the HP-SEE infrastructure provides a good model and a useful practice. Currently, this procedure is performed with the help of the Application Review Committee (ARC) and involves both the scientific assessment (mainly performed by the leaders of the Virtual Research Communities) and the technical evaluation - which is done by HPC experts.

The procedure for getting access to HPC resources consists of the following steps:

1. The applicant fills in a questionnaire regarding the technical requirements and the scientifically relevant aspects, which is sent to the ARC mailing list.

2. After reviewing the application, ARC makes the appropriate decision, which is communicated to the applicant and, if it is positive, the request is forwarded to appropriate(s) HPC center(s) for further evaluation of the technical compatibility aspects.

3. The technical staff of the centre(s) analyse the request, interacting by e-mail with the applicant for the clarification of technical details, if necessary.

4. After getting a positive answer from a HPC centre, the applicant will have to fill in the appropriate registration form that will be provided by the centre staff.

At a next stage, the procedure will be implemented on a web access portal, but the steps above will remain practically unchanged.

Despite showing an obvious delay compared to other EU countries, the current quasiabsence of national assessment systems in SEE can also be seen as an advantage, as this offers the opportunity to apply the most advanced models and procedures that were found in PRACE and other international projects (e.g. in CINECA's studies above), on the extent in which they are appropriate to each country.

In this process it is very likely that the assessment and the set of guiding principles of the peer review will be close versions, at the national scale, of the PRACE models, but the role played by the peer reviewing in the access policy could slightly change from one country to another. Indeed, as shown in a recent IDC study (*D2 Interim Report: Development of a Supercomputing Strategy in Europe* – 2010), most of the interviewed EU funding agencies and HPC datacenters supported the idea that EU-sponsored centres should be allowed to allocate a part of the compute time according to their own priorities, not through a central peer review process. Moreover, opinions were expressed regarding the frequent rejection from funding of innovative projects by reviewers supporting traditional fields and viewpoints.

Transposed at national level, this would mean that many centrally financed hosting institutions would prefer to allocate a (minor) quota of the compute time according to procedures different from central peer review.

In the following, we will present two case studies from PRACE countries, which are very instrumental, before we proceed with the SEE countries analysis.

#### Switzerland:

Compute time on the national systems is given as a competitive grant through peer review. The peer review process is managed by the Swiss National Supercomputing Centre [5] (CSCS), under the supervision of the National HPC and Networking (HPCN) Steering Committee. The allocation process is run twice a year for all national systems for compute time and associated storage. It consists of the following steps:

- 1. Technical review: Carried out by CSCS. Assessment of feasibility and readiness as well as of justification of resource request size.
- 2. Scientific review: Carried out by at least two international experts (not from Switzerland). CSCS maintains a pool of more than 140 external reviewers. Each project proposal is given to two experts from the scientific field of the proposal. The reviewers assess the scientific merit of the proposal, taking associated grants by the National Science Foundation or the European Research Council (ERC) into account. The also assess whether the chosen computational approach is feasible. The reviewers grade the proposal on a scale of six different values.
- 3. All graded proposals are then ranked together by a panel at a meeting. The panel also proposes the allocated CPU time and storage.

The CSCS director can make changes to the panel's decision (although this almost never happens) and informs the researchers on the allocation decision.

#### France:

GENCI [15] coordinates the global allocation of national HPC resources to French researchers on the 3 national centres. There is a common portal to apply for resources from all 3 national centres (https://www.edari.fr/).

Assessment is performed by 10 Scientific Thematic Committees (CT), organized around the main topics of scientific interest.

The mechanism is that applications are examined by the CTs, ranked through a scientific evaluation, twice a year, for allocations in January and June. The CTs each have a President and a number of experts.

An Evaluation Committee builds an allocation plan proposal based on the output of the CTs. This Committee is composed of the President of CSCI (Comité Stratégique du Calcul Intensif, a national advisory board for HPC) and the Presidents of the CTs; the computing centres directors and a representative from each of GENCI's associates are also invited but are not voting members.

An Allocation Committee then makes the final allocation decision, based on the input from the Evaluation Committee.

In the following, we will present case studies from SEE countries. The responses to a survey regarding application assessment and peer reviewing in the HP-SEE partner countries led to the following conclusions:

- In general, there is no central peer reviewing of the HPC applications (although the assessment of the scientific projects is performed through peer reviewing in most cases).

- The partners that provide HPC resources have local access procedures for the computing centres, which involve the scientific assessment performed by a group of experts / committee - most often associated to specific projects. The peer reviewing of the applications is accomplished in the more experienced centres at NIIFI [29] and in Bulgaria (in the framework of the supporting projects).

- The beneficiaries of the HP-SEE HPC resources don't need special scientific assessment for running their small-scale applications in their home institutes.

Several cases of HP-SEE resource providers, respectively consumers, are presented below.

#### Bulgaria:

For each of the systems the peer review process is defined during the provisioning process according to the project or other source of funding. For the HPC clusters it is usually a review committee whose members are defined in the project proposal. For the biggest HPC resource in Bulgaria so far it is again a scientific committee. In most cases such committees include not also leading scientists, but also people with technical background. The access is granted based on access forms. After the allocated resource is used a report is requested and the same committee performs assessment. Usually there is a defined period (6 months) to use the allocated usage quota. Such procedures are not followed in smaller HPC clusters, which are obtained for the needs of a particular research group and are not open for outside utilization.

#### Romania:

Although there is no peer review at the national scale, the access policy to the mediumsize HPC systems is governed by local assessment rules.

The procurement and instalation of the HPSC clusters and support systems was funded from R&D projects carried out by the hosting institutions and/or EC structural funds for supporting their R&D infrastructure, while operation and maintenance are funded from various non-regular sources of the hosting institutions. Therefore the decision factors regarding the usage policy are members of the local R&D groups involved in procurement (that perform the scientific assessment of the applications), the local HPC experts (for technical evaluation), and the management of the hosting institutions (whose consent is required for supporting the cost of utilities, such as electric power, etc.).

At the submission of access request, technical requirements and scientific details are provided by the applicants. These are analysed in technical and scientific reviews, respectively, and the access is granted if both reviews are positive.

The resources being mainly targeted towards specific scientific activities developed at the host institution, their use by external researchers not involved in collaborations with the host institution is seldom. Therefore, most often the scientific assessment of the applications does not require external experts.

The reporting of scientific results obtained through the use of the application is part of the project reports. The resouce usage per project is monitored, and technical reports are issued by the IT management at regular time intervals and at the end of the projects.

A global peer-review access procedure will be necessary when the supercomputing resources will become available together with a national funding project to suport their operations. In this respect, the HP-SEE and PRACE projects, together with some more advanced national HPC ecosystems (like in Germany) provide good models.

