

Access to regional High Performance Computing (HPC) resources



HP-SEE

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

**South Eastern
Europe (SEE)**

**IMI ASM
RENAM**

www.math.md
www.renam.md

Nicolai ILIUHA





What types of tasks (Applications) can be run on a usual multi-core computer (desktop or notebook)?

Sequential Application - application runs on one computer and it's run time (wall time) depends on the capacity of the computer

Parallel Application – Application runs on all cores of one processor

Distributed Application (parametric sweep) – the same Application runs on several cores with different input parameters

Task flow – several tasks (perhaps one and the same program with different inputs) are run in sequence

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Server

Server (hardware) is a computer, dedicated to performing any service tasks without direct human intervention.

Servers are distinguished from a group of personal computers or from a group of specialized computer equipment.

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A **cluster** is a group of computers connected by high-speed communication channels (1-2 Gbit/s) and representing, from a user's point of view, a single hardware resource.

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20 — 120 Gbit/s



A **supercomputer** is a multiprocessor complex with ultra-fast data transmission channels within the complex.

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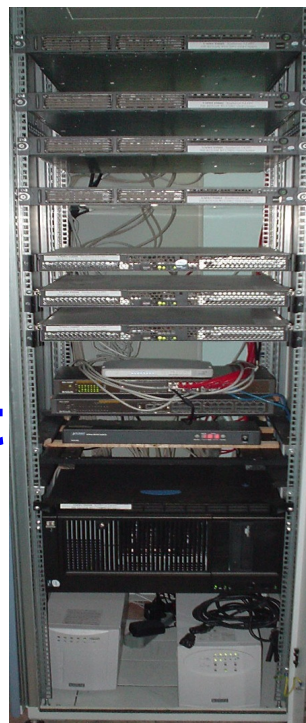
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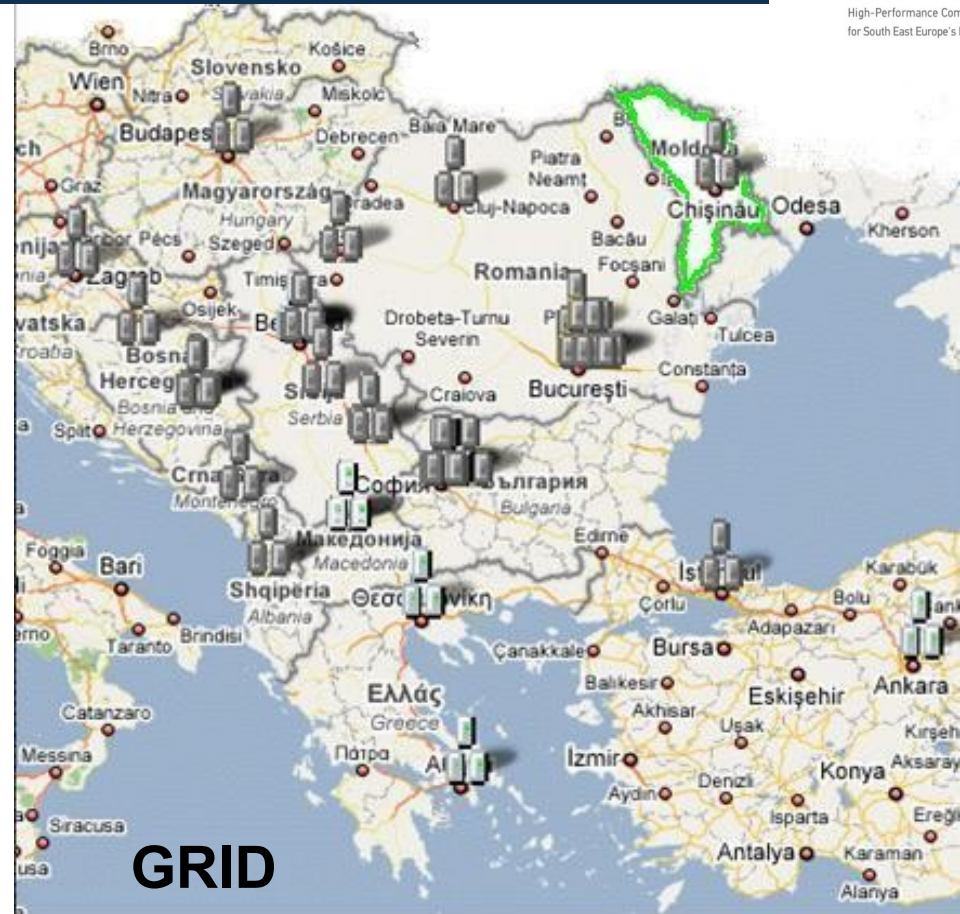
+
**Software-
Middleware**

