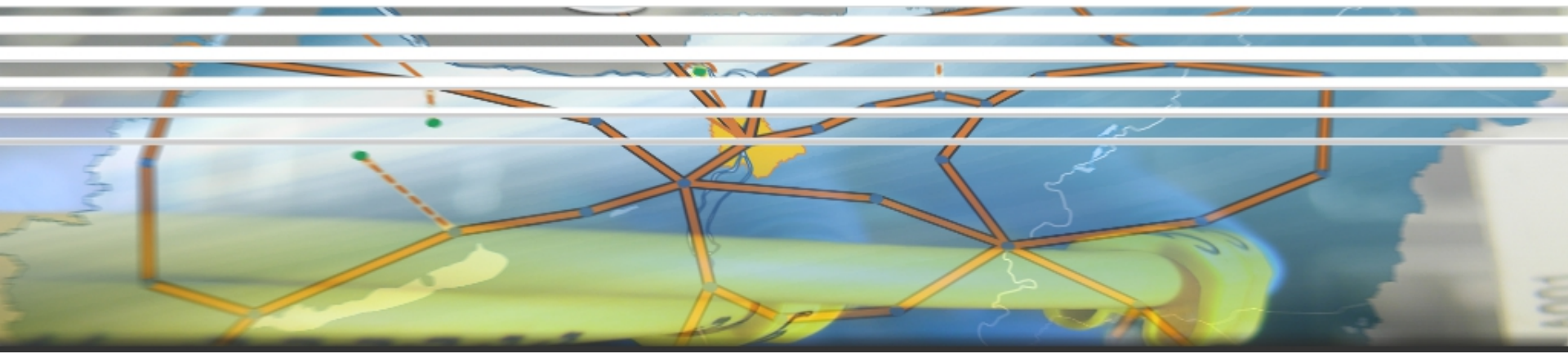


HP-SEE projekt eredményei



2013. március 26.
Networkshop 2013
Sopron



Róczei Gábor
roczei@niif.hu

HP-SEE projekt

- High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE)
- PRACE mintájára jött létre
- Délkelet-Európában még nincs jelentős HPC múlt
- Nagy számítási/adattárolási igény
- Dedikált szuperszámítógépek
- 2010 szeptember – 2013 augusztus
- Európai Unió támogatja, FP7
- Greek Research and Technology Network (GRNET) a koordinátor
- Grant agreement no: 261499

