



E-infrastructure shared between Europe and Latin America

Biomed Applications in the EELA Project

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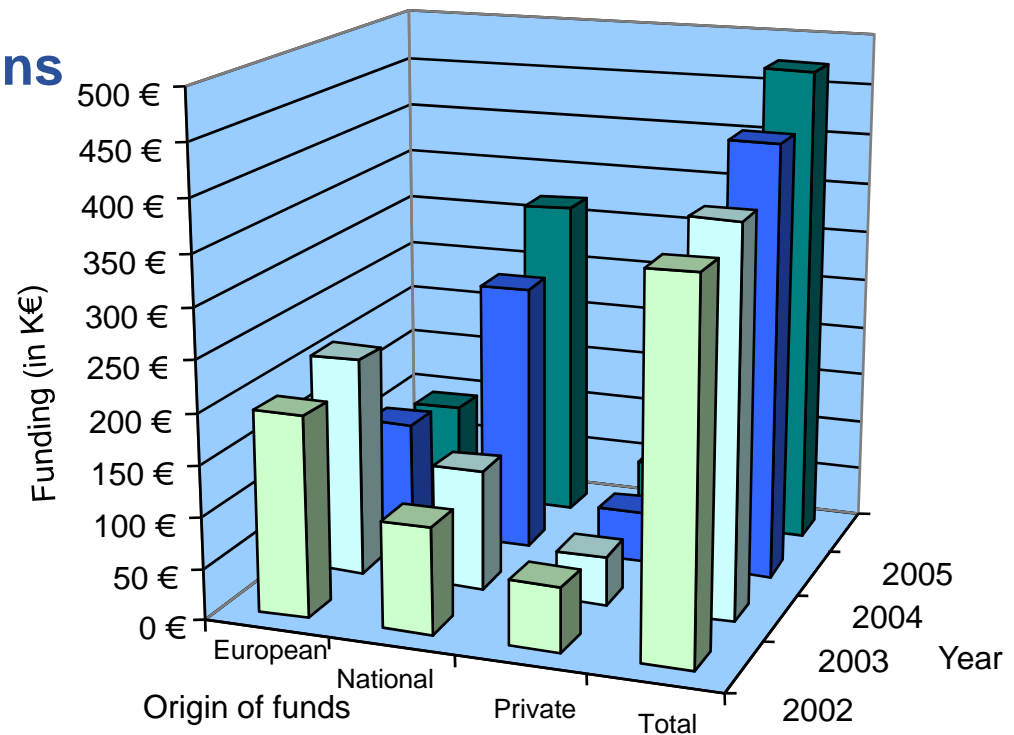
BioinfoGrid School
Varenna - Italy

- **The GRyCAP.**
- **The EELA Project.**
- **The Biomed Applications in EELA.**
 - GATE.
 - WISDOM.
 - BiG Processing Service.
 - Phylogenetics
- **Future Plans.**
- **Summary and Conclusions.**



The GRyCAP in a Slide

- A Research Group Funded by Vicente Hernandez, with 20 Years of Existence and Comprising 30 Researchers.
- The GRyCAP has Participated in 17 European Projects, Being the Coordinator in 10 of Them (7 Of them on the Medical Sector).
- The GRyCAP is Integrated in the Institute of Applications of Advanced Information Technologies and Communications (ITACA) and the Network Centre of Biomedical Engineering (CRIB).
- Ignacio Blanquer is the Responsible Person of the Medical Technologies Area of this Group.



<http://www.grycap.upv.es>



The Activity of the GRyCAP in HealthGrids

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- **Participant in EGEE-I and EGEE-II in the Development of Biomedical Applications.**
- **Responsible of Task 3.1 “Biomed Applications” in EELA.**
- **Other Relevant Activities**
 - Responsible of the Development of the HealthGrid Applications Roadmap in the SHARE (“Supporting and structuring HealthGrid Activities & Research in Europe: developing a roadmap”) Project.
 - Coordinators of CVIMO (Cyber-infrastructure for Medical Imaging in Oncology in Valencia Region).
 - Members of the Board of Directors of the HealthGrid Association.