#### Hungary:

The scientific users can sign up for the HPC facilities operated by NIIFI by using the HPC project and HPC user registration forms. These are web-based forms that can be used

both for printing applications in PDF and also for directly transfer user registration data from the registration databases to the user authentication and authorization databases, thus facilitating both written and electronic user registration processes. The application process for HPC resources is as follows:

- First the users submit a project application describing the purpose and objectives of accessing HPC resources.
- Then the user submits individual user registration forms corresponding to the project. Both project and user registration forms should arrive in courier, though they also arrive in electronic mails.
- The application forms are then evaluated by the HPC team and is approved by the appointed HPC responsible person (or his deputy).
- User and group accounts are then created and the application forms are filed.
- The users are contacted via telephone.
- The users are informed about the operation messages and HPC news on a mailing list dedicated for this purpose.

The applications are peer reviewed every year and a report is requested for each project summarizing the annual progress being done on the HPC resources.

#### Serbia:

Serbia does not have a peer review system at the national level. Access to each HPC cluster is granted to national research projects based on the local access form. The management team of the cluster is in charge of the allocation of resources. The access is also granted to users from international projects, where usually the allocation is done by the corresponding scientific committee of the project. In the future, a unified national peer review system is planed for access to the resources of the national HPC center. It will be based on a two-step procedure:

- Technical assessment, done by the application support and HPC administration teams, focusing on the assessment of the code implementation, compiling/installation, benchmarking and scalability.
- Scientific assessment, done by the peer review scientific committee, focusing on the scientific and societal impact of the proposed research.

Peer review scientific committee will consist of leading experts from various fields of science.

#### Albania:

There is no official system/practice for the scientific assessment. A peer review phenomenon exists only as paper review in few scientific journals (Scientific Bulletins published by some faculty or university, and the Albanian Journal of Natural and Technical Sciences of Academy of Sciences), and in a lower degree in some local conference. Funding resources are managed by universities and programme committees of bodies funding the research (ministries and Agency for Research Technology and Innovation). In the latter case projects are evaluated by the technical board.

#### Macedonia, FYR:

Macedonia does not have a peer review system at the national level. This is one of the tasks that should be performed by the National HPC Initiative. So far, access to resources (non-HPC) is managed by the NGI, through supported VOs. It is hoped to produce most of this documents and procedures within this project, and use them to govern the upcoming HPC resource.

#### Montenegro:

Montenegro does not have a centralized peer review system at national level. There are individual scientific assessments for all national projects, scientific conferences (IT & INFOFEST), magazines and scientific journals. Assessments are performed by University professors from related disciplines, members of MREN [58] or by external reviewers. Scientific and technical assessments related HPC projects are performed by MREN (Montenegro Research & Education Network).

#### Georgia:

There is no real peer review mechanism in the country, scientific importance and technical capabilities are analyzed by GRENA [27] with the support of universities staff. Until now we have only two research groups that expressed their needs in HPC. For both of them review is done at first stage locally and then in the framework of HP-SEE project. Scientific assessment is done by GRENA and universities staff. For this a small description of the application is requested from the research group.

#### Moldova:

There is no official regulation of applications peer-review in Moldova. All analysis and selection procedure is effectuated at present by MD-GRID NGI members that are representing leading universities and research institutes of ASM. Now MD-GRID NGI covers all deals with national research communities that express their necessity to gain access to Grid and HPC infrastructures.

Every team that proposes their application for scientific assessment first of all is asked to fill application questionnaire, which template is base on HP-SEE applications survey. Also they are requested to provide description of there project, sources of funding, other information about thematic area the team involved, description of the expected impact of the research results from the project that originated requirements for HPC resources utilization.

# 3.1. Guidelines for the peer review at the national level

While there is not much experience in the scientific peer review for HPC applications in the countries of the SEE region, almost each country has in place a peer review scheme for the assessment of national research projects, and thus the necessary experience in assessing the scientific quality of the proposed projects for HPC access. Based on such experiences as well as the PRACE approach, a number of guidelines can be identified:

- Scientific steering committee should be appointed as a part of the governance model of a national HPC initiative. It should consist of HPC experts with the background from various scientific fields, representing fairly all major user communities in the country. The committee opens calls for access to national HPC resources, defines procedures, creates the appropriate questionnaires and forms for the calls, and makes decisions on the priorities/quotas assigned to each scientific field.
- The work of the scientific steering committee and/or assessment of proposals is usually organized through a number of expert panels, representing major scientific areas and priority fields for the country. Each panel can appoint additional experts, which are involved in the assessment of proposals for HPC access at the national level.
- Prior to the scientific peer review of research proposal, each project has to successfully pass a technical review, done by the operational personnel at the HPC centre where resources are requested. The technical review should establish if the proposal is associated with a working application code, which can be

compiled and correctly executed at the assigned HPC resources, as well as that its performance reasonably scales at the requested level of computing resources, and does not present significant bottlenecks, including I/O ones.

- Scientific steering committee and each panel should carefully follow up the results of the projects that are granted access to national HPC resources, and take necessary measures if the applied approach and the quality of the obtained results is not deemed satisfactory. The panels should report back to the Scientific steering committee, which will discuss regularly the results of each call for proposals and refine the procedures and access criteria based on the feedback from panels as well as from the user advisory board.
- Proposals that do not pass technical review should be advised to apply for preparatory access at one of national HPC centres. If the number of such requests is seen to be high, then Scientific steering committee may organize preparatory access calls, and award such support (usually done by the user support teams at national HPC resources) only to selected proposals, based on the available support personnel. Otherwise, if the overall number of such requests is not high, research teams may be advised to contact directly user support teams at HPC centres.
- Based on the results of the peer review, Scientific steering committee can also provide feedback regarding technical and operational requirements to the technical director/manager and/or technical coordination board.

# 4. HPC Centre Coordination

There is a variety of HPC centre coordination models in the region and in Europe. The nature of HPC favors concentration of resources, but more distributed approaches are also possible, especially for smaller HPC resources that could be closer to the prospective users. In this chapter we will describe various organizational aspect of HPC centers, including technical support, training, dissemination, European coordination and interoperability, and user support. The organizational structure of various HPC centers should be designed to reflect all these important functions, taking also into account numerous funding and policy constraints.

The following two examples of such types of organization illustrate the complexities.

#### Switzerland:

In Switzerland, the main HPC center is CSCS [5], which is organized in the following units:

- Scientific Computing Research: research on parallel programming methods, algorithms, mathematical methods, system architectures.
- Technology Integration: Collaboration with vendors, hardware and software testing, prototyping, hardening of technical solutions.
- National Supercomputing Service: operation of national supercomputers and associated systems (storage, pre- and postprocessing), user support, application support.
- HPC Co-Location Services: Hosting mandates for end.to.-end HPC solutions, e.g. the Swiss Weather Service.
- Business Services: Internal administrative support, building infrastructure, networking & Cybersecurity, internal IT support.

#### **Bulgaria:**

HPC initiative in Bulgaria is formed from structural parts of larger legal entities. The biggest supercomputer resource in Bulgaria is the supercomputer BlueGene/P located at the Executive Agency for Electronic Communication Networks and Information Systems. For some smaller HPC resources (clusters) the overall administrative control is concentrated at one institution while the technical/scientific control is distributed among a consortium of partners in a large scientific project.