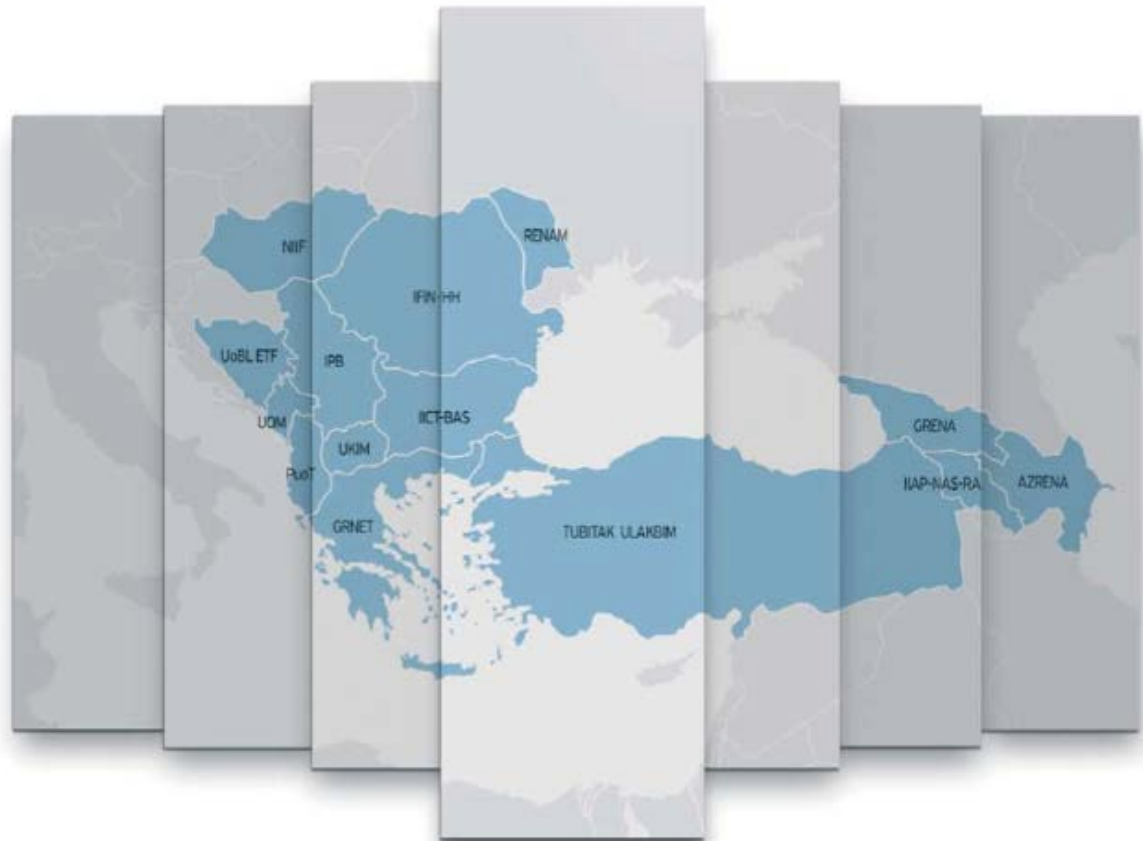


Főbb célok:

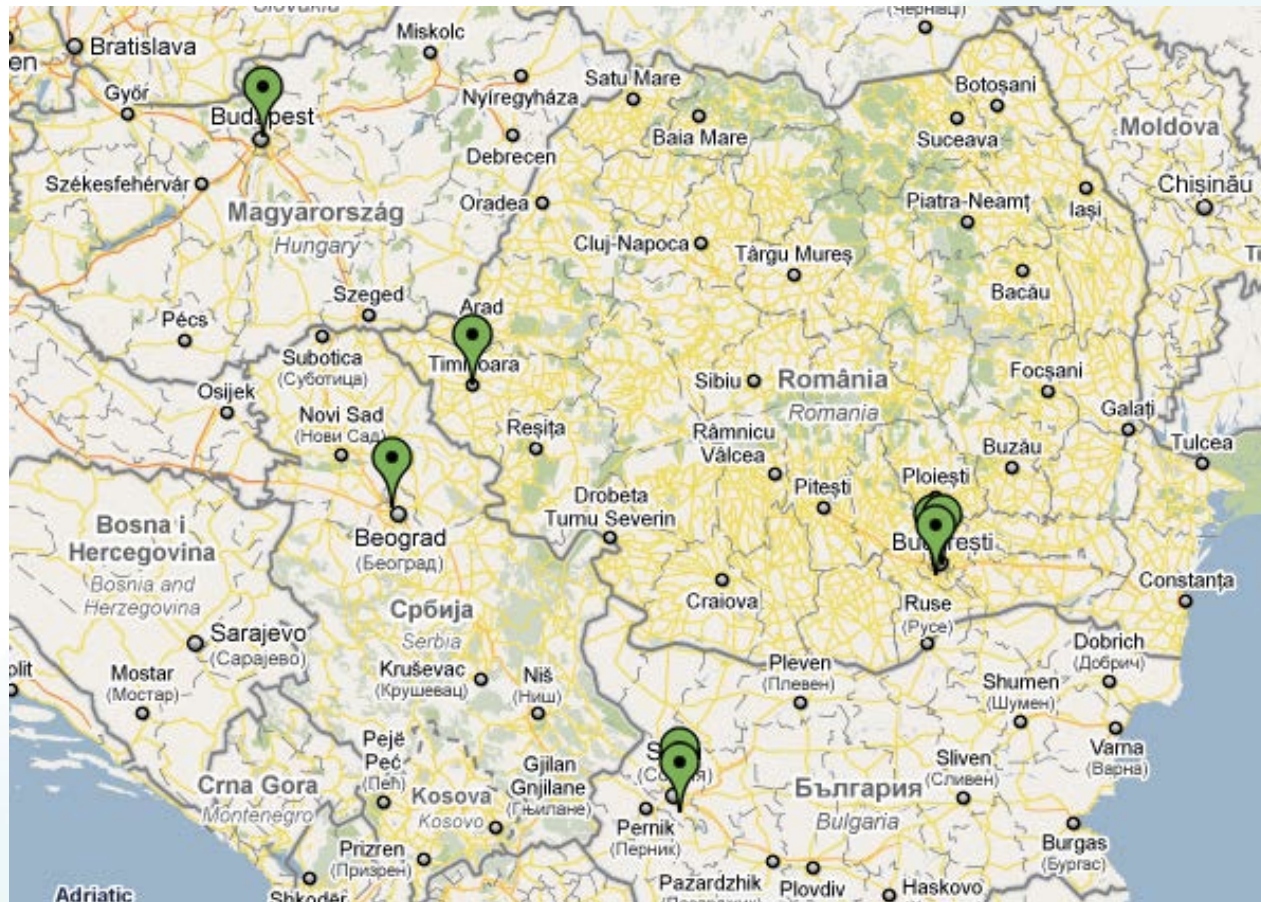
- Szuperszámítógépes központok összekapcsolása és üzemeltetése Délkelet-Európában
- Kutatói közösségek támogatása
- Gigabit European Academic Networking Technology (GEANT) kapcsolat kiépítése Dél-Kaukázussal