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- **E-Infrastructures Shared Between Europe and Latin America**
 - Build a Bridge Between Consolidated E-infrastructure Initiatives In Europe And Emerging Ones In Latin America.
 - Create a Collaboration Network to Deploy a Large Portfolio of Scientific Applications on a Well Supported Pilot Test-Bed.
 - Set up a Pilot e-Infrastructure in Latin America, Interoperable with the Existing one in Europe (EGEE).





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The EELA Web Site

<http://www.eu-eela.org>

ee la E-INFRASTRUCTURE SHARED BETWEEN EUROPE AND LATIN AMERICA Contract no. 026409

Collaborate with FFI A or become an EELA Member?

please, come in

Latest News
Itacuruza 4-13 December 2006 (Brasil)
→ 1st EELA Conference Videos

Argentina
Brazil
Chile
Cuba
Mexico
Peru
Venezuela
CLARA
Italy
Portugal
Spain



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EELA Partners

Italy: INFN

Portugal: LIP

Spain: CIEMAT, CSIC, Red.ES, UC, UPV

CERN



- 10 Countries
- 21 Partners

Argentina: UNLP

Brazil: CEDERJ, RNP, UFF, UFRJ

Chile: REUNA, UDEC, UTFSM

Cuba: CUBAENERGIA

Mexico: UNAM

Peru: SENAMHI

Venezuela: ULA

CLARA



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EELA Infrastructure

- **Resources**
 - EELA Pilot Test-bed with 16 Sites Integrated.
 - High quality network (GÉANT, RedCLARA, NRENs).
 - 734 CPUS, 61.2 TB Storage.
- **Certification Authorities**
 - 7 Certification Authorities and 1 Registration Authority have Been Set-up in Latin America (No Grid CAs nor RAs Before)
- **EELA Test-bed Evolving Towards Production Quality.**

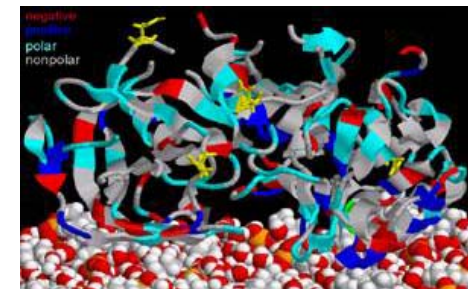




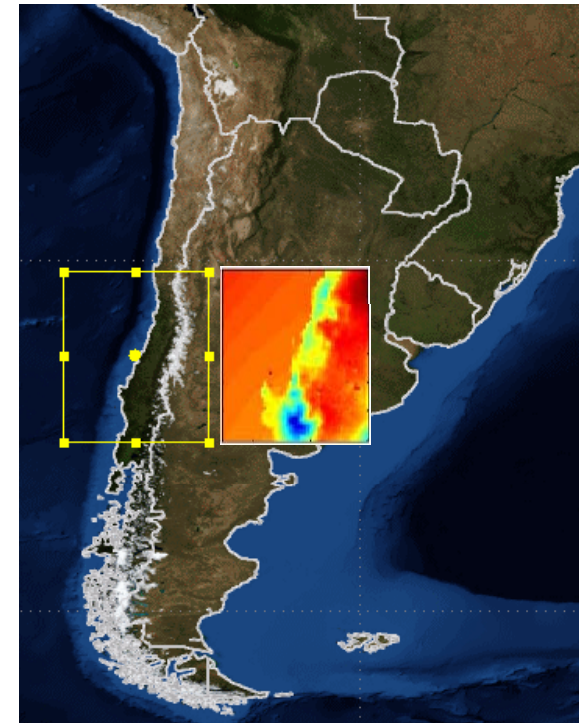
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Biomedical Applications in EELA

- **Application Workpackage Coordinated by CIEMAT.**
- **Biomed Applications are Coordinated by UPV with the Participation of CUBAENERGIA and ULA.**
- **Grid Biomedical Applications Typically Fall into Four Categories**
 - **Bioinformatics Applications**
 - BLAST in Grids.
 - Phylogeny.
 - **Computational Biochemical Processes**
 - Wide in-Silico Docking on Malaria (WISDOM).
 - **Biomodels Simulation**
 - GATE.



