

Running a successful VO

Status of the GridUnesp project

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Open Science Grid - 2011 All Hands Meeting
Harvard Medical School

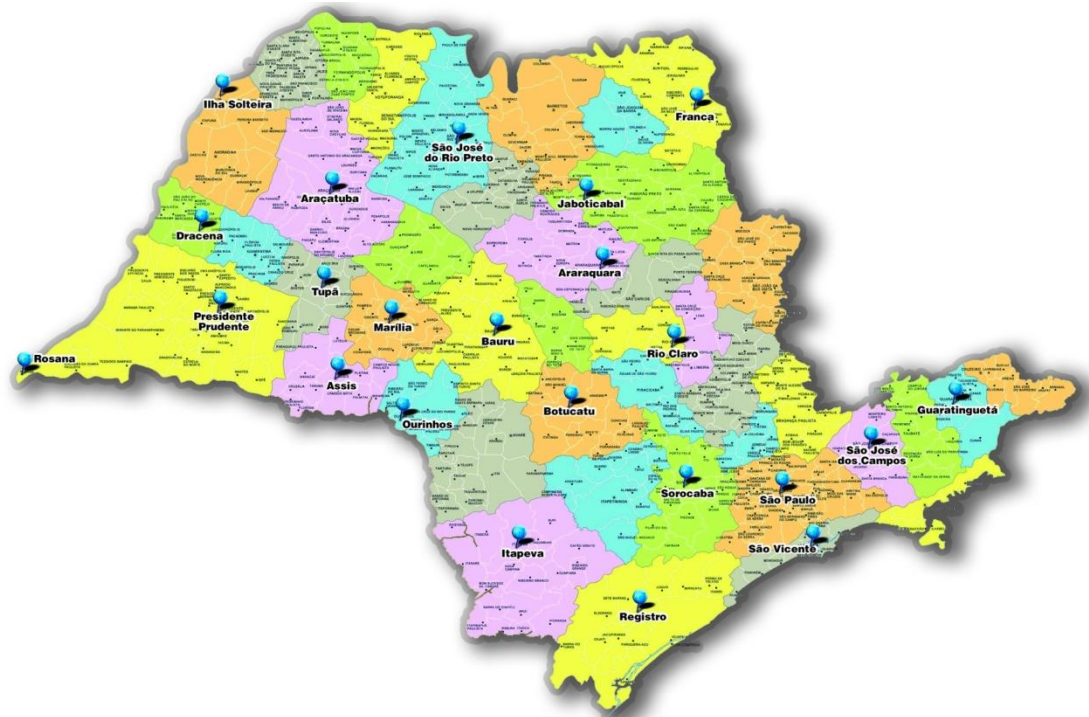
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The São Paulo State University

33 institutes, colleges and schools on 23 campuses distributed throughout the State of São Paulo

Second largest university in Brazil; part of the state of São Paulo public higher education system



GridUnesp scope and evolution

A distributed computational system for scientific computing with resources dispersed over a wide geographic area

A production-quality, multi-campus Grid → one of the largest campus Grid infrastructures in Latin America



Started in 2004 with a call for Scientific Proposals sent to UNESP researchers

Formal proposal submitted to FINEP by the end of 2005 and approved by the middle of 2006

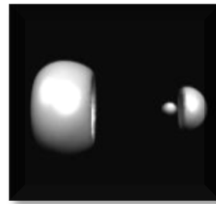
Hardware acquisition process finished by the end of 2008; operations started in 2009



