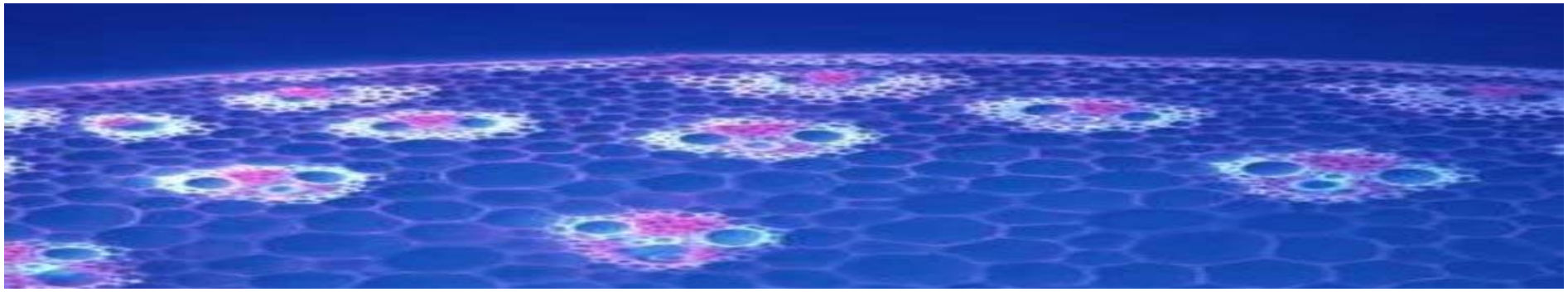

ShareGrid

a Peer-to-Peer Desktop Grid for scientific applications federating small research laboratories

- ***Guglielmo Girardi, TOP-IX, guglielmo.girardi@topix.it***
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Outline

- Introduction
  - Scientific computational needs and possible solutions
  - Small research laboratories... Peer-to-Peer Grids
  - OurGrid Design Principles & Architecture
- ShareGrid an open Community
  - The project
  - Participants
  - Using ShareGrid...
  - How to join the ShareGrid Community
- Conclusions
  - ShareGrid, a Community where you share relationships and projects

Introduction

ShareGrid: a Peer-to-Peer Desktop Grid for scientific applications federating small research laboratories

Scientific computational needs

- Computers are changing scientific research
  - Enabling collaboration
  - As investigation tools (simulations, data mining, etc...)
- In many scientific areas, the use of computers to carry out research has become essential.
- The availability of computing infrastructures is therefore fundamental for the achievement of scientific results.
- Grid computing conceived as the answer to the computation needs:
  - use of a set of resources geographically dispersed and belonging to different organizations as a single computing platform

Grid Computing: classical solutions

- "Big Iron" solution
  - Individual entities contribute with their resources to what is called a Virtual Organization (VO)
    - temporary association of individual entities
    - resource sharing by out-of-band agreements
  - Typical Grids aggregate high-end, always online and continuously maintained resources
  - Globus is the de facto standard middleware
  - But...
    - highly specialized skills and complex off-line negotiations
- Volunteer Grid computing
  - A type of distributed computing in which individual computer owners donate their computing resources
  - Popularized by highly visible projects SETI@home, FightAIDS@home, Folding@home, YouNameIt@home
  - But...
    - good support team to run "the server", good deal of effort in "advertising", very high visibility project, prestigious institution

Small research laboratories...

- the labs
  - are small
  - do not have resources to invest in publicity,
  - do not belong to top Universities
  - cannot rely on cutting-edge computer support team
- the projects
  - focus their research on some narrow topic
  - are unable to catch the attention of a large community
- the possible approach
  - can federate their resources and use them cooperatively according to the peer-to-peer computing paradigm:
    - each participant lets other members use its resources when it does not need them, provided that they do the same.

