Institutul de Matematică şi Informatică
Institutul de Economie,Finanţe şi Statistică

HP-SEE

# Scientific computing – current state and perspectives of development

Dr. Petru Bogatencov

IMI ASM,
RENAM

www.math.md

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

# Scientific Computing - definitions

- Computing facilities based on Parallel Architectures including:
  - Cluster systems,
  - Grid systems,
  - Supercomputers,
  - Scientific Clouds…
- Parallel Algorithm Design and Programming
- Parallel Computing Applications Development
- Scientific Computing architecture is a bridge for building modern virtualized computing systems

# Importance of Scientific Computing for Research

- *"Although the fastest computers can execute millions of operations in one second, they are always too slow. This may seem a paradox, but the heart of the matter is: the bigger and better computers become, the largest are the problems scientists and engineers want to solve."*

  **A. Jaffe, Ordering the Universe: The Role of Mathematics, SIAM Review, 1984**

- *"Computing has become a third branch of research, joining the traditional practices of theorization and laboratory experimentation and verification. Due to the expense and complexity of actually performing experiments in many situations, simulation must be done first."*

  **C. C. Douglas, G. Haase, U. Langer, A Tutorial on Elliptic PDE Solvers and their Parallelization, SIAM, 2003**

# The knowledge triangle at work

**To be a genuinely competitive in the knowledge economy, one must be better**

- in producing knowledge through research
- in diffusing it through education
- in applying it through innovation