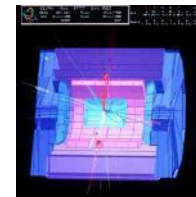
GridUnesp main research areas



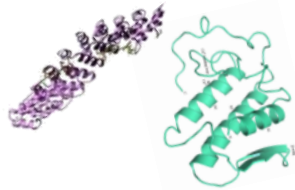
**Biological
Networks**



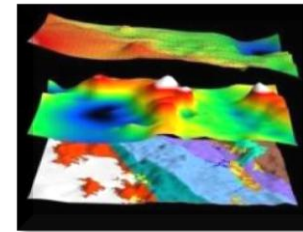
**Relativistic
Chemistry**



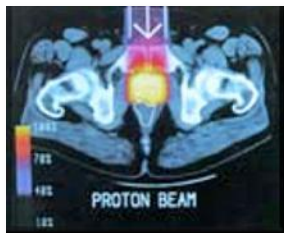
**High Energy
Physics**



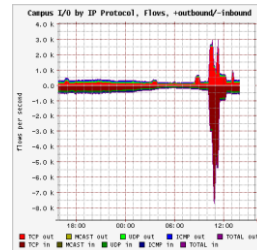
**Molecular
Dynamics**



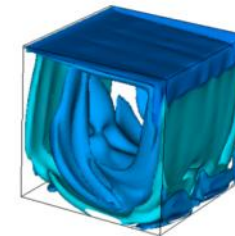
**Geological
Modeling**



