# HP-SEE

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

**HP-SEE User Forum, 17th October 2012**

www.hp-see.eu


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


The HP-SEE initiative is co-funded by the European Commission under the FP7 Research Infrastructures contract no. 261499

# Pan-EU e-Infrastructures vision

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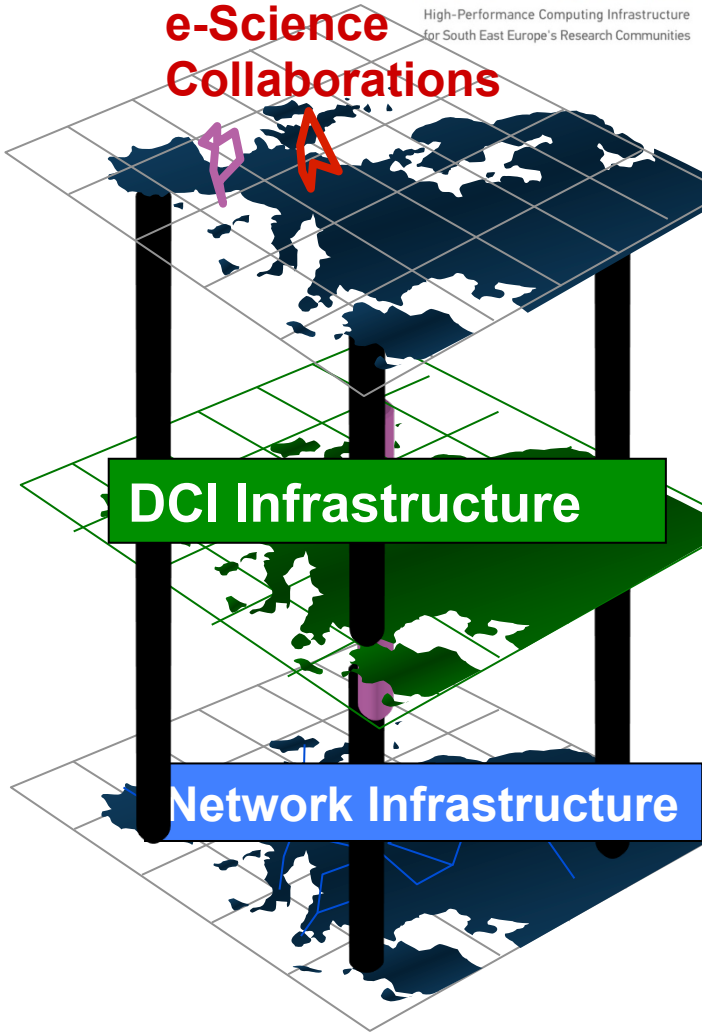
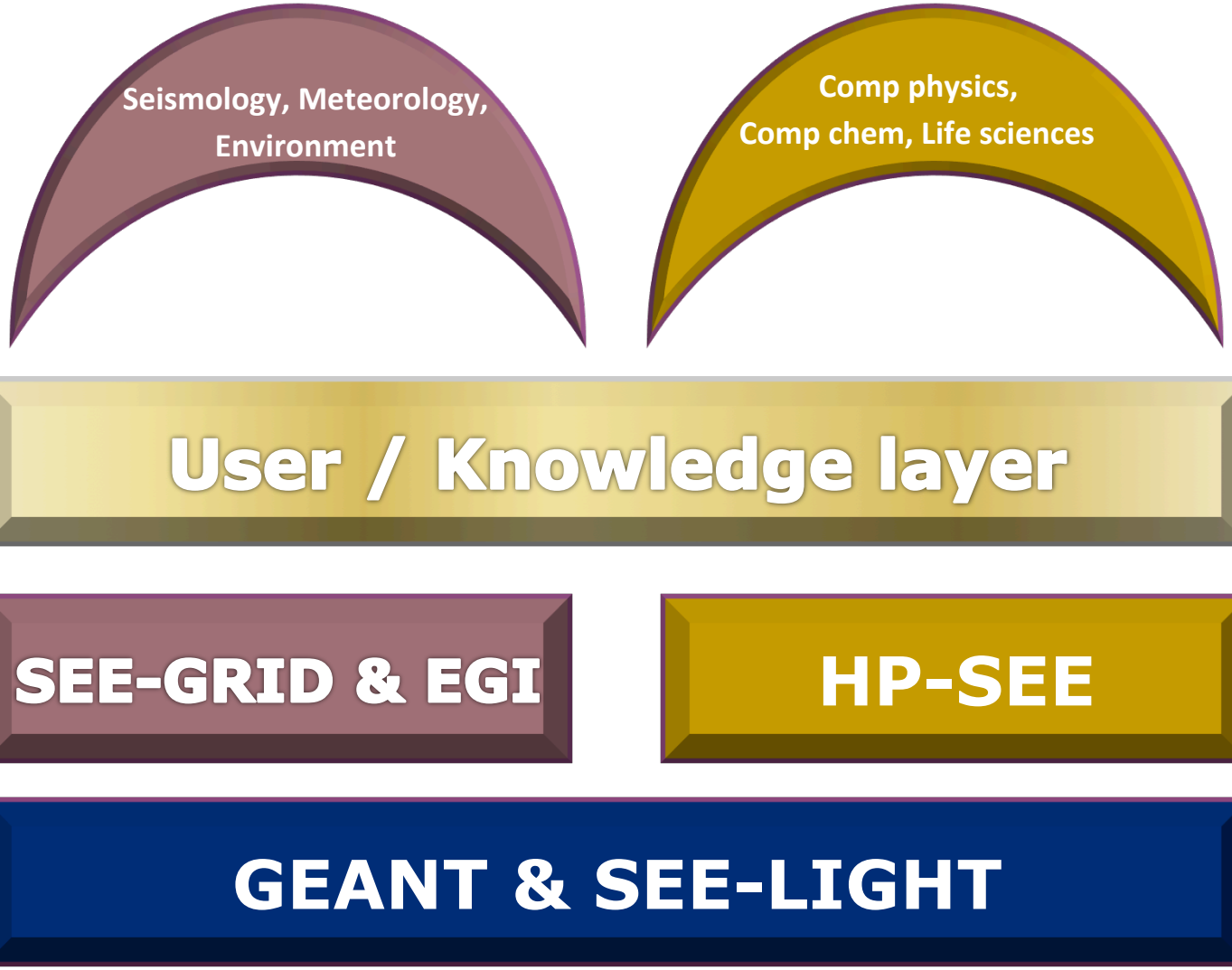
- The Research **Network infrastructure** provides fast interconnection and advanced services among Research and Education institutes of different countries
- The Research **Distributed Computing Infrastructure (Grid, HPC)** provides a distributed environment for sharing computing power, storage, instruments and databases through the appropriate software (middleware) in order to solve complex application problems
- This integrated environment is called **electronic infrastructure (eInfrastructure)** allowing new methods of global collaborative research - often referred to as **electronic science (eScience)**