+...+
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InterNet



+
**Software-
Middleware**

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Grid is a computational infrastructure that provides access through Internet to computing power and storage resources distributed across the globe.

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How is the GRID forms ? What GRID gives to users?

NGI_MD Total number of jobs by VO and DATE.

ALL VOs. March 2012 - May 2012.

The following table lists the sites that have not published accounting data to GOC during the last 3 months. This probably indicates a major problem in the accounting system of the site so listed sites are encouraged to take the appropriate measures to correct it.

sites NOT publishing accounting data to GOC in the last 3 months

Region	Sites
--------	-------

The following table shows the distribution of Total number of jobs grouped by VO and DATE.

Total number of jobs run by VO and DATE

VO	Mar 12	Apr 12	May 12	Total	%
atlas	0	3	5	8	0.26%
biomed	129	449	139	717	23.33%
dteam	1	0	0	1	0.03%
mdgrid	10	0	0	10	0.33%
ops	286	700	1,351	2,337	76.05%
Total	426	1,152	1,495	3,073	
Percentage	13.86%	37.49%	48.65%		

[Click here for a CSV dump of this table](#)

[Click here for XML encoded data](#)



What types of tasks (Applications) can be run on a High Performance Resources ?

Sequential Application - application runs on one computer and it's run time (wall time) depends on the capacity of the computer

Parallel Application – Application runs on all cores of one processor or on multiply processors (cores) of one or more computers

Distributed Application (parametric sweep) – the same Application runs on several cores on one or more computers.

Task flow – several tasks (perhaps one and the same program with different inputs) are run in sequence (automatically)



