

# HP-SEE

## Regional eInfrastructure Development for South East Europe's Research

Workshop on e-Infrastructures in Eastern Partnership Countries

11th December 2012  
[www.hp-see.eu](http://www.hp-see.eu)



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# HP-SEE

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

# HP-SEE



## HP-SEE

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

- ❑ **Contract n°:** RI-261499
- ❑ **Project type:** CP & CSA
- ❑ **Call:** INFRA-2010-1.2.3: VRCs
- ❑ **Start date:** 01/09/2010
- ❑ **Duration:** 24 + 12 months
- ❑ **Total budget:** 3 885 196 €
- ❑ **Funding from the EC:** 2 100 000 €
- ❑ **Total funded effort, PMs:** 539.5
- ❑ **Web site:** [www.hp-see.eu](http://www.hp-see.eu)



## HP-SEE

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# HP-SEE Partnership



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## Contractors (14)

GRNET	Coordinating Contractor	Greece
IICT-BAS	Contractor	Bulgaria
IFIN-HH	Contractor	Romania
TÜBİTAK-ULAKBİM	Contractor	Turkey
NIIFI	Contractor	Hungary
IPB	Contractor	Serbia
UPT	Contractor	Albania
UOBL ETF	Contractor	Bosnia-Herzegovina
UKIM	Contractor	FYROM
UOM	Contractor	Montenegro
RENAM	Contractor	Moldova (Republic of)
IIAP NAS RA	Contractor	Armenia
GRENA	Contractor	Georgia
AZRENA	Contractor	Azerbaijan

**Third Party / JRU mechanism used**  
associate universities / research centres

# HP-SEE Project Objectives



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- ❑ Objective 1 – Empowering multi-disciplinary virtual research communities
  
- ❑ Objective 2 – Deploying integrated infrastructure for virtual research communities
  - ❑ Including a GEANT link to Southern Caucasus
  
- ❑ Objective 3 – Policy development and stimulating regional inclusion in pan-European HPC trends
  
- ❑ Objective 4 – Strengthening the regional and national human network

# HPC Systems in the region



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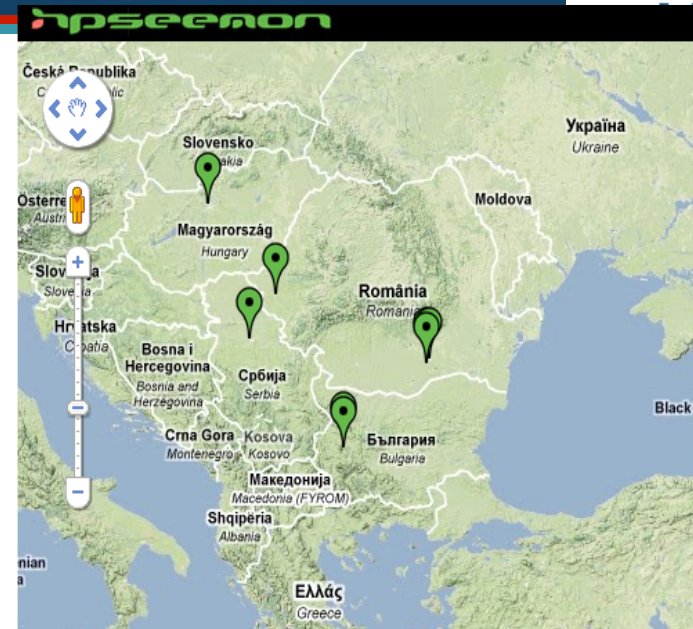
Workshop on e-Infrastructures in Eastern Partnership Countries – Chisinau, Moldova 11<sup>th</sup> December 2012