# SEE Model: Converged communication & service infrastructure for the region

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# SEE eInfrastructure partners

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- "Provider/manager" partners:
  - National Research and Education Networks – NRENs – bodies that provide network connectivity to universities, schools, research institutes, etc.
  - National Grid Initiatives – NGIs – consortium of computing providers in the country; includes HPC providers
- Affiliated "Stakeholder" partners:
  - Research institutes, universities
- Policy makers:
  - Ministries, agencies, research councils

- Western Balkans, Greece, Turkey, Bulgaria, Romania, Moldova, Southern Caucasus.

# SEE eInfrastructure projects

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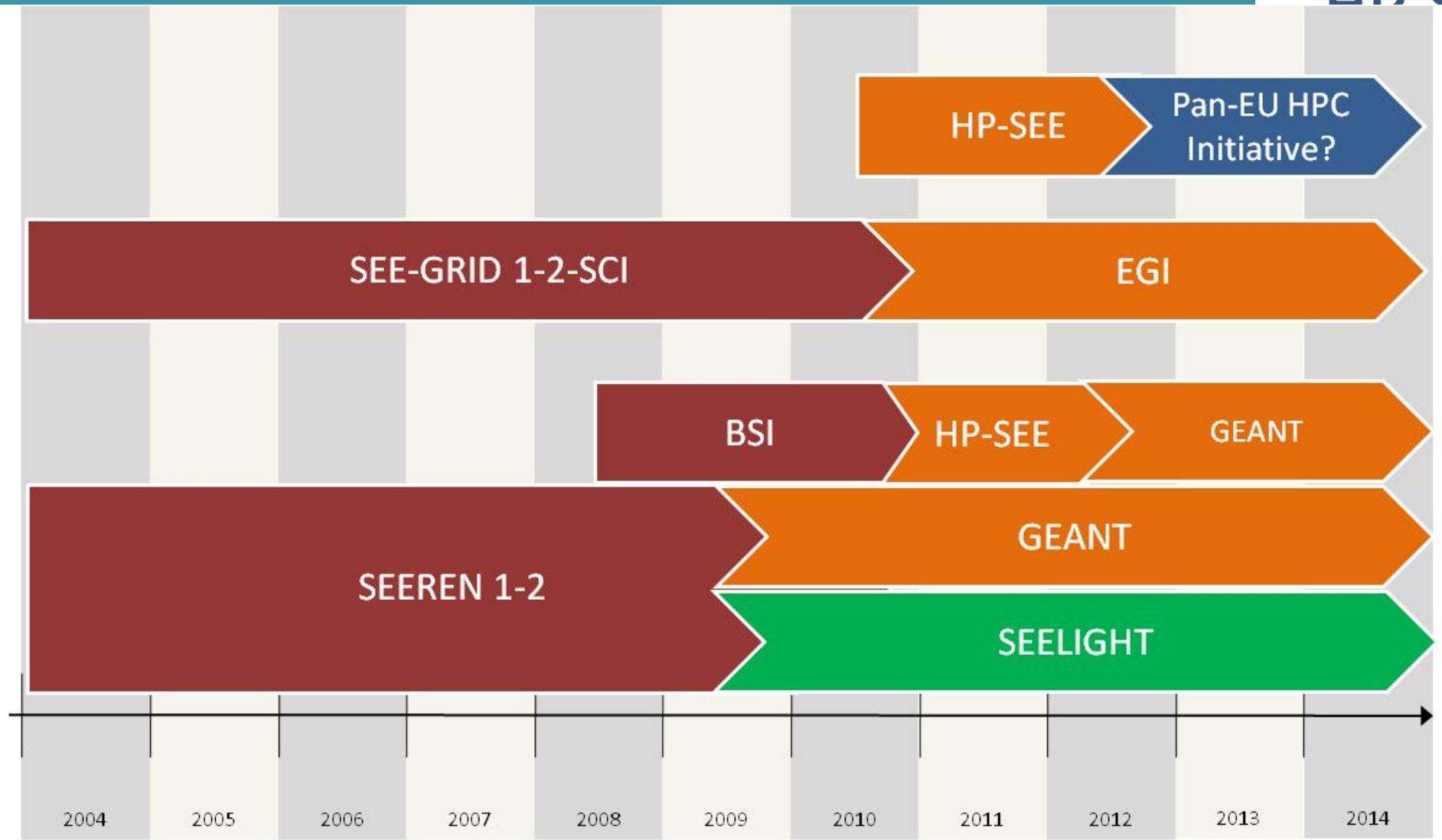
- **SEEREN1/2:** regional inter-NREN connectivity and GEANT links [DGINFSO]
- **BSI:** Southern Caucasus links [DGINFSO]
- **SEELIGHT:** lambda facility in SEE [Greek HiperB]
- *Result: sustainable national & regional networks, most countries in GEANT*

- **SEEGRID1/2:** regional Grid infrastructure, building NGIs and user communities
- **SEE-GRID-SCI:** eInfrastructure for large-scale environmental science user communities: meteorology, seismology, environmental protection. Inclusion of Caucasus. [DGINFSO]
- *Result: sustainable national Grids, regional coordination, all countries within European Grid Initiative*