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

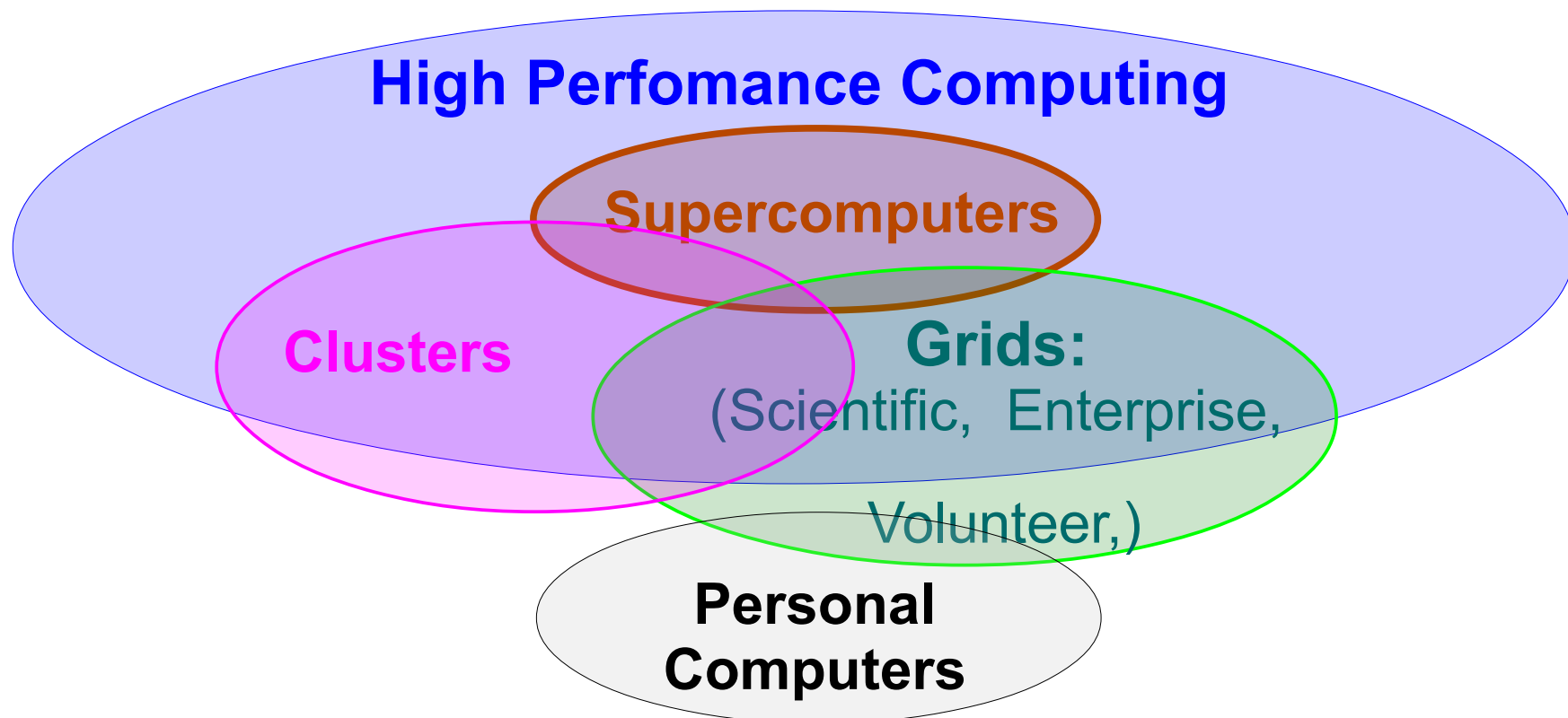
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High-performance computing is a branch of applied computer science that is dealing with the finding of solutions to problems that require a large amount of computing resources.



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South Eastern
Europe (SEE)

IMI ASM
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HP-SEE (under contract number 261499)**

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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.

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HP-SEE project brings together 14 partners from the South-East European region, more than 10 institutions involved in the project as third parties...

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**
5. **Hungary** National Information Infrastructure Development Office
6. **Serbia** Institute of Physics Belgrade
7. **Albania**
8. **Bosnia and Herzegovina**
9. **Former Yugoslav Republic of Macedonia** SS. Cyril & Methodius University of Skopje
10. **Montenegro**
11. **Moldova (Republic of)**
12. **Armenia**
13. **Georgia**
14. **Azerbaijan**

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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	TFI ops	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	2.050.39	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

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HPCG cluster located at ICT 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 μ s
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

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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 μ s
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

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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	2xGigabit 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	

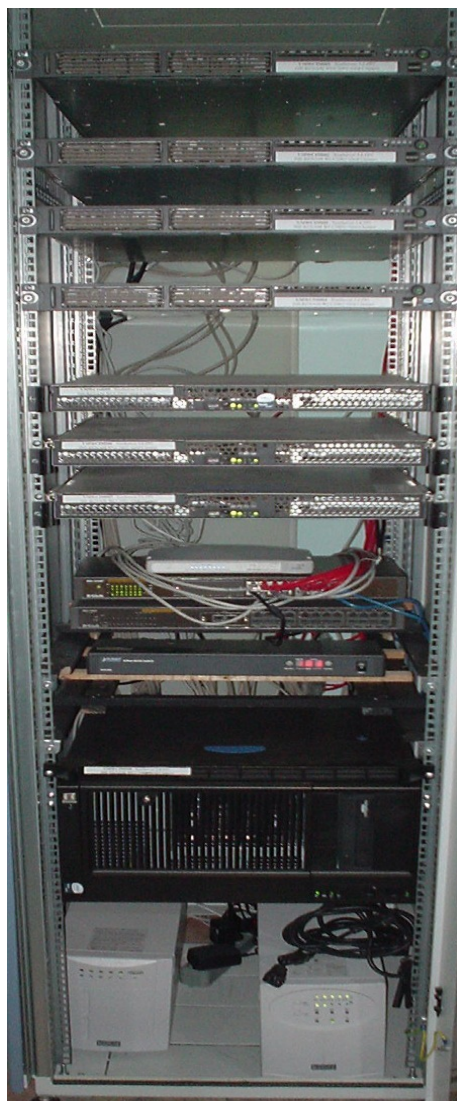
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48-core IMI-RENAM cluster