federating & using resources in a peer-to-peer computing paradigm

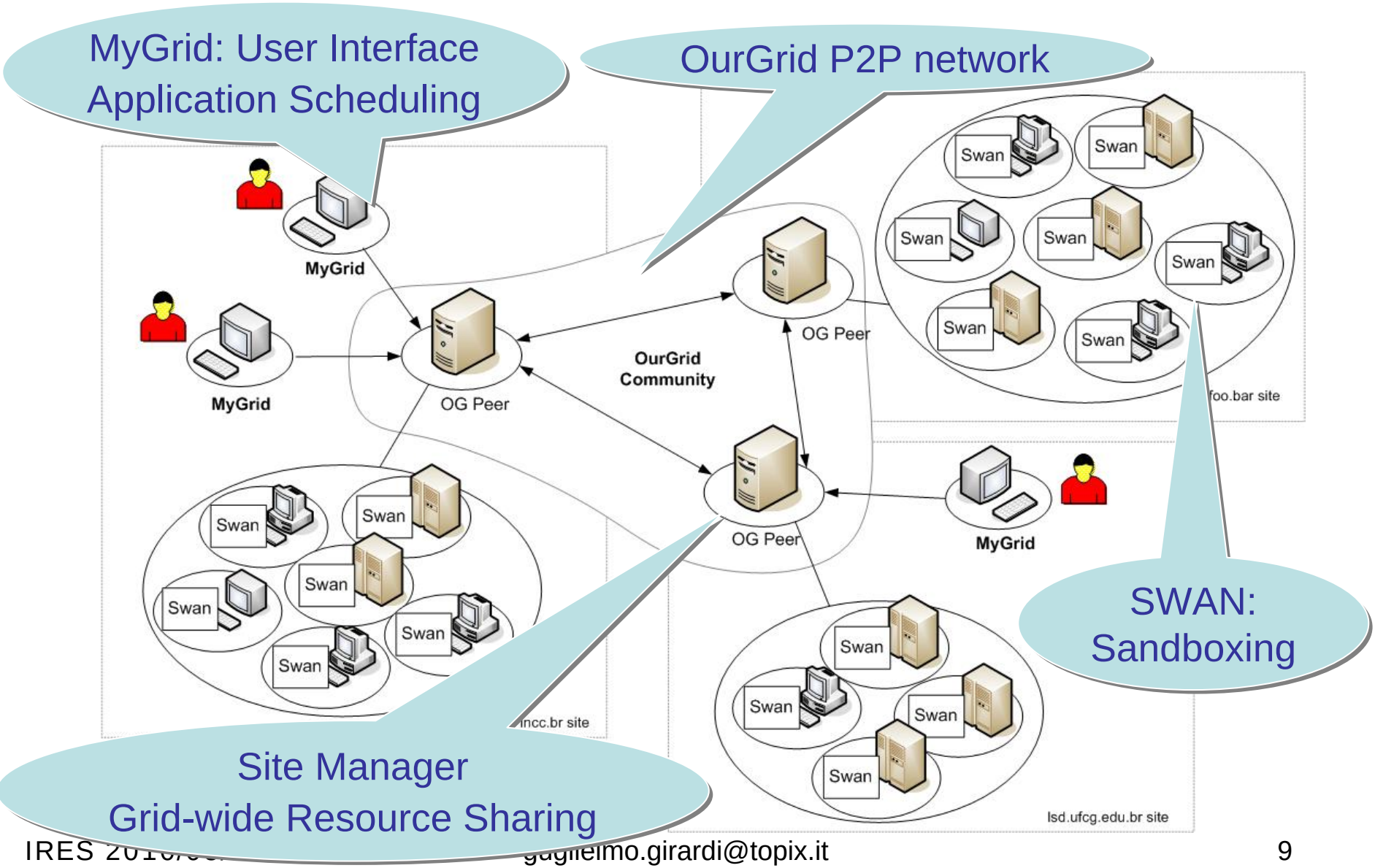
Peer-to-Peer Grids

- Grids in which participant join spontaneously, without prior agreements/negotiations, and may leave without prior notice
  - alternative to VO concept
- Focus on cooperative resource sharing: “I will let you use my resources (when I don’t need them) if I can use yours”
- Approach pioneered by the Brazilian OurGrid project
  - carried on at the Universidad Federal de Campina Grande (http://www.ourgrid.org)
  - sponsored by HP Brazil
  - started in 2003, currently very active
  - deployed on a public testbed that can be used by anyone interested