Résztvevő országok

- ❑ Albánia
- ❑ Azerbajdzsán
- ❑ Bosznia-Hercegovina
- ❑ Bulgária
- ❑ Görögország
- ❑ Grúzia
- ❑ Macedón Köztársaság
- ❑ Magyarország
- ❑ Moldovai Köztársaság
- ❑ Montenegró
- ❑ Örményország
- ❑ Románia
- ❑ Szerbia
- ❑ Törökország



HPC erőforrások



- ❑ Bulgária
- ❑ Magyarország
- ❑ Románia
- ❑ Szerbia

http://hpseewiki.ipb.ac.rs/index.php/HP-SEE_Wiki#HPC_Centers

HPC erőforrások - Bulgária



IBM Blue Gene/P



HPC erőforrások - Szerbia



HPC erőforrások - Románia



HPC erőforrások - Magyarország



HPC erőforrások

	Sebesség
Bulgária	40 Tflops (CPU)+ 20 Tflops (GPU)
Románia	35 Tflops (CPU) + 25 Tflops (GPU)
Magyarország	50 Tflops (CPU)+ 10 Tflops (GPU)
Szerbia	20 TFlops
Összesen	145 Tflops (CPU)+ 55 Tflops GPU

Milyen problémákat kell megoldani?

- Heterogén rendszerek, különböző architektúrák, operációs rendszerek
- Eltérő szoftver komponensek vannak telepítve az egyes HPC központokban
- Ugyanazon alkalmazásból, függvény könyvtárból több verzió
- Nincs telepítve egy adott szoftver
- Az alkalmazások nem használják ki a több processzort
- A felhasználók nem tudják hatékonyan használni a rendszereket, mert nincs meg a szükséges tudásuk

HP-SEE szoftver környezet (2/1)

	NIIF Szeged, HUN	NIIF Pécs, HUN	NIIF Debrecen, HUN	NIIF Budapest, HUN	BG Blue Gene/P, BG	HPCG,BG	IFIN_BC, RO	IFIN_Bio, RO	InfraGRID, RO	UVT Blue Gene/P, RO	NCIT-Cluster, RO	PARADOX, RS	FINKISC, Macedonia
Minimal software stack													
bash	*	*	*	*	*	*	*	*	*	*	*	*	*
tcsh	*	*	*	*	*	*	*	*	N/A	N/A	*	*	N/A
GNU compiler (C, C++, Fortran)	*	*	*	*	*	*	*	*	*	N/A	*	*	*
Java compiler	*	*	*	*	*	*	*	*	N/A	N/A	*	*	*
Vendor compiler (C, C++, Fortran)	*	*	*	*	*	*	N/A	N/A	*	*	*	*	N/A
OpenMP	*	*	*	*	*	*	*	*	*	*	*	*	*
MPI	*	*	*	*	*	*	*	*	*	*	*	*	*
CUDA	*	N/A	N/A	N/A	N/A	*	N/A	N/A	N/A	N/A	N/A	N/A	N/A
BLACS	*	*	*	*	*	*	*	*	*	*	*	*	*
BLAS	*	*	*	*	*	*	*	*	*	*	*	*	*
FFTW	*	*	*	*	*	*	*	*	*	*	*	*	*
Scalapack	*	*	*	*	*	*	*	*	*	*	*	*	*
MPIBLAST	*	*	*	*	N/A	N/A	*	*	*	*	*	*	*
LAPACK	*	*	*	*	*	*	*	*	*	*	*	*	*
Profiler	*	*	*	*	*	*	*	*	*	*	*	*	*
Debugger	*	*	*	*	*	*	*	*	*	*	*	*	*
Perl	*	*	*	*	*	*	*	*	*	*	*	*	*
Python	*	*	*	*	*	*	*	*	*	*	*	*	*
Tcl	*	*	*	*	*	*	*	*	N/A	N/A	*	*	*
Middleware	*	*	*	*	*	*	IP	IP	*	N/A	N/A	*	*

