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ACCESS TO THE REGIONAL SCIENTIFIC COMPUTING INFRASTRUCTURE

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

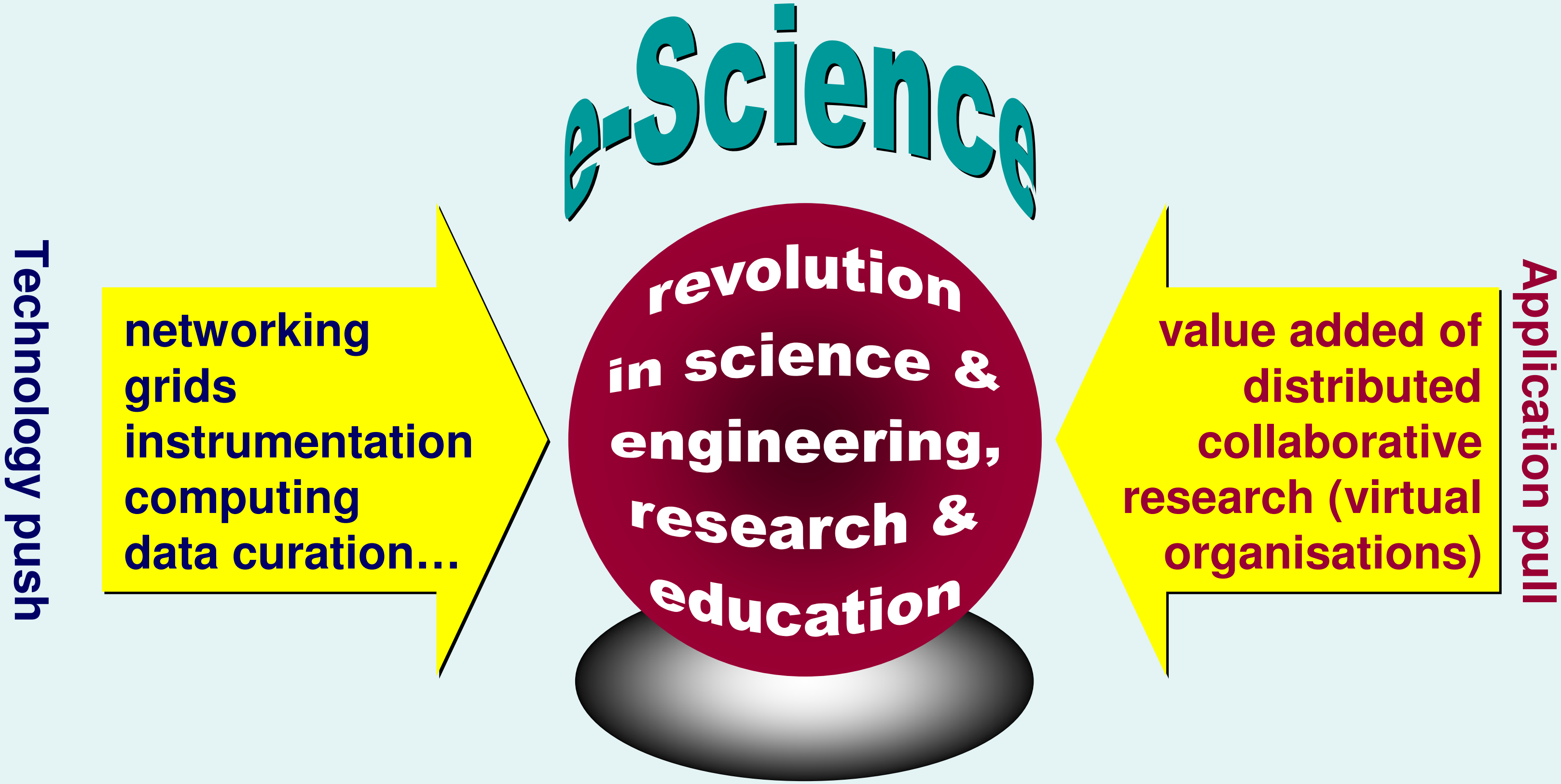
RENAM Association,

Institute of Matematics and Computer Science

Importance of e-Science

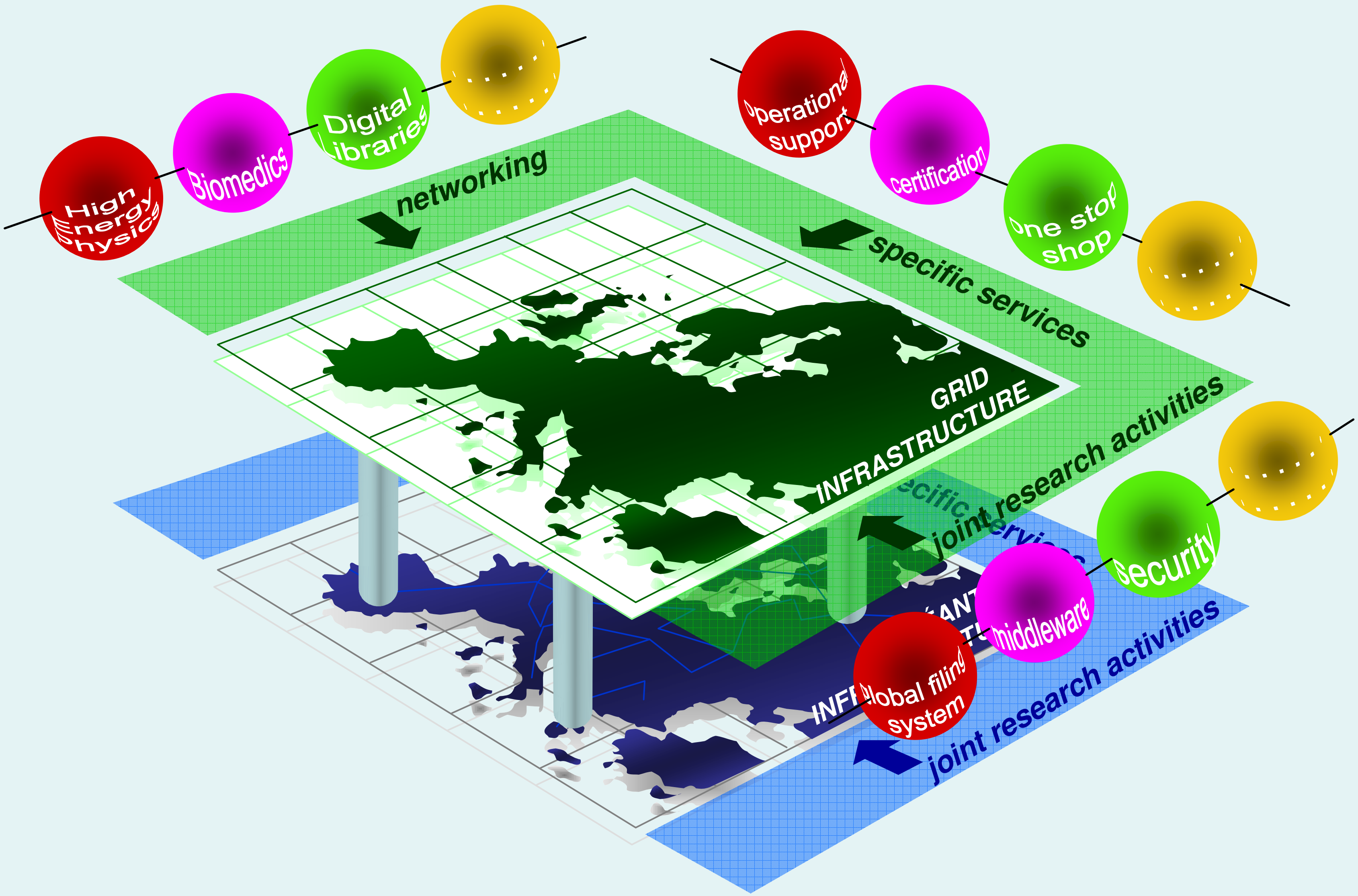
- The transition of the traditional science to e-Science is fueled by the ever increasing need for processing of exceedingly large amounts of data and exponentially increasing computational requirements: in order to realistically describe and solve real-world problems, numerical simulations are becoming more detailed, experimental sciences use more complicated instruments to make precise measurements;
- Shift from the individuals-based science work towards collaborative research model now starts to dominate.
- The role of scientific computing that comprises Grid, High Performance Computing (HPC) and intensively developing scientific clouds in the modern research is crucially increasing. It considerably determines the level of development of the knowledge based society.
- Mathematical modeling forms a solid theoretical and applied basis in describing, simulating and studying the complex problems. The regional and European cooperation in the field of scientific computing repre-sents an important factor for developing of the research activities and determine perspectives of integration the in the European Research Area.

eInfrastructure - new way of doing Science



a new way for all scientists to work on research challenges that would otherwise be difficult to address

e-Infrastructure - Implementation blocks



Scientific Computing - definitions

- Computing facilities based on Parallel Architectures and used for running complex applications:
  - HPC - Clusters' systems;
  - HPC - Supercomputers;
  - Distributed computing – Grids;
  - Scientific Clouds…
- Parallel Algorithms Design and Programming
- Complex Computing Applications Development
- Scientific Computing architecture is a bridge for building modern virtualized computing systems – scientific clouds

