Utilization of the Computational Resources Provided by HP-SEE Project

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

IIS 2013

South Eastern Europe (SEE)

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In september 2010 new project started:
High-Performance Computing Infrastructure for South East Europe's Research Communities

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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.

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	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 +	SC Linux 5.5	53.1 TB

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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.

AMR_PAR application is ready in OpenMP mode and was tested locally on small AMR grids (up to128x128x128 cells, 5 layers) on MS Windows Compute Cluster 2003.

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

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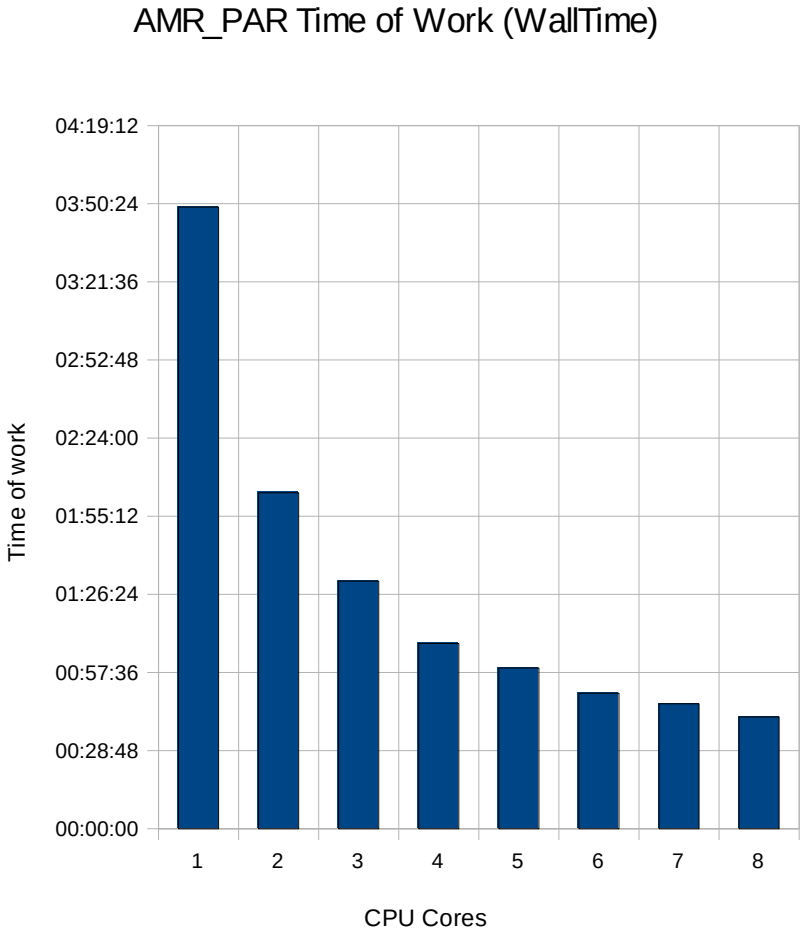
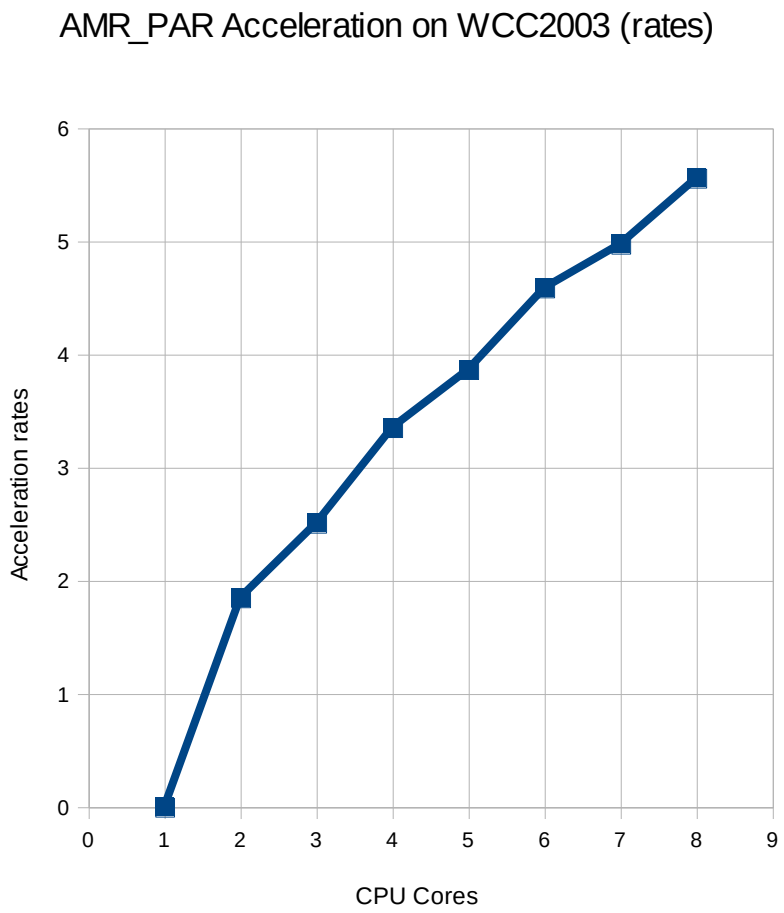
Results of AMR_PAR application execution