- **High Energy Physics**
 - Mainly Alice and LHCb Experiments from the LHC.
- **Climate**
 - Simulation of “el Niño” and “La Niña” Weather Phenomena.
- **eLearning**
 - Video on Demand, Cuban Grid for Learning and Laboratorio Experimental Multidisciplinario a Distancia (LEMDist).
- **More than 100 Users on 2 Vos.**



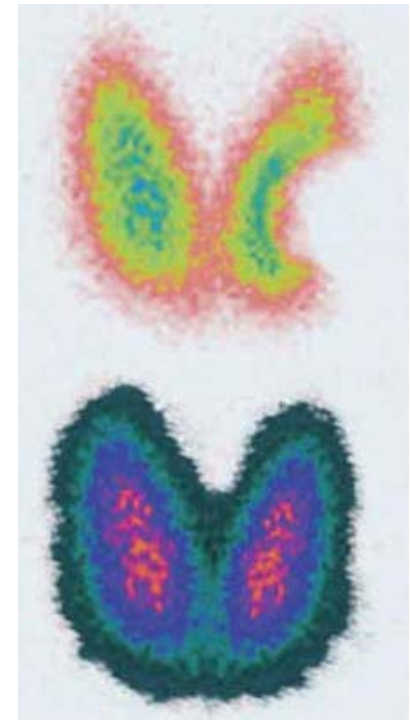


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GATE

GEANT4 Application to Tomographic Emission

- **Geant4 Application to Tomographic Emission (GATE)**
- **GATE is an Environment for the Monte-Carlo Simulation of Particle Physics Emission in the Medical Field Developed in the Frame of the OpenGate Collaboration (<http://www-lphe.epfl.ch/GATE>).**
- **The Interest of the LA Community is Led by CUBAENERGÍA**
 - It is Focused Towards Two Main Oncological Problems:
 - Thyroid Cancer.
 - Treatment of Metastasis with P^{32} .
 - 9 centers in Cuba are Interested (5 Hospitals and 4 Oncological Centers and Institutions)





- **Resources Available**

- UPV (ramses.dsic.upv.es; GATE-1.0.2-3)
- CIEMAT (ce-eela.ciemat.es; GATE-1.0.0-3)
- UFF (ce-eela.ic.uff.br; GATE-1.0.0-3)
- UFRJ (ce-eela.uf.ufrj.br; GATE-1.0.0-3)

- **User Communities**

- Cuban Centres have Problems with Bandwidth
 - A Local Deployment is Being Developed.
 - This Local Grid will be Used Rather for Training than for Production.
 - It However Comprises all the Necessary Elements for a Pilot Test-Bed.



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WISDOM

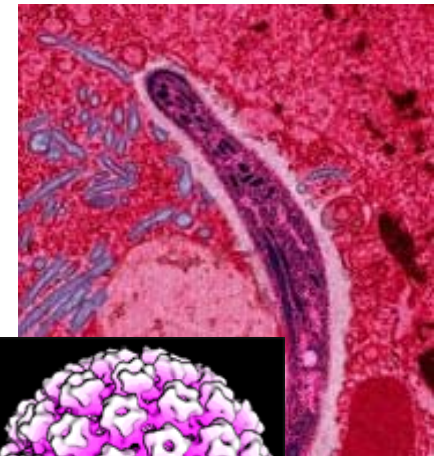
Wide in Silico Docking on Malaria



Status of Mature Applications: WISDOM

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- **WISDOM (Wide In-Silico Docking Of Malaria) is a Deployment of a High-Throughput Virtual Screening Platform in the Perspective of In-Silico Drug Discovery for Neglected Diseases.**
- **The In-Silico Docking is Faster and Much Cheaper than the Experimental Docking, Which is Restricted to the Most Successful Ligands Obtained After the Simulation Process.**
- **The Initial Objective of WISDOM is the Proposition of New Inhibitors for a Family of Proteins Produced by a Protozoan Parasite (Plasmodium Falciparum) that Causes Malaria.**
- **ULA has Selected New Targets of Plasmodium Vivax which have been Included in Large-Scale Docking Experiments.**