## 4.1. Technical support

The countries with HPC installation deploy their own solutions for technical support, mostly based on helpdesk with a layered organization of the support units. The experience of some countries with HPC installations is outlined below:

#### Switzerland:

Technical support is in general second-level support (or third-level). This means that it typically occurs when a ticket has been escalated from first-level support (helpdesk) because it requires deeper investigation and does not have an obvious solution. Second-level support directly communicates with the user once it has received a request.

#### Bulgaria:

In the case of Bulgaria each HPC resource has their own ticketing system or email lists for support to the users. Due to established personal relationship during workshops and trainings phone support is also effectively available in some cases. In many cases support is required in the application porting phase and the problems can require deeper understanding of the software being used, even being able to correct bugs in publicly available software packages.

#### Hungary:

Technical support team for HPC facilities can be accessed in two ways:

- The team calls NIIFI [29] call center who in turn submits a ticket into the central issue tracking system. Here the operator on duty assigns the ticket to whoever is available from the HPC user support team. He/she then contacts the user in 1 hour and begins processing the issue.
- The users can directly contact the HPC team via dedicated support mailing lists. Such SLA, like the 1-hour callback is not guaranteed in this case.

The support team offers basic user support including the following activities: compiling and job execution issues, core profiling and performance analysis, code porting and using the different available tools. The support does not cover high-level numeric modeling and parallelization.

### 4.1.1. System management

In HPC installations system monitoring and pro-active management are essential for achieving good overall effectiveness. Good working relations with the vendors of the hardware are important for achieving this. It is natural to use the tools and services that the vendors provide as part of their offering, if this is economically feasible. These considerations entail a wide variety of software deployed and organization of the system management. Example of such arrangements is shown later in this section.

There is variety of free or open source tools that can be a good alternative for system administrators. Many tools manage both installation and configuration, but there are some tools that do only one of these tasks.

For the installation part we note the following tools, some of which are also used for reconfiguration and monitoring:

- **Oscar:** OSCAR [59] consists of a fully integrated and easy to install software bundle designed for high performance cluster computing (HPC). Everything needed to install, build, maintain, and use a modest sized Linux cluster is included in the suite, making it unnecessary to download or even install any individual software packages. OSCAR is the first project by the Open Cluster Group. For more information on the group and its projects, visit its website.
- <u>Rocks</u>: Rocks [60] is an open-source Linux cluster distribution that enables end users to easily build computational clusters, grid endpoints and visualization tileddisplay walls. Many so-called "rolls" exist related to popular software packages or libraries, speeding-up deployment.
- **Perceus:** Perceus [61] is an installation and configuration tool that is mainly geared towards diskless node installations, where the easiest reconfiguration method is via a reboot. It includes its own Linux distribution but also can work with CentOS or other RedHat derivatives.
- **<u>Xcat:</u>** xCAT [62] (Extreme Cluster Administration Toolkit) is open-source distributed computing management software used for the deployment and administration of clusters. It can:
  - create and manage diskless clusters.
  - install and manage many Linux cluster machines in parallel.

- set up a high-performance computing software stack, including software for batch job submission, parallel libraries, and other software that is useful on a cluster.
- cloning and imaging Linux and Windows machines xCAT is the default systems management tool of the IBM Intelligent Cluster solution.

For the configuration we note the following tools that are in heavy use today:

- <u>Cfengine:</u> Cfengine [63] is one of the most popular data center automation solutions available today with an estimated 5.000 companies running Cfengine on more than 1 million machines. It can be used for all life-cycle phases from Build, to Deploy, to Manage, to Audit, with continuous maintenance and repair, on or offline. It has been shown to scale to tens of thousands of machines and is very versatile and dependable solution.
- **Pdsh:** Pdsh [64] is a an efficient, multithreaded remote shell client which executes commands on multiple remote hosts in parallel. Pdsh implements dynamically loadable modules for extended functionality such as new remote shell services and remote host selection.

The monitoring of the system can be accomplished by integrating relevant sensors in Nagios [65], Ganglia [66] or any other tools.

Monitoring of system utilization should be based on collecting and processing accounting data for each job. More advanced setups would correlate accounting data with monitoring data, e.g. from ganglia in order to obtain better view of patterns of resource utilization of the applications.

We now present three case studies from the SEE region.

#### Bulgaria:

For each HPC resource there is a team of administrators that are supporting its operations. The team is using state-of-the-art operational tools to monitor the functional status of the system, system security and environment (electrical power supply, temperature, cooling, etc.) and to perform installations and other administrative work. For the IBM Blue Gene/P supercomputer there is an additional arrangement, where an IBM support personnel is monitoring the system remotely and reacting to problems when required.

#### Romania:

As a rule, the management of the HPSC clusters is performed by the local administration teams of the hosting institutions. Occasionally, when a host cannot afford to support a professional team, the management is performed remotely by some institution with more specialized human resources like, for instance, technical universities (e.g. UPB [48]). Cases of HPSC system management by companies are not known.

The management teams ensure the operational and monitoring services and, in many cases, monitor the support systems too (i.e. cooling & power supply).

The system management of the recently purchased BlueGene/P supercomputer hosted at UVT [49] is not fully decided yet, but is expected to involve both the IT personnel at UVT and IBM support.

#### Hungary:

All HPC sites are operated by NIIFI [29] with the help of local operators. A dedicated HPC team has been set up for this purpose. Open source monitoring tools are used to inspect the most descriptive resource parameters as well as the environment such as the air conditioner, fire extinguisher, the room temperatures, the power supplies, etc. Several parameters are measures, accumulated, and aggregated by free tools. As for all the sites a 5-years of vendor support and warrantee are available, the administrator team

consults the vendor support team in case of any significant issues, such as the security updates, version changes, or major failures.

### 4.1.2. Technical application assessment

The process of *technical application assessment* provides a basis for application acceptance and further management of allocated resources. It is complementary to the scientific application assessment with a peer review process. Partners providing HPC resources have their procedures for technical application assessment, which allows readjustment of allocated resources and also re-configuration of the system when required, based on the outcome.

The process of technical application assessment is continuous in most cases because most applications evolve from technical and scientific view point. The initial technical assessment should provide basis for directing the proposal to an existing HPC center or rejecting the proposal proving the reason for rejection and suggestions for improvement. Several aspects of the application should be considered within this initial phase.

First of all the list of required software should be considered. It is especially important to determine if there are any applicable licensing restrictions for software that is not open sourced. The technical review panel could suggest alternative software or libraries if there is a problem.

The storage requirements of the application should be investigated and matched with the available resources. The type of utilization of storage – permanent versus scratch space should be well understood. It is important at this point to make sure that the regular production use of the application will not impact the every-day work of other users – information about any patterns of storage use that can lead to high load on the regular /home directories should be noted. In most HPC centers there is a clear distinction between high performance storage for parallel computations and permanent storage where input and output data is stored and users should have good understanding of how to properly utilize storage space.