OurGrid Design Principles

- Labs can freely join the system without any human intervention
  - No need for negotiation; no paperwork
- Clear incentive to join the system
  - One can't be worse off by joining the system
  - Free-riding resistant
- Basic dependability properties
  - Some level of security
  - Some resilience to failures
  - Scalability
- Easy to install, configure and program
  - No need for specialized support team
  - Script-based programming is natural
- Focuses on Bag-of-Tasks (BoT) applications
  - No communication among tasks
  - facilitates scheduling and security enforcement
  - Simple fail-over/retry mechanisms to tolerate faults
  - No need of QoS guarantees

OurGrid Architecture



ShareGrid an open community

ShareGrid: a Peer-to-Peer Desktop Grid for scientific applications federating small research laboratories

Sala Convegni IRES Piemonte - Via Nizza, 18 - Torino - 11 Maggio 2010

ShareGrid, the project...

- management
  - TOP-IX: general coordination and relationships with Regione Piemonte
  - Computer Science Department, Università del Piemonte Orientale: technical and scientific coordination
  - Computer Science Department, Università di Torino: application support and operational management
- funding
  - Regione Piemonte within the framework of TOP-IX's Development Program (a consortium plan devoted to foster innovation activities and related business)
- goals
  - implementation of a distributed computing platform
  - facing the need of users from universities and research labs
    - small laboratories with computing resources to be optimized and shared
    - individual researchers
  - locallly based on the regional wideband network infrastructure
- implementation guides
  - instance of OurGrid

ShareGrid, step by step

- 2007
  - platform set-up
  - start collecting laboratories and forming the community,
    - TOP-IX' s data center as main seed: machines devoted to computational purposes
    - Department of Drug Science, Faculty of Pharmacy, University of Turin
    - University of Piemonte Orientale
  - first intensive use: Department of Drug Science Department of Economic and Financial Sciences of University of Turin
- 2008
  - keep the community alive and growing
  - application support for individual users/researcher/projects
  - debugging OG3
  - SG Portal for job submission: implementation and community test
- 2009
  - keep the community alive and growing
  - application support for individual users/researcher/projects
  - SG Portal for job submission: maintenance
  - availability of SGVirtual ShareGrid Virtual instances (peer & user agent)
  - ToSM (Torino Software & Systems Meeting)

ShareGrid 2010

- Project management:
  - general / technical / scientific coordination
- Keep the community alive and growing
  - meetings, seminars, workshops
- Application support for individual users/researcher/projects
- TOP-IX seeds (peer – user agents):
  - minimal and extended configuration/set-up from T-Cloud
- Communication and Dissemination of the results:
  - specific papers / presentations, seminars, etc
- OurGrid 4: assessment & deployment
- SG Portal OG3 to OG4
- Operational management:
  - technical relationships among participants (basic FAQs)
  - P2P platform maintenance

Remarks on activities and fundings

- management
  - out-of-band agreements
  - complex off-line negotiations
- resources
  - buying high-end clusters and/or mainframes
- education
  - highly specialized skills to run “servers” to manage high-end clusters...

- management
  - simply install OG peer and workers
  - work at once: MyGrid – Portal
- resources
  - share your own resources as many as you want
- education
  - read & learn how to install OG peer-workers

No funding for...

ShareGrid solution...