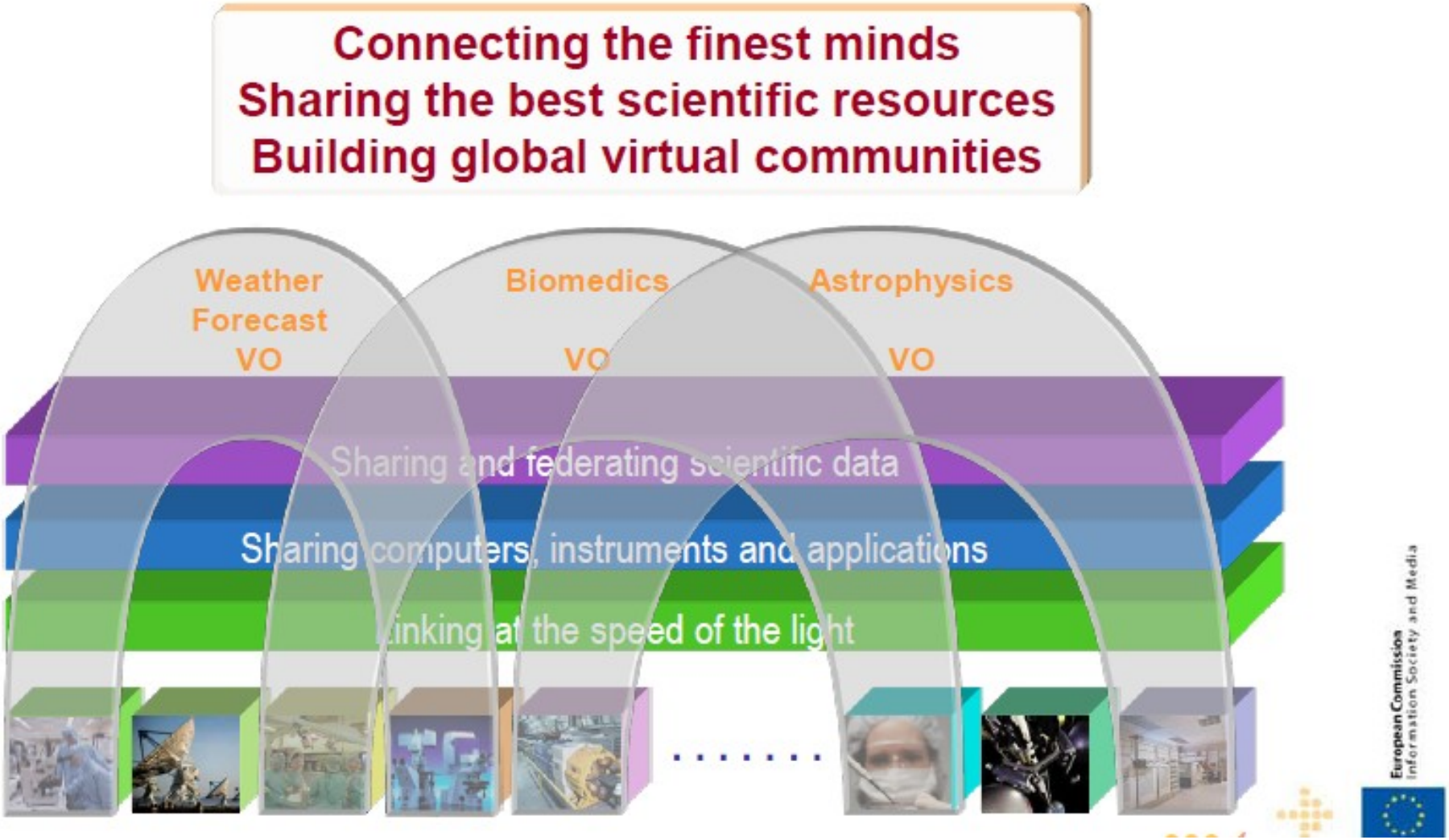
# A Role of Scientific Computing

## A new vision for Science:

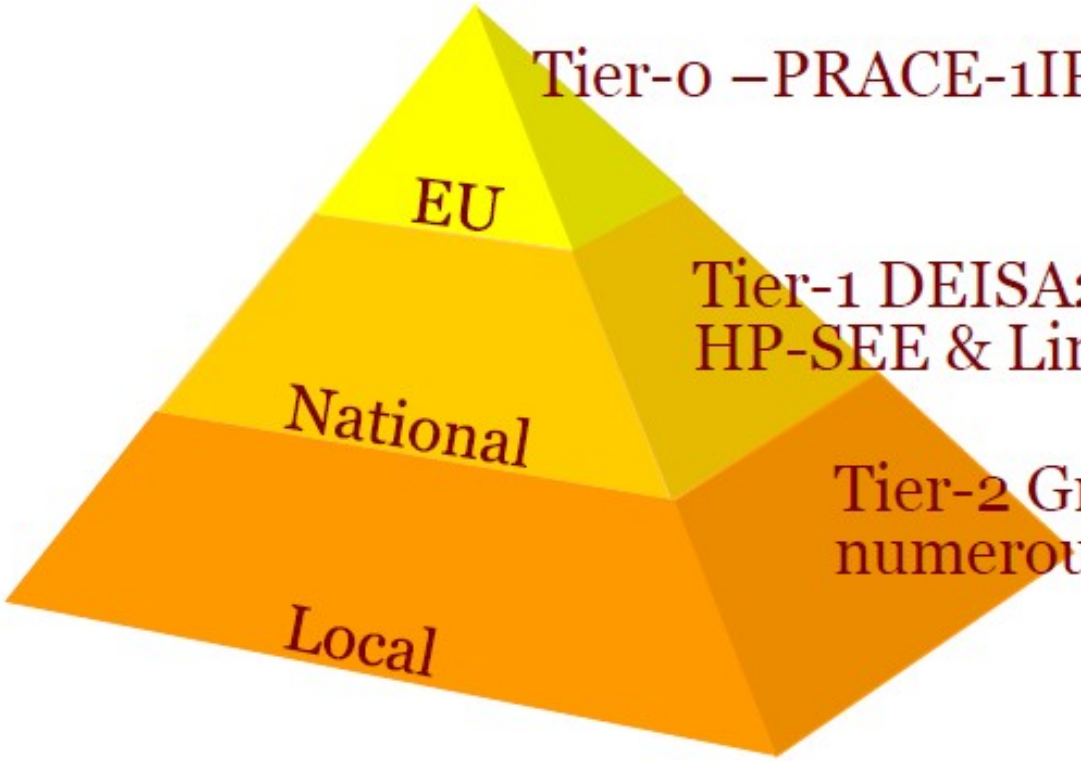
- Collaboration between European and worldwide research teams; remote access
  - Global virtual research communities
- Data-intensive science and innovation
  - Use and manage exponentially growing sets of data
- Experimentation *in silico*, simulation
  - **Use of High-Performance Computing**