Importance of Scientific Computing

- *"Although the fastest computers can execute millions of operations in one second, they are always too slow. This may seem a paradox, but the heart of the matter is: the bigger and better computers become, the largest are the problems scientists and engineers want to solve."*

  A. Jaffe, Ordering the Universe: The Role of Mathematics, SIAM Review, 1984

- *"Computing has become a third branch of research, joining the traditional practices of theorization and laboratory experimentation and verification. Due to the expense and complexity of actually performing experiments in many situations, simulation must be done first."*

  C. C. Douglas, G. Haase, U. Langer, A Tutorial on Elliptic PDE Solvers and their Parallelization, SIAM, 2003

Scientific computing development in South-East Europe

- In Eastern Europe the eIfrastructure components such as Grids, HPC and Scientific clouds in general are less developed than in Western Europe
- In the past years the European Commission has funded, through a number of targeted initiatives, creation of new regional e-Infrastructures and user communities and enabling collaborative research across a number of fields.
- Advancing the Information Society in areas such as South-East Europe, strengthening of the local eInfrastructures, activating new user communities and enabling collaborative research across a number of fields, would strongly contribute to closing the existing technological and scientific gap, and thus bridging the digital divide, stimulating research and consequently alleviating the brain drain in the region.

European Projects for Scientific Computing development support

- PRACE (Partnership for Advance Computing in Europe – www.prace-project.eu)
- DEISA (Distributed European Infrastructure for Supercomputing Applications - www.deisa.eu)
- EGEE I-III projects (Enabling Grids for eScinse)
- EGI-InSPIRE (European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe – www.egi.eu)
- Enabling Clouds for e-Science

- SEE-GRID-1 project (May 2004 - May 2006)
- SEE-GRID-2 project (May 2006 - May 2008)
- SEE-GRID-SCI project (May 2008 - May 2010)
- HP-SEE project (High-Performance Computing Infrastructure for South East Europe's Research Communities)

  www.hp-see.eu

Grid and HPC Initiatives. MD-Grid NGI Aims and Tasks

- **MD-Grid NGI** participates in strategic European Programs for the development of transnational grids and in initiatives for the completion of SEE eInfrastructures. The operation of the MD-Grid NGI implements the general EU policy on the development of national initiatives for the coordination of actions related to eInfrastructures and Grids.
- **The integration** of Grid actions (infrastructures, middleware and applications) with the broadband research and technology network into a standard e-Infrastructures system. Optimization of exploitation of advanced network resources and services, which can serve the new e-Science generation and will attract the greater users community of the Information Society to the mass adoption of advanced services provided by Grid architectures.
- **Permanent development** and administration of Grid infrastructure in Moldova
- **Organization access** for national R&E community to the regional and European computational resources (HPC, Grid, scientific clouds, etc.)
- **Preparing** (educational, training events organization) and **support** of national users' communities

Access to regional High Performance Computing (HPC) resources

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

The aim of the **HP-SEE** project - combine existing and developed in the region **HPC**-resources in a single infrastructure.

For participating countries without their **HPC**-resources to provide access to these resources in virtual research organizations in the areas of computational physics, chemistry and life sciences.

Project started in 2010. Project duration - 3 years.

The project involves 14 countries.

RENAM and **IMI ASM** participate in the project from the Republic of Moldova.

HP-SEE project partners

1. **Greece -** Greek Research & Technology Network
2. **Bulgaria -** Institute for Parallel Processing, Bulgarian Academy of Sciences
3. **Romania -** "Horia Hulubei" National Institute of Research and Development for Physics and Nuclear Engineering
4. **Turkey - ** ULAKBIM
5. **Hungary -** National Information Infrastructure Development Office
6. **Serbia -** Institute of Physics Belgrade
7. **Albania -** UPT
8. **Bosnia and Herzegovina**
9. **Former Yugoslav Republic of Macedonia -** SS. Cyril & Methodius University of Skopje
10. **Montenegro -** UoM
11. **Moldova (Republic of)** – RENAM and IMI ASM
12. **Armenia -** IIAP NAS RA
13. **Georgia -** GRENA
14. **Azerbaijan -** AZRENA

HP-SEE Infrastructure current status and plans of development

Country	TFlops			
	2010	2011	2012	2013
Greece	0	0	40	80
Bulgaria	25	31+8GPU	31+20GPU	40+20GPU
Romania	10	26+4GPU	30+20GPU	30+20GPU
Hungary	1	48	48+12GPU	48+12GPU
Serbia	6	6	20	20
OVERALL	**42**	**111 + 12 GPU**	**169 + 52 GPU**	**218 + 52 GPU**