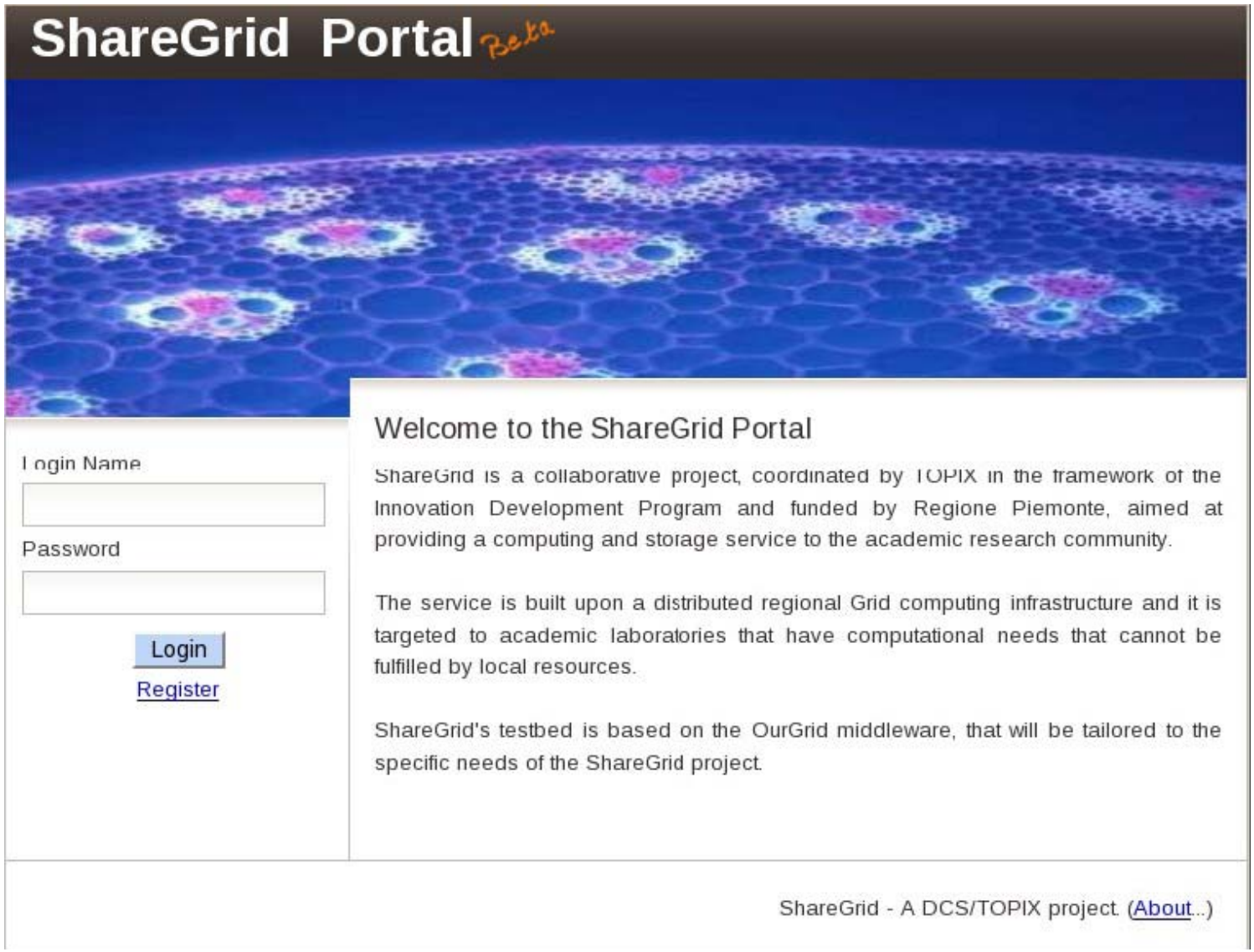
Participants sharing resources

- University of Turin,
  - Department of Drug Science, Faculty of Pharmacy
  - Department of Economic and Financial Sciences
  - Academic Network and Telecommunications

- TOPIX, Internet traffic exchange point in northwest, Italy, Alessandria node
- University of Piemonte Orientale, Department of Computer Science
- University of Turin, Department of Computer Science