HP-SEE szoftver környezet (2/2)

	NIIF Szeged, HUN	NIIF Pécs, HUN	NIIF Debrecen, HUN	NIIF Budapest, HUN	BG Blue Gene/P, BG	HPCG, BG	IFIN_BC, RO	IFIN_Bio, RO	InfraGRID, RO	UVT Blue Gene/P, RO	NCIT-Cluster, RO	PARADOX, RS	FINKI SC, Macedonia
Recommended software stack													
SPRNG						*						*	
Atlas	*	*	*	*		*	*	*			*	*	*
charm++						*							
GotoBLAS	*	*	*	*	*								
Octave	*	*	*	*	*								*
GROMACS	*	*	*	*	*	*						*	*
AMBER					*	*							
GAMESS					*	*							*
NAMD	*	*	*	*	*	*						*	*
VMD	*	*	*	*	*	*							
ROOT	*	*	*	*									
CPMD					*	*						*	*

HP-SEE module környezet

```
[loginnode.szeged:~]$ module load hce
```

```
[loginnode.szeged:~]$ module list
```

Currently Loaded Modulefiles:

- | | | |
|--------------------------|--------------------------------|-------------------|
| 1) jdk/1.7.0_13 | 7) scalapack/2.0.2-gnu | 13) namd/2.9-smp |
| 2) open64/4.2.4 | 8) atlas/3.10.1-gnu | 14) vmd/1.9.1 |
| 3) openmpi/1.4.3 | 9) acml/5.1.0 | 15) root/5.34-gnu |
| 4) blacs/1.1-gnu-openmpi | 10) mpiblast/1.6.0-openmpi-gnu | 16) arc/1.1.1 |
| 5) gotoblas2/1.13-gnu | 11) octave/3.0.5 | 17) cuda/5.0 |
| 6) fftw/3.3.3-gnu | 12) gromacs/4.5.5 | 18) hce |

```
[loginnode.szeged:~]$ █
```