**Scientific Computing is a fundamental enabler for research & innovation**

# Virtual Research Organizations



# European Scientific Computing Eco-System




Tier-0 –PRACE-1IP/exa-scale – €55 M

Tier-1 DEISA2/PRACE-2IP – €30 M
HP-SEE & LinkSCEEM2

Tier-2 Grids EGI – €50 M
numerous other projects

# European HPC Development Actions

- Implement a common Supercomputing Strategy in Europe
- Strengthen the European industrial base for the supply of HPC systems, technologies and services
- Support the setup of an HPC European Technology Platform
- Make Europe more attractive through the provision of a world-class HPC infrastructure
- Establish a wide ranging HPC training scheme
- Use mechanisms for the joint (pre-commercial) procurement

European Commission
Information Society and Media

# MD-Grid NGI Members

- **RENAM - Coordinator**
- **Institute of Mathematics and Computer Science of Academy of Sciences of Moldova**
- **Faculty of Radioelectronics and Telecommuni-cations of Technical University of Moldova**
- **Institute of Geophysics and Seismology of ASM**
- **State Hydrometeorological Service**
- **School of Public Health. State Medical and Pharmacy University of Moldova**
- **Institute of Applied Physics of ASM**

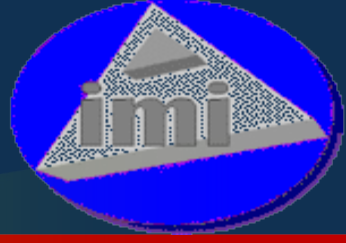
## Potential MD-Grid NGI extension

- **State University of Moldova**
- **Institute of Ecology and Geography of ASM**
- **Academy of Economical Studies**
- **Institute of Economy, Financing and Statistics of ASM**
- **…**
- ***The list is open for any others …. Welcome!***

# MD-Grid NGI Aims and Tasks

- **MD-Grid NGI** participates in strategic European Programs for the development of transnational grids and in initiatives for the completion of SEE eInfrastructures. The operation of the MD-Grid NGI implements the general EU policy on the development of national initiatives for the coordination of actions related to eInfrastructures and Grids.
- **The integration** of Grid actions (infrastructures, middleware and applications) with the broadband research and technology network into a standard e-Infrastructures system. Optimization of exploitation of advanced network resources and services, which can serve the new e-Science generation and will attract the greater users community of the Information Society to the mass adoption of advanced services provided by Grid architectures.
- **Permanent development** and administration of Grid sites infrastructure in Moldova

# European GRID Evolution



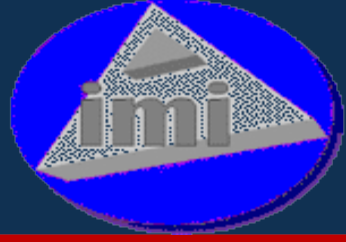

**National**

**European e-Infrastructure**

**Global**

**Testbeds** → **Productive Use** → **Utility**

# European Grid Initiative




**Goal**:

- Long-term sustainability of grid infrastructures in Europe
- through establishment of a new federated model bringing together NGIs to build the EGIorganization

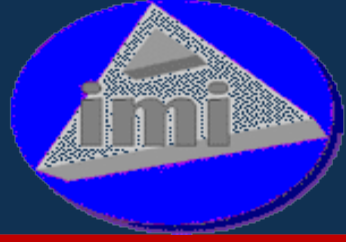
**EGI Organization**:

