



The GENIUS Grid Portal : some success stories!

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- EnginFrame framework
- The GENIUS Grid Portal
- Some Integrated Applications
- References

RiginfoGRID

A grid portal: why and how

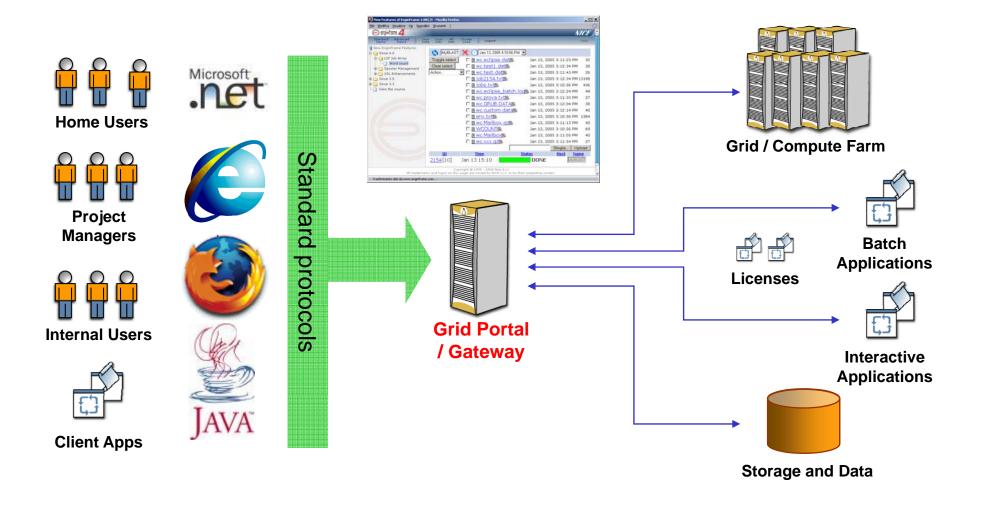
- It can be accessed from everywhere and by "everything" (desktop, laptop, PDA, cell phone).
- It can keep the same user interface to several backends.
- It must be redundantly "secure" at all levels:
 - 1) secure for web transactions,
 - 2) secure for user credentials,
 - 3) secure for user authentication,
 - 4) secure at VO/VOMS level.
- All available grid services must be incorporated in a logic way, just "one mouse click away".
- Its layout must be easily understandable and user friendly.



- A Grid Portal improves usability of Grids
 - Lowering end-user requirements for accessing the Grid
 - Hiding the complexity of data and job services management in the Grid
- A Grid Portal improves utilization of Grids
 - Making the Grid (r)evolution transparent to the enduser
 - Providing an appealing user-friendly Web interface
 - Enforcing Grid utilization policies



The Grid Portal / Gateway





- Grid Portals technology
- EnginFrame Framework
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- It is a web-based technology able to expose Grid services running on Grid infrastructures
- It allows organizations to provide application-oriented computing and data services to both users (via Web browsers) and applications (via SOAP/WSDL and/or RSS)
- It's a Grid *gateway*
- It greatly simplifies the development of Web Portals exposing computing services that can run on a broad range of different computational Grid systems

Who uses EnginFrame?

Mechanical

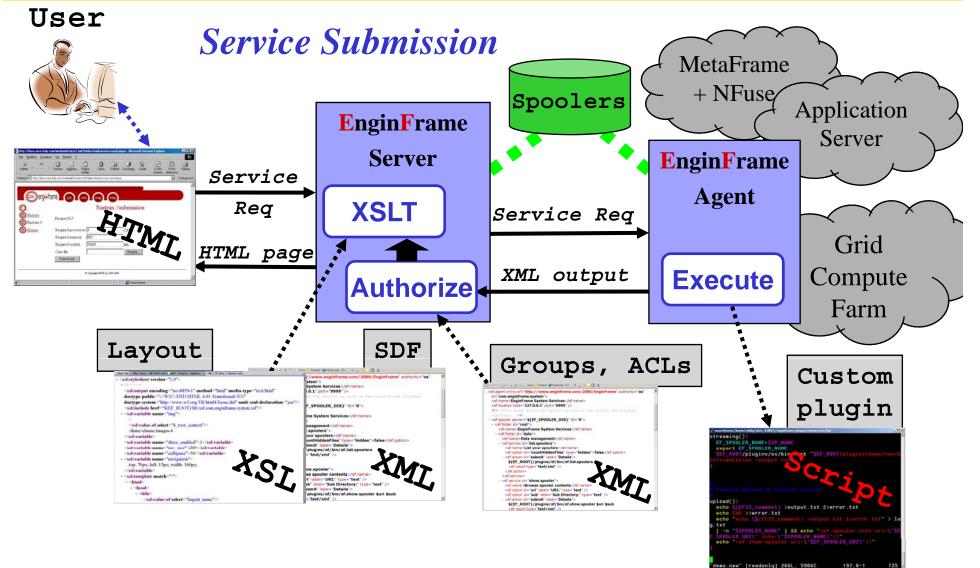
RiginfoGRID

- Ferrari, Audi, BMW, FIAT Auto, Elasis, Magneti Marelli, P+Z, Swagelok, Toyota, TRW
- Manufacturing
 - Bridgestone, Procter & Gamble, Galileo Avionica
- Oil&Gas
 - Slavneft, Schlumberger, TOTAL, VNIIGaz
- Electronics
 - STMicroelectronics, Accent, SensorDynamics, Motorola
- Biotech
 - ENEA, EGEE LS community

- Telecom
 - Telecom Italia
- Research
 - INFN, ASSC, CCLRC, CERN, CILEA, CINECA, CNR, CNRS/IN2P3, ENEA, FzU, ICI, IFAE, ITEP, JSC G.G.M., KU Leuven, SSC-Russia, SDSC
- Education
 - Dresda University, Ferrara University, ITU, Messina University, Politecnico of Milan, Technische Universität Dresden, Trinity College Dublin, Salerno University, S-PACI