- **HP-SEE**: regional HPC interconnection and 2nd generation Caucasus link
- *Expected result: stable national HPC centers, (hierarchical) model in collaboration with PRACE and DEISA*

- **SEERA-EI:** regional programme managers collaboration towards common eInfrastructure vision, strategy and regional funds [DGRTD]
- *Result: influencing national agendas, setting common regional policy, identifying regional funds to complement EC funds*

# Timeline & funding modalities: synergy and complementarity



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# Network

# Network: SEELIGHT

- SEEREN projects set up regional NREN connectivity and GEANT links
- SEE-LIGHT: South-East European Lambda Network Facility for R&E
- Deployment of an advanced regional network infrastructure, fibres and equipment
- Under the Hellenic Plan for the Economic Reconstruction of the Balkans – HiPERB (80-20)
- Serbia implementation stage, Bulgaria tender stage, Romania on own funds, FYR of Macedonia ongoing
- SEENet: a management body for SEELIGHT

# Network: regional benefits

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- Exploit economy of scale
  - Connectivity
  - Common operations
- Being on a par with EU
- Common development path for ICT
- Joint platform for advanced services
- Policy support for cross-border links by governmental agencies through SEERA-EI

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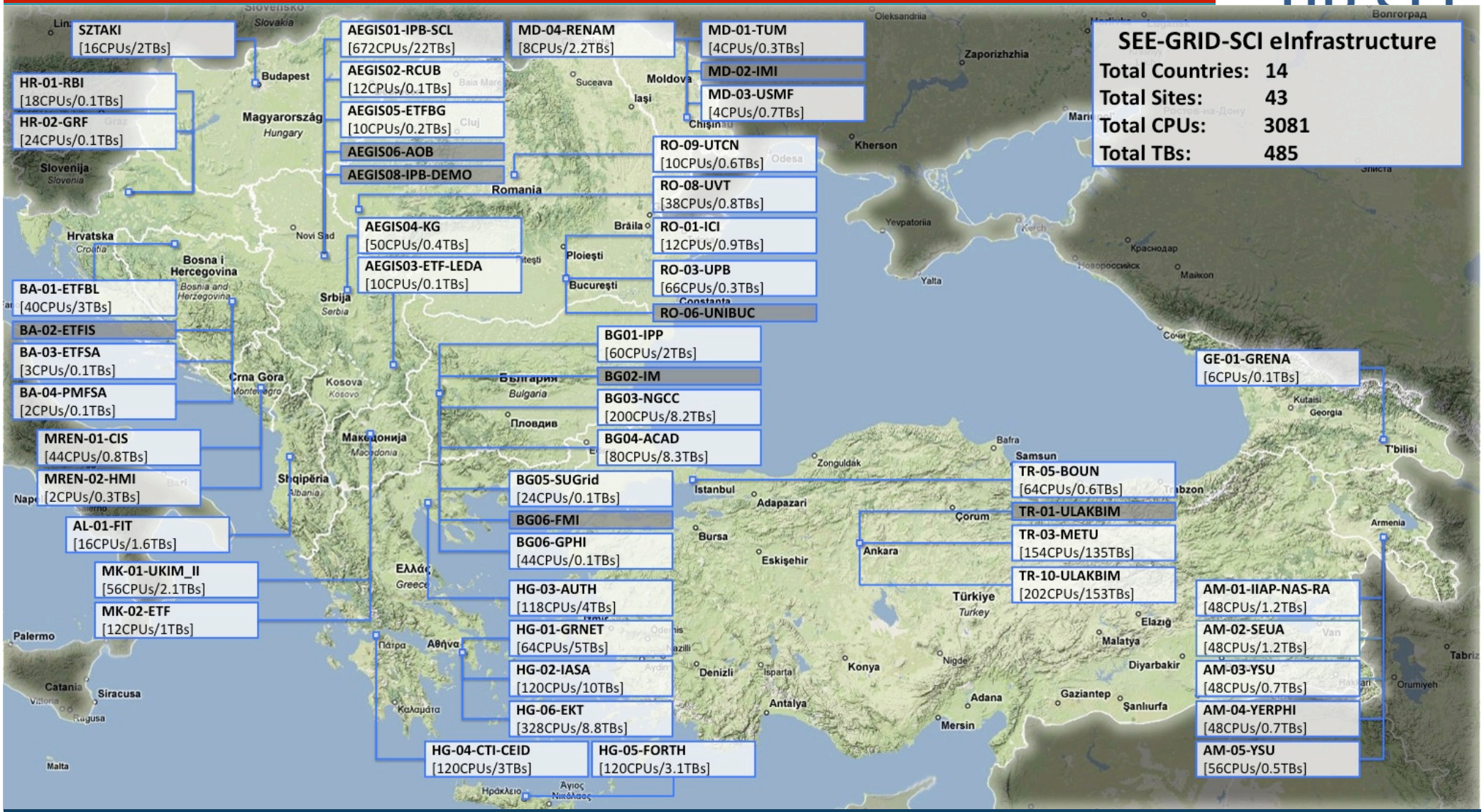
# Grid Computing