# High-Performance Computing



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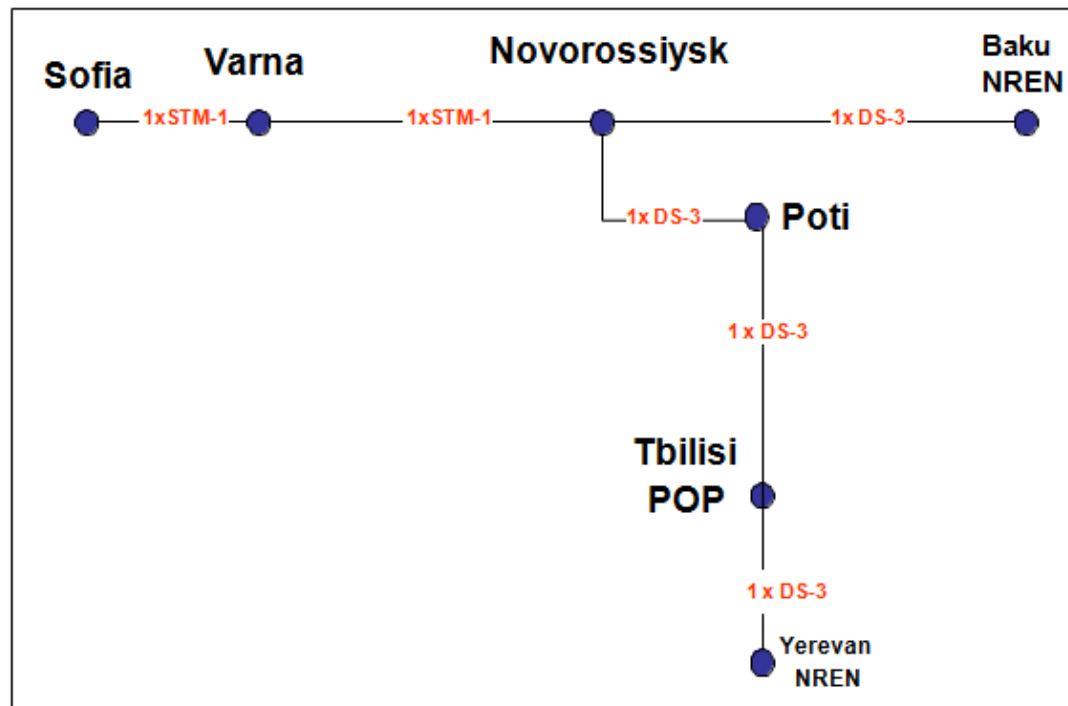
- ❑ 120 Tflops aggregate
- ❑ 2 BlueGene machines
- ❑ Bulgaria, Romania, Serbia, Hungary, FYRoM offering resources
- ❑ Procurements coming - Greece and Serbia
- ❑ 26 applications in 3 VRCs
- ❑ Envisaged as bridge to PRACE
- ❑ Joint operations centre studied and assessed



# Topology of GÉANT link to the South Caucasus



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- The beneficiaries in Armenia are ASNET-AM, ARENA and Armenian National Grid Initiative.
- The beneficiaries in Azerbaijan are the most of the universities and research centers (Azerbaijan Technical University, Azerbaijan Oil Academy, Azerbaijan Architecture and Construction University, National Academy of Science (Grid initiative))