- Coordination and operation of a common multi-national, multi-disciplinary Grid infrastructure
- to enable and support international Grid-based collaboration,
- to provide support and added value to NGIs,
- and to liaise with corresponding infrastructures outside Europe

# Clouds for Research - Current Situation

- Cloud Computing is currently at an early stage of adoption within higher education, and even more so within research computing.
- Those who are using cloud facilities for research are typical for early adopters of any new technology –
  - they have technical backgrounds,
  - they enjoy investigating new technologies, and
  - they are self-reliant problem solvers, and
  - they are mostly addressing "hard science" problems.
- At present, the vast majority of research computing use of Cloud Computing has been funded by Amazon

# Enabling Clouds for eScience (ECEE)




Open collaboration spot for cloud projects in Europe

- VENUS-C (Italy, Germany, UK, Spain, Sweden, Greece, Israel)
  - VENUS-C is co-funded by European Commission, as one of six European Distributed Computing Infrastructures (DCIs). VENUS-C is combining experiences in Grid infrastructures and Cloud computing to capitalise on EU investments. VENUS-C brings together 14 European partners.
  - Supporting basic research disciplines:
    - Biomedicine: Integrating widely used tools for Bioinformatics, System Biology and Drug Discovery into the VENUS-C infrastructure
    - Data for Science: Integrating computing through VENUS-C on data repositories. In particular focus will be on Marine Biodiversity through Aquamaps.
    - **...**

# Enabling Clouds for eScience (ECEE)

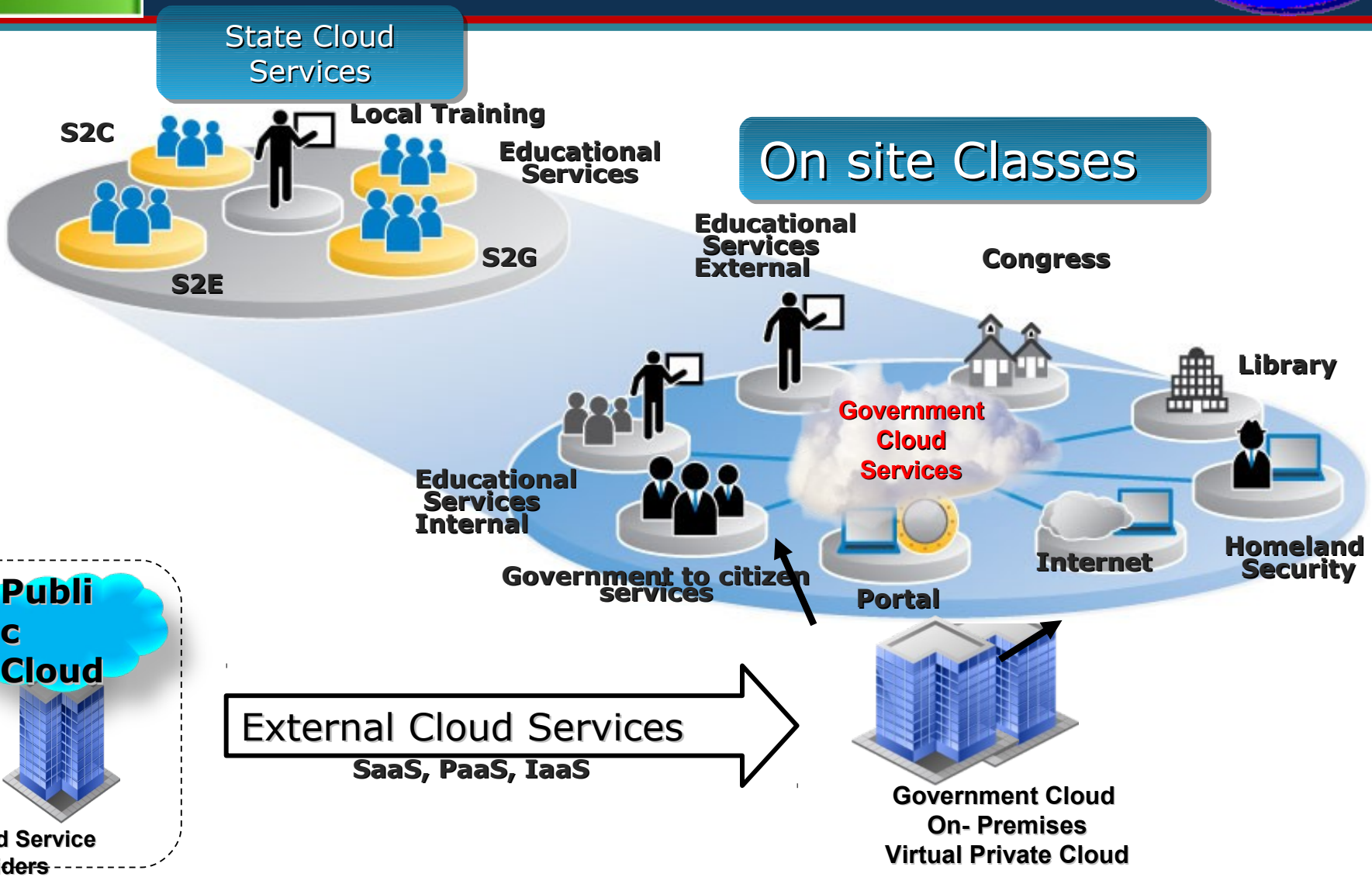
- StratusLab (France, Greece, Switzerland, Spain, Ireland), FP7 funded project
  - Enhancing Grid Infrastructure with Virtualization and Cloud Technologies;
  - Developing a complete, open-source cloud distribution that allows grid and non-grid resource centers to offer and to exploit an "Infrastructure as a Service" cloud.
- NGS (United Kingdom)
  - Cloud@NGS – The NGS Cloud Prototype is expected to be available until September 2011
- GRNET cloud (Greece)
  - Offering Cloud Services to Greek Research Community
- SARA cloud (The Netherlands)
  - HPC cloud computing
  - With the newly developed High Performance Computing Cloud environment researchers get access to their own Virtual Private HPC Cluster.