# Grid: the SEE-GRID series



# Grid: the SEE-GRID series

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- Regional infrastructure and operations built through 3 projects
- User community buy-in secured
- National structuring via NGIs
- All countries in European Grid Initiative
- Key to success: distributing operations and supporting cross-border communities

# Grid: regional benefits

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- Being on a par with EU
- Know-how exchange through regional operations and user support
- Common development path for computing
- Strong regional user communities
- Know-how for national-level organization models

- Policy support for regional resource sharing by governmental agencies through SEERA-EI
- Stimulation of national-level projects

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# High Performance Computing

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- **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

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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-ULAKBIM | 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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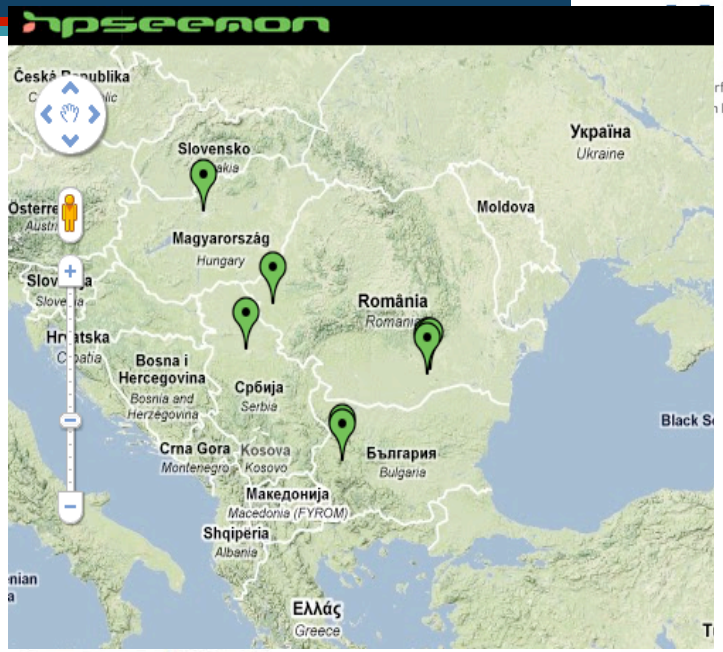
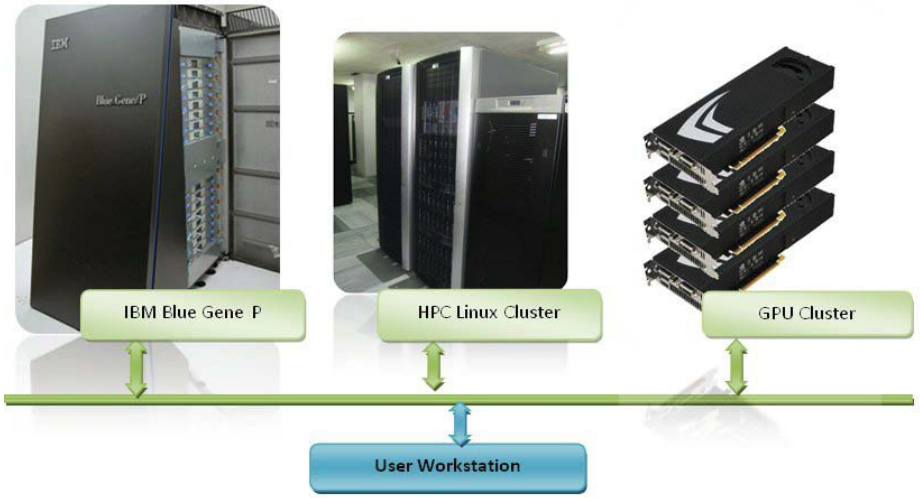
# High-Performance Computing