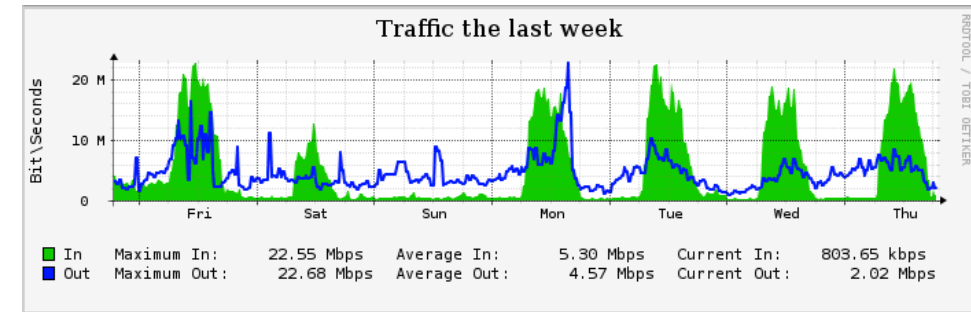
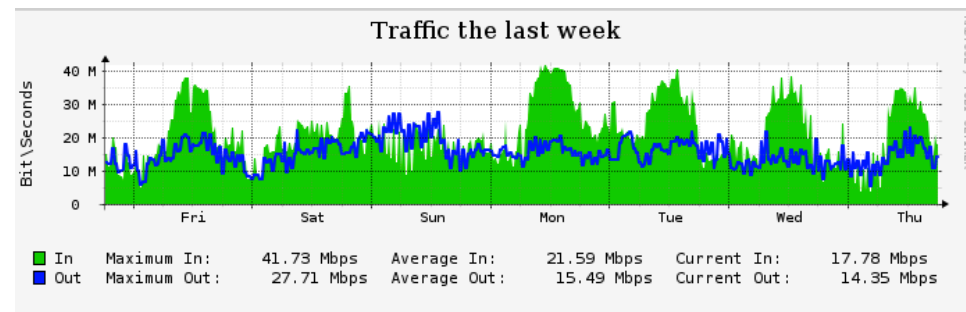
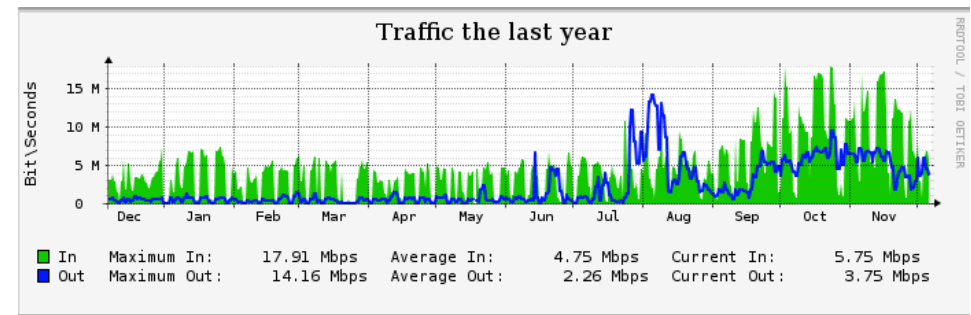
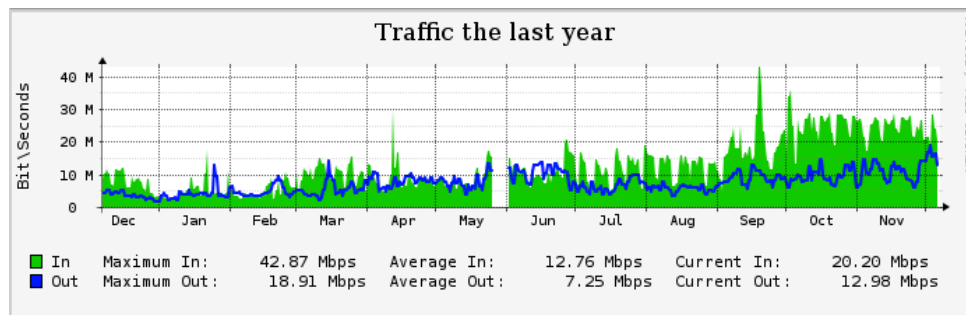
# GÉANT link Traffic Statistics



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## Yerevan-Sofia

## Baku-Sofia



<http://hp-see.ulakbim.gov.tr/hp-see/index.php?name=yerevan-sofia>

<http://hp-see.ulakbim.gov.tr/hp-see/index.php?name=baku-sofia>

Nagios®





# Applications: key results



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- ❑ Supported applications within **Virtual Research Communities**
- ❑ Computational Physics  
6 countries  
12 applications
- ❑ Computational Chemistry  
6 countries  
7 applications
- ❑ Life Sciences  
5 countries  
7 applications

Country	Physics	Chemistry	Life Sciences	TOTAL
Albania	2			2
Armenia			1	1
Bosnia-Herzegovina	1	1		2
Bulgaria	3	2		5
Georgia			1	1
Greece		1	2	3
Hungary			2	2
Moldova	1			1
Montenegro			1	1
FYR of Macedonia	1	1		2
Romania	3	1		4
Serbia	1	1		2
<b>TOTAL</b>	<b>12</b>	<b>7</b>	<b>7</b>	<b>26</b>

# Computational Physics VRC



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- ❑ Applications Areas
  - ❑ High Energy and Particle Physics
  - ❑ Plasma Physics
  - ❑ Physics of Condensed Matter
  - ❑ Atomic Physics
  - ❑ Computational Fluid Dynamics
- ❑ Indicative Applications range
  - ❑ Nano-electronics
  - ❑ Micro-devices optimization and modeling of robotic devices for biomedicine
  - ❑ Feature detection in satellite images
  - ❑ Modeling of electron transport
  - ❑ Complex gas dynamics and convection