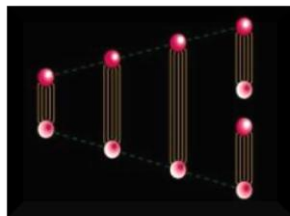
**Medical
Physics**



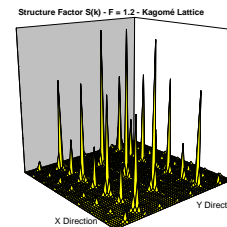
**Network
Security**



Turbulence

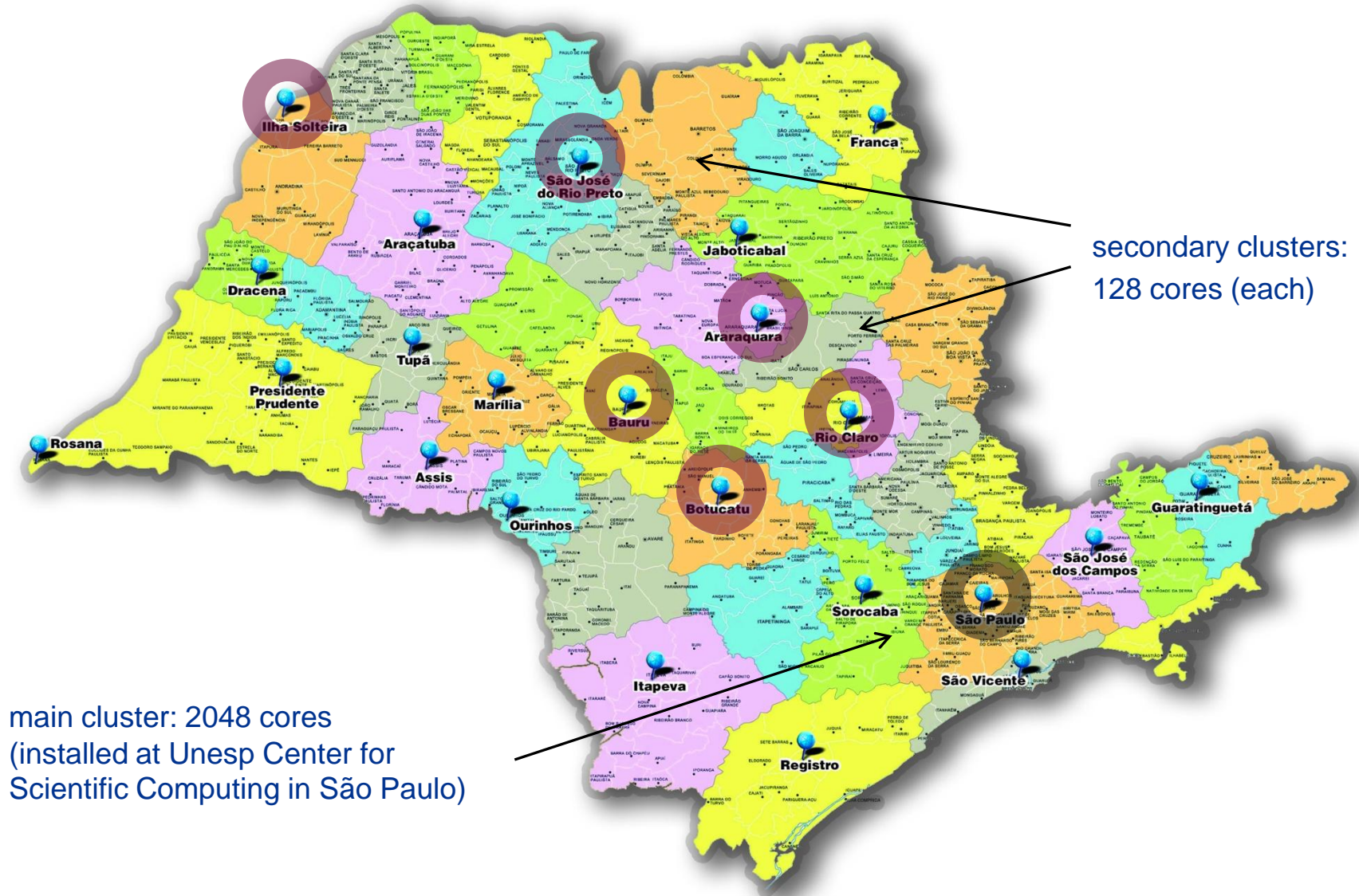


**Lattice
QCD**



**High Tc
Superconductivity**

GridUNESP sites



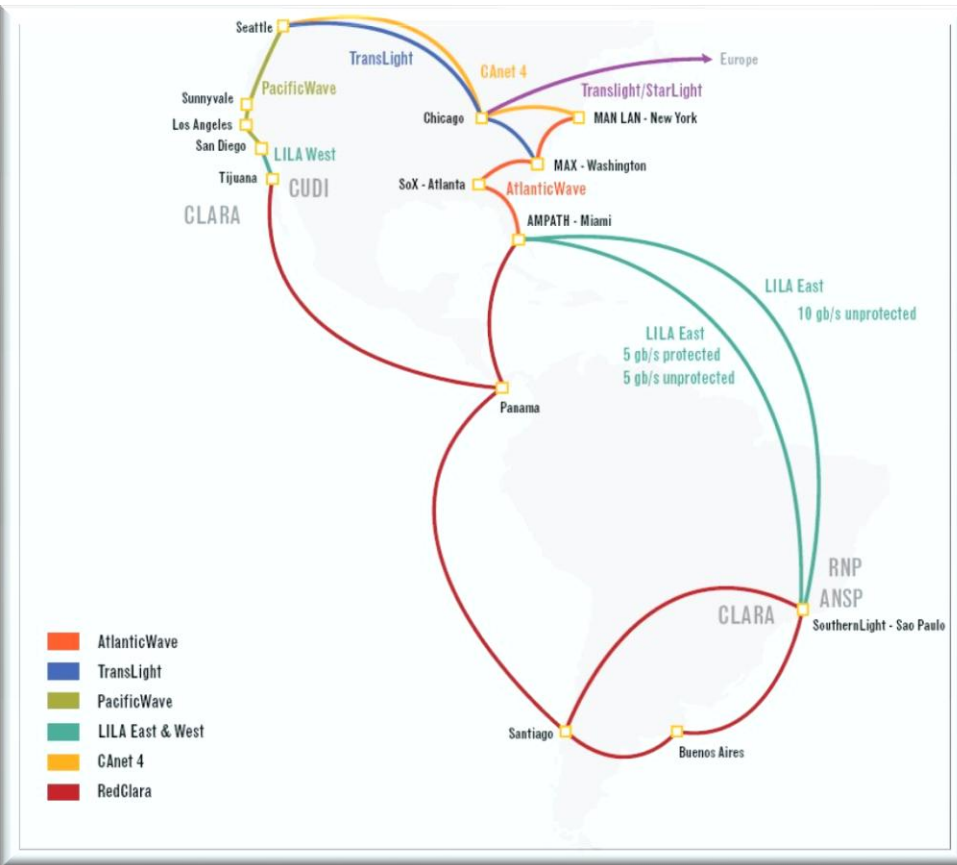
main cluster: 2048 cores
(installed at Unesp Center for
Scientific Computing in São Paulo)

secondary clusters:
128 cores (each)