- 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



# 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** |
| Greee | | 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** |
| **TOTAL** | **12** | **7** | **7** | **26** |

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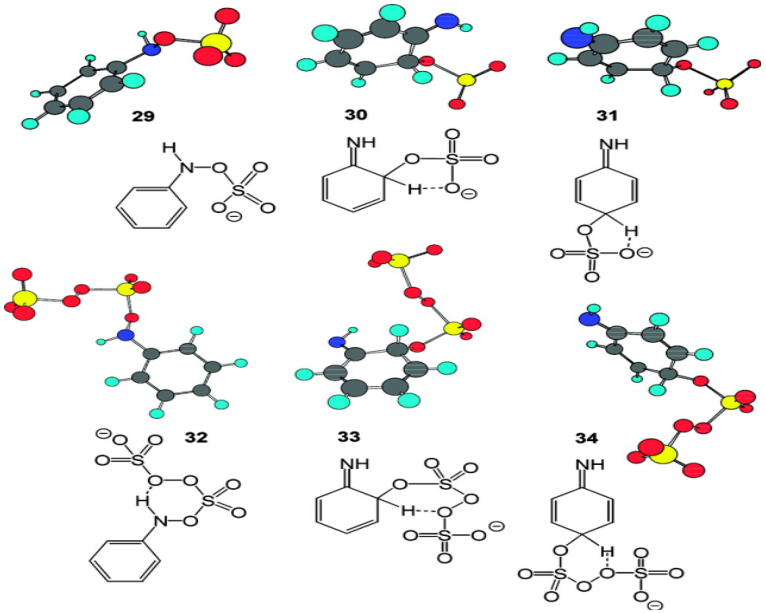
- Numerical study of ultra-cold quantum gases
- Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation in chemistry
- Searching for novel miRNA genes and their targets tems



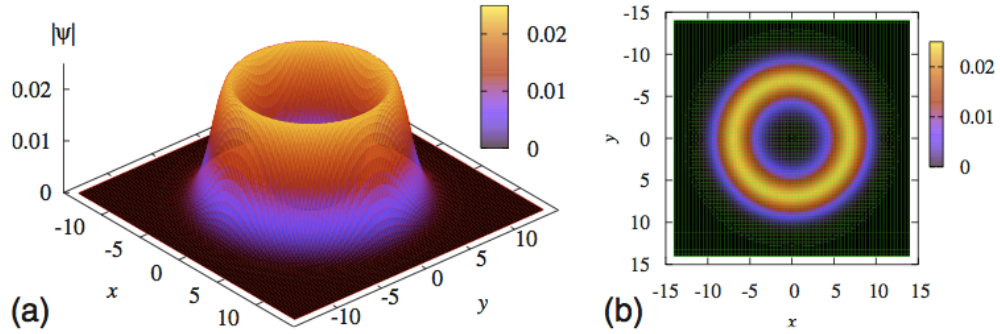
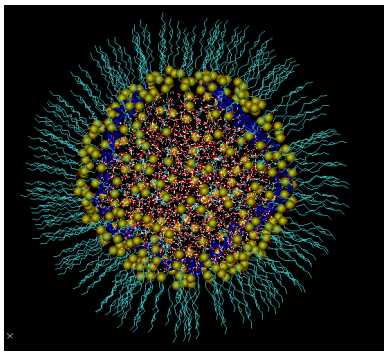




FIG. 6. (Color online) Ground state (as a three-dimensional plot on the left, and as a density plot on the right) of a rotating gas of $^{87}$Rb atoms in a $d$=2 anharmonic trap obtained using $p$=21 effective action. The parameters are $r$=1.05, $g$=$g_{exp}$, $L$=20, $\Delta$=0.25, $t$ =0.2.