# Computational Chemistry VRC



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- ❑ Applications Areas
  - ❑ Molecular dynamics and simulations
  - ❑ Material science
- ❑ Indicative Applications range
  - ❑ Study of physicochemical properties of compounds
  - ❑ Molecular design of platinum complexes
  - ❑ Material design for photonic applications
  - ❑ Molecular-orbital simulations
  - ❑ Design of chemical reactors, burners, boilers
  - ❑ Quantum mechanical simulation of Condensed Phases

# Life Sciences VRC



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- ❑ Applications Areas
  - ❑ Neuroscience
  - ❑ Proteomics
  - ❑ Genomics and DNA sequence analysis
- ❑ Indicative Applications range
  - ❑ Network models of short and long term memory
  - ❑ Identification of novel miRNA genes
  - ❑ Genomics / sequence analysis
  - ❑ Molecular Dynamics
  - ❑ Synthesis of nucleotide bases

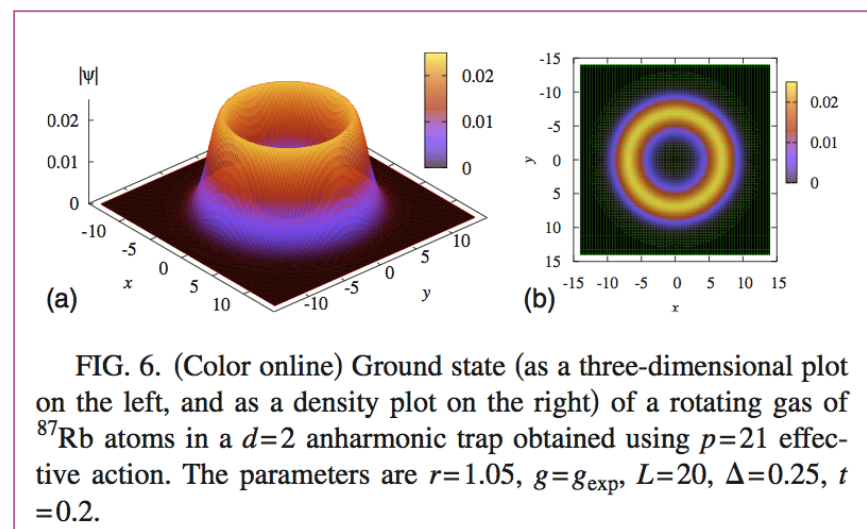
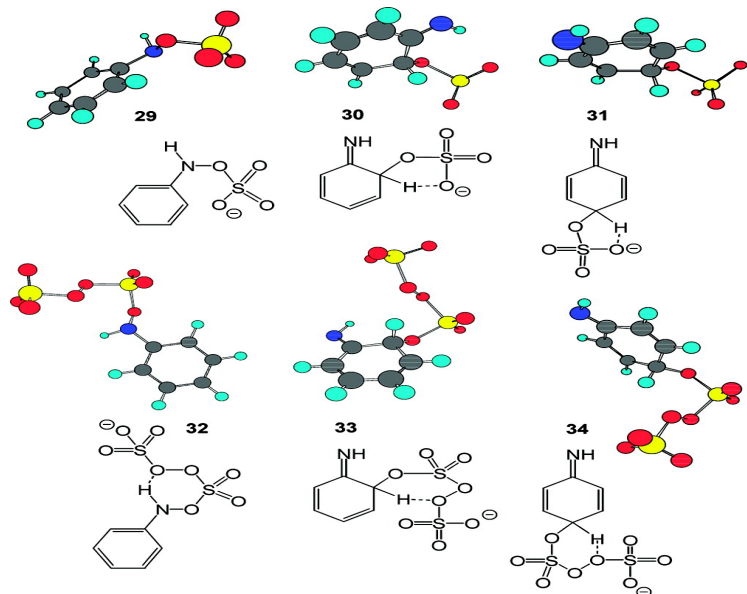
# HPC: application examples



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- Numerical study of ultra-cold quantum gases
- Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation in chemistry
- Searching for novel miRNA genes and their targets tems