EnginFrame Working Environment

BioinfoGRID



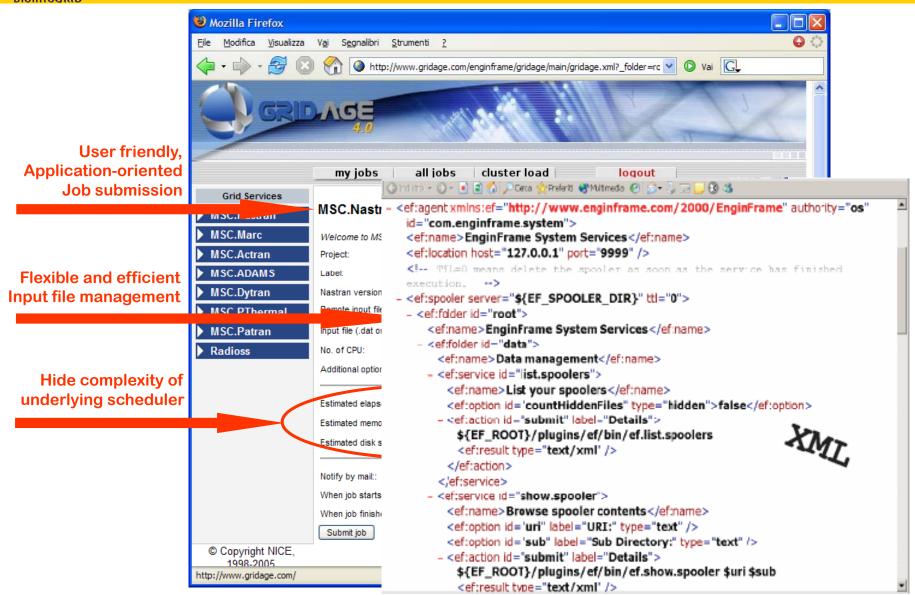


Service example

BioinfoGRID <ef:service id="gzip"> <ef:name>qzip sample</ef:name> <ef:option id="level" label="Compression level" type="list"> <ef:option id="9">maximum</ef:option> <ef:option id="4">medium</ef:option> <ef:option id="0">none</ef:option> </ef:option> <ef:option id="FILE" label="File to compress" type="file"/> <ef:action id="submit" label="Submit job"> EF SPOOLER NAME="gzip \$file" export EF SPOOLER NAME \${EF ROOT}/plugins/lsf/bin/bsub -o output.txt gzip -\$level \"\$FILE\" <ef:result type="text/xml"/></ef:action> </ef:service> (e) 'Remote' Agent demonstration - Microsoft Internet Explorer - 🗆 × <u>File M</u>odifica <u>V</u>isualizza <u>Preferiti Strun</u>enti <u>?</u>)enginframe) local (gzip samples azio sample Simple test Compression level maximum 🔻 Choice test File to compress Stoglia.. 🔇 <u><embed> test</u> Submit job Execute command S View the source Copyright NICE srl, 1998-2001 ۲ 🥝 Internet 🥙 Operazione completata



Usability & Input Management





- Grid Portals technology
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- GENIUS is a powerful Grid Portal that allows scientists to exploit Grid resources only using a conventional Web browser
- It's a gateway to European EGEE Project middleware
- It has been built on top of the EnginFrame framework
- It allows to expose gLite-enabled applications via Web-browser as well as Web Services



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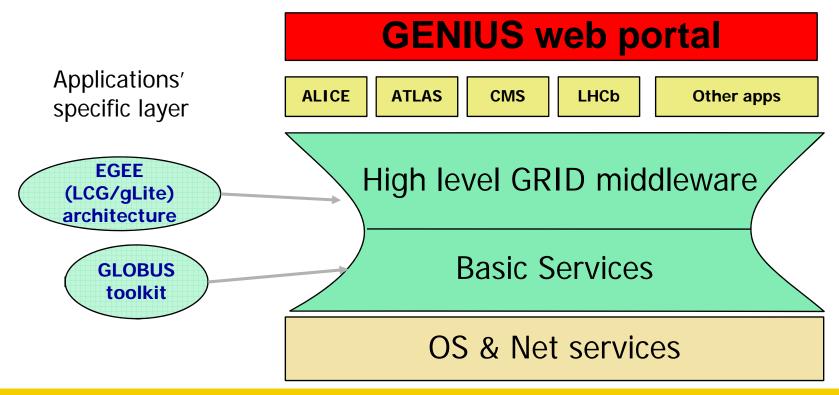
The GENIUS hourglass model