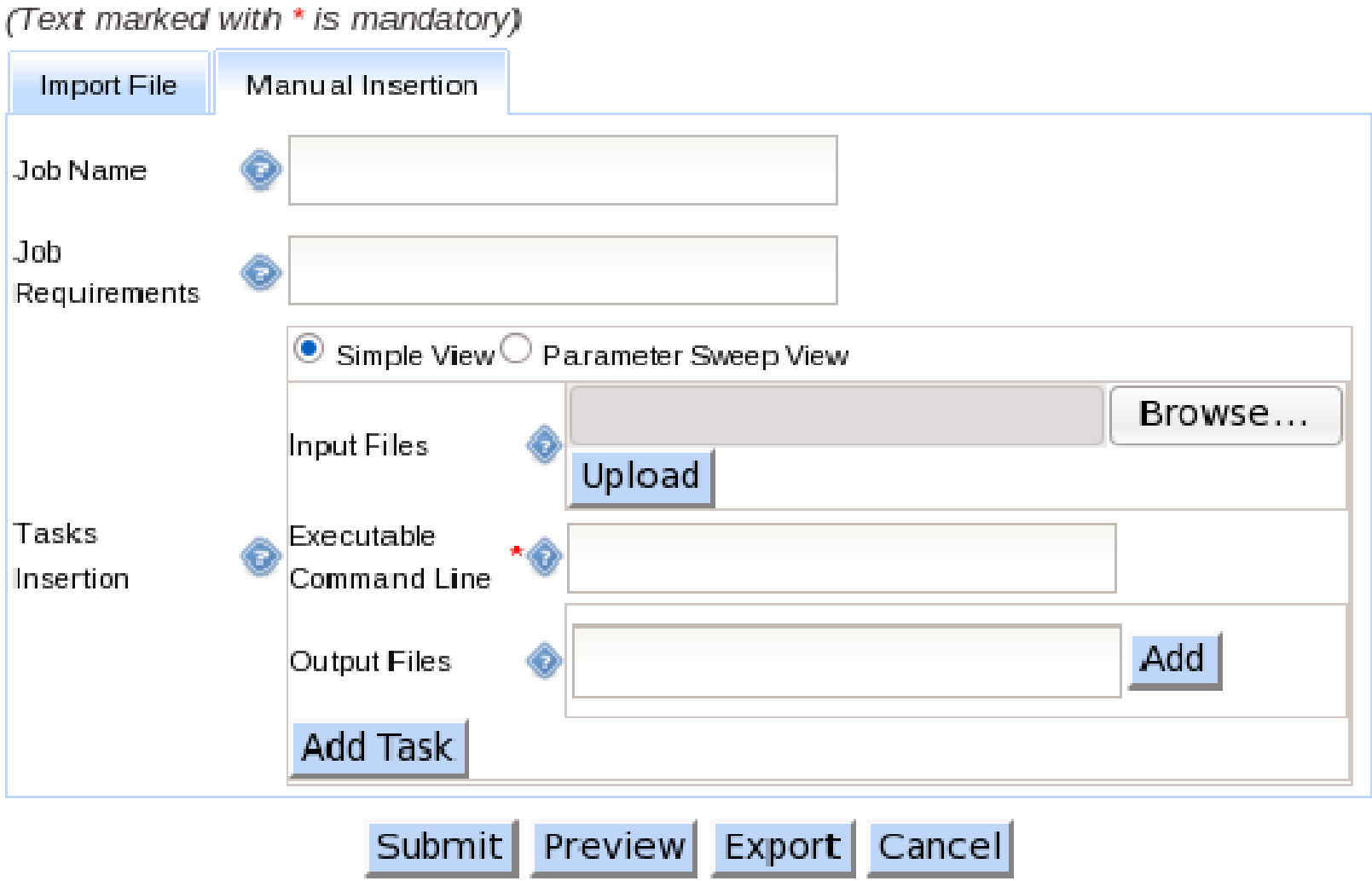
- University of Genova, Department of Computer and Information Science
- University of Padova, Centro di Calcolo di Ateneo
- CSP's render and computing farm