# `Producing results / scientific publications

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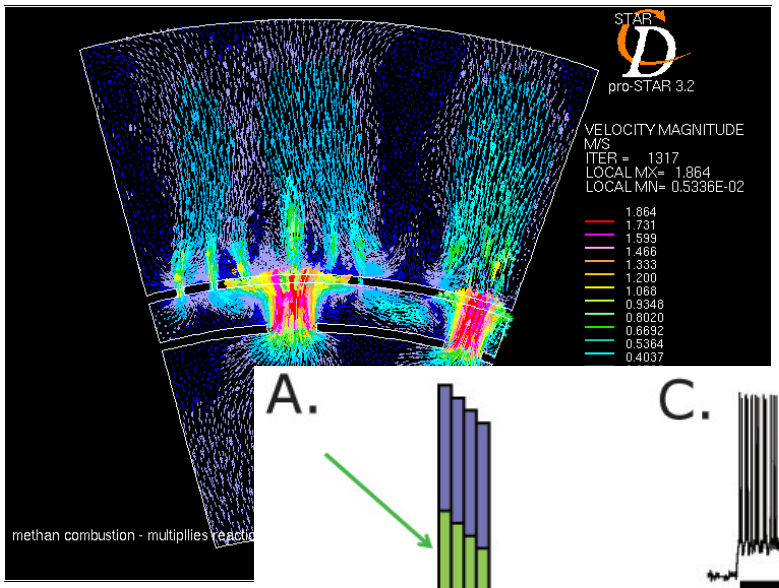