GENIUS

Grid Enabled web eNvironment for site Independent

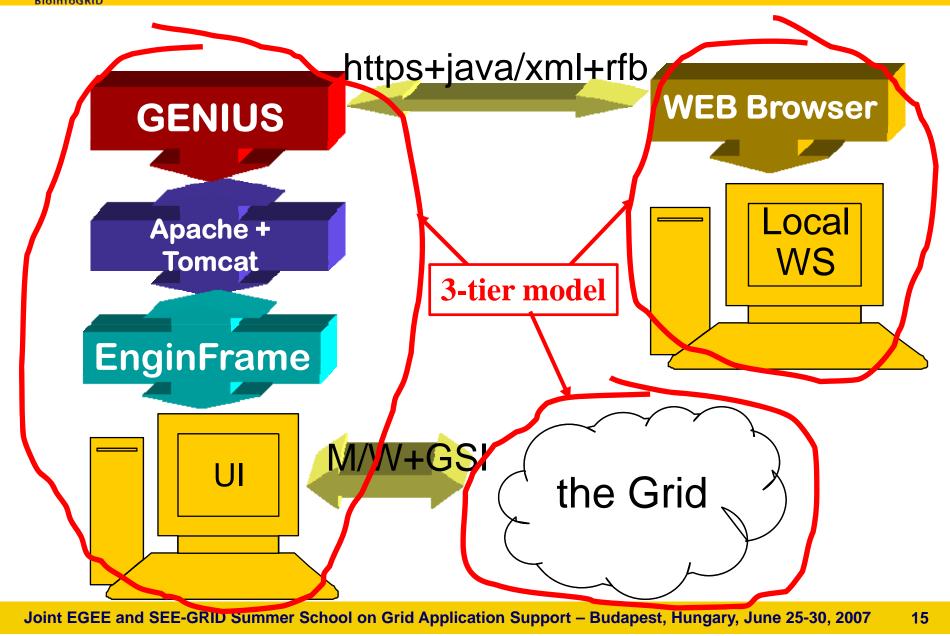
User job Submission

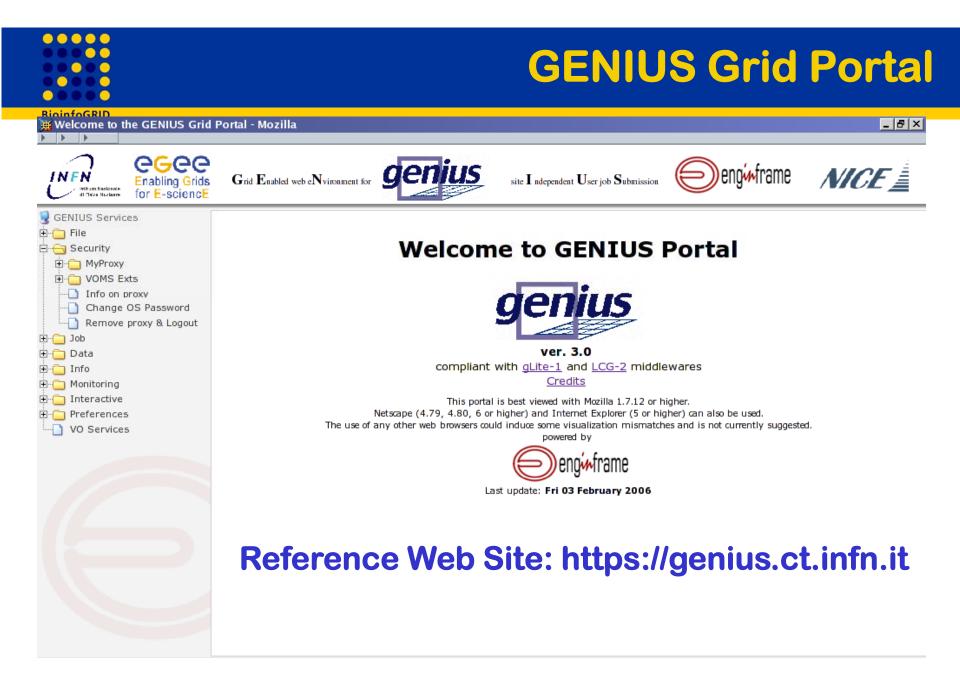
INFN / NICE Collaboration





GENIUS Architecture





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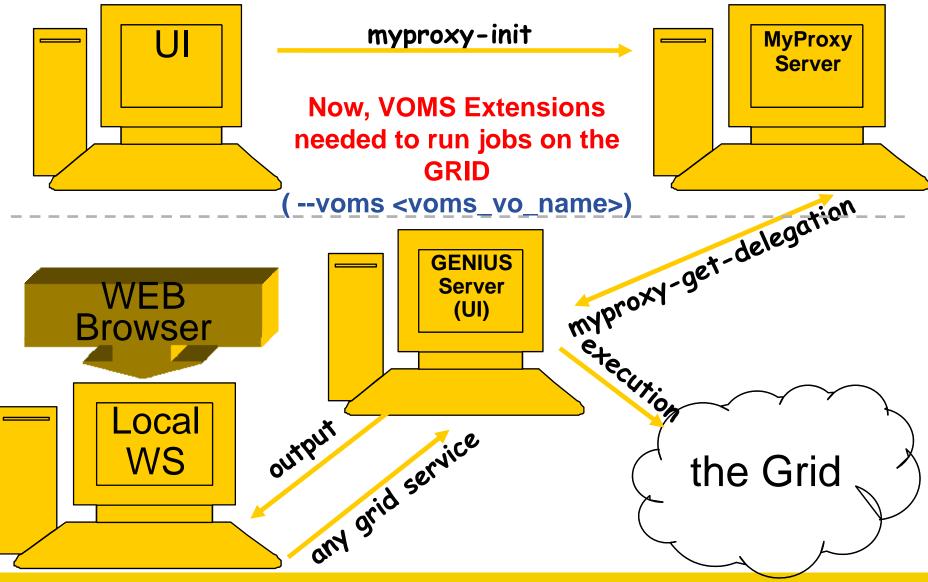
GENIUS : Security Infrastructure