The most difficult part of the technical assessment is usually the scalability and performance analysis of the application. It is advisable to maintain a list of experts in the use of some popular software packages so that their opinion can be obtained. Even with the help of experts it can be difficult for the users to estimate precisely the amount of computational time and the number of processors that they require at a point where they have not yet access to the system. That is why it is advisable for the users to follow a path from local cluster to bigger high-performance cluster and then supercomputer so that they can use the experience gained at the previous step in moving to the next step. When the main percentage of prospective CPU utilization could attributed to a wellknown software package or library it is expected that publicly available benchmark can serve as a basis for this assessment. If the application is based on in-house developments, then some benchmark data should be provided to the panel in order to assess the suitability of the application for the available systems. It should be made clear to the applicants that they will not be allowed to run applications that do not achieve certain acceptable scalability. If the applicants provide justification for not meeting such thresholds, then the case should be forwarded to the scientific review committee to decide if the other merits of the application justify the underutilization of the parallel capabilities of the system.

The acceptance or rejection of the application should also depend on the suitability of the application for alternative ways of computing that are usually cheaper, because usually the HPC resources are the most difficult to obtain vs. Grid or other possibilities.

After the positive conclusion of the technical assessment and provided the application starts production utilization the phase of continuous technical monitoring of the application is started. In this phase it is important to note immediately and correct any negative impact of the application on other users or the system as a whole or any deviation from the stated parameters. In order to be able to detect such deviations, for example from the stated scalability parameters it is important to have appropriate monitoring and accounting data. This data will serve as a basis of discussion with users and if necessary with the scientific committee if necessary.

It is obvious that such review should be done at regular basis of every few months and each application has to be fully re-assessed after 6 months to 1 year to take into account any changes and progress made.

By policy the scientists should provide reports at such periods (we suggest 6 months) detailing also the scientific progress being made.

We now present three case studies from the SEE region.

#### **Bulgaria:**

When users apply for access to the HPC resources, they also provide detailed explanations about required resources and any unusual characteristics of their applications that may impact system performance. The administrators take these into account and perform changes in the system configuration if these are required. Example of such requests is: jobs that require the use of all of the Blue Gene/P processors – such jobs require administrator action; high amount of storage in the range of Terabytes for some applications at the HPC cluster in IICT-BAS [33]. Some unusual patterns of resource utilization are noticed via monitoring tools when the production utilization starts and appropriate actions are taken if necessary, for example providing assistance to users about better ways to submit their jobs. For the HPC cluster at IICT-BAS the users are required to submit a technical report upon exhausting their usage quota, which allows for better evaluation and improvement of resource utilization.

#### Romania:

The technical assessment of the applications is the first step towards getting access to the HPSC clusters. This is ensured by the local management personnel that gets a summary description of the application requirements (in terms of number of cores, RAM/core, storage, bandwidth/latency of interconnects, software environment, resource usability, etc.), attached to the request of use of the cluster.

The publishing of cluster guides, such as those realized by the managers of the NCIT/UPB [67] centre (<u>http://cluster.grid.pub.ro/images/clusterguide-v3.0.pdf</u>), were proven to be very helpful in providing information on cluster access, enhancing technical support for the applicants and shortening the technical assessment period.

In many cases, after a first evaluation the managers need more technical details from applicants in order to make a decision, and e-mail dialogue with them is initiated. The decision also depends of the current usage of the cluster resources by other applications, and sometimes the queuing of the requests might be necessary. The full granting of access for production can eventually be issued only after a test period, in which the usage of resources is evaluated and suggestions regarding application optimization can be provided.

#### Hungary:

Based on initial user surveys NIIFI [29] has collected a list of popular scientific applications that the user communities are willing to use. Such applications are installed centrally on all sites optimized to the particular platforms. Besides these there are two commercial applications licensed to only two sites: the latest version of Gaussian [68] that is used by a broad range of chemistry-oriented user communities, and Matlab [69] Distributed Computing Environment that needs client side licenses to be able to use.

Users are allowed to install any applications into their user space as long as they adhere to NIIF's HPC AUP. In case of licensed applications users must provide valid licenses.

Users may also request central application installations by contacting the technical team. Such requests are followed by a technical and system dependency evaluation and if there are no technical impediments, then the software is compiled, optimized, packaged and installed.

# 4.2. Training

Training activities related to HPC, distributed and parallel programming in the SEE region are usually organized and planned within the framework of various regional or EU-wide projects, since national HPC initiatives are still being formed, and are mainly focused on infrastructure and technical aspects of the establishment of HPC centers. For this reason, the support for training from such HPC-related projects, especially HP-SEE and PRACE are seen as essential for the development and activation of user communities in the region.

The intense collaboration by the SEE partners in organization of training events, including the national-level ones for which speakers and lecturers are regularly invited from around the region, presents one of the important results of the series of projects on e-Infrastructures in the South Eastern Europe. The human network built in the past 6-7 years now provides assistance to all interested parties and leads the way towards inclusion of HPC topics into curricula of universities in the region. Several use-cases presented below illustrate training activities in SEE countries.

#### **Bulgaria:**

The training of users is performed in several ways. Introductory training events are performed at relatively regular intervals, approximately 6 months. Usually they are intended for general audience of scientists with appropriate background (knowledge of programming languages C/C++ and/or FORTRAN, knowledge of Linux or Unix). Some additional training is performed at a request of specific institutions or projects and is focused on their specific needs. Topics like HPC computing or parallel algorithms are thought at universities or at the Bulgarian Academy of Sciences at the level of master or Ph.D. students. New master programs that include similar topics are under active development. Since many national or European projects require the use of HPC resources, the practice is that they include such trainings or training courses in their DoW and then they ask for experts that can perform these trainings for them.

#### Romania:

The regular training of the application developers is traditionally performed by academic institutions, like UPB [48] and UVT [49], and is seen as an essential mean for improving the access to the HPC capacities, the quality of the code, and the optimization of the resource usage. These universities have quite recently adapted the curriculum to include trainings in multi-core programming, and make available hibrid clusters providing various types of hardware, that are ideal for code testing and training (e.g. NCIT [67] cluster). Also, trainings in IBM, Intel, Microsoft or Cisco technologies which are relevant for the HPC applications have been provided. A major regular training event is the *NCIT Summer School* (http://cluster.grid.pub.ro/index.php/workshops-and-training-events) - which takes place annually in the training laboratories of NCIT, and is now in its 8<sup>th</sup> edition. Recently, the training of the potential users of the HPC resources was also initiated by the advanced programmers from the R&D institutes such as ISS, which gave introductory courses in CUDA programming and general GPGPU technology.

#### Hungary:

There are no dedicated HPC trainings in Hungary. There are grid tutorials, grid trainings, summer schools and also written user documentations available for the community.

#### Serbia:

HPC training events are mainly related to the international collaboration, in particular HP-SEE and PRACE projects, whose NA3 activities are organizing a number of trainings at the national, regional and European level. IPB and other HPC stakeholders are involved in organization of such events, and significant number of young researchers participate in HPC schools. For more than 5 years, IPB is also involved in the organization of HPC and Grid schools at the International Centre for Theoretical Physics "Abdus Salam" (ICTP) in Trieste, Italy. Such schools have strong participation from the region, and IPB provides teaching and tutoring staff, and also serves as co-organizer. In April 2011, ICTP Advanced school on HPC and Grid computing has received support from ICTP, PRACE and HP-SEE, and has involved more than 60 participants from all over the world. We also plan to organize HPC software design school in February 2012, which was already approved for funding by ICTP.