<http://modules.sourceforge.net>

Nagios monitorozás

	bash	OK	03-26-2013 14:56:26	14d 2h 42m 9s	1/3	OK - GNU bash, version 3.2.25(1)-release (x86_64-redhat-linux-gnu) Copyright (C) 2005 Free Software Found
	blacs	OK	03-26-2013 14:56:26	14d 2h 42m 1s	1/3	OK - BLACS version:
	blas	OK	03-26-2013 14:52:48	1d 21h 14m 57s	1/3	OK - BLAS version: 3.2.2-gnu
	fftw	OK	03-26-2013 14:49:19	14d 2h 38m 26s	1/3	OK - FFTW version: 3.1.2
	gnu_compiler	OK	03-26-2013 14:56:24	14d 2h 42m 34s	1/3	OK - gcc (GCC) 4.1.2 20080704 (Red Hat 4.1.2-51)
	gotoblas	OK	03-26-2013 14:56:26	14d 2h 42m 4s	1/3	OK - GOTOBLAS version: 1.13
	lapack	OK	03-26-2013 14:52:53	1d 21h 14m 52s	1/3	OK - LAPACK version: 3.4.2-gnu
	mpi	OK	03-26-2013 14:49:50	14d 2h 37m 55s	1/3	OK - gcc (GCC) 4.1.2 20080704 (Red Hat 4.1.2-51)
	mpiblast	OK	03-26-2013 14:54:23	1d 22h 43m 22s	1/3	OK - MPIBLAST version: mpiBLAST/1.6.0-gnu
	namd	OK	03-26-2013 14:50:21	14d 2h 37m 24s	1/3	OK - NAMD version: NAMD/2.8
	perl	OK	03-26-2013 14:52:50	1d 21h 14m 55s	1/3	OK - This is perl, v5.8.8 built for x86_64-linux-thread-multi Copyright 1987-2006, Larry Wall Perl may be copied the terms of either the Artistic License or the GNU General Public License, which may be found in the Perl 5 sc Complete documentation for Perl, including FAQ lists, should be found on this system using "man perl" or "perl you have access to the Internet, point your browser at http://www.perl.org/, the Perl Home Page.
	python	OK	03-26-2013 14:50:20	14d 2h 37m 25s	1/3	OK - 2.4.3 (#1, May 5 2011, 18:44:23) [GCC 4.1.2 20080704 (Red Hat 4.1.2-50)]
	scalapack	OK	03-26-2013 14:57:41	14d 2h 40m 4s	1/3	OK - SCALAPACK version: 2.0.2-gnu
	tcsh	OK	03-26-2013 14:52:51	1d 21h 14m 54s	1/3	OK - tcsh 6.14.00 (Astron) 2005-03-25 (x86_64-unknown-linux) options wide,nls,d1,a1,kan,sm,rh,color,filec
see-ldap.grid.niif.hu	LDAP	OK	03-26-2013 14:57:28	11d 13h 15m 20s	1/3	LDAP OK - 0.136 seconds response time
ui.ipb.ac.rs	LOOKUP	OK	03-26-2013 14:57:26	53d 13h 22m 0s	1/3	DNS OK: 0.061 seconds response time. ui.ipb.ac.rs returns 147.91.84.247
	PING	OK	03-26-2013 14:57:29	0d 1h 6m 16s	1/3	PING OK - Packet loss = 0%, RTA = 0.53 ms
	SSH	OK	03-26-2013 14:57:26	11d 13h 15m 20s	1/3	SSH OK - OpenSSH_5.3 (protocol 2.0)
	atlas	OK	03-26-2013 14:51:22	26d 16h 16m 23s	1/3	OK - ATLAS version: atlas/3.8.4
	bash	OK	03-26-2013 14:52:23	26d 16h 15m 52s	1/3	OK - GNU bash, version 4.1.2(1)-release (x86_64-redhat-linux-gnu) Copyright (C) 2009 Free Software Found License GPLv3+: GNU GPL version 3 or later <http://gnu.org/licenses/gpl.html> This is free software: you are change and redistribute it. There is NO WARRANTY, to the extent permitted by law.
	blacs	OK	03-26-2013 14:56:26	25d 2h 31m 56s	1/3	OK - BLACS version: blacs/1.1-gnu-openmpi
	blas	OK	03-26-2013 14:52:24	26d 16h 15m 21s	1/3	OK - BLAS version: 3.2.2-gnu
	debugger	OK	03-26-2013 14:53:01	26d 16h 14m 51s	1/3	OK - GNU GDB version: 7.3-0.6
	fftw	OK	03-26-2013 14:53:27	26d 16h 14m 20s	1/3	OK - FFTW version: fftw/3.2.1
	gnu_compiler	OK	03-26-2013 14:53:55	26d 16h 13m 49s	1/3	OK - gcc (GCC) 4.1.2 20120305 (Red Hat 4.1.6-4)

PRACE ekvivalense: INCA

Infrastruktúra – HP-SEE RMS portál



HP-SEE

Welcome, Dobromir M. Georgiev

HP-SEE username: **dgeorgiev**

[Profile](#) [HPC Centres](#) [Requests](#) [Resources](#) [Support](#)