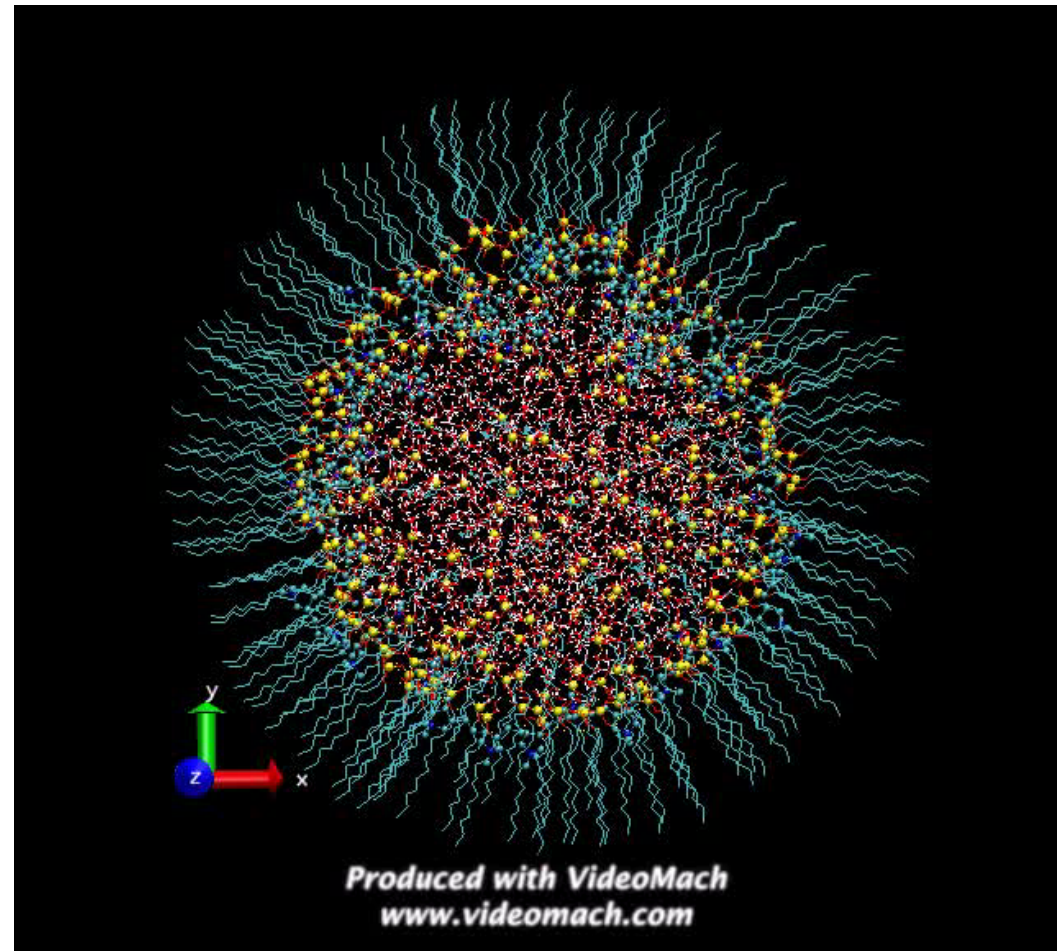
# HPC: application example for Armenia



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## Molecular Dynamics Study of Complex Systems (MDSCS)

**Introduction:** The parallel molecular dynamics simulation of complex system consisting of surfactant/polymer mixtures has been carried out. The molecular dynamics results together with experimental findings help to understand the mechanism of interactions in physical point of view and, which is most important, will give us an important information concerning the conformation and localization of system components (polymer, surfactant, water, etc.).