	Max processes	CPU type	Nodes	TFlops	Batch system	OS	Total storage
Blue Gene, BG	8192	IBM Power PC	2048	23.42	Load leveler	Compute Node Linux (CNL)	12 TB
HPCG cluster, BG	576	Intel Xeon X5560	36	3	Torque + maui	SC Linux 5.3	30 TB
Pécs SC, HUN	1152	Intel Xeon X7542	1	10	SGE 6.2u5	SuSELinux ES 11 SP1	160 TB
Debrecen SC, HUN	3072	Intel Xeon X5680	128	18	SGE 6.2u5	SuSELinux ES 11 SP1	152 TB
Szeged SC, HUN	2112	AMD Opteron 6174	44	14	SGE 6.2u5	Red Hat ELS 5.4	230 TB
InfraGrid, RO	400	Intel Xeon E5504	50	2,15	Condor 7.4.4	CentOS 5.5	10 TB
IFIN_Bio, RO	256	Intel Xeon E5430	32	1,2	PBS Torque	CenOS 5.5	180 GB
IFIN_BC, RO	368	IBM PowerXCell 8i, AMD Opteron 2376	26	2.05 0.39	PBS Torque	Fedora 9	120 GB
NCIT cluster, RO	562	Xeon E5504, Opteron 2435, PowerXCell 8i, Xeon E5630		1,04	SGE 6.2u5, PBS Torque	SC Linux 5.5	13,1 TB
ISS_GPU, RO	4x480	Nvidia		4	PBS	Ubuntu 10.10	
PARADOX, RS	672	Intel Xeon E5345	84	5,25	Torque 2.3.6 + Maui 3.2.6	SC Linux 5.5	53.1 TB

HPC Resources, available for MD application deploying

HPCG cluster located at IICT of Bulgarian Academy of Sciences.
576 computing cores. The storage and management nodes have 128 cores.

Number of nodes	36
CPU	Intel Xeon X5560 @2.8Ghz
RAM	24GB per node
Max number of parallel processes	576
Interconnect type	DDR Infiniband
Interconnect latency	2.5 μs
Interconnect bandwidth	20Gbps
Peak performance (Tflops, double precision)	3.23
Achieved performance (Tflops, double precision)	3
Operating system	Scientific Linux 5.3 64 bit
Batch system	torque + maui

HPC Resources, available for MD application deploying

SGI UltraViolet 1000 supercomputer at NIIFI, located in Pecs, Hungary. 1152 cores, 6057 GByte of memory

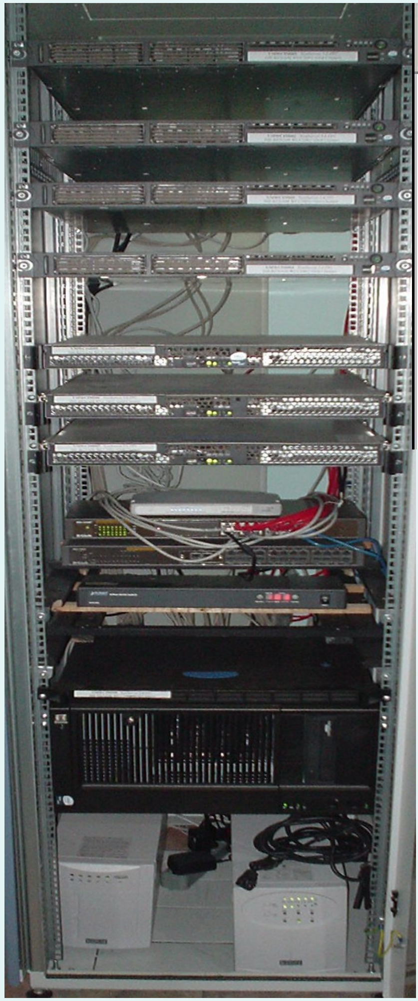
Number of nodes	1
CPU	Intel Xeon X7542 (Nehalem EX), @ 2.67GHz
RAM	6 TByte
Max number of parallel processes	1152 cores
Interconnect type	NUMAlink 5, paired node 2D torus
Interconnect latency	<1 μs
Interconnect bandwidth	15 GByte/sec
Peak performance (Tflops, double precision)	10
Achieved performance (Tflops, double precision)	10
Operating system	SUSE Linux Enterprise Server 11 SP1 (x86_64)
Batch system	Sun Grid Engine 6.2u5