Connectivity between sites: the KyaTera network



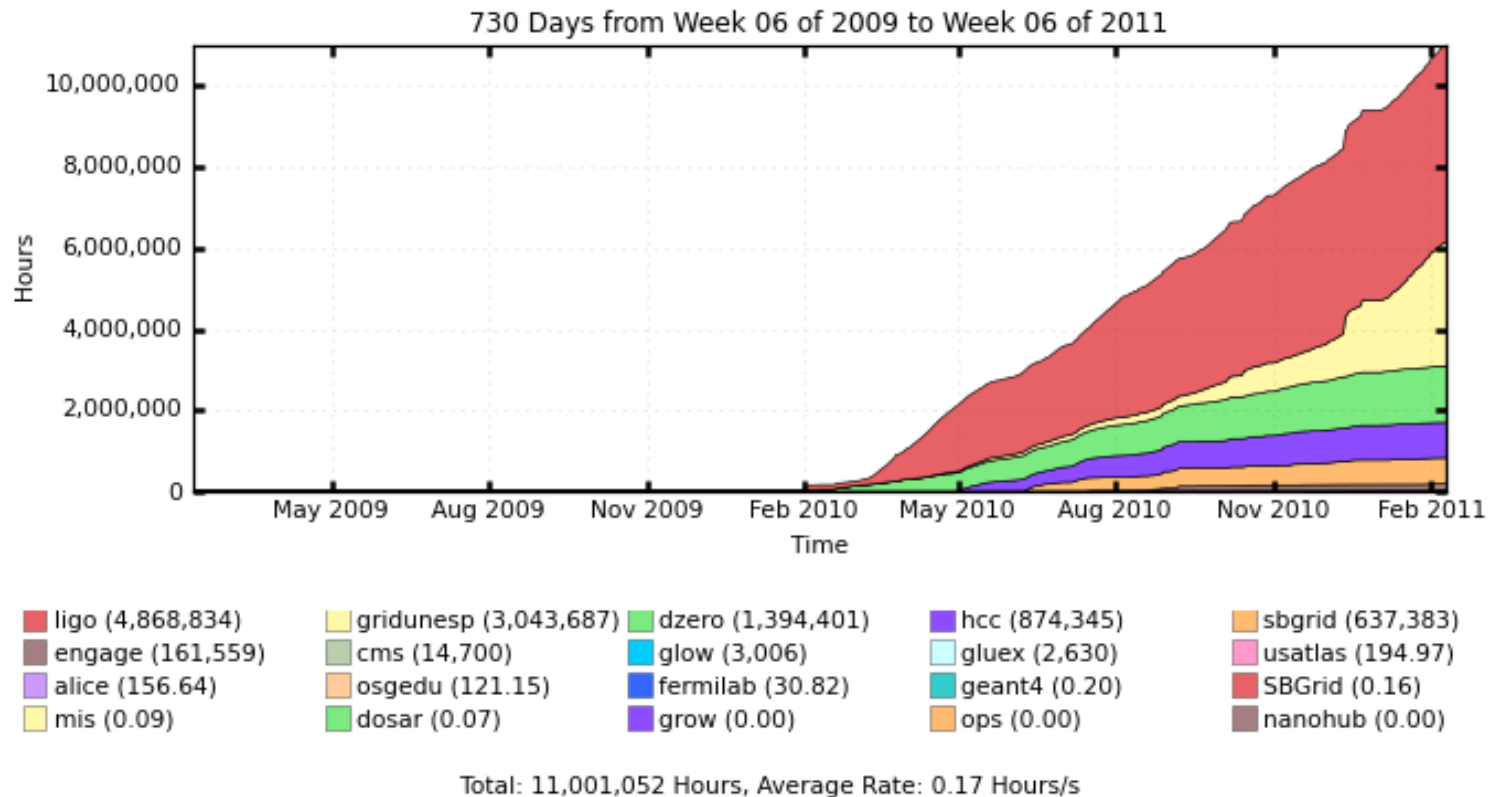
International connectivity



Hardware & software infrastructure

- **Main cluster**
 - 2048 processing cores, 4 data servers (24 TB each), SAN storage system (36 TB), InfiniBand and gigabit switches
- **Secondary clusters (7)**
 - 128 processing cores, SAN storage system (6 TB), gigabit switch
- **Software / middleware**
 - Intel software: C/C++/Fortran compilers, VTune, MKL, MPI, Cluster Toolkit
 - Grid middleware: Open Science Grid
 - formal agreement w/ OSG Executive Board
 - establishment of the 'GridUNESP VO'
 - GridUnesp is the first OSG VO outside U.S.