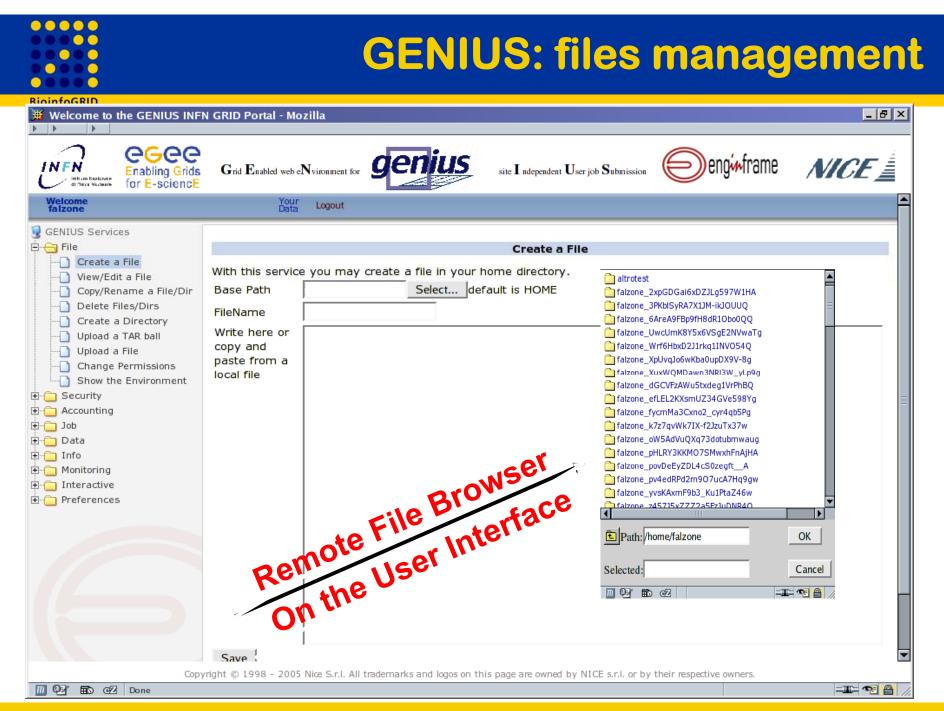
- All web transactions are executed under the Secure Socket Layer (SSL) via HTTPS
- The user must have an account on the User Interface
- When the user wants to interact with the file-system of the UI, GENIUS will prompt for the username and password of user's account on that machine
- Grid authentication in GENIUS is currently based on the concept Proxy