Available HP-SEE training resources

Country	Partner	Number of Nodes	Number of Cores	CPU Architecture	Interconnection	Batch System
BG	**IICT**	4	1920	GPU/NVIDIA	**2xGigabit Ethernet**	Torque
RO	**UVT**	50	400	x86_64	**QDR 4xInfiniband**	SLURM
RO	**UPB**	48	544	X86_64/Cell	**4xGigabit Ethernet QDR 4xInfiniband**	Sun Grid Engine
RO	**ISS**	4	2100	GPU/Fermi NVIDIA	**2xGigabit Ethernet**	Rocks Clusters
RS	**IPB**	2	16	x86_64 2.0GHz	**Gigabit Ethernet Infiniband**	Torque
RS	**IPB**	2	16	POWER6 4.0GHz	**Gigabit Ethernet Infiniband**	Torque
RS	**IPB**	2	16	PowerXCell 8i	**Gigabit Ethernet Infiniband**	Torque
RS	**IPB**	1	16	Nehalem	**Gigabit Ethernet Infiniband**	Torque
BA	**UOBL ETF**	2	16	x86_64	**Gigabit Ethernet**	Torque
MD	**RENAM**	1-6	8-20	x86_64	**Gigabit Ethernet**	CCS2003
AM	IIAP NAS RA	6	48	x86_64	**Gigabit Ethernet**	Torque
AM	IIAP NAS RA	24	48	x86_64	**Gigabit Ethernet**	Torque
AM	IIAP NAS RA	1	240	Tesla 1060	**GPU**	

Local HPC resources for training, applications testing and debugging

48-core IMI-RENAM cluster



MS Windows Compute Cluster 2003

Cluster Status Last Refreshed: 24.05.2011 13:02:02

Compute Nodes:

Ready nodes:	8
Paused nodes:	0
Unreachable nodes:	0
Pending for approval nodes:	0
Total nodes:	8

Processors:

Processors in use:	14
Idle processors:	8
Total processors:	22

Name	Status	Jobs Run...	CPUs	CPUs in Use	OS Vers...	Total Memory
VMWCIMI01	Ready	0	4	0	5.2.3790	2043
VMWCIMI02	Ready	1	4	4	5.2.3790	4091
VMWCIMI03	Ready	1	4	4	5.2.3790	2043
VMWCIMI04	Ready	1	4	4	5.2.3790	2043
VMWCIMI05	Ready	0	2	0	5.2.3790	507
VMWCIMI06	Ready	1	2	2	5.2.3790	507
VMWCIMI07	Ready	0	1	0	5.2.3790	507
VMWCIMI08	Ready	0	1	0	5.2.3790	507

Access to the regional HPC resources

How the application should be prepared to run on a High Performance Resources ?

- No user interface — computing part only
- The application must be debugged - should work without error.
- It is necessary to make an executable module - the application must be compiled on Linux or Windows.
- It is advisable to calculate how much the application need computing time and other resources

HP-SEE project. Moldavian application deploying in regional HPC-infrastructure

AMR_PAR application (Parallel algorithm and program for the solving of continuum mechanics equations using Adaptive Mesh Refinement), being developed in the Institute of Mathematics and Computer Science of the Academy of Sciences of Moldova.

AMR_PAR 64-bit application was developed in MS Visual Studio 2010.

Now AMR_PAR application is ready in OpenMP mode and was locally tested on small AMR grids (128x128x128 cells, 5 layers) on MS Windows Compute Cluster 2003 (4-8 Nodes, 4-22 Cores (QuadCore Intel Xeon E5335, E5310 CPU)

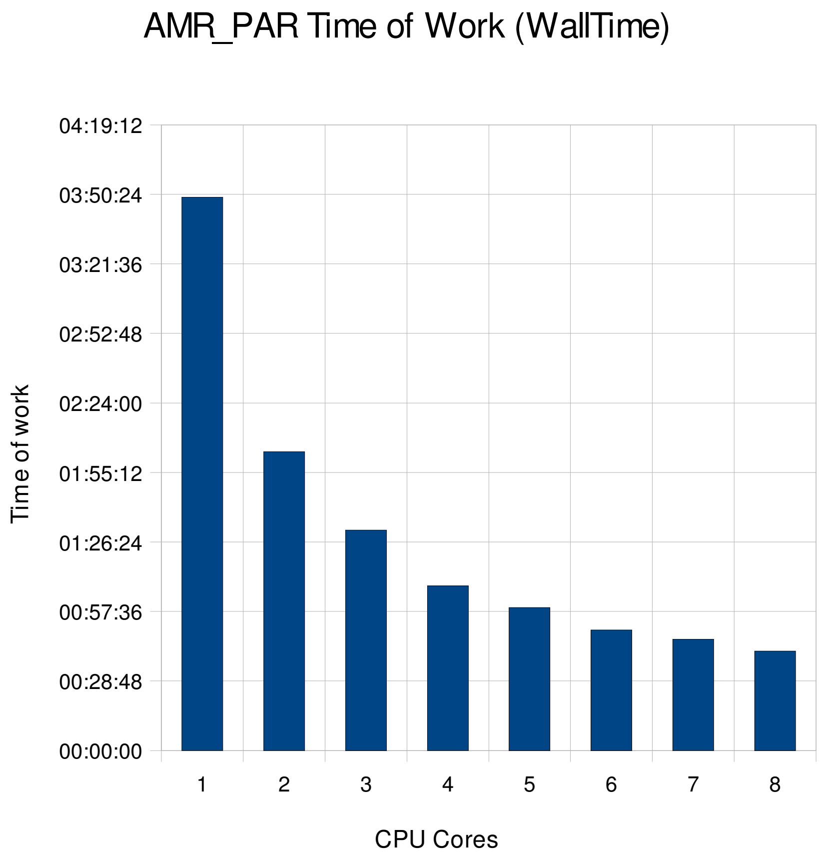
Application was ported to Linux, compiled and tested on front-end computer ***HPCG cluster located at IICT of Bulgarian Academy of Sciences*** and at the front-end computer of ***SGI UltraViolet 1000 supercomputer at NIIFI, located in Pecs, Hungary***.