GridUnesp site usage



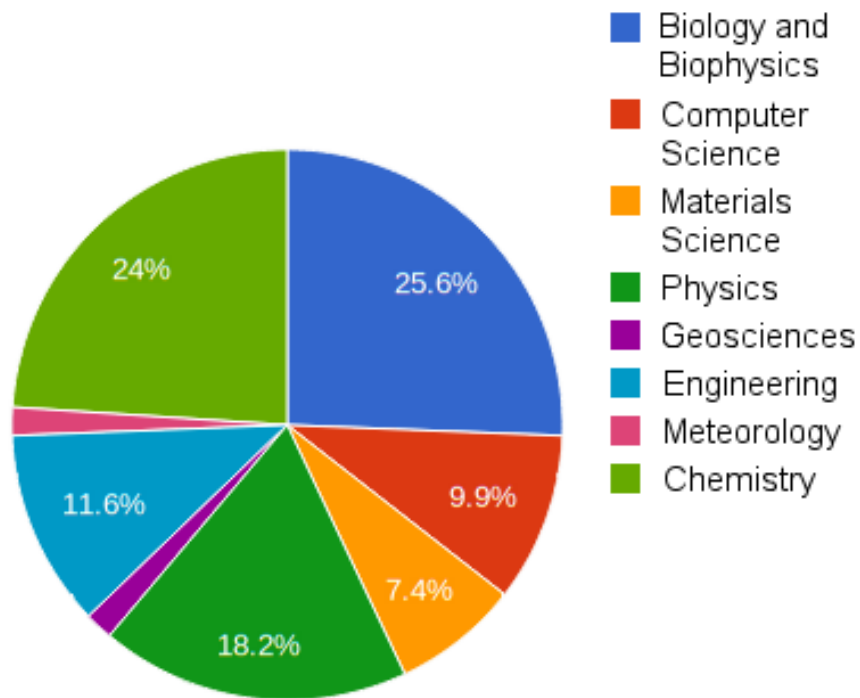
Main cluster usage approaching 12 million CPU hours
(usage is coming closer to its maximum capacity - 90% in Feb)

Projects and users registration progress

GridUnesp is a multipurpose VO: 29 projects from different scientific disciplines and around 170 users (researchers and students)

User distribution per scientific disciplines

Latest User Distribution per UNESP Project Area.



Extensive work has been done on assisting users on porting and adapting cluster applications to the Grid environment

GridUnesp and the São Paulo State Grid initiative



GridUnesp - Complex user requirements

Most of GridUnesp users come from the HPC community

→ efforts centered at transforming their needs into grid-friendly workflows

→ we successfully run typical HPC applications like Gromacs, Gaussian, Gamess, MrBayes, etc, with MPI support

Local applications have complex and challenging requirements

→ support for MPI, multithreaded (SMP) jobs, large memory jobs and long run jobs (> 20 days)

→ main cluster batch scheduler switched to Torque/Maui to better support long run queues and complex job requirements

Conclusions and perspectives

One vision for the future of HPC: a Grid of high-performance clusters interconnected by advanced optical metro/wide area networks - GridUNESP project designed with this vision in mind

→ it is providing the means for researchers to work on scientific projects that demand a great deal of computing power

Hardware and network infrastructure fully under our control

Building a multidisciplinary infrastructure is challenging

Next steps include:

→ integration of the inter-cluster WAN infrastructure

→ deployment of a Certificate Authority for the state of São Paulo

→ training courses and workshops for researchers & developers

References

GridUnesp and OSG Agreement

<http://osg-docdb.opensciencegrid.org/cgi-bin/ShowDocument?docid=827>

R. L. Iope, S. F. Novaes, *GridUnesp and the São Paulo State Grid initiative*

<http://osg-docdb.opensciencegrid.org/cgi-bin/ShowDocument?docid=1020>

J. Caballero, H. Severini, R. Gardner, *Employing Open Science Grid to support National Grid Initiatives in South America and South Africa*, CHEP 2010 Conference Proceedings

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References

R. L. Iope, *The São Paulo State University Campus Grid Initiative*, in Proceedings of the Second EELA-2 Conference, eds. R. Mayo et al (CIEMAT 2009), 25-27 November 2009, Choroní, Venezuela, pp. 257-266.

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R. L. Iope, N. Lemke, G. A. von Winckler, *GridUNESP: a multi-campus Grid infrastructure for scientific computing*, in Proceedings of the 3rd Latin American Conference on High Performance Computing (CLCAR 2010), 25-28 August 2010, Gramado, Brazil, pp. 76-84.

Slides available at

<http://gppd.inf.ufrgs.br/CLCAR2010files/slides/32.pdf>