on the WCC2003 cluster of IMI in OpenMP mode,cores from 1 to 8
(2 x QuadCore Intel Xeon E5310, 1600 MHz, 8 GB of RAM)





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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	24 GB per node
Max number of parallel processes	**576 cores**
Interconnect type	DDR Infiniband
Interconnect latency	2.5 μs
Interconnect bandwidth	20 Gbps
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
Libraries	BLAS, LAPACK
Development and application software available	MVIAPICH 1, MVIAPICH 2, OPENMPI, gcc, gfortran, etc.

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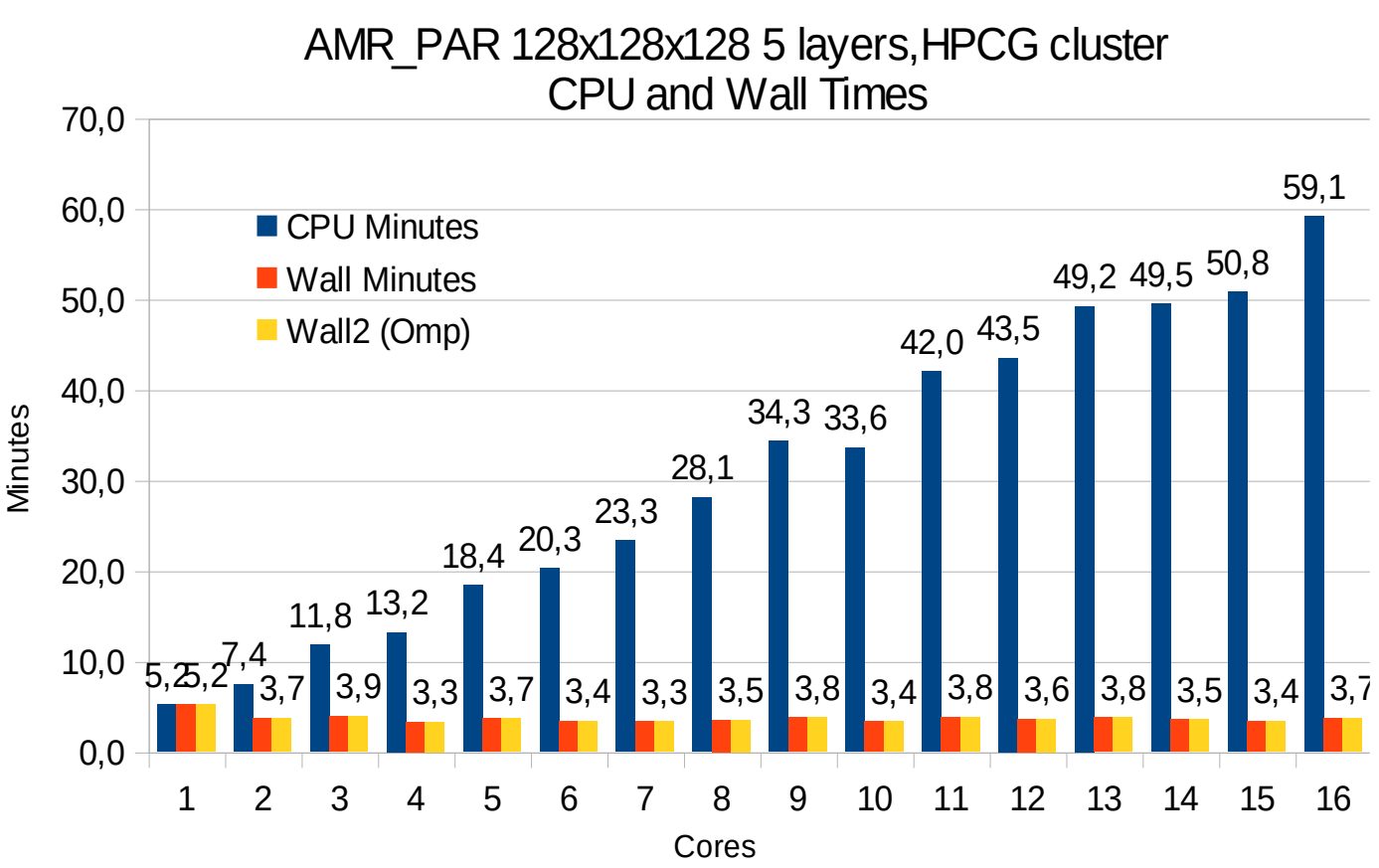
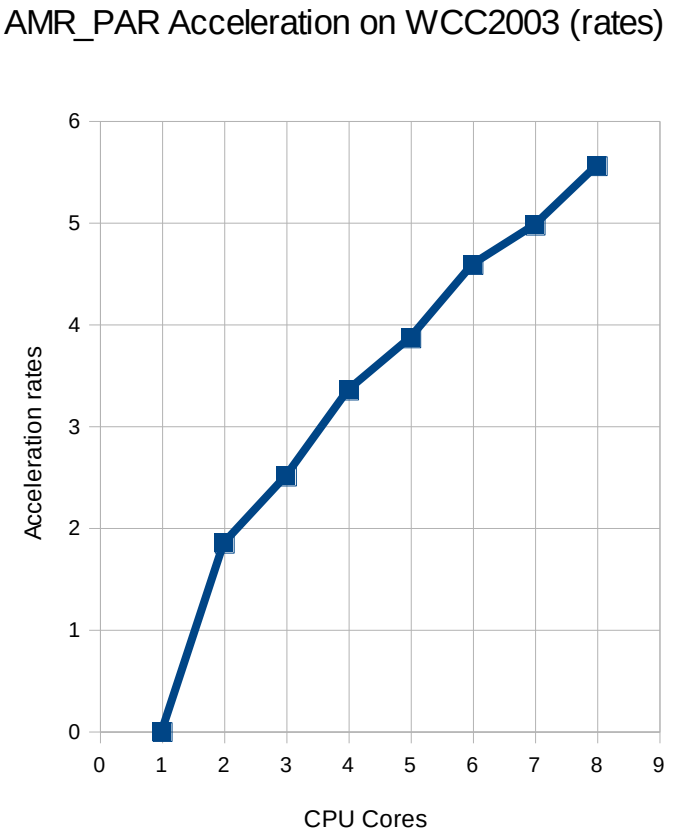
Benchmarking activities:

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





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Scientific results:

Figure 1 shows the analytical solution for the gravitational potential, obtained from equation (4).

Figure 2 - the numerical results,

Figure 3 - two-dimensional cross-section of the X-axis of Fig.2

Figure 1.