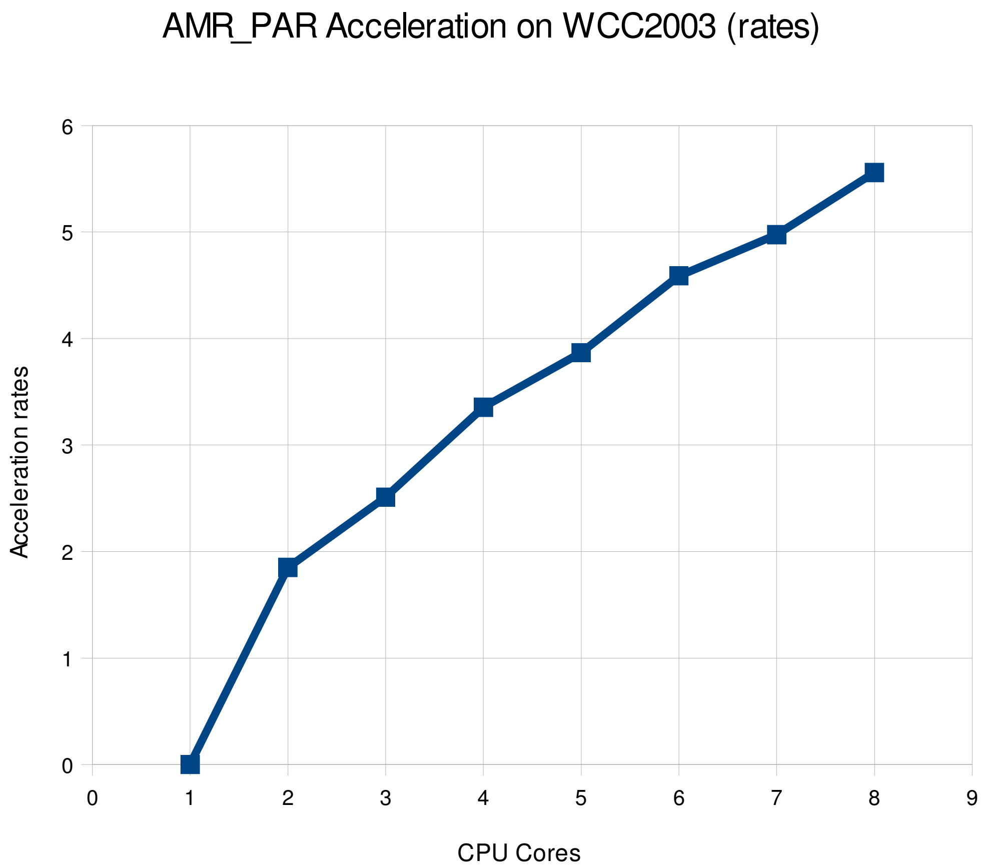
AMR_PAR application for the solving of continuum mechanics equations using Adaptive Mesh Refinement

- The AMR_PAR application is considering a continuum mechanics problem, and namely the problem of modeling the explosion of a supernova type II and, for this example, created the algorithm and parallel program using the AMR method
- Adaptive Mesh Refinement method can be applied to any other nowadays problem of continuum mechanics - to calculate the aerodynamics of aircraft, the calculations of the air flow of cars, a large number of other problems of mathematical modeling – the calculation of the flow of blood through the vessels, the calculations of the heart valves, etc. In all these cases, at the beginning of the problem we define a way to highlight areas in which we need to construct the grid, then the program builds a sequence of grids and makes a decision on them. The social impact depends on the problem to be solved, the use of AMR_PAR being of interest for heavy industry (e.g. car body design and development, aircraft aerodynamics), or for healthcare industry.