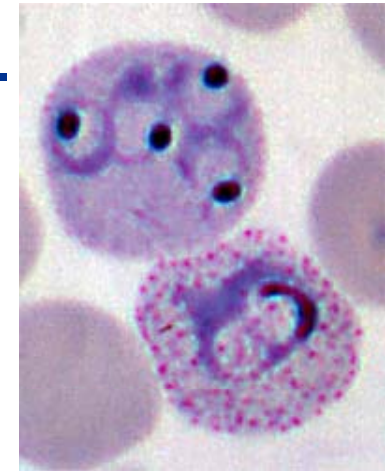




First EELA WISDOM Data Challenge

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- **Outcome:**
 - 2 Targets proposed by ULA.
 - DC operated and coordinated by UPV.
 - Starting date: October the 23rd, 2006.
 - Ending date: January the 1st, 2007.
 - Number of original jobs of the first target: 2422.
 - Average computing time per job: 34,4 hours.
 - Total effective running time: 228 CPU.days.
 - Results obtained: 53 Gbytes.





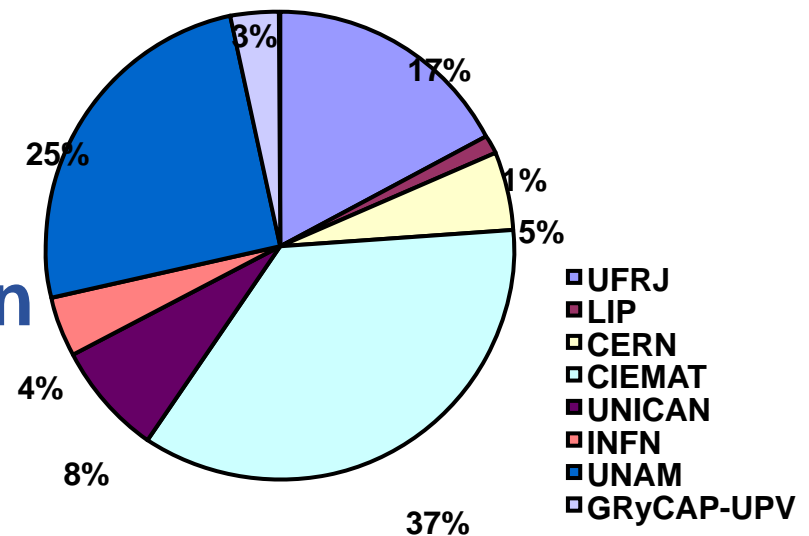
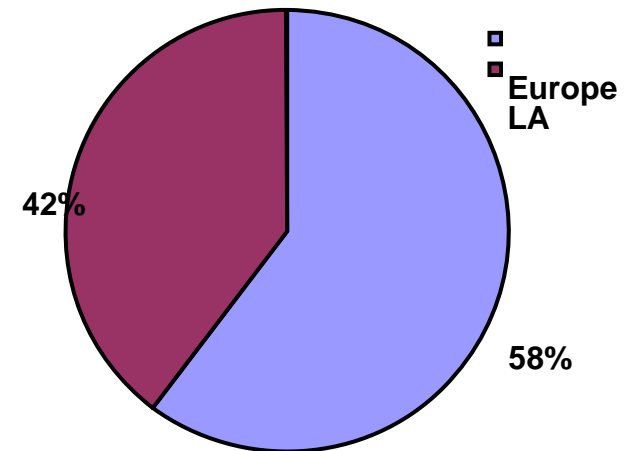
First EELA WISDOM Data Challenge

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- **Sites used:**

- Spain: CIEMAT, GRYCAP-UPV UNICAN.
- Italy: INFN.
- Portugal: LIP.
- Mexico: UNAM.
- Brazil: UFRJ.
- Internat: CERN.