# Enabling Clouds for eScience (ECEE)

- UCM (Spain –as part of the OpenNebula Project)
  - OpenNebula.org is an open-source project aimed at building the **industry standard open source cloud computing tool** to manage the complexity and heterogeneity of distributed data center infrastructures.
- SEECCI (Slovenia, Croatia, Serbia, Bosnia and Herzegovina, Montenegro, Kosova, FYRo Macedonia, Albania, Romania, Bulgaria)
- CESGA Spain –as part of the Open Cirrus project
  - Open Cirrus is an open cloud-computing research testbed designed to support research into the design, provisioning, and management of services at a global, multi-datacenter scale
- NEON (Sweden, Norway, Denmark, Finland, Iceland)
  - Northern Europe Cloud Computing
  - The aim with the NEON project is to review the promises and summarize the overall offering cloud computing could give to the Nordic eScience community
- BalticCloud (Estonia, Latvia, Lithuania, Belarus, Poland)
  - BalticCloud is a subproject of the BalticGrid project aimed at developing cloud infrastructure in Baltic states and Belarus

# Applicability of cloud technologies to research problems

- Two major areas have emerged as being currently unsuitable for migration to a cloud platform.
  - These are situations in which an extremely large amount of data needs to be processed/stored, and for large-scale fine-grained parallel jobs.

1. Large-scale data handling and processing is currently likely to prove unaffordable due to charging models used by commercial cloud service vendors.
2. Fine-grained/tightly-coupled parallel processing for example using OpenMP or MPI is currently likely to suffer unacceptable performance overheads from virtualisation into a cloud.

# Clouds for Future National Level Services