BioinfoGRID

Grid authentication with MyProxy



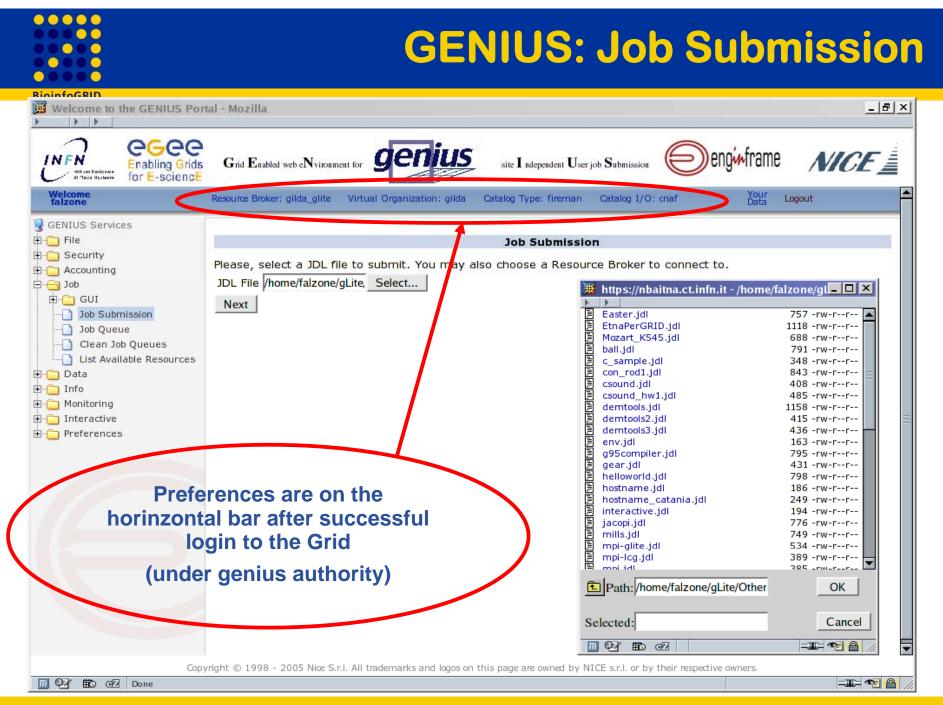


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GENIUS: Job Queue

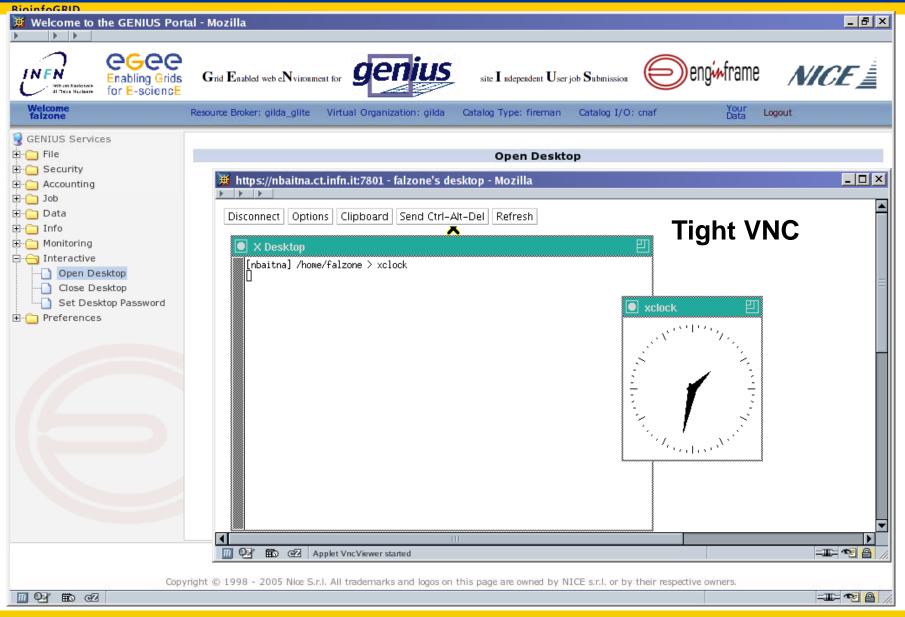
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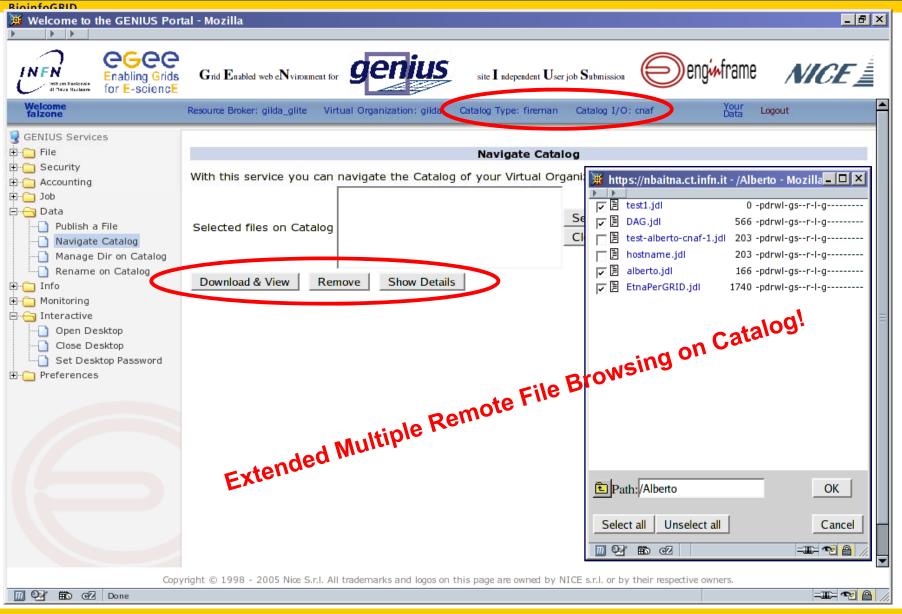
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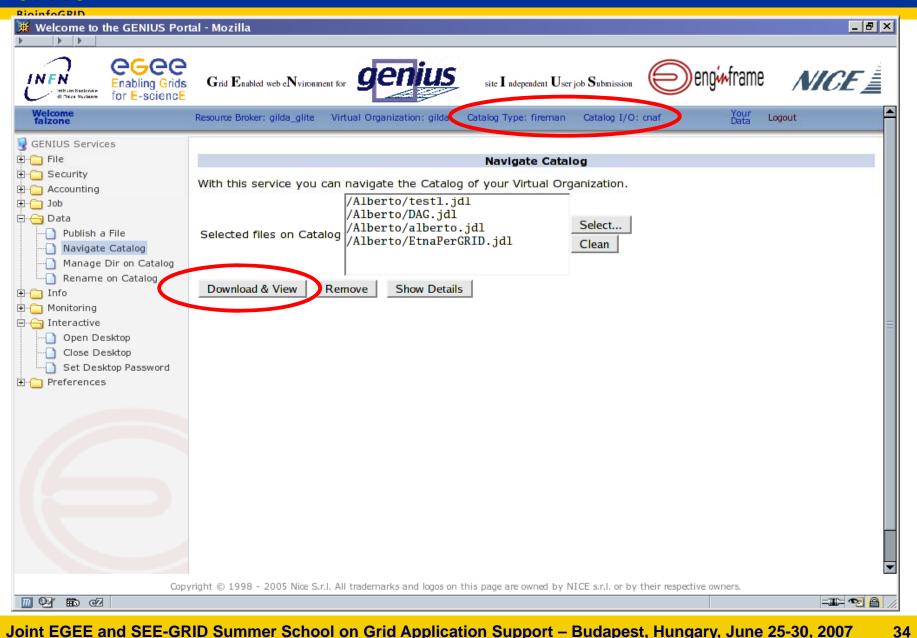
GENIUS: Data & Grid Catalogs

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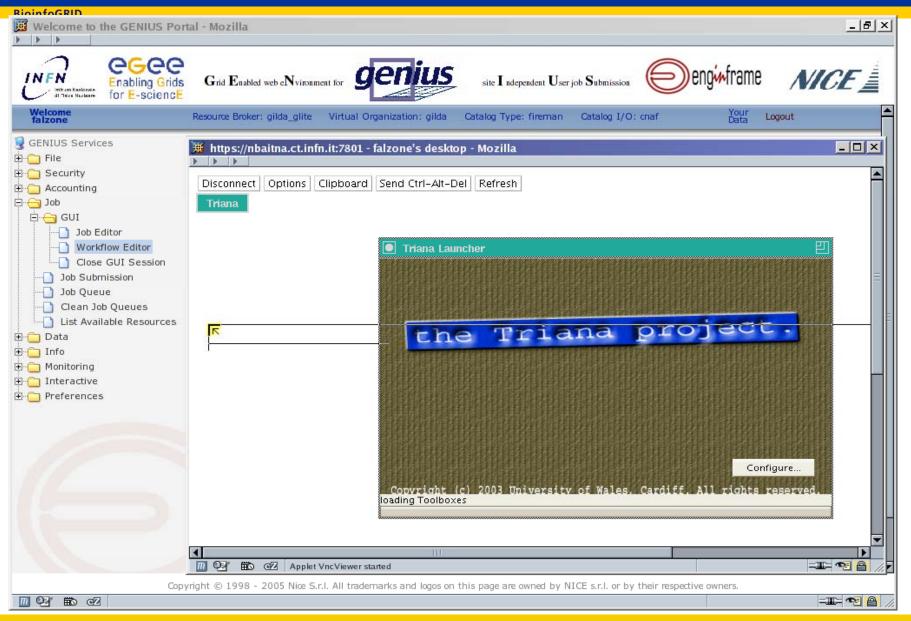
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GENIUS: Data & Grid Catalogs