- **More than 40% of the jobs were effectively executed in LA sites**





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BiG BLAST in Grids



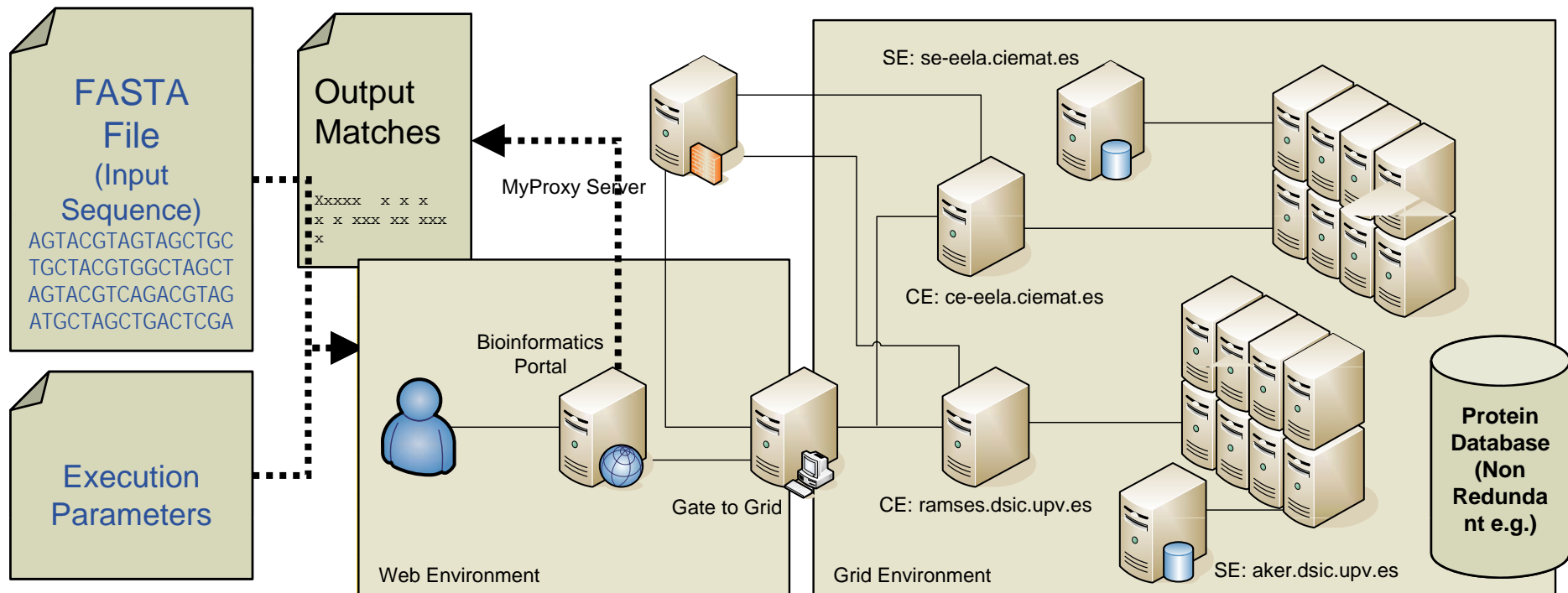
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Status of New Applications: BiG

- **BiG: BLAST in Grid is a Grid-enabled BLAST Interface.**
- **BLAST (Basic Local Alignment Search Tool) is a Bioinformatics Procedure Applied to Identify Compatible Protein and Nucleotids Sequences in Protein and DNA Databases.**
- **User Community**
 - The Bioinformatics Ibero-American Network and Portal (<http://portal-bio.ula.ve>).
 - This Portal Also Provides Several On-Line Applications for Registered Users.
 - It Currently has Almost 600 Registered Users from 70 Countries (Although 90% Come from 10 Countries).