#### Albania:

Training on parallel programming is organized in few cases in framework of past SEE-GRID initiative, and actually in framework of HP-SEE.

# 4.3. Dissemination

As is the case with training activities, dissemination of information on HPC developments in the region are also mostly done through the international projects, as well as through the participation and presentations at national and regional scientific conferences and workshops. Usually, intense dissemination is also included during the training events, where information on HPC infrastructure on the national, regional and pan-European level are presented to interested participants. Significant effort is also invested by all partners to reach general public, and in particular young students, in order to raise awareness and interest for careers in HPC and technology.

Another important aspect of dissemination is communication of important information to policy makers, and their involvement in further dissemination through participation in public events, articles in the press, TV and radio shows, internet presentations etc. In this regard, HP-SEE and PRACE projects offer valuable support and visibility, especially by organizing dedicated dissemination events for policy makers at the regional and EU level. We illustrate dissemination activities in the SEE region through several use cases below.

#### Bulgaria:

Apart from using general forms of dissemination like participation in scientific conferences and workshops, scientific publications and production of brochures and posters, there is a tradition of holding once a year an annual meeting of the consortium defined in the National Roadmap for Scientific Infrastructure with accent on participation of young scientists in HPC activities. There have been many TV and radio appearances and the Bulgarian newspapers and media has broad coverage of the important events in HPC like the inauguration of the Blue Gene/P, the acceptance of the National Roadmap for Scientific Infrastructure and so on. The regional supercomputing conference in December 2010, organized by: the Ministry of Transport, Information Technology and Communications, the National Centre for Supercomputing Applications, the Center of Excellence "Supercomputing Applications" [32], IBM, and Rila Solutions attracted more than 300 participants and was a resounding success. Training and other technical materials are being produced and made available.

#### Romania:

The R&D results related to HPC and HPC infrastructure usage are disseminated through papers in scientific publications. An image of the international visibility of Romanian research in this field can be obtained through the search in an international database of publications, such as SCOPUS [70]. For instance, a search over the string "parallel computing" OR "parallel algorithm" OR "parallel implementation" OR "parallel program" OR "parallel architecture" reveals 101 institutional contributions to papers published between 2008-2010.

Dissemination is also performed via workshops, conferences and symposia at national or international scale. Recent examples are the *Workshop on High Performance Computing with application in environment* (http://synasc11.info.uvt.ro/workshops/hpce-2011), organized by UVT, and the *High Performance Computing* workshop organized by UPB (http://cluster.grid.pub.ro/index.php/workshops-and-training-events/hpsc/hpsc2010).

Under current investigation is the organization of a free annual workshop for the national developers community, in which the major HPC centres will present their new development and operating environments and will organize hands-on sessions of programming, profiling and tuning of the applications proposed by the potential beneficiaries.

#### Hungary:

The main HPC achievements are disseminated in both oral and written forms. On the most relevant national events there is always at least one HPC oriented presentation, and we publish the use of resources and the most interesting application examples in the 3-times-a-year released NIIF News.

#### Serbia:

IPB organizes various dissemination activities related to HPC through regular channels: news releases on the occasion of important events (training, visits, hardware upgrades, new projects, application milestones etc.), public presentations at conferences, workshops and public events, participation in press interview, TV and radio shows, broad dissemination of all activities through the web site. In addition to this, dissemination is also done in conjunction with other activities. One of the examples is this year's celebration of 50 years from the establishment of IPB. A month-long exhibition was organized in the Gallery of Science and technology of the Serbian Academy of Sciences, with more than 10 presentations and public lectures, including the participation in the "Night of Museums" activity in Belgrade. This has brought large audiences to the exhibition, which prominently featured activities of IPB's Scientific Computing Laboratory and its involvement in HPC an HP-SEE and PRACE projects. Numerous articles in the press, TV and radio reports also followed up the celebration.

A significant step further for dissemination activities in Serbia has been put forward by the new cycle of national research project for the period 2011-2015. Each project (including basic research, technology and integrated projects) is now obliged to use 5% of its national funding for dissemination of main results of the project. This practice will be also followed by the national HPC programme, once the Blue Danube center is established.

#### Albania:

Dissemination of information about HPC possibilities are included in training events, and also mentioned in different presentations on participation of the country in regional initiatives and EC Framework Programmes.

#### Georgia:

GRENA as a co-organizer of the First ATLAS/South Caucasus Software/Computing Workshop & Tutorial took part in preparation and conduction of the event. Workshop was held in Tbilisi, Georgia during October 25 – 29, 2010 (<u>http://dmu-atlas/web.cern.ch/dmu-atlas/2010/</u>). R. Kvatadze made presentation at the workshop.

# 4.4. European coordination and interoperability

The variety and diversity of the requirements of the South Eastern Europe HPC users communities, as it has been observed both from the HP-SEE applications questionnaire and documented in D4.1 [71] as well as from the individual SEE countries experience,

necessitates the deployment and use of a diverse set of HPC architectures. Furthermore the increasing demand for computational resources, at different time periods, increases the challenge of the national HPC centers to offer adequate resources to cover the user communities' needs. To overcome the above problems there is a need and had become a common practice in Europe as well as worldwide for different HPC centers to share exchange resources as well as expertise.

On the European level the Distributed European Infrastructure for Supercomputing Applications (DEISA) [53] operates a distributed HPC infrastructure consisting of leading European Tier-1 centers aiming at delivering a turnkey operational solution for the European HPC ecosystem. On the top level of supercomputing in Europe, PRACE [4], the Partnership for Advanced Computing, has been created as a not for profit association in May 2010 as a permanent pan-European High Performance Computing service providing world-class systems for world-class science. The PRACE infrastructure implements the Tier-0 HPC research infrastructure for Europe. In 2011 DEISA will be integrated to PRACE and therefore PRACE will operate both the Tier-0 and Tier-1 infrastructures in Europe, thus integrating the European HPC ecosystem covering all the needs for HPC. In the US Teragrid [72] is an open scientific discovery infrastructure combining leadership class resources at eleven partner sites to create an integrated, persistent computational resource. It is therefore similar in concept and objectives to DEISA.

In the region of South Eastern Europe the HP-SEE project aims at providing HPC resources to the scientific communities of the SEE region capitalizing on the existing and planned HPC infrastructure in the region and integrating those resources making it easier for the end users to port and deploy their applications into the infrastructure.

The above initiatives aim to provide a coordinated, integrated and interoperable infrastructure where resource sharing, among the participating countries, is taking place fostering scientific usage of HPC resources.