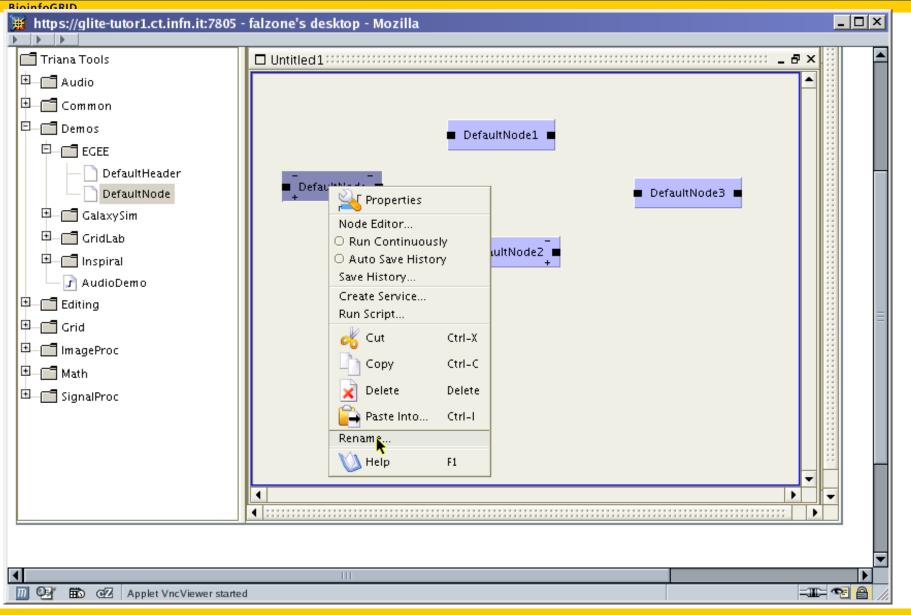


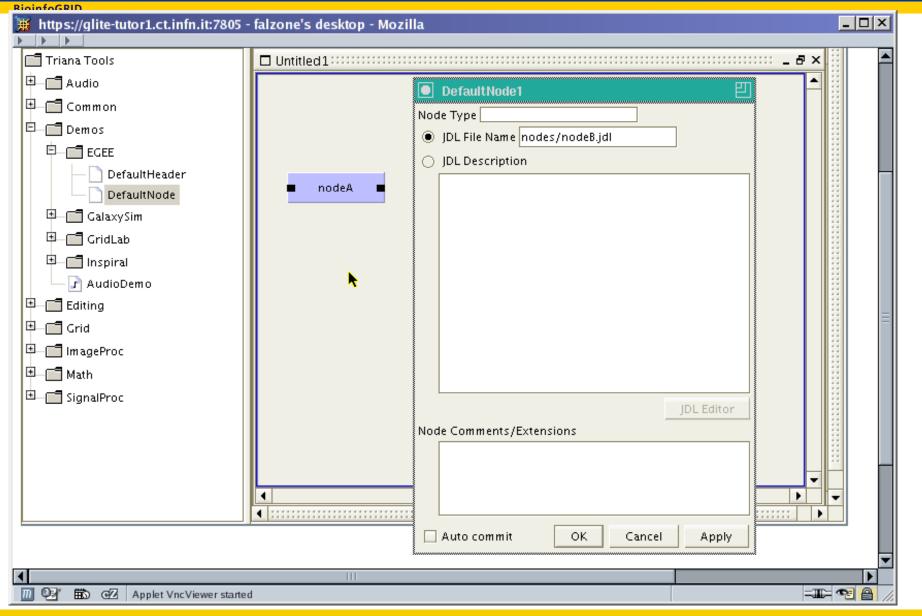
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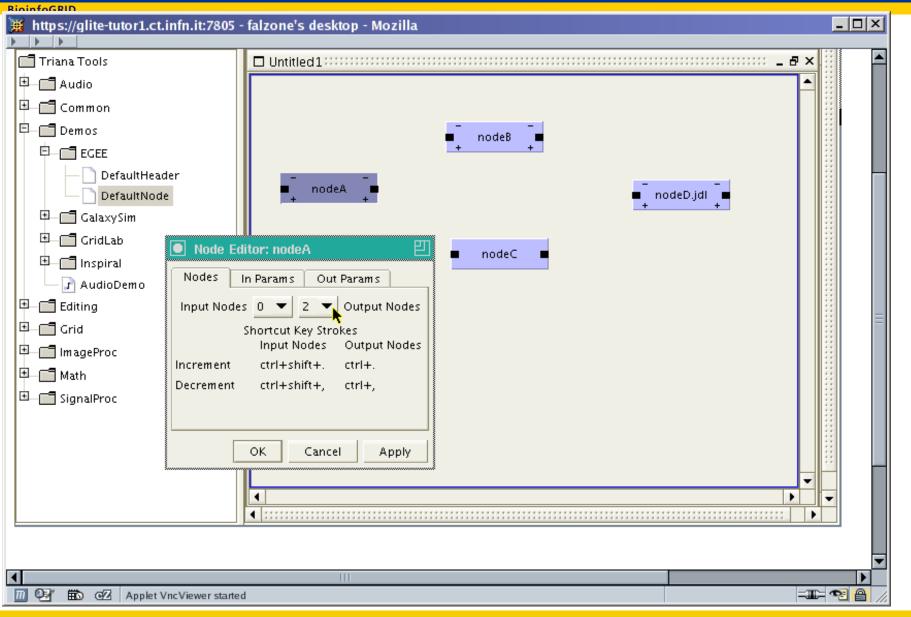
GENIUS & TRIANA /2