Remaining resources

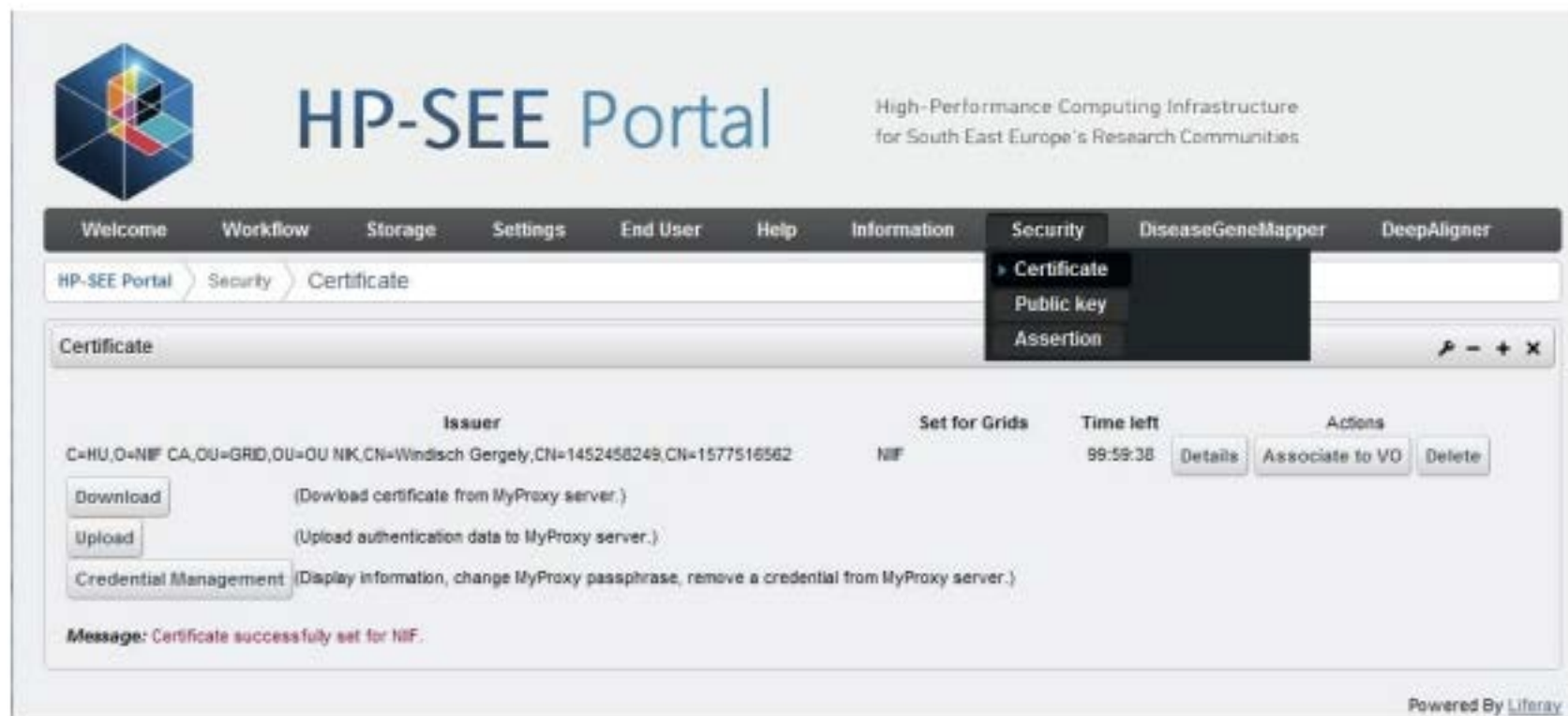
Approved resource requests

Request information	Status	Used CPU time	JobCount	Remaining CPU time
HPC centre: HPCG CPU time: 3000 hours Storage: 232GB Applications: HMLQCD	Approved	1698.8919	699	1301.1081

Pending resource requests

Request information	Status
HPC centre: BG CPU time: 8754 hours Storage: 522GB Applications: HMLQCD	Pending