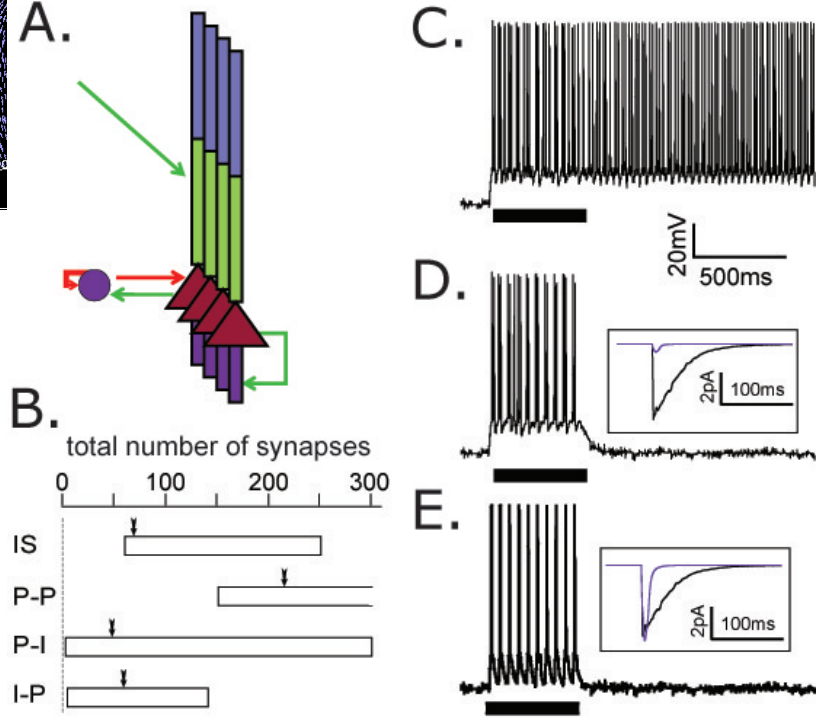


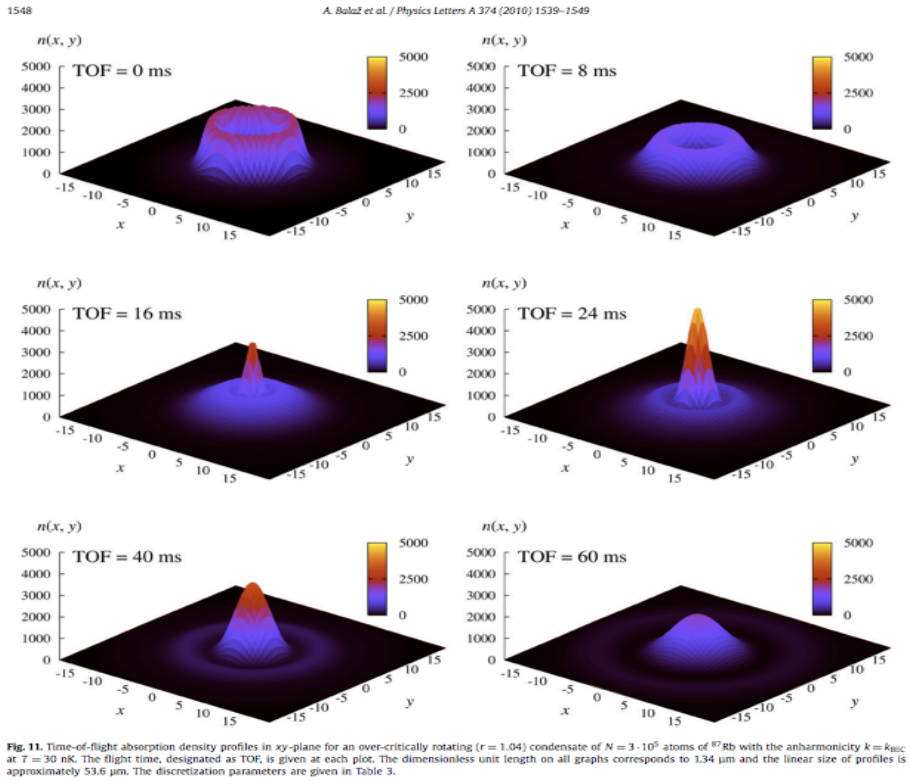


Fig. 11. Time-of-flight absorption density profiles in $xy$-plane for an over-critically rotating ($r = 1.04$) condensate of $N = 3 \cdot 10^5$ atoms of $^{87}$Rb with the anharmonicity $k = k_{BEC}$ at $T = 30$ nK. The flight time, designated as TOF, is given at each plot. The dimensionless unit length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

# New Access Mechanisms

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- Pilot call for access to resources
  - Call closed -> 5th 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

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# Policy

# SEERA-EI

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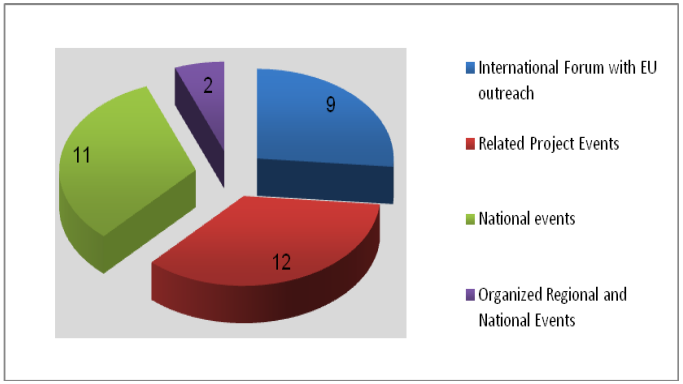
- **Core Objective:** Develop and strengthen the coordination and cooperation of national eInfrastructures programmes in the region of South-East Europe.
- National programme Best Practices identification
- National programme Cookbook
- Studies on long term strategy for major eInfrastructures



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# Long Term Vision

# Long Term Vision

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- 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