# HPC: application example for Armenia



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## MDSCS Publications 2012

- ❑ A. Shahinyan, et al., The study of lyotropic liquid crystal structure using the molecular dynamics method, Journal of Molecular Crystals and Liquid Crystals, 2012, DOI:10.1080/15421406.2012.687174
- ❑ Armen Poghosyan, et al., A Molecular Dynamics Study of Intermediate Phase of Long Chain Alkyl Sulfonate/Water Systems, Langmuir Journal, American Chemical Society, 2012, DOI: 10.1021/la302378r
- ❑ A. Poghosyan, L. Arsenyan, H. Astsatryan, et al, NAMD Package Benchmarking on the Base of Armenian Grid Infrastructure, Journal of Communications and Network, Scientific Research Publishing, Vol. 4 No. 1, 2012, pp. 34-40, doi: 10.4236/cn.2012.41005
- ❑ A.A.Shahinyan, L.H.Arsenyan, A.H.Poghosyan, The Study of Phase Diagram of the Surfactant/Water System by Molecular Dynamics Simulation, Book of Abstracts of 5th Japan – Russia International Workshop "Molecular Simulation Studies in Material and Biological Sciences", Joint Institute for Nuclear Research, Dubna, Russia, September 9 – 12, 2012.
- ❑ A.H. Poghosyan, L. H. Arsenyan, H.V. Astsatryan, NAMD Benchmarking of Complex System on Bulgarian BlueGene/P, IEEE Proceedings of MIPRO 2012 - Jubilee 35th International Convention, Opatija, Croatia, pp. 319-321.



# Producing results / scientific publications



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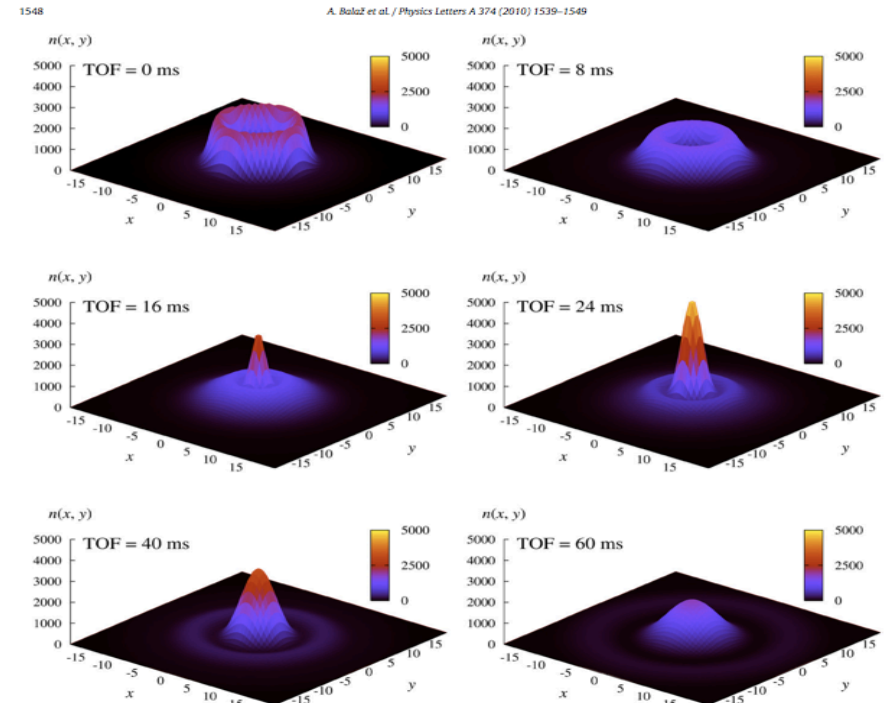
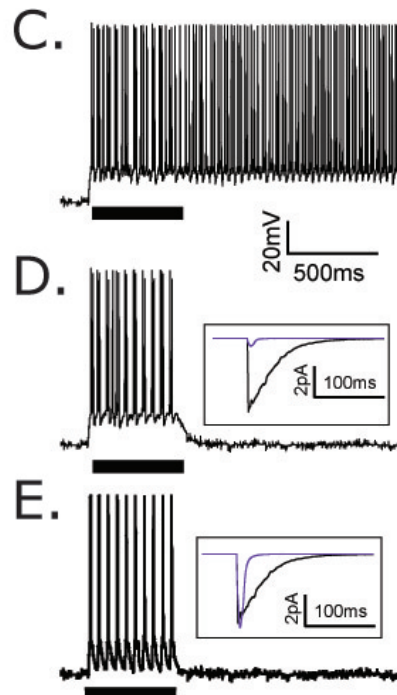
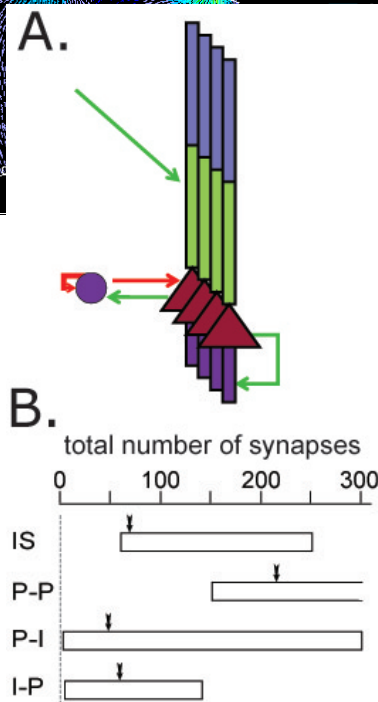
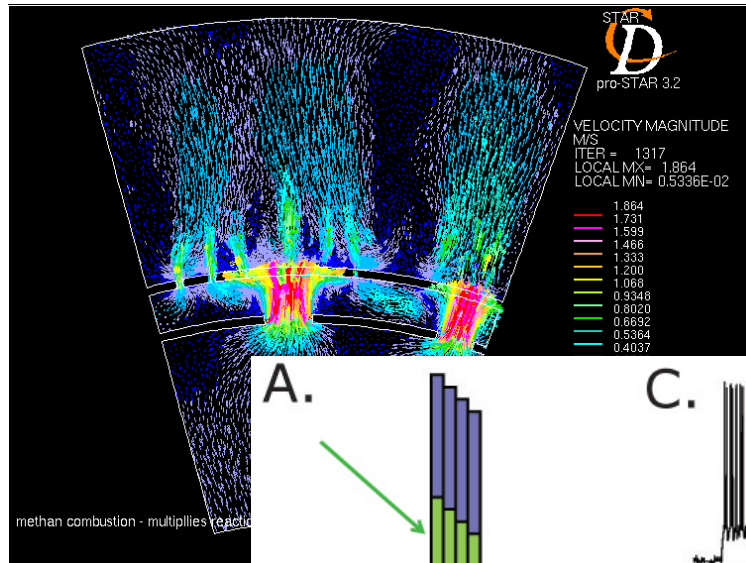