Blast in Grids: Approach

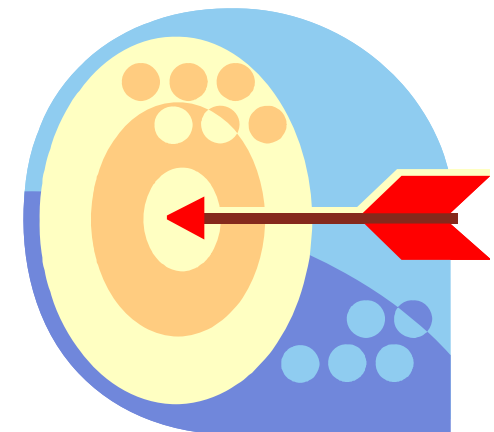




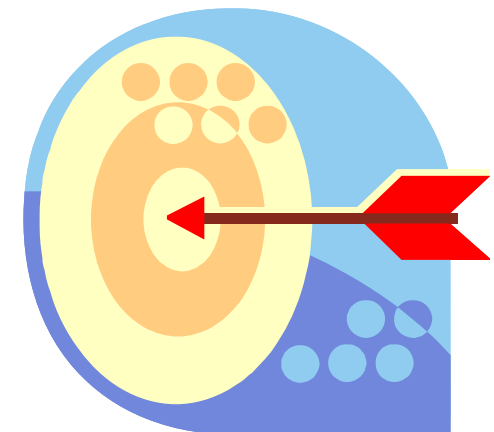
Design Objectives and Requirements I

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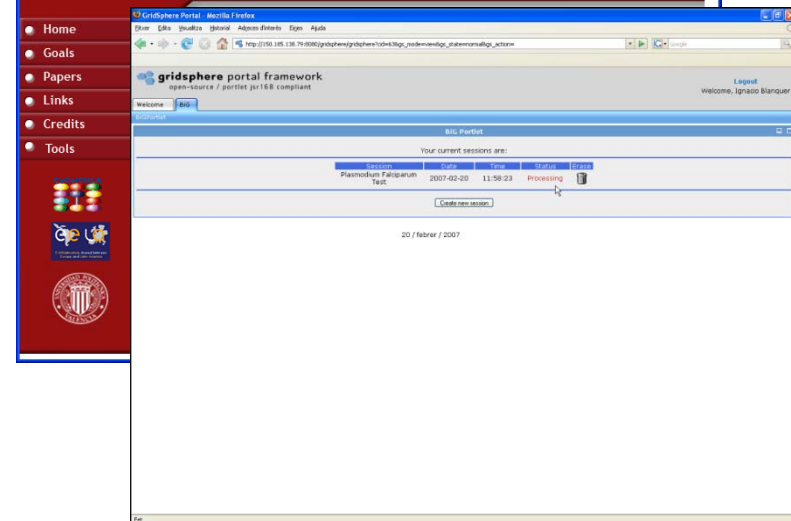
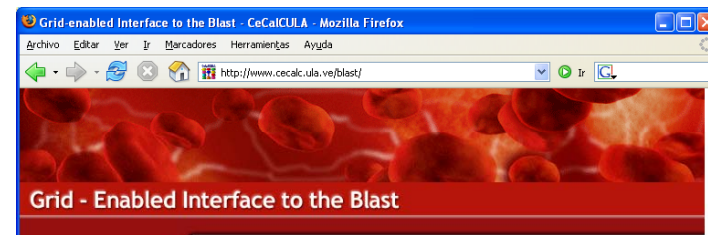
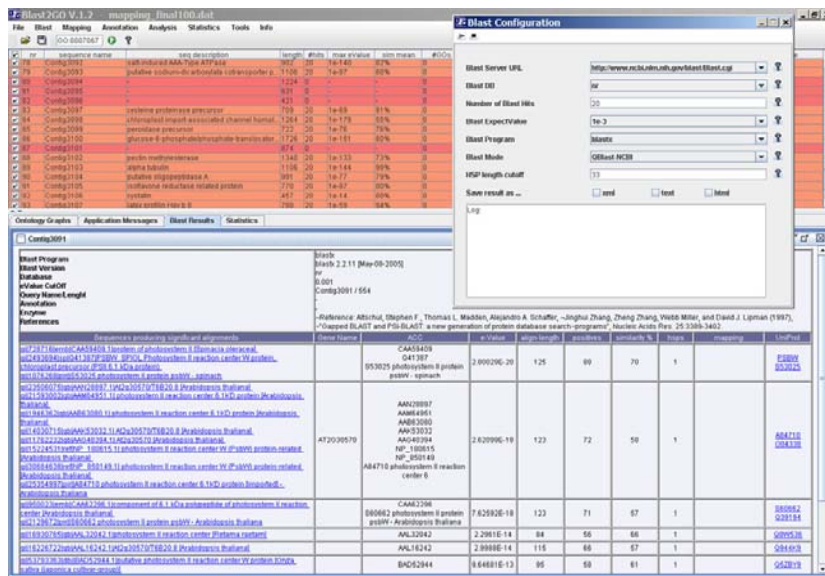
- **Easy Interface with High Compatibility (Web Service + NCBI Based)**
 - Same Parameters as NCBI BLAST.
- **Portable**
 - Sessions Could Be Independent of the Server.
- **Secure and Efficient**
 - Users can Provide Grid or Portal Credentials.
 - Portal Credentials are Mapped to Gate-to-Grid Credentials.
 - Credentials are Stored in a MyProxy Server to Avoid Security Leakages.
 - Credentials are Automatically Renewed for Long Jobs.