Infrastruktúra – Biológusokat támogató portál



The screenshot displays the HP-SEE Portal interface. At the top left is a hexagonal logo with colorful geometric shapes. The title "HP-SEE Portal" is prominently displayed in the center, with the subtitle "High-Performance Computing Infrastructure for South East Europe's Research Communities" to its right. A navigation bar below the title contains links: Welcome, Workflow, Storage, Settings, End User, Help, Information, Security, DiseaseGeneMapper, and DeepAligner. The "Security" link is active, and a sub-menu is open showing "Certificate", "Public key", and "Assertion". The "Certificate" sub-menu item is selected. Below the navigation bar, the breadcrumb trail shows "HP-SEE Portal > Security > Certificate". The main content area is titled "Certificate" and contains a table with one row of certificate information. The table has columns for Issuer, Set for Grids, Time left, and Actions. The Issuer column contains the text "C=HU,O=NIF CA,OU=GRID,OU=OU NIK,CN=Windisch Gergely,CN=1452458249,CN=1577516562". The Set for Grids column contains "NIF". The Time left column contains "89:59:38". The Actions column contains buttons for "Details", "Associate to VO", and "Delete". Below the table, there are three buttons: "Download" (with the description "(Download certificate from MyProxy server.)"), "Upload" (with the description "(Upload authentication data to MyProxy server.)"), and "Credential Management" (with the description "(Display information, change MyProxy passphrase, remove a credential from MyProxy server.)"). At the bottom of the main content area, a message states "Message: Certificate successfully set for NIF." The footer of the page indicates "Powered By Liferay".

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

Welcome Workflow Storage Settings End User Help Information **Security** DiseaseGeneMapper DeepAligner

HP-SEE Portal > Security > Certificate

Certificate

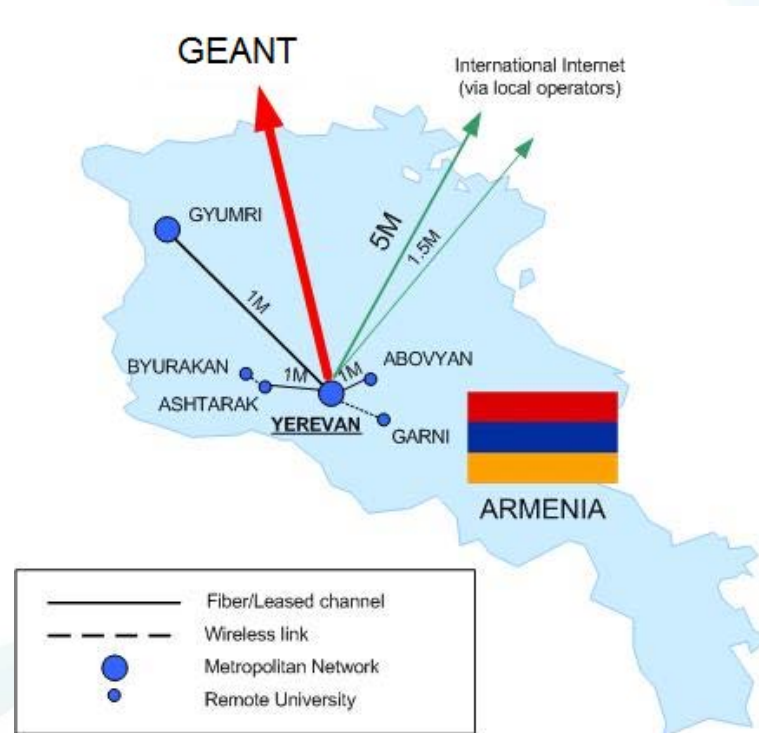
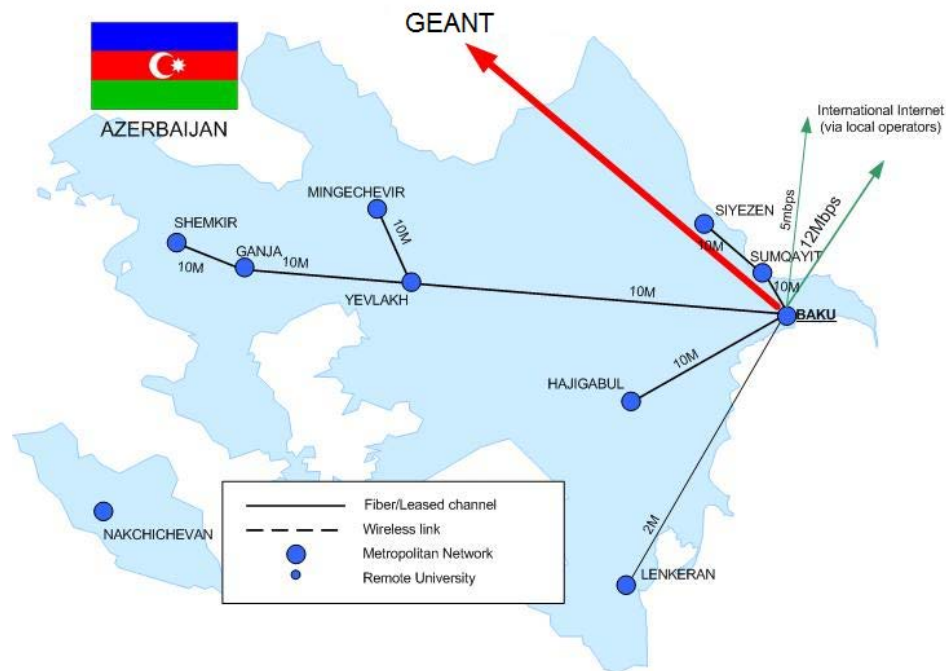
Issuer	Set for Grids	Time left	Actions
C=HU,O=NIF CA,OU=GRID,OU=OU NIK,CN=Windisch Gergely,CN=1452458249,CN=1577516562	NIF	89:59:38	Details Associate to VO Delete