ShareGrid Portal

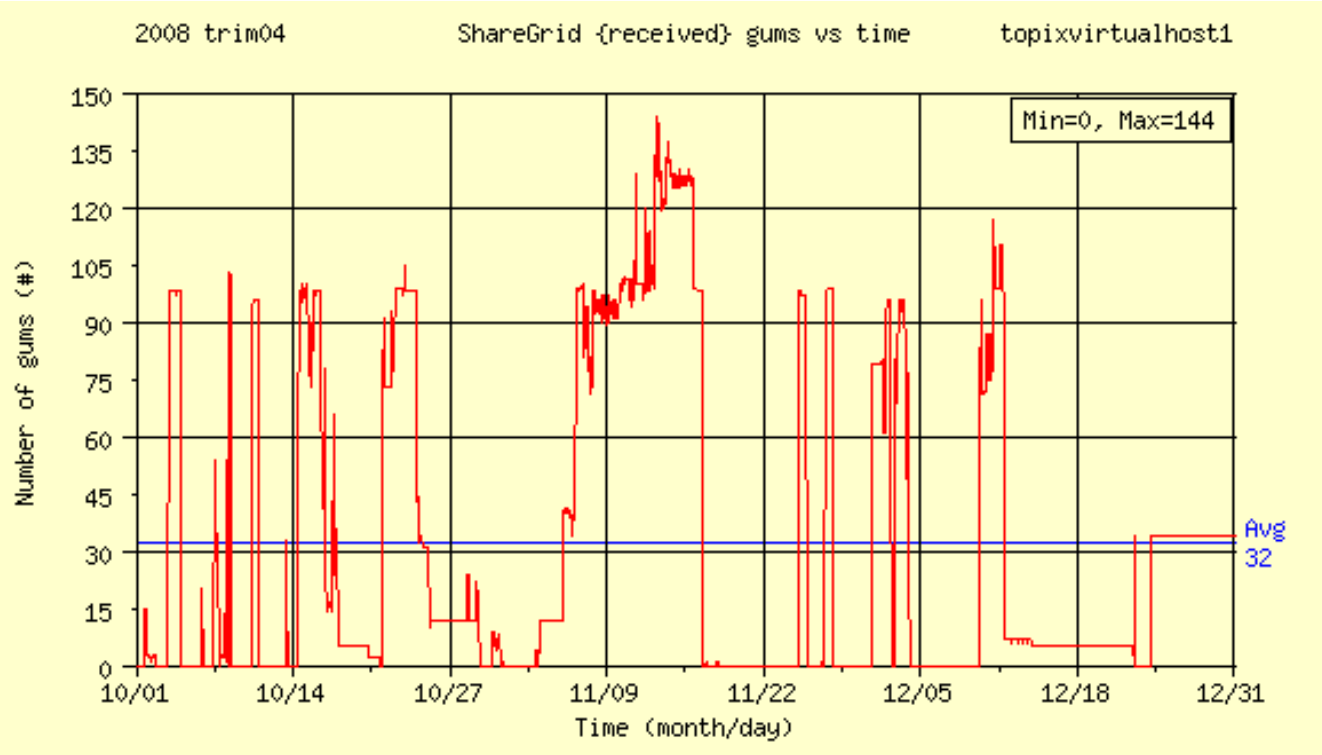


http://ramses.di.unipmn.it:8080/sgportal/faces/index.jspx

ShareGrid Portal, Job Submission



Using ShareGrid...



- Image processing
- Distributed rendering
- Simulation of economic systems
- Simulation of molecular systems
- Simulation of scheduling algorithms for distributed systems
- Evaluation of Classifier Systems
- Evaluation and suppression of noise caused by flows over a cavity

Cover Picture of ChemMedChem 6/2009

- Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin
- Paolo Tosco & Loretta Lazzarato
  - Department of Drug Science, Faculty of Pharmacy, University of Torino, Italy

izzate 40% Roma. We gratefully acknowledge the ShareGrid management team for the computing power provided through the ShareGrid distributed platform.[36] *3D Representations of mol-*

Open3DQSAR

J Mol Model
DOI 10.1007/s00894-010-0684-x

SOFTWARE REPORT

Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields

Paolo Tosco · Thomas Balle

authors of their later extensions [16, 21-23]. We gratefully acknowledge the ShareGrid management team for the computing power provided through the ShareGrid distributed platform. Finally, P.T.