Fig. 11. Time-of-flight absorption density profiles in  $xy$ -plane for an over-critically rotating ( $r = 1.04$ ) condensate of  $N = 3 \cdot 10^5$  atoms of  $^{87}\text{Rb}$  with the anharmonicity  $k = k_{\text{BEC}}$  at  $T = 30$  nK. The flight time, designated as TOF, is given at each plot. The dimensionless unit length on all graphs corresponds to  $1.34 \mu\text{m}$  and the linear size of profiles is approximately  $53.6 \mu\text{m}$ . The discretization parameters are given in Table 3.



# User Requirements in EP countries – HEP Armenia



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- Grid site (6 nodes/48 cores – Dell PE1950 III) located in Yerevan Physics Institute supports ATLAS and ALICE VO communities

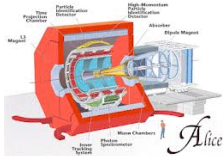
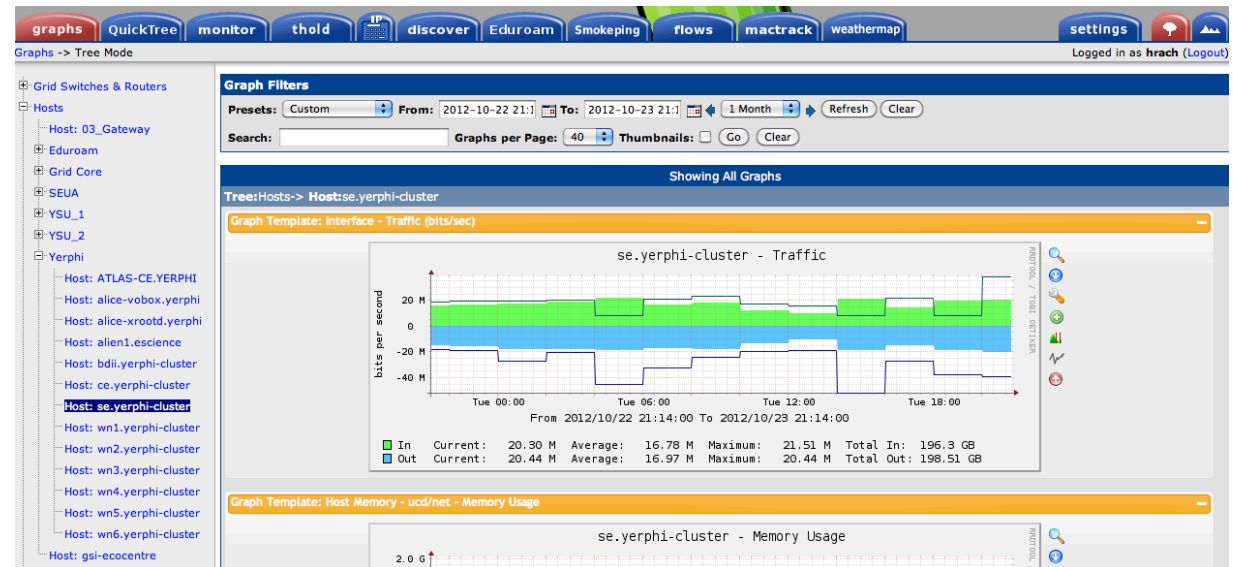
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ANALY_AM-04-YERPHI	voatlas215	5	0	0	2	2	1
ANALY_AM-04-YERPHI	voatlas214	8	0	0	0	0	0
ANALY_AM-04-YERPHI	voatlas213	8	0	0	1	1	1

Factory	job	state	payload?	created	last modified
voatlas214	9456029.0	CREATED	-	4 hrs ago	4 hrs ago
voatlas213	9146699.0	CREATED	-	18 hrs ago	12 hrs ago
voatlas213	9145778.0	CREATED	-	19 hrs ago	13 hrs ago
voatlas213	9144699.0	CREATED	-	20 hrs ago	14 hrs ago
voatlas213	9056403.0	FAULT	-	4 days ago	17 hrs ago
voatlas215	9034450.0	CREATED	-	23 hrs ago	17 hrs ago
voatlas213	9145693.0	DONE	miss	19 hrs ago	19 hrs ago
voatlas215	8941120.0	FAULT	-	5 days ago	19 hrs ago
voatlas214	9438463.0	CREATED	-	1 day ago	22 hrs ago
voatlas215	9034319.0	DONE	miss	1 day ago	23 hrs ago
voatlas215	9034031.0	DONE	miss	1 day ago	23 hrs ago
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voatlas213	9124789.0	CREATED	-	1 day ago	1 day ago



- After 80 additional servers upgrade (from DESY)?



# New Access Mechanisms



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- ❑ Pilot call for access to resources
  - ❑ Call closed -> 5<sup>th</sup> of October
  - ❑ Resources to be offered: 4.6 Million Core hours, 1.8 Million GPU hours
  - ❑ Allocations for 1 year – starting December 2012
  - ❑ Peer review based
  - ❑ Access to the resources from all countries of the region
  
- ❑ Fast track access mechanism
  - ❑ Limited resources provided
  - ❑ 2 Month allocation period
  - ❑ Suitable for: New user communities – Non experienced users

# HP-SEE: Other services



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- ❑ Support for the development of national and regional organizational models
- ❑ Distributed operations
- ❑ Technology watch and infrastructure deployment strategies
- ❑ Scalability and interoperability studies
- ❑ User and Applications support
- ❑ Training
- ❑ Dissemination to scientific but also wider communities

# HPC: regional benefits



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- ❑ Mutual support in HPC technology
- ❑ Know-how exchange through regional operations, procurement know-how
- ❑ Regional user communities
- ❑ Platform to entry-level for PRACE
- ❑ Know-how for national-level organizational models
  
- ❑ Policy support for regional resource sharing by governmental agencies through SEERA-EI
- ❑ Concrete support of hosting agencies materialized through a common pilot call for applications
- ❑ Stimulation of national-level projects

# Long Term Vision



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

- ❑ Being on the technological par with the rest of Europe
- ❑ Enabling local scientists to use their potential
- ❑ Integrating the region into pan-European e-Infrastructure landscape
- ❑ Role-model for regional developments
- ❑ Leading the way in wider contexts