[Download](#) (Download certificate from MyProxy server.)
[Upload](#) (Upload authentication data to MyProxy server.)
[Credential Management](#) (Display information, change MyProxy passphrase, remove a credential from MyProxy server.)

Message: Certificate successfully set for NIF.

Powered By [Liferay](#)

GEANT hálózat bővítése



Alkalmazás optimalizáció

Elért skálázódás (CPU core)	HPC alkalmazás
4096	SET
1024	GIM
512	FMD-PA
258	NUQG
256	DNAMA
256	DeepAligner
256	DiseaseGeneMapper
128	CompChem
64	HC-MD-QM-CS
64	MSBP
60	GENETATOMICS
48	SFHG
32	CFDOF
16	AMR_PAR

HPC környezet kipróbálása

<http://www.hp-see.eu/hp-see-fast-track>

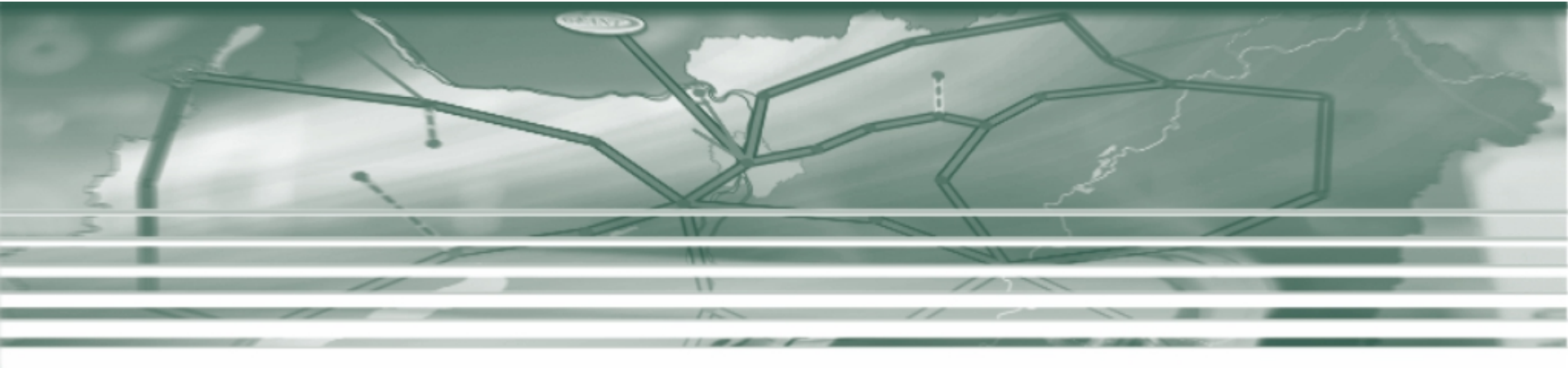
- Maximum 2 hónap

Hasznos linkek

HP-SEE-ről bővebben:

- <http://www.hp-see.eu/material/61>
- http://hpseewiki.ipb.ac.rs/index.php/HP-SEE_Wiki
- <http://indico.ipb.ac.rs/categoryDisplay.py?categId=3>

Köszönöm a figyelmet!



Rőczei Gábor