Received: 25 December 2009 / Accepted: 1 February 2010

E5530 workstation equipped with 24 GB 1066 MHz ECC DDR3 RAM. Program testing was carried out taking advantage of the ShareGrid distributed platform [26]. Some algorithms described by other authors have been imple-

How to join the ShareGrid Community

- access the project web page: http://dcs.mfn.unipmn.it/sharegrid/
- download and fill-in a questionnaire describing:
  - the application(s) you are going to submit
  - the laboratory you are going to share (if any)
- send the questionnaire and your references to <sharegrid.admin@topix.it>
- read the directions on how to download/install the needed software (peer and/or client) and install the needed software
- learn how to submit your jobs using whatever you want
  - myGrid client
  - ShareGrid portal from http://ramses.di.unipmn.it:8080/sgportal/faces/index.jspx
- start and interact with the working group <sharegrid@di.unito.it>
- expected results in general are
  - test of the applications and of the laboratory as a component of the entire system
  - active participation to ShareGrid user meetings
  - aknowledgments while presenting the results

"The author(s) acknowledge(s) the support graciously provided by the ShareGrid project and its management team, that donated a significant amount of computing power without which this research would not have been possible."

"More information on the ShareGrid project can be found at http://dcs.di.unipmn.it/sharegrid"

Conclusions

ShareGrid: a Peer-to-Peer Desktop Grid for scientific applications federating small research laboratories

ShareGrid, an Open Computing Community

- ShareGrid is a peer-to-peer desktop grid matching the computing needs of small research laboratories (initially located in the Piedmont area in Northern Italy but today being extended to Liguria and Veneto).
- Share-Grid adopts a cooperative approach, in which each participant allows the others to use his/her own resources on a reciprocity basis.
- ShareGrid is based on the OurGrid middleware, that provides a set of mechanisms enabling participating entities to quickly, fairly, and securely share their resources.
- ShareGrid comprises more than 300 machines (including both desktop-class and server-class computers), shared by University research labs (Alessandria, Torino, Genova, Padova) and two private institutions (TOP-IX, CSP)
- ShareGrid is used to run applications including Distributed Rendering, Simulation of economics systems, Simulation of molecular systems, Simulation of scheduling algorithms for distributed systems, Evaluation of Classifier Systems.

A Community for sharing relationships and projects

ShareGrid, a Community where you share relationships and projects

- the cooperation is implicitly achieved as soon as you install the OurGrid middleware Software (join the Community without hard paperwork)
- research projects committed to university departments are actually carried out in several (not directly owned) laboratories (use other's "idle" resources)
- widen the space of resources where experimental projects can be carried out without extra costs
- enables large scale experiments without additional costs (eg buying new equipment tailored to a specific project and used only for a limited amount of time)
- enables tuning up projects and innovative solutions assessing in advance the costs of future industrial implementations
- provides solutions tested in a best effort environment but easily applicable to a quality of service controlled environment (same middleware)

A Community for sharing relationships and projects

The ShareGrid management team

- TOP-IX
  - Guglielmo Girardi, TOP-IX, guglielmo.girardi@topix.it
  - TOP-IX's staff
- Department fo Computer Science, Universita' del Piemonte Orientale, Alessandria
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  - {cosimo.anglano,massimo,canonico,marco.guazzone}@unipmn.it
- Department fo Computer Science, Universita' di Torino
  - Marco Botta, Sergio Rabellino
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User contributions and papers