Results of AMR_PAR application execution on the WCC2003 cluster of IMI

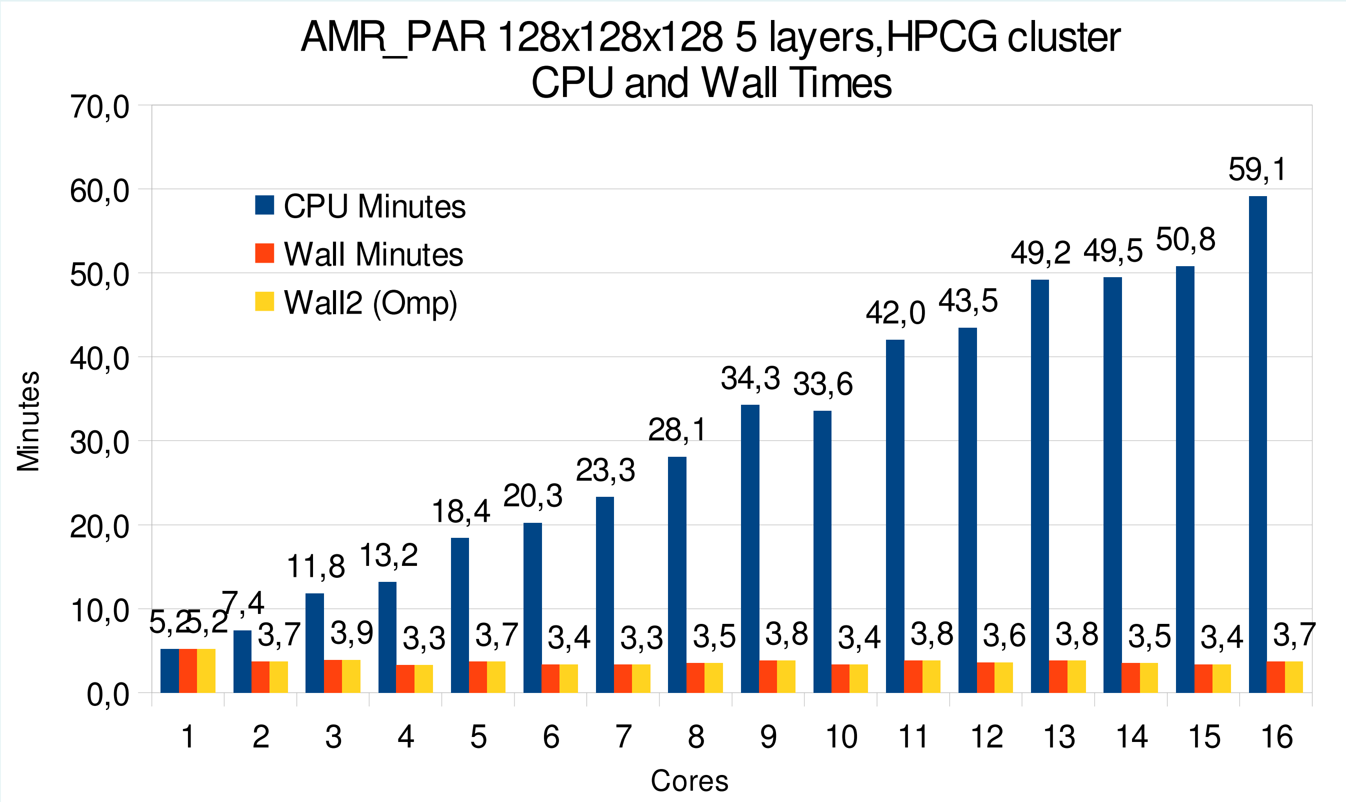
AMR_PAR Acceleration — results of testing in OpenMP mode, cores from 1 to 8 (2 x QuadCore Intel Xeon E5310, 1600 MHz, 8 GB of RAM)





Results of AMR_PAR application execution on HPCG cluster, IICT of the Bulgarian Academy of Sciences.

Acceleration and Run Time dependences from CPU cores.
For 128x128x128 dimention best number of cores — 4.
4 cores - walltime - 3,3 min, CPU time -13,2 min.
16 cores - walltime - 3,7 min, CPU time - 59,1 min



Calculated requirements of computational resources for the current OpenMP version of AMR_PAR application.

