



Enabling Grids for E-sciencE

Introduction to cluster computing and Grid environment

Antun Balaz antun@phy.bg.ac.yu Scientific Computing Laboratory Institute of Physics Belgrade, Serbia













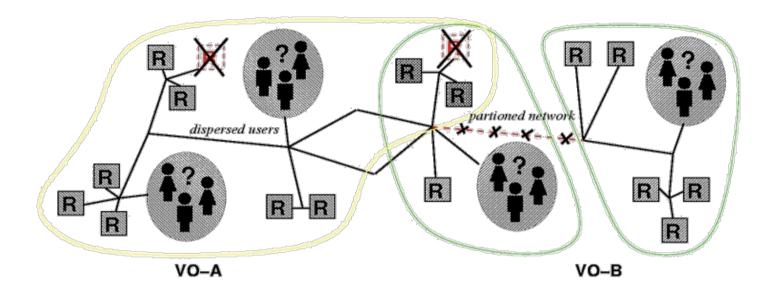


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Unifying concept: Grid



Resource sharing and coordinated problem solving in dynamic, multi-institutional virtual organizations.





What problems Grid addresses

- Too hard to keep track of authentication data (ID/password) across institutions
- Too hard to monitor system and application status across institutions
- Too many ways to submit jobs
- Too many ways to store & access files/data
- Too many ways to keep track of data
- Too easy to leave "dangling" resources lying around (robustness)





Requirements

- Security
- Monitoring/Discovery
- Computing/Processing Power
- Moving and Managing Data
- Managing Systems
- System Packaging/Distribution
- Secure, reliable, on-demand access to data, software, people, and other resources (ideally all via a Web Browser!)



- Right balance of push and pull factors is needed
- Supply side
 - Technology inexpensive HPC resources (linux clusters)
 - Technology network infrastructure
 - Financing domestic, regional, EU, donations from industry
- Demand side
 - Need for novel eScience applications
 - Hunger for number crunching power and storage capacity





Supply side - cluster

- The cheapest supercomputers massively parallel PC clusters
- This is possible due to:
 - Increase in PC processor speed (> Gflop/s)
 - Increase in networking performance (1 Gbs)
 - Availability of stable OS (e.g. Linux)
 - Availability of standard parallel libraries (e.g. MPI)
- Advantages:
 - Widespread choice of components/vendors, low price (by factor ~5-10)
 - Long warranty periods, easy servicing
 - Simple upgrade path
- Disadvantages:
 - Good knowledge of parallel programming is required
 - Hardware needs to be adjusted to the specific application (network topology)
 - More complex administration
- Tradeoff: brain power $\leftarrow \rightarrow$ purchasing power
- The next step is GRID:
 - Distributed computing, computing on demand
 - Should "do for computing the same as the Internet did for information" (UK PM, 2002)





Supply side - network

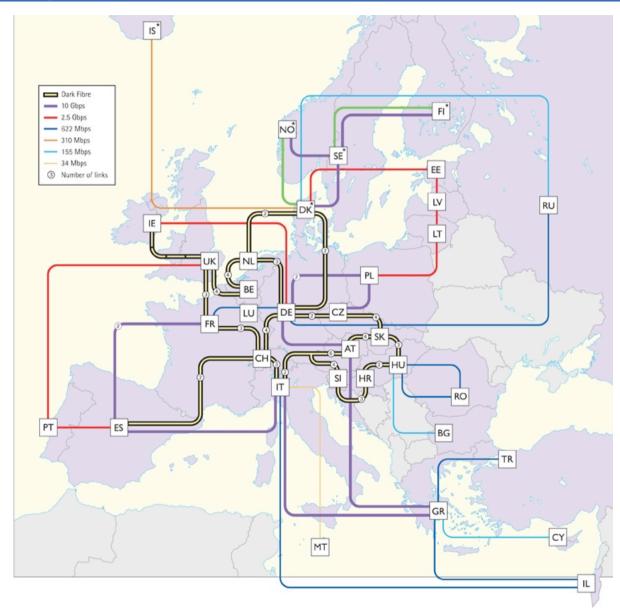
Needed at all scales:

- World-wide
- Pan-European (GEANT2)
- Regional (SEEREN2, ...)
- National (NREN)
- Campus-wide (WAN)
- Building-wide (LAN)
- Remember it is end user to end user connection that matters





GÉANT2 Pan-European IP R&E network





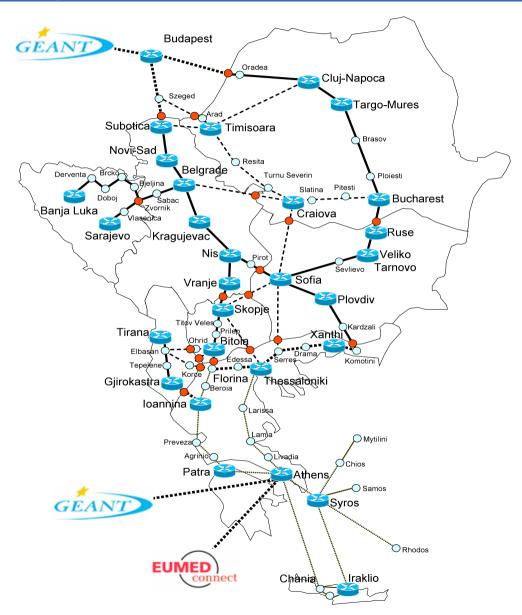


GÉANT2 Global Connectivity





Future development of regional network







Supply side - financing

- National funding (Ministries responsible for research)
 - Lobby gvnmt. to commit to Lisbon targets
 - Level of financing should be following an increasing trend (as a % of GDP)
 - Seek financing for clusters and network costs
- Bilateral projects and donations
- Regional initiatives
 - Networking (HIPERB)
 - Action Plan for R&D in SEE
- EU funding
 - FP6 IST priority, eInfrastructures & GRIDs
 - FP7
 - CARDS
- Other international sources (NATO, ...)
- Donations from industry (HP, SUN, ...)





Demand side - eScience

- Usage of computers in science:
 - Trivial: text editing, elementary visualization, elementary quadrature, special functions, ...
 - Nontrivial: differential eq., large linear systems, searching combinatorial spaces, symbolic algebraic manipulations, statistical data analysis, visualization, ...
 - Advanced: stochastic simulations, risk assessment in complex systems, dynamics of the systems with many degrees of freedom, PDE solving, calculation of partition functions/functional integrals, ...
- Why is the use of computation in science growing?
 - Computational resources are more and more powerful and available (Moore's law)
 - Standard approaches are having problems
 Experiments are more costly, theory more difficult
 - Emergence of new fields/consumers finance, economy, biology, sociology
- Emergence of new problems with unprecedented storage and /or processor requirements





Demand side - consumer

- Those who study:
 - Complex discrete time phenomena
 - Nontrivial combinatorial spaces
 - Classical many-body systems
 - Stress/strain analysis, crack propagation
 - Schrodinger eq; diffusion eq.
 - Navier-Stokes eq. and its derivates
 - functional integrals
 - Decision making processes w. incomplete information
 - ...
- Who can deliver? Those with:
 - Adequate training in mathematics/informatics
 - Stamina needed for complex problems solving
- Answer: rocket scientists (natural sciences and engineering)