To accommodate the efficient resource sharing and usage, several governance, organizational, operational and user support models have to be implemented and coordinated on the international level and individual countries are required to implement such mechanisms. On the European level the coordination is mainly achieved through PRACE-RI and its supporting EC co-funded projects (PRACE Preparatory, and PRACE 1<sup>st</sup> and 2<sup>nd</sup> implementation projects). PRACE-RI through its Statutes and the Agreement for the initial period sets the governance rules for countries participating to the PRACE AISBL, while the Implementation Projects coordinate the infrastructure operations, resource sharing, training and dissemination, user and applications support, industrial cooperation and applications support activities on the European level setting the common activities required for supporting the operation and efficient access to European level researchers.

In this context the countries of the region, via their participation to the HP-SEE project and the participation of Greece, Bulgaria, Serbia and Turkey in PRACE, are already in the process of developing a strategy for European collaboration and interoperability. More specifically:

- This deliverable proposes national level organizational models for the creation national HPC initiatives taking into account the best practices in the European context and of PRACE in particular aiming at bringing the countries of the region on par with the rest of the European countries.
- Furthermore the HP-SEE project is already in the process of creating an integrated interoperable distributed infrastructure providing also the countries of the region with expertise in operating such an infrastructure. On this level a set of integrated services is being created where all countries participate in their implementation. More specifically HP-SEE is taking care of services such as: a common Helpdesk and user support procedures, regional training services, resource allocation policies, HPC access services, AAI service, software installation, data transfer services, network connectivity, monitoring of resources,

application porting, optimization, scalability and support, security services and technology watch. The details and requirements of such services have been provided in deliverables [73], [74] and [71] as well as in the projects wiki pages [75].

• In the near future the partners of the project will collaborate towards the establishment of a regional Memorandum of Understanding, a resource sharing model for the region, a peer review process and a study of the benefits and methodology for joining the pan European research infrastructure aiming at providing the scientific communities of the region with the expertise and the opportunities to utilize high level computing resources for their research.

HP-SEE through the activities of porting, optimization and support of applications to be deployed in the regional infrastructure enables regional scientists to use advanced computing infrastructures and facilitates the technical readiness of the applications for possible access to the PRACE infrastructure.

# 4.5. User support

In this section we plan to give generic guidelines as well as best practices on establishing professional user support around HPC services. This kind of service is a significant added value since HPC users often get their very first impression on the HPC center through the user support services, and the good experience and the feeling of confidentiality might further influence their use of resources and they can better exploit the systems' capabilities.

When setting up a support team one needs to consider the scope first. It is important to clarify what kind of expertise is available within the future support team. The users' most important expectation is the competence here, which means that the support team must either offer reasonable solutions to the particular issues, or must declare that there is not enough knowledge to properly address it and let the user go and ask help from any other sources (i.e. application or vendor support).

The scope of support might vary within a broad range. One of the most elementary offers in this field is the HPC resource usage support in which the use of different system components, such as schedulers, grid middleware, compilers, and high performance libraries are covered. This basic support is often extended by application execution analysis services, including debugging help, and code optimization for particular platforms. Moving one step further the support team might also cover some higher-level support, like providing consultation service on parallel programming, numerical modeling and algorithms. The highest scope contains applications and also science-specific support, for example including a bioinformatics expert in a service offered for bioinformatics oriented user communities. It is easy to see that the scope is directly associated to the targeted user audience, so defining it is often preceded by a thorough user analysis performed either via direct face-to-face inspections or through questionnaires. As the most common user needs in this context are related to either the operations or to the user applications we give further guidelines and case studies on these in dedicated subsections.

As soon as the scope is determined the support activities are classified into different groups depending on their severity. For example generic user job execution issues might represent a low severity group as it requires minimal platform specific knowledge and a user-oriented attitude, while making an application ten times faster on the platform might be a more concerned issue requiring deep and extensive technical knowledge about the hardware and coding. This step is necessary for the future assignments of issues to personnel and also for rational use of human HPC expertise.

Moving one step further a helpdesk or a customer relationship manager tool needs to be established. This mixture of organizational model and tools typically contain

- a mail gateway enabled issue-tracking system for registering issues and their follow-ups,
- an issue synthesizing tool for generalizing and sharing knowledge learned from the already solved issues,
- a portal that helps the users efficiently finding solutions to their potential issues,
- archived mailing lists for storing the written communication,
- a phone operator that can receive and escalate calls within a specified time frame, most often on 24/7 basis.

Establishing legal and organizational backgrounds are as important as the technical infrastructure here. The key organizational aspect is how the personnel are organized into a coherent and fully functional team, what the responsibilities are within, and how the group of people is structured (leaderships, deputies, rights delegations). The team needs to be legally justified within the organization, by having properly specified work descriptions and appropriate operational financial resources assigned to.

Defining workflows to the most common issue types is also useful and helps congealing the further processing. A default workflow might also be established for tackling any unexpected problems. Workflows corresponding to alarms taken from monitoring and measuring systems are particularly important, as they often require immediate actions even beyond labor-time (part replacements, reconfiguration, etc.).

Last, but not least an internal policy is also required to help to lay down basic disciplines

- on how to keep the relationship with the users,
- on what kind of communication is recommended, and
- on what kind of information can and cannot be exposed.

In multilingual environment the communication language and the language use policy are also determined (e.g. try to avoid using particular expressions, forbidden to use vulgar, etc.).

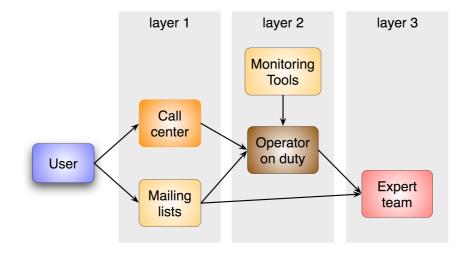
If all the ingredients are ready, the technical infrastructure should be set up, pertaining to the corresponding disciplines and policies.

From now on we show case studies on how operational support and application support is performed in different organizations being involved or being close to the project.

### 4.5.1. Operational support

As soon as the operations support team is up it performs two major activities: operations support and applications support. While the former mostly concentrates on keeping the HPC infrastructure and the corresponding services in operation, the latter focuses on aiding the users in exploiting the hardware facilities the most efficient way. The two are deemed to need different skills, so in most of the contemporary HPC centers they are also treated by separate teams or by at least separate workflows.

The most typical operations support cover continuous service monitoring, and periodic physical hardware health check that often means inspecting the hardware looking for suspicious signs, like red LEDs, and flashing information panels. In Figure 4.1 the most typical operations support workflow is illustrated.



### Figure 1: Operations support workflow and escalation.

As it is shown, the operations support is often subdivided into support layers. Each layer represents a different service level, severity class, and also technical expertise. The issues often enter at the lowest layer (layer1), and if they are not solved there, they are escalated to higher levels. The chart shows that there are two major sources of issues: on the one hand users and operators can notice any disorder by physical inspection, on the other hand, the automated monitoring and measuring tools can also trigger alarms or warnings. The human-originated announcements are submitted either at a service call center, or in email. The call center often transforms the announcement into a ticket. Both the mailing lists and the ticketing system are frequently and periodically checked by a team of operators. In addition, the operator must also inspect monitoring and measuring tools (Nagios [65], Munin, or any vendor-specific tools) for not only the HPC resource itself, but also for the environment, i.e. cooling, power supply systems, room temperature, cameras. The operators attempt to solve the issue first based on their initial experience and the available internal documentations. If they fail, they forward the issue to the expert team that might involve senior HPC operators or product-specific vendor experts. Involving vendor support is considered to be the final step in the escalation chain.