- **High Performance**
 - Grid Computing + MPI Parallel Jobs in Dedicated Clusters.
 - MPI Blast Provides Results Quicker.
- **Scalability**
 - Scalability of MPIBlast Strongly Affected by Network.
 - Data Partition in Grid Approach Gives Scalability with Huge Quantities of Data.
- **Support to Searching Simultaneously on Multiple Databases**
 - Parallel Process on Multiple Databases.
- **Robust**
 - Fault Tolerance on Server and Client.

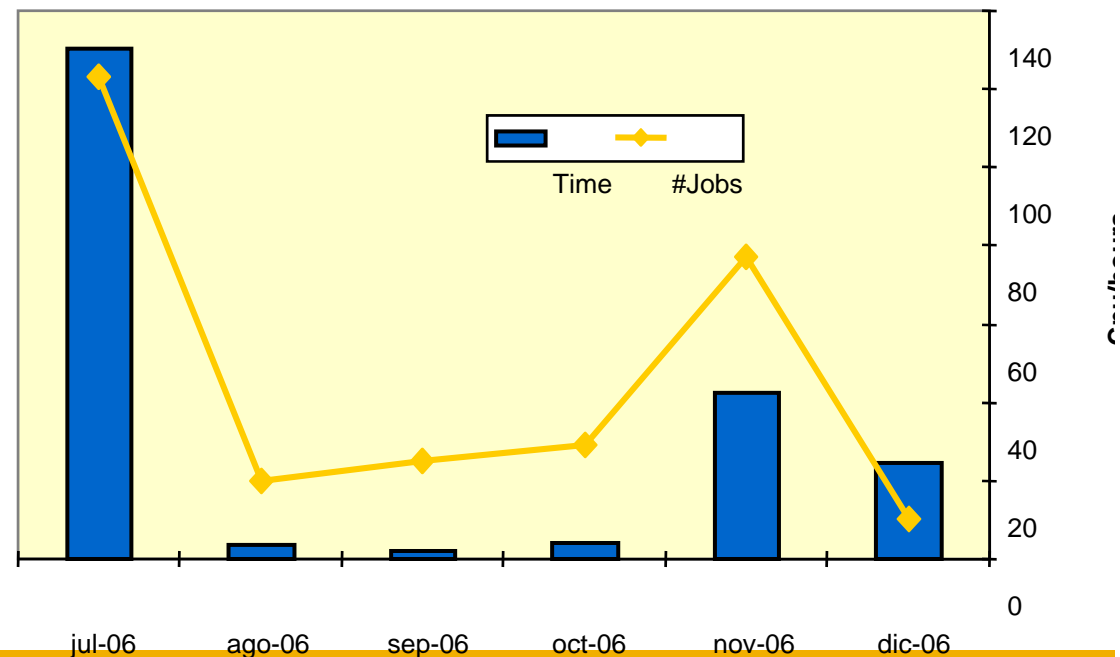


- Users Access the System Through Stand-Alone Applications or Web Portals. Currently
 - BLAST2GO: www.blast2go.org.
 - Web from CeCalcula: <http://portal-bio.ula.ve>.
 - Even CLI.