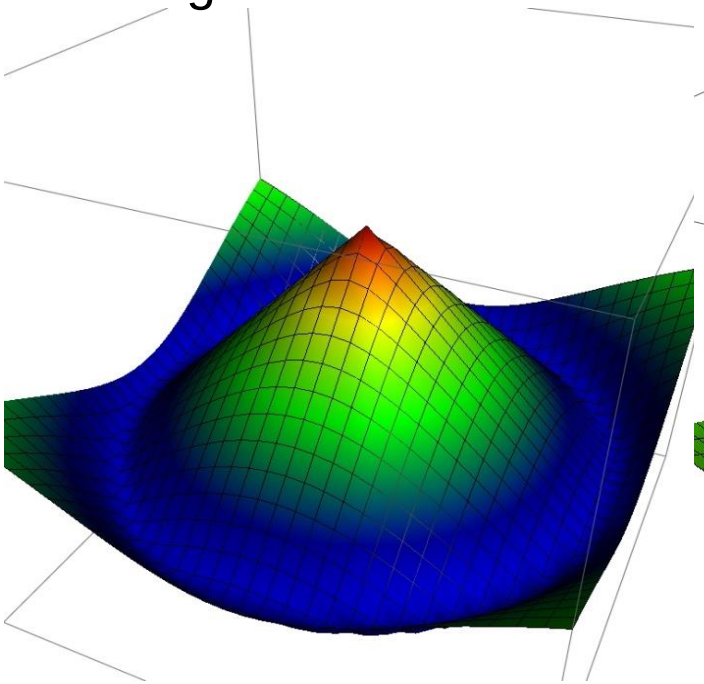


Figure 2.

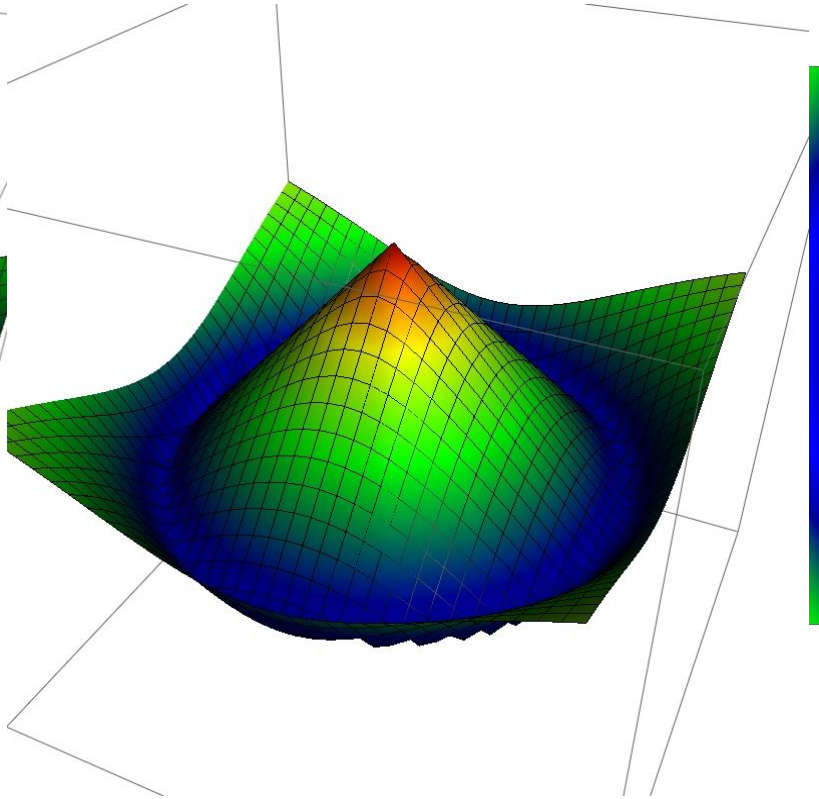
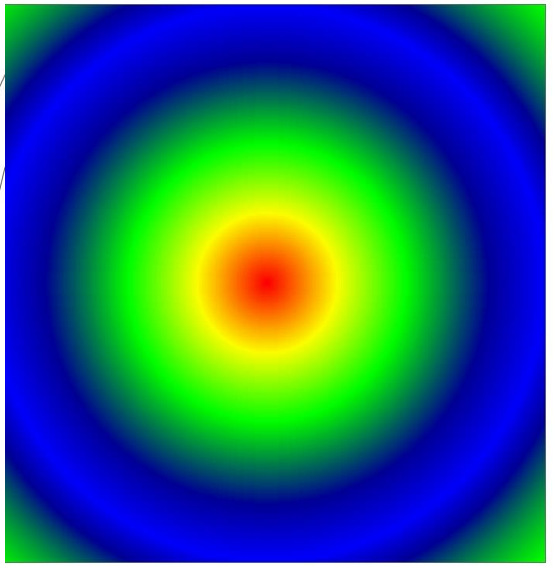