In the rest of the section we provide use cases on how operations support is organized at different HPC sites that the project has insight.

#### **Bulgaria**:

Operational problems are usually detected by monitoring tools like Nagios and when a respective alarm is received it is acted upon. Sometimes operational problems are reported by users. This usually indicates that a specific condition is affecting this particular user and requires tracing of the respective job and detailed view of the conditions of execution. The usual response time in both cases is within the same working day, but the resolution time can be larger because some problems are result of hardware failures that require communication and reaction from the vendor. Other problems are related to outside conditions. Networking problems are usually forwarded to the NREN support, which is also very responsive and the resolution time is rather low.

The most difficult problems are those related to instability of a service, which require rethinking of the setup of this service and then reinstallation or upgrade to achieve more stable condition.

#### Romania:

Due to the fact that the major resource providers for the Romanian HPSC activities were first involved in the national Grid, there is a considerable experience in advanced

computing operational support and monitoring. The provision of the required quality of service is locally ensured by means of the implementation and adaptation of the tools developed in the European framework to the specific conditions of the HPC clusters. In this framework, the adoption of common operational and monitoring standards in the framework of the HP-SEE project is welcome.

The high operational availability of the resources is also supported by the NREN RoEduNet (<u>http://www.roedu.net</u>), which offers 10 Gbit/s external connectivity within the country and to GEANT.

#### Hungary:

Operational problems are either detected by automatic monitoring tools (central Nagios, log file processors, Munin measures) or by human parties, mostly by operators, and rarely by users. In either case first the issue is registered finto the local ticketing system, and then the exact failure conditions are examined. This is often performed by a person being on duty 24 hours a day. Then the issue is assigned to the person (or group of persons) that are believed to be the best suitable and to have the most knowledge in this respect. Then steps are made to recover the problem, which might also include a vendor consultancy call, or even involvement of the vendor support based upon the 6-years of support contract established before. Each step being significant on the way of solving the issue is registered in the ticketing system. In case of operations problems there are no first level support, i.e. the call center is not involved in the escalation process. If a suitable solution is found, then the whole team as well as the announcing party is informed and the ticket is closed.

Severe issues that are either representing a high risk (i.e. that needs machine shutdown or restart) are communicated on the all-users mailing list, including the site downtime schedule.

As NIIFI [29] is also the Hungarian NREN, security issues are treated in tight cooperation with the data network operator team.

### 4.5.2. Application support

The purpose of applications support is to aid the users in utilizing the hardware resources in the most efficient way. Compared to the operations support this requires different expertise and different attitude in user care. Compared to operations it is not a 7/24 exercise, no quick reactions are needed, as the issues might not cover the whole site, but particular software or services. Also the initiator here is always the user who submits a well-phrased problem description often regarding to porting an application to the used platform, getting it executed, and process or even visualize the execution outcome. In some cases they want to get the code optimized to boost executions.

In this subsection we show case studies on how application specific support is covered in different organizations and countries. We mostly focus on porting and code optimization for the national and international resources.

#### Bulgaria:

Problems corresponding to porting and optimal usage of specific applications are resolved after identifying the available experts in the particular application or field and then collaborating with them until appropriate solution can be found. Applications that either have large user base, or are deemed important for other reasons, e.g. because of high social or scientific impact, are ported and installed centrally, in such a way that all application users can get uniform access to the ported version. Other applications are ported by the respective scientific group with some guidance and help from the administrators or other experts. For some important applications there have been specific grants for application porting, optimization, installation and production of appropriate documentation (in Bulgarian). The result of this process is a long list of supported applications for each of the HPC resources. The actual production utilization of the applications produces feedback that is used when reconfiguring and adjusting the system. For example, some applications require long execution times even when using maximum number of CPUs. This condition has led to the addition of appropriate batch queues. Unfortunately, the high cost of loss of machine time in such cases, when machines are rebooted, imposes a restriction on the operations, i.e. it is not possible to introduce configuration changes at once by simple reboot of all nodes. The frequent contact between operational and management teams with the users, not only related to reporting problems, but also at workshops and scientific conferences, improves the mutual understanding and coordination of the use of HPC resources.

#### Romania:

Given the absence of a national coordination, the support of the application running on the HPC clusters is currently provided by members of the technical staff as well as programmers associated to the clusters, following local rules. In the nearest future, on the extent of the standardization of the procedure of accessing to the major resource centers, by making use of compatible job submitting schemes, storage and archiving best practices following the HP-SEE model, the application developers will be helped in porting their applications in a straightforward manner. Thus, they will be able to focus on the scientific aspects of their applications, rather than the scalability and optimization aspects targeted by technical experts.

#### Hungary:

Application support is limited to porting user applications into the currently used platforms, and also to perform executable optimization based on the available profiling and debugging tools. We also offer execution failure analysis. The most frequent user request in this sense is to migrate some ancient Fortran applications into the contemporary execution environment. Such cases always include compiling the code with multiple Fortran compilers, then to link them to the efficient HPC libraries being available on all platforms, and then to perform test executions both from command line and on the scheduler. Another typical application support issue is to configure checkpointing/restarting mechanism into the code, mostly on the library level. The third most typical application issue is rather related to the use of the local scheduler and its different execution environments.

Each issue is registered by either the call center in the proper branch of the ticketing system, or on the pertaining mailing lists, where each issue is updated and closed whenever solved or terminated.

## 4.6. Guidelines for the HPC centre coordination

Coordination of an HPC centre is a complex task, whose workflow has to be carefully managed and adapted for each country based on various parameters, our of which the most important ones are: size, structure and maturity of user communities, availability, hardware structure and amount of HPC resources, number of personnel and available effort of operational and user support teams. On top of these major criteria, the technical coordination has to provide the following functions:

- Technical support/hardware management HPC centre system management at the fabric/hardware level, as well as at the base OS services level, is done by the technical support team. It coordinates its work with the operational and user support teams.
- Operational support
   Management and monitoring of HPC services as well as a support for resolving of
   issues and problems identified by end users is performed by the operational
   support team, which can be organized jointly with the technical support team. In

collaboration with the user support team, operational support develops, provides and deploys additional HPC services and user-level tools, requested by the users. It also deploys/adapts libraries, modules etc. based on the user communities' needs.

• User support

User communities and researchers whose proposals are granted access to HPC centres, local HPC centre users, as well as those preparing, porting and developing their HPC applications, are served by a user support team. This team is a first line of support, and should accept all requests from users, routing them if necessary to other support units.