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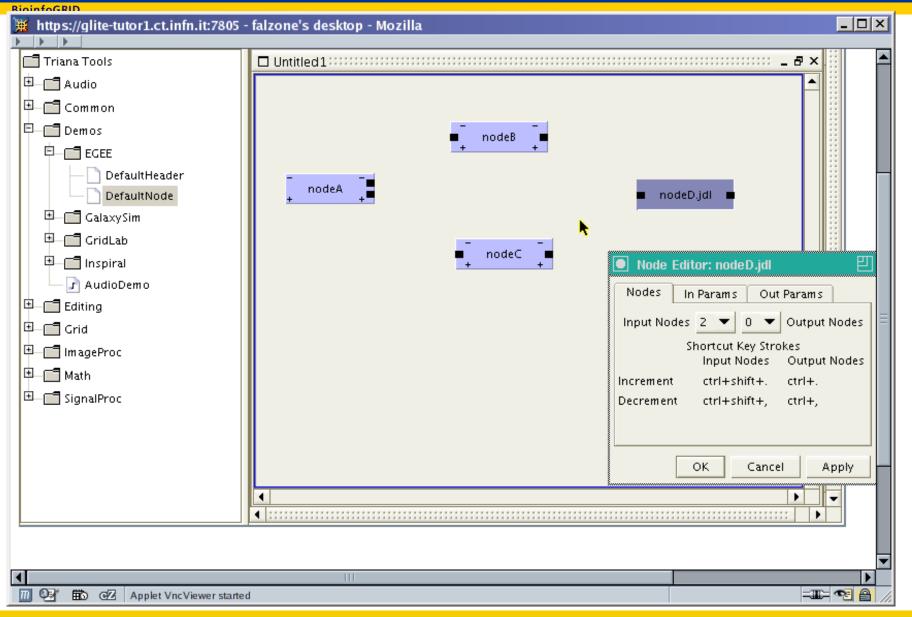


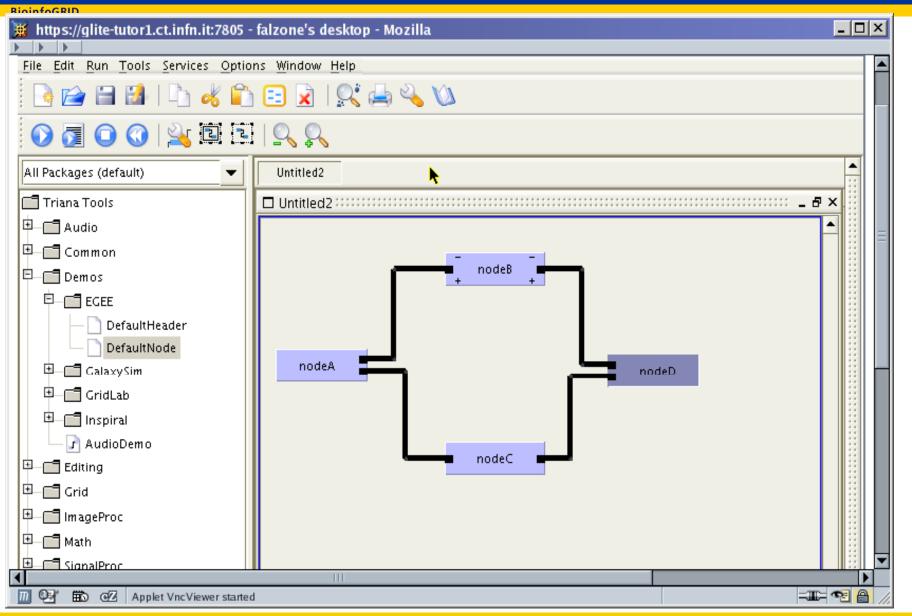


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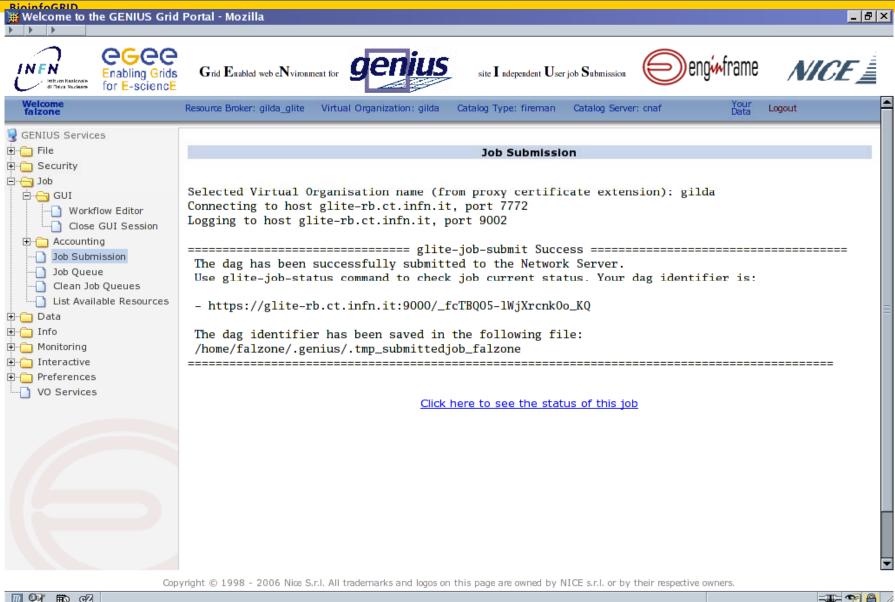
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- Grid Portals technology
- EnginFrame Framework
- The GENIUS Grid Portal

• Some Integrated Applications

References



This is a work supported in part by the <u>LIBI</u> and the <u>BIOINFOGRID</u> project.

What is **BLAST**?

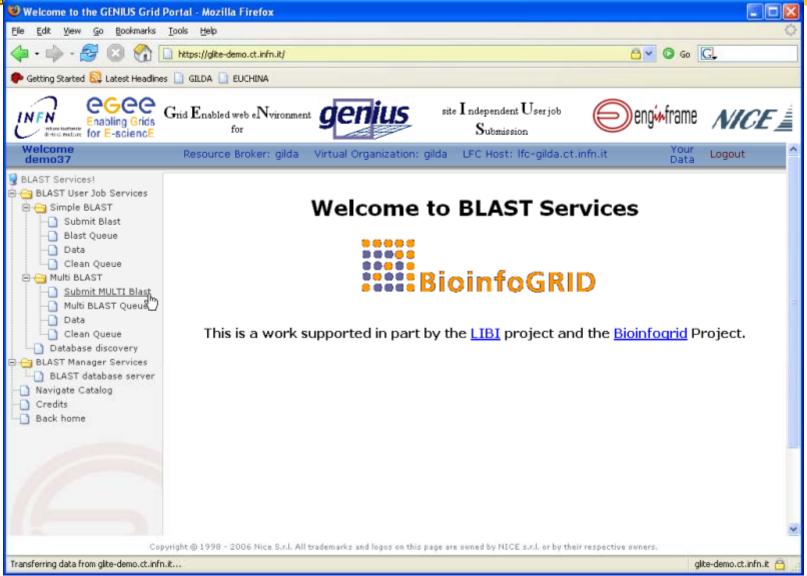
BLAST (Basic Local Alignment Search Tool) is an algorithm used to compare biological sequences, such as the amino-acid of different proteins or the nucleotides of DNA sequences.