For HPCG cluster located at the Institute of Information and Communication Technologies of Bulgarian Academy of Sciences maximum grid dimension for 5 layers is 384x384x384, approximate time of calculations – 5 hours, optimal number of cores – 8

For grid dimensions more than 384x384x384 require up to 3 Tb of RAM

Dimension	Layers	Max Iteration per level	Cores	RAM Gb	CPU minutes	WallTime minutes
128x128x128	5	200000	4	0,789	28	3,5
256x256x256	5	200000	4	5,972	273	68
256x256x256	5	200000	8	6,062	527	66
256x256x256	5	200000	12	6,068	807	68
384x384x384	5	200000	8	19,2	2110	270
448x448x448	5	200000	8 — 16	37,7	~ 4500	~ 500
512x512x512	5	200000	8 — 16	~ 55,6	~ 130 hours	~ 17 hours
1024x1024x1024	5	200000	16 — 32	~ 415	~ 2000 hours	~ 248 hours
2048x2048x2048	5	200000	32 — 64	~ 3250	~ 1200 days	~ 154 days

AMR_PAR application for the solving of continuum mechanics equations using Adaptive Mesh Refinement

Foreseen Activities:

For further optimization of AMR_PAR application, we plan collecting statistics of calculations' acceleration dependences from different number of cores - up to 64 (or more). It is necessary to produce investigations to find optimal number of cores for fastest calculations for large-scale grid dimensions. As a result of this research we plan to modify application to use OpenMP more effectively.

Next step is to run application using HP-SEE regional resources for large-scale grid dimensions – up to 2048x2048x2048, 5-7 layers. After obtaining results of the modified application execution, it will be possible to make new benchmarking (due to long time of forecast calculations) and propose new recommendations for application optimization. The results of calculations will be visualized in 2-D images and 3-D models.

Memorandum of Understanding for High-Performance Computing resource sharing in the region of South Eastern Europe

- This Memorandum of Understanding (MoU) is made on February 23rd 2012 hereinafter referred to as the "effective date"
- BETWEEN Resource Coordinators and Beneficiaries:
- For Moldova: RESEARCH AND EDUCATIONAL NETWORKING ASSOCIATION OF MOLDOVA
- The following principles will be followed within this resource sharing model:

A. *Partners should allocate as a minimum 5% of the total core hours of their HPC systems offered for resource sharing, per year for regional use.*

B. Cycles are allocated to users via the peer review system.

C. Calls for access can be either continuous or are announced periodically (yearly or twice a year), based on the demand and the capacity of the peer review system.

- This MoU is intended to remain into effect for at least 3 years from the effective date.
- The duration of the MoU is automatically extended for one year after the end of the initial 3 years period or after the end of each yearly extension.

Perspectives of Scientific Cloud Computing Infrastructure Deployment

- Development of scientific clouds is rather new, but perspective direction of computational technologies development.

  For SEE region needs in cloud technologies deployment were analyzed during execution of SEERA-EI project funded by EC ERA-NET Programme. The analysis produced had shown strong interest of the regional research communities in scientific clouds technologies deployment. In many countries this perspective direction is supported by governmental strategies as new technological approach for providing wide range of e-governmental services. As a resulting outcome of SEERA-EI project was recommendation to launch regional Pilot Call for projects in the area of scientific cloud computing. This Call was announced (http://www.seera-ei-pjc.asm.md/) and one of its priority topics is feasibility study of approached for scientific clouds integration to the announced e-government cloud infrastructures in the region.
- For finding optimal solutions for scientific clouds deployment in SEE region, investigations within SEERA-EI project were carried out. On the base of these work it was argued and proposed approaches for scientific clouds integration to the announced e-government cloud infrastructures in the region.
- The carried out analysis within framework of SEERA-EI project had shown strong interest of the regional and especially Moldovan research communities in scientific clouds technologies deployment. In many countries, and Moldova is one of them, clouds are supported by governmental strategies as a perspective technological approach for providing wide range of e-government services. In 2010 the Government of Moldova launched the national initiative known as "M-Cloud Initiative: Providing IT Services for Society." The Initiative consists of and covers many compartments, directions and projects. Key points of the M-Cloud Initiative are:

✓ All citizens (including research and educational community) deserve high quality e-services operated by a modern, reliable and cost efficient platform.

✓ e-Services provided by M-Cloud respond for the satisfaction of all society needs and Government demands.

✓ M-Cloud architecture is based on the leading edge Cloud Computing technology and service-oriented architecture.

✓ Modernized ICT regulatory framework may speed up Moldova's integration into European Union.

✓ The Initiative supports the implementation of e-Transformation Agenda that is the national priority.

- One of the main goals of developing now initiatives in the area of Scientific Clouds is the determination of optimal technological solutions for finding standard platform to facilitate the interoperability and to support the interactions of Governmental Clouds (like M-Cloud) and possible open source Scientific cloud solutions

Thank you!

Questions?

www.math.md

www.renam.md
www.grid.md