Blast in Grids: Usage Report

- **Period: Jul'06-Dec'06.**
- **Usage Statistics:**
 - Number of Jobs: 284.
 - CPU Consumed: 173 CPU/Days.
 - Resources Used: ramses.dsic.upv.es:2119/jobmanager-pbs-biomedg.
 - BiG is Being Used at the University of Los Andes to Work on the Complete Genome of the Plasmodium Falciparum for the Identification of DHFR Antigenic Proteins.





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MBG

MrBayes in Grids

- **Problem Addressed**

- A Phylogeny is a Reconstruction of the Evolutionary History of a Group of Organisms. Very Important for the Analysis of the Resistance to Treatments.
- Phylogeny Tools Consumes Much Memory And Computing Time.

- **User Community**

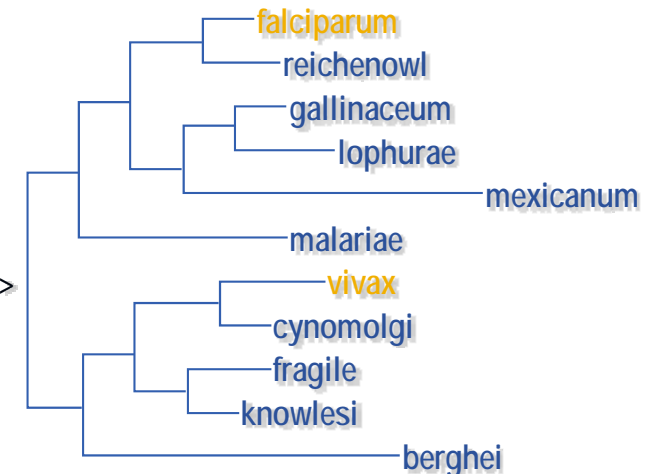
- The Bioinformatics Ibero-American Network and Portal (<http://portal-bio.ula.ve>).

- **Solution proposed**

- Use an Mpi-enabled Version of a Widely used Bayesian Inference Application For Phylogeny (MrBayes).

- **Achievements**

- A Grid-service to Run Parallel MrBayes Executions is Currently Available at UPV.





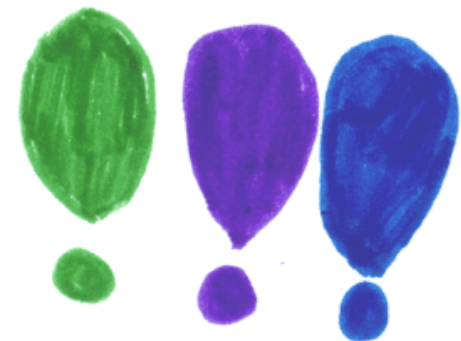
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Future Plans



- **To Enlarge the User Community**
 - New Users from LA and European Countries have been Contacted and Access to BiG and MrBayes will be Provided.
- **To Increase the Portfolio of Applications**
 - Complete Phylogenetic Process.
- **To Address other Biomedical Areas**
 - Recently Submitted, EELA-2 Proposal Aims at Epidemiology as a New Application Area for HealthGrids.
 - PharmaEpidemiology and Molecular Epidemiology Also Requires Intensive Computing.

- **EELA Aims at Bridging the Research Between Europe and Latin America Through the Usage of Common eInfrastructures.**
- **Users in LA Have very Similar Needs, Although they Suffer from More Technical Problems.**
- **However, there are Key Research Centres in LA that Produce Scientific Excellence in Many Areas of Bioinformatics.**
- **Applications Deployed in EELA could be of Interest to European Users.**





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