The program requires a query sequence (also called *target sequence*) and a database.

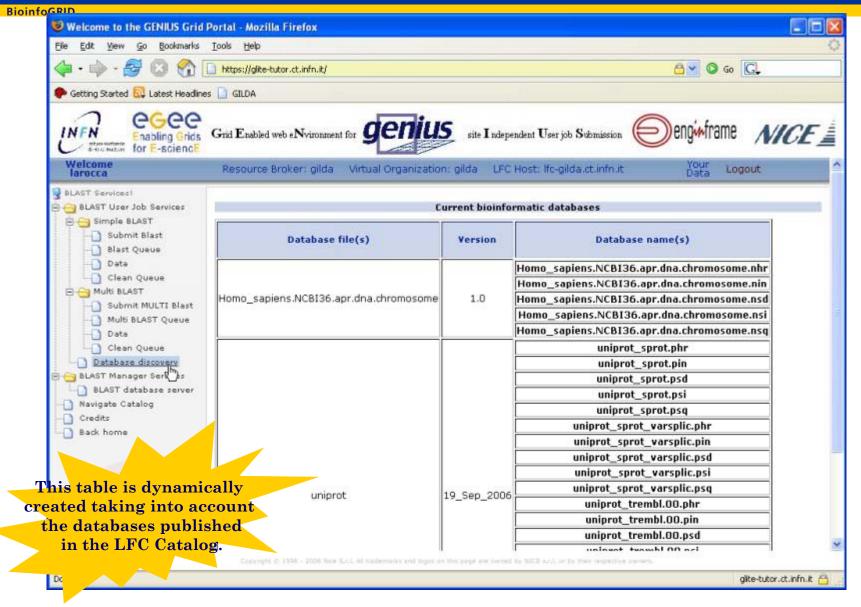
Its identifies all the sub-sequences of the target query that are similar to the sub-sequences in the database.



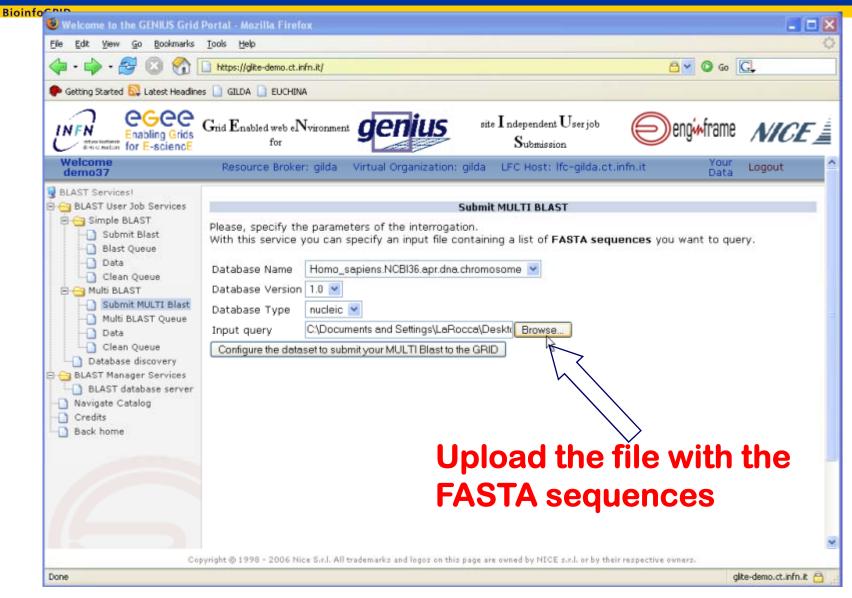




Bioinformatics databases

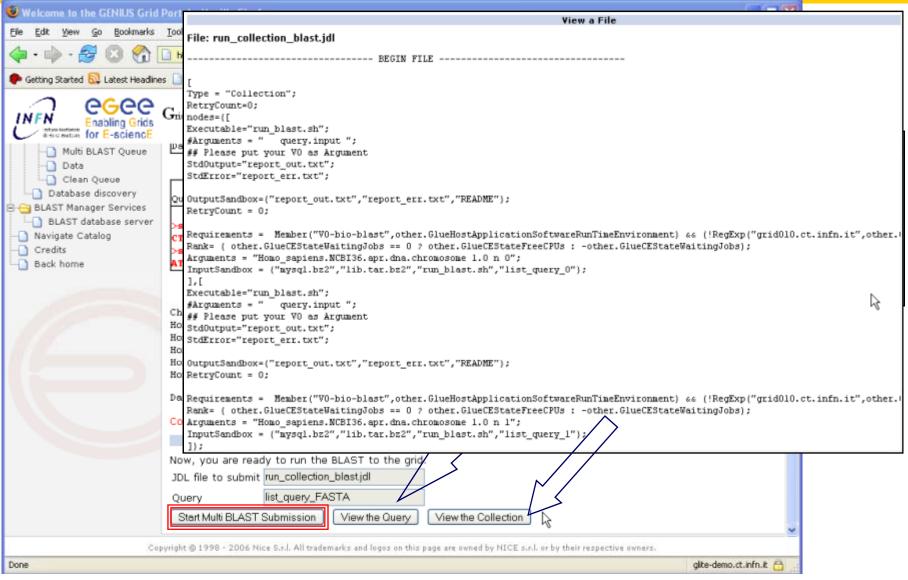


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