- Planning of support teams
   While technical and operational support teams should be sized according to the
   amount of available hardware, the size of the user support team should critically
   depend on the size of active user communities, as well as the number and
   necessary effort to support them. Other activities, such as support to users in
   porting, benchmarking and optimizing their scientific codes can also necessitate
   additional personnel.
- Technical assessment of applications
   User support team, in collaboration with the operational support, should be
   responsible for technical assessment of applications. A clearly established
   procedure for this should be defined.
- Support system (helpdesk)
   For each of the support teams, on-line troubleshooting tracking system should be deployed (helpdesk), such that end users and members of the support teams could easily access it, and that the trouble tickets can be easily exchanged between different units. Ideally, the on-line support system should be also able to communicate with other support systems at the national level, as well as with the other support systems of relevance.

 Training coordination HPC centre should organize regular training activities for its users and support personnel. For this reason, a dedicated person should be appointed as a training coordinator, and be responsible for organization of local training events, as well as collaboration with other HPC centres at the national, regional and EU-level on training activities.

Dissemination coordination

HPC centre should also appoint a person responsible for dissemination of information on centre's activities, as well as scientific dissemination. Public relations and relations with the media are an important element, and significant effort should be invested into outreach. This applies also to participation in public events, organization of visits to HPC centre, promotion of its results and achievements, popularization of scientific computing in general, and dissemination of relevant, interesting or otherwise visually attractive scientific results. Dissemination coordinator should be also responsible for organization of events for policy makers and high profile visits to HPC centre.

#### • National and European coordination and interoperability

Coordination of activities of the centre with other centres from the country, region or from EU-wide infrastructures (PRACE) is an important element for the successful operation of a national HPC centre. This applies to all types of activities, including the management, technical coordination and interoperability, provisioning of operational and user support, organization of training and dissemination activities. Technical manager/coordination of HPC centre should be responsible for this task overall, while coordinators of each particular activity within the centre should be in charge of interoperability and collaboration within their domains.

# 5. Conclusions

In this deliverable we have analyzed and presented various organizational aspects of national HPC initiatives and task-force modeling guidelines. The analysis was based, on one hand, on the inputs from several PRACE countries, representing the experiences of the well-developed HPC initiatives and infrastructures, and on the other hand, on experiences, inputs and plans from the core HP-SEE countries (Greece, Bulgaria, Romania, Hungary, Serbia), as well as other general partners in the project, which are currently working on the establishment of national HPC initiatives from the technical and organizational/policy point of view. This deliverable should serve as a guideline to SEE countries in creating their own organizational model and in planning of their HPC activities. It should also facilitate collaboration in the region, and collaboration with the PRACE initiative, by sharing the experiences and dissemination information on the organization model and activities of PRACE partners.

In particular, this deliverable has investigated possible governance structures for HPC initiatives, and identified several models, which include MoU-based entities, initiatives coordinated by the designated research institute or university, centers of excellence, consortia, and legal entities with mixed ownership. The details are presented in Chapter 2, and can serve as a starting point in planning of HPC initiatives in the SEE countries. In particular, the following key guidelines for the governance of national HPC initiatives are identified:

- Coordination: managed by a council (board) and by a director/chair/coordinator of the initiative, technically coordinated by a technical director/manager.
- Scientific steering committee to be established to carry out the peer review of proposal for access to national HPC resources.
- User advisory/representation body to be formed as a responsible to give recommendations and feedback regarding all aspects of the operation of HPC infrastructure.

Chapter 3 gives exhaustive analysis on peer review scientific assessment of proposals for the use of HPC resources. Peer review is an important requirement, and it presents a corner stone for building the scientific excellence in e-Science. Various assessment models are presented, which can be adopted by SEE countries. At present, peer review in the region is done by the NA4 activity of HP-SEE project for computational physics, computational chemistry and life sciences, but as more HPC resources are procured and national HPC centers are established, national peer review systems will have to be organized. Experiences of PRACE countries from national calls, as well as from the PRACE access calls are therefore valuable inputs, and were presented here together with the inputs from HP-SEE partners. Analyzing the collected inputs, Chapter 3 identifies the most important principles to be followed by peer review process, as well as typical steps in the organization of the application assessment. The key guidelines identified:

- Scientific steering committee should be appointed, consisting of HPC experts with the background from various scientific fields, representing fairly all major user communities in the country. The committee opens calls for access to national HPC resources, defines procedures, creates the appropriate questionnaires and forms for the calls, and makes decisions on the priorities/quotas assigned to each scientific field.
- Prior to the scientific peer review of research proposal, each project has to successfully pass a technical review, done by the operational personnel at the HPC centre where resources are requested.
- Scientific steering committee should carefully follow up the results of the projects that are granted access to national HPC resources, and take necessary measures

if the applied approach and the quality of the obtained results is not deemed satisfactory.

And finally, Chapter 4 considers HPC centre coordination through various aspects, including organization of the technical support, training and dissemination, European coordination and interoperability, user support, including both operational and application support. Specific guidelines are given for the organization of the technical support and system management, where a number of tools were presented. Guidelines were also given for carrying our technical application assessment, which is part of the peer review process for HPC access proposals. Here we summarize the key guidelines identified. Regarding the organization of the HPC centre, the deliverable identifies the following conclusions:

- Technical support/hardware management HPC centre system management at the fabric/hardware level, as well as at the base OS services level, is done by the technical support team. It coordinates its work with the operational and user support teams.
- Operational support Management and monitoring of HPC services as well as a support for resolving of issues and problems identified by end users is performed by the operational support team, which can be organized jointly with the technical support team.
- User support
   User communities and researchers whose proposals are granted access to HPC centres, local HPC centre users, as well as those preparing, porting and developing their HPC applications, are served by a user support team.

Regarding the organization of activities and workflows of the HPC centre, the deliverable identifies the following guidelines:

• Planning of support teams

While technical and operational support teams should be sized according to the amount of available hardware, the size of the user support team should critically depend on the size of active user communities, as well as the number and necessary effort to support them. Other activities, such as support to users in porting, benchmarking and optimizing their scientific codes can also necessitate additional personnel.

- Technical assessment of applications User support team, in collaboration with the operational support, should be responsible for technical assessment of applications.
- Support system (helpdesk) For each of the support teams, on-line troubleshooting tracking system should be deployed (helpdesk), such that end users and members of the support teams could easily access it, and that the trouble tickets can be easily exchanged between different units.
- Training coordination HPC centre should organize regular training activities for its users and support personnel. For this reason, a dedicated person should be appointed as a training coordinator, and be responsible for organization of local training events, as well as collaboration with other HPC centres at the national, regional and EU-level on training activities.
- Dissemination coordination HPC centre should also appoint a person responsible for dissemination of information on centre's activities, as well as scientific dissemination. Dissemination coordinator should be also responsible for organization of events for policy makers and high profile visits to HPC centre.
- National and European coordination and interoperability Coordination of activities of the centre with other centres from the country, region or from EU-wide infrastructures (PRACE) is an important element for the

successful operation of a national HPC centre. Technical manager/coordination of HPC centre should be responsible for this task overall, while coordinators of each particular activity within the centre should be in charge of interoperability and collaboration within their domains.