Figure 3



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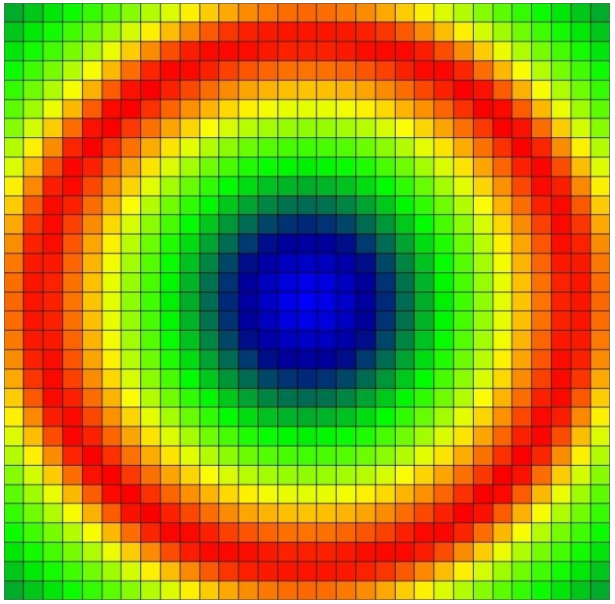
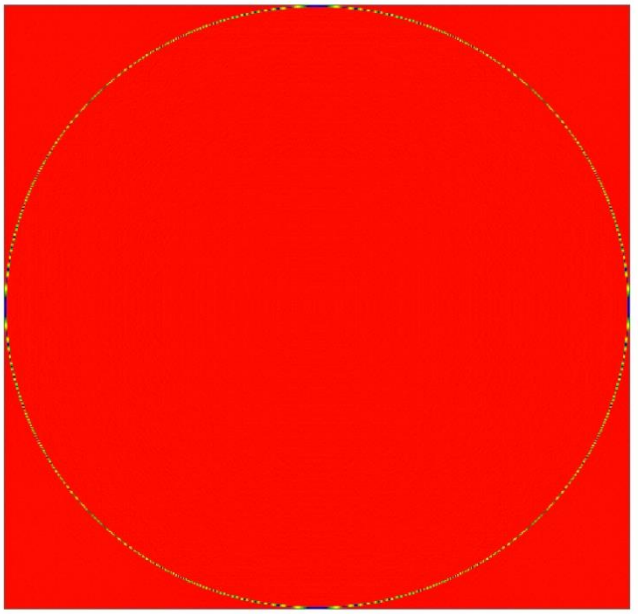
Scientific results:

The difference between the analytical and numerical solutions:

for the grid of 32x32 and two levels of grid



for the grid of 512x512 and 5-level grid



It should be mentioned the significant refinement of result and consequently decreasing of the error by four orders of magnitude. These results show the importance of applying the AMR method for raising accuracy of the solutions of multidimensional partial differential equations.

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

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

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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 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

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Within the framework of "Fast Track Process for Access to HP-SEE Resources", application from Moldova was submitted, successfully evaluated and passed the procedure of gaining access to HPC resources:

- Application's name: "The electronic structure, optical and transport properties of layered transition-metal dichalcogenides and their intercalated compounds";
- Acronym of the software application: **TMDC**;
- Scientific domain: **Computational Physics**;
- Contact person: **Dr. Yurii Chumakov**, Institute of Applied Physics Academy of Sciences of Moldova.

Before starting the procedure of the access, the application developer had possibility to run the application in test mode on resources of HPCG cluster located at **IICT-BAS, Bulgaria**.

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Questions ?

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