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

22 Virtual CPU on 8 Virtual Machines

Name	Status	Jobs Run...	CPUs	CPUs in Use	OS Vers...	Total Memory
VMWCIM101	Ready	0	4	0	5.2.3790	2043
VMWCIM102	Ready	1	4	4	5.2.3790	4091
VMWCIM103	Ready	1	4	4	5.2.3790	2043
VMWCIM104	Ready	1	4	4	5.2.3790	2043
VMWCIM105	Ready	0	2	0	5.2.3790	507
VMWCIM106	Ready	1	2	2	5.2.3790	507
VMWCIM107	Ready	0	1	0	5.2.3790	507
VMWCIM108	Ready	0	1	0	5.2.3790	507

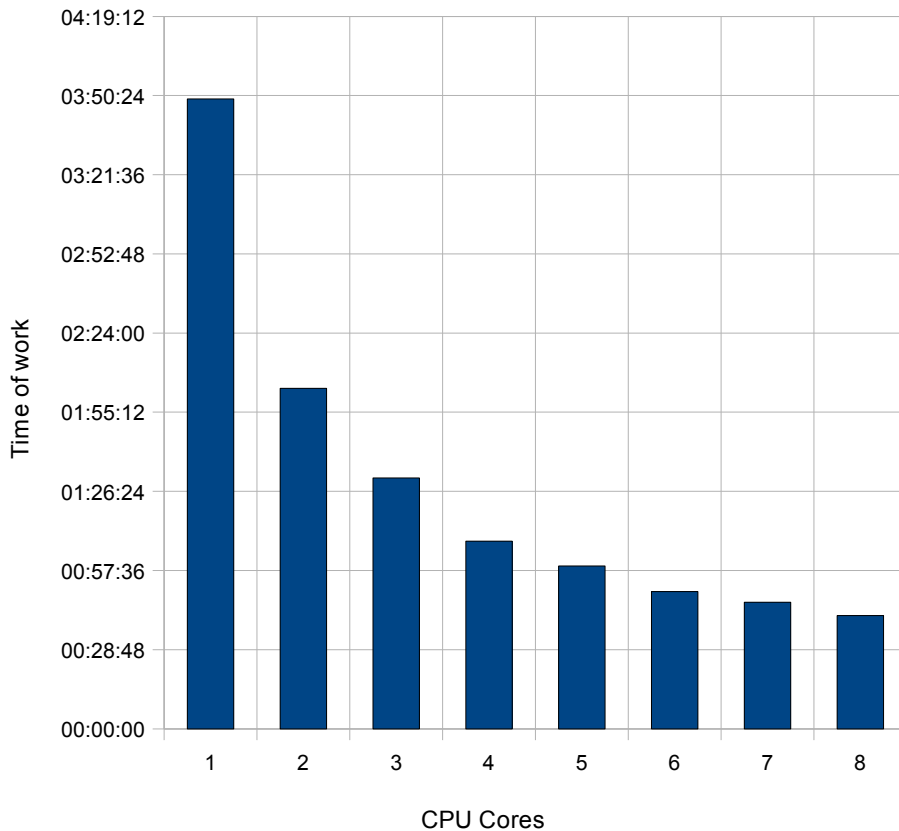
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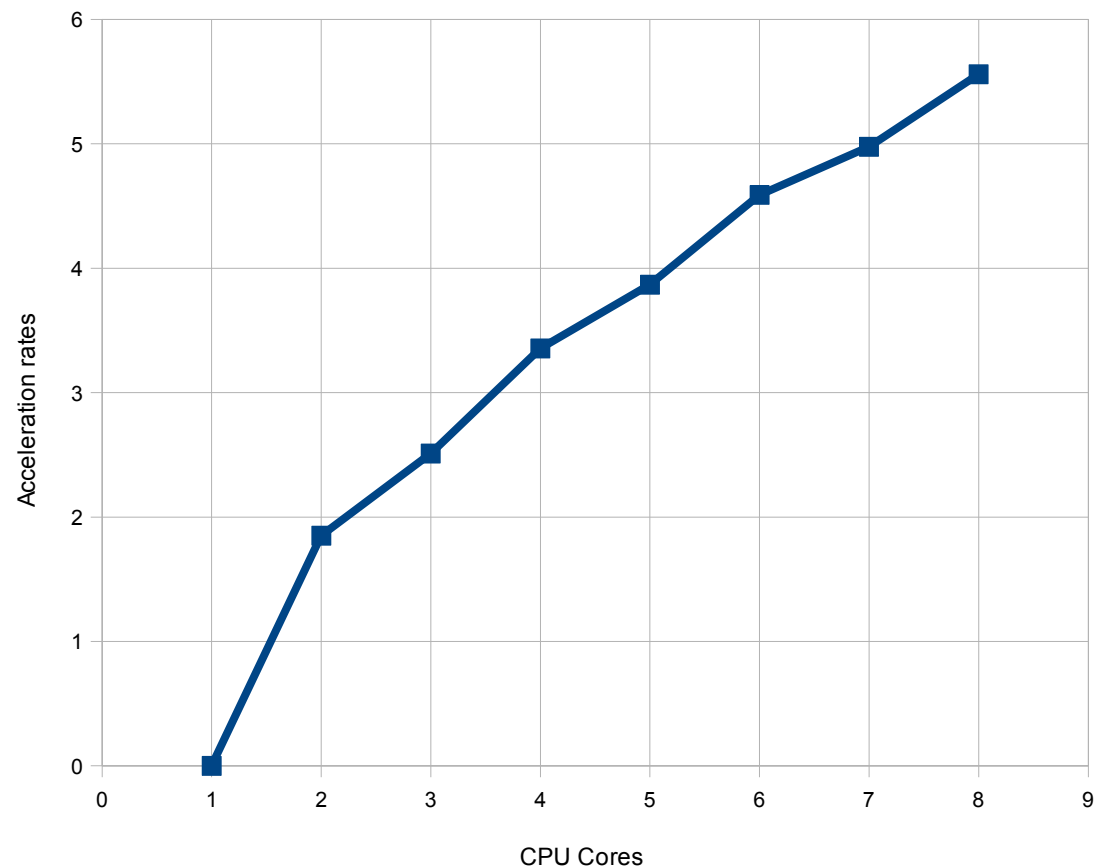
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Parallel computing B.Rybakin's task of IID simulation on the WCC2003 cluster of IMI

TVD_IID WCC2003 Test



TVD_IID ACceleration WCC WallTime



EGI-InSPIRE - European Grid Initiative:

Integrated Sustainable Pan-European Infrastructure for Researchers in Europe.

Supports „grids“ of high-performance computing (HPC) and high-throughput computing (HTC) resources

Supports integration into a seamless production infrastructure of new Distributed Computing Infrastructures (clouds, supercomputing networks and desktop grids)

Continued support for current heavy users of the infrastructure in earth science, astronomy and astrophysics, fusion, computational chemistry and materials science technology, life sciences and high energy physics as they move to sustainable support models for their own communities

A 4-year project, started in 2010

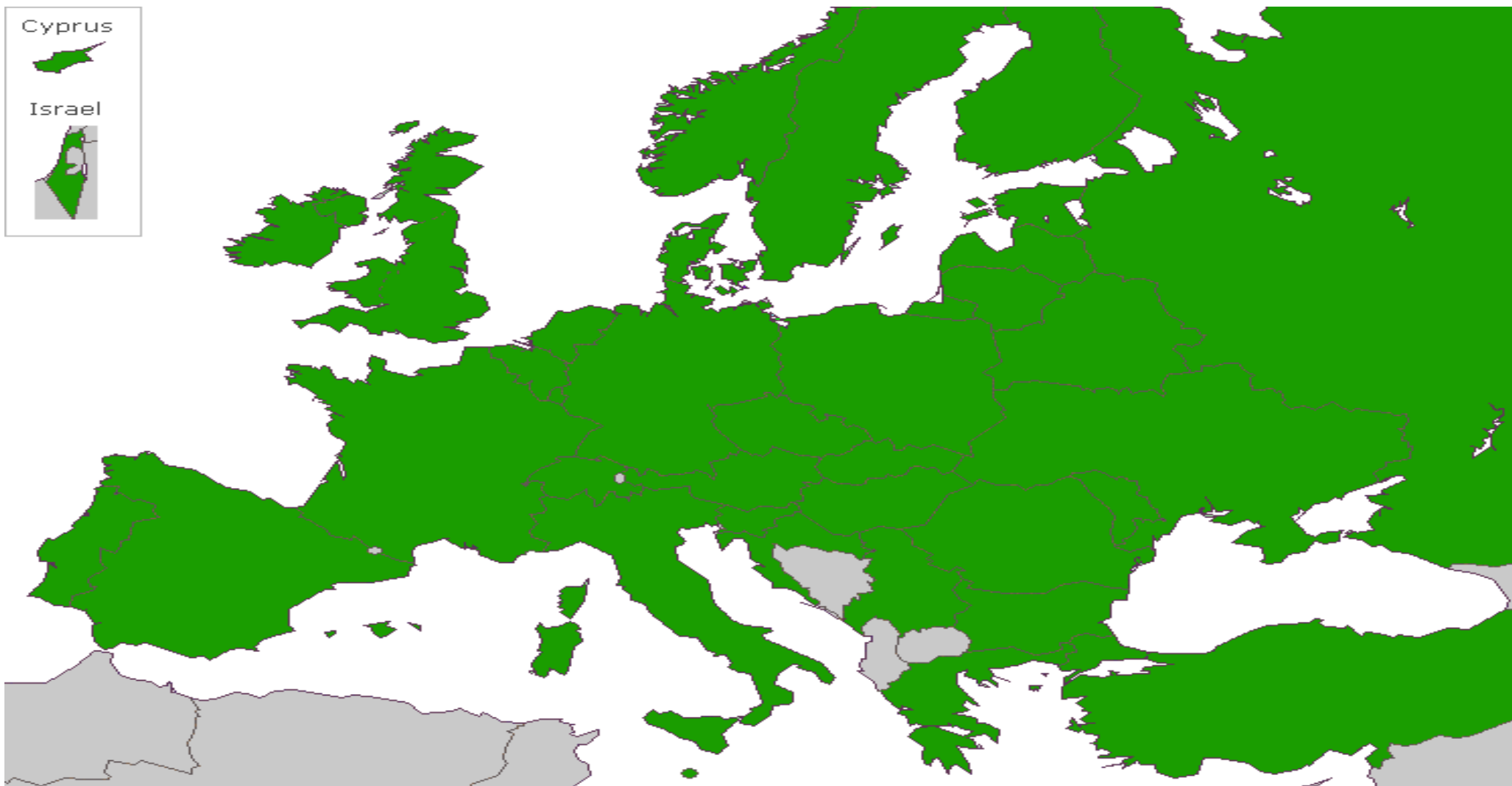
Many countries have launched National Grid Initiatives (**NGI**) to establish National grid infrastructures.

MD-Grid — National Grid Initiative of Moldova was officially inaugurated on the plenary session of RENAM "Users Conference – 2007" on **May, 14 2007**

Now the **European Grid Initiative (EGI)** is an organisation being developed to coordinate the European Grid Infrastructure, based on the federation of individual **National Grid Initiatives (NGI)**, to support a multi-disciplinary user community.

EGI will unite the National Grid-organisations of Europe.

NGI from **37** countries (coloured in green) are partners in **EGI-InSPIRE** Project



Задачи и цели EGI:

- Гарантировать долговременную устойчивость европейской e-инфраструктуры;
- Координировать интеграцию и взаимодействие между Национальными Grid Инфраструктурами;
- Создать общеевропейскую производительную грид-инфраструктуру для широкого спектра научных дисциплин на основе Национальных Grid Инфраструктур;
- Интегрировать, тестировать, утверждать и формировать, делать широкодоступным программное обеспечение от ведущих проектов по разработке и развитию Grid ПО;
- Создавать документацию и обучающие материалы по ПО и работе с ним (Национальные Grid организации обеспечат их перевод на соответствующий язык);
- Связать европейскую инфраструктуру с аналогичными инфраструктурами во всем мире;
- Тесно сотрудничать с индустриальными, технологическими и сервисными поставщиками, а также с пользователями Grid для обеспечения быстрого и успешного понимания и внедрения Grid-технологий в европейскую промышленность.

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 <p>1D_H2 MPI code for a 1D hydrogen molecule model</p>	 <p>2d-ANACONDA 2d-ANALYSIS of COpy Number DATA</p>	 <p>2D-MC-MOSFET 2D Monte Carlo Double G Silicon on Insulator MOS simulator</p>
 <p>3D_H2+ MPI code for a 3D Hydrogen molecular ion</p>	 <p>AA-GISSmodelE Academy of Athens-NASA-Goddard Institute for Space Studies modelE</p>	 <p>Abaqus by SIMULIA Abaqus by SIMULIA</p>
 <p>ABC ABC</p>	 <p>ABINIT ABINIT</p>	 <p>ADAP Advanced Diagnostics of Astrophysical Plasmas</p>
 <p>ADF First principles electronic structure package</p>	 <p>AERMOD (GISELA) AMS (American Meteorological Society) / EPA (Environmental Protection Agency...)</p>	 <p>AeroVANT (EPIKH) Engineering / Aerospace manufacturing</p>
 <p>Aiuri (GISELA) Aiuri</p>	 <p>ALICE ALICE</p>	 <p>AliRoot AliRoot</p>

Available in EGI Database:

368 Applications

37 Tools



ALMOST
almost - all atom molecular simulation toolkit



MD-Grid NGI resources

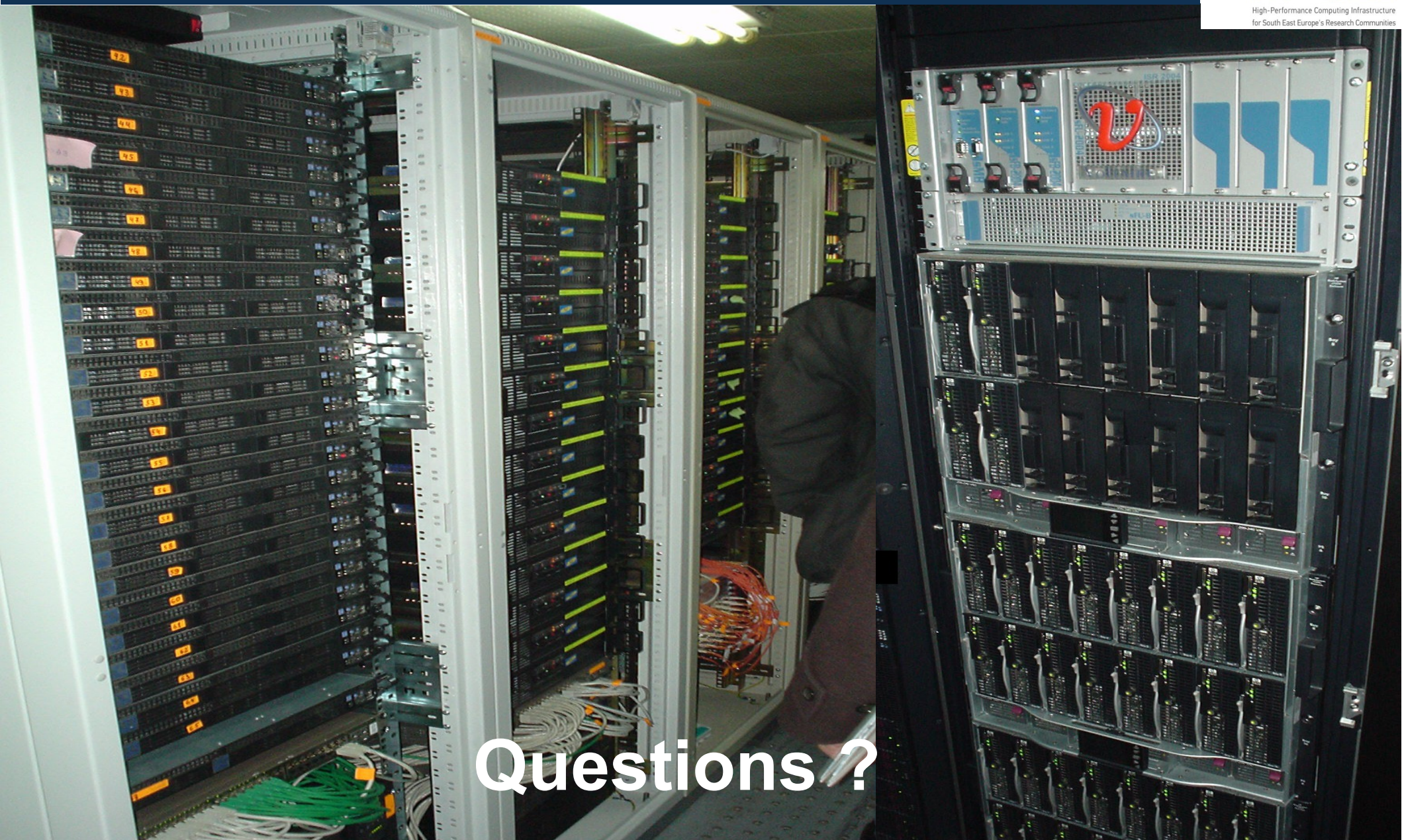
MD-GRID NGI site	Available CPUs	Available storage	Network
Certified sites			
MD-01-TUM	5 Intel P-IV 3,0 GHz CPUs	320 GB on Storage Element	100 Mbit Ethernet
MD-03-SUMP	5 x CPU AMD Athlon 64 X2 6000+ (3.0GHz)	650 GB on Storage Element	100 Mbps Ethernet
MD-04-RENAM	6 Quad Core Xeon 5130 CPUs	2 TB on Storage Element	100 Mbit Ethernet
MD-02-IMI	6 Quad Core Xeon 5130 CPUs	1 TB on Storage Element	100 Mbit Ethernet
Planned to be integrated into MD-GRID NGI			
MD-05-SUM	4x2xAMD 275 Dual-Core 2.2GHz and 3x2xAMD 280 Dual-Core 2.4GHz CPUs	2x500GB 7.2k SATA and 4x80 GB 7.2k SATA	100 Mbit Ethernet

COMPUTATIONAL RESOURCES OF THE REGIONAL SOUTH-EAST EUROPE HIGH PERFORMANCE COMPUTING INFRASTRUCTURE



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Questions?