User contributions

- Idleness on Solaris and Windows (upgrade of OurGrid middleware)
  - Sergio Rabellino, Head of ICT Services, Computer Science Department, University of Torino
  - *ourgrid-src-3.3.2-WinSol-RabSer.zip* [*2007-08-29*] [*18 MB*]
- Scheduler wrapper of MyGrid application
  - Paolo Tosco, PhD, Dipartimento di Scienza e Tecnologia del Farmaco
  - ptosco-scheduler 0.42_03082007 [*2007-07-10*] [*100.84 KB*]
- JDF Java Writer (A Java class for automatically writing .jdf files for the repetition with different values of random seed)
  - Riccardo Boero, Università di Torino - Facoltà di Economia
  - Boero-GridlabJDFWriter [*2007-07-10*] [*1.37 KB*]
- DcsShareGridBlender: Distributed Rendering in ShareGrid with Blender (an add-on for the ShareGrid infrastructure useful for performing distributed rendering in ShareGrid with the Blender application)
  - Marco Guazzone, Universita' del Piemonte Orientale - Dipartimento di Informatica
  - DcsShareGridBlender.zip [*2008-03-16*] [*6.99 MB*]

Project documents

- Massimo Canonico, Marco Guazzone
  - project web site, http://dcs.mfn.unipmn.it/sharegrid/
- Marco Guazzone,
  - DCS Grid Blender v.1.0, User Manual, 28 September 2007
- Marco Guazzone,
  - Studio di fattibilità per l'integrazione tra OurGrid e EnginFrame, 13 novembre 2007
- DCS Team,
  - Configuring ShareGrid components in a Virtual Machine, 6 maggio 2008 (VM-ShareGrid-configuration.pdf)

Papers on ShareGrid

- C. Anglano, M. Canonico, M. Guazzone, M. Botta, S. Rabellino, S. Arena, G. Girardi.
  - Peer-to-Peer Desktop Grids in the Real World: the ShareGrid Project.
  - In Proc. of the 8th IEEE International Symposium on Cluster Computing and the Grid (CCGRID'08), Lyon (France), May 2008, IEEE Press.
- C. Anglano, M. Canonico, M. Guazzone.
  - The ShareGrid Portal: an easy way to submit jobs on computational Grids.
  - Technical Report. University of Piemonte Orientale, Italy, October 2008.

Papers and acknowledgements

- Riccardo Boero (Università di Torino)
  - Simulazioni di interazioni fra le unità produttive del Piemonte, con particolare riferimento alla provincia di Biella: metodo e risultati.
  - Progetto di ricerca nazionale Prin-2004, “Creazione di valore e crescita economica in reti economiche dinamiche”, Università di Trento, Torino, Genova
  - Convegno finale, Biella, 12 e 13 giugno 2007
- Paolo Tosco, Dr., Elisabetta Marini, Dr., Barbara Rolando, Dr., Loretta Lazzarato, Dr., Clara Cena, Prof. Dr., Massimo Bertinaria, Dr., Roberta Fruttero, Prof., Marianne Reist, Dr., Pierre-Alain Carrupt, Prof. Dr., Alberto Gasco, Prof.,
  - Structure-Antioxidant Activity Relationships in a Series of NO-Donor Phenols,
  - in ChemMedChem, Volume 3 Issue 9, Pages 1443 – 1448,
  - Published Online: 14 Jul 2008, http://dx.doi.org/10.1002/cmdc.200800101
- Konstantin Chegaev, Clara Cena, Marta Giorgis, Barbara Rolando, Paolo Massimo Bertinaria, Roberta Fruttero, Pierre-Alain Carrupt, and Alberto,
  - Edaravone Derivatives Containing NO-Donor Functions, in J. Med. Chem.,
  - Article ASAP • DOI: 10.1021/jm8007008, http://dx.doi.org/10.1021/jm8007008

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Paolo Tosco

Papers and acknowledgements

- Paolo Tosco, Loretta Lazzarato
  - Cover Picture: Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin (ChemMedChem 6/2009)
  - ChemMedChem, vol. 4, num. 6, pag. 588, 2009
- Paolo Tosco, Loretta Lazzarato
  - Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin
  - ChemMedChem, vol. 4, num. 6, pag. 939-945, 2009
- Paolo Tosco, Elisabetta Marini, Barbara Rolando, Loretta Lazzarato, Clara Cena, Massimo Bertinaria, Roberta Fruttero, Marianne Reist, Pierre-Alain Carrupt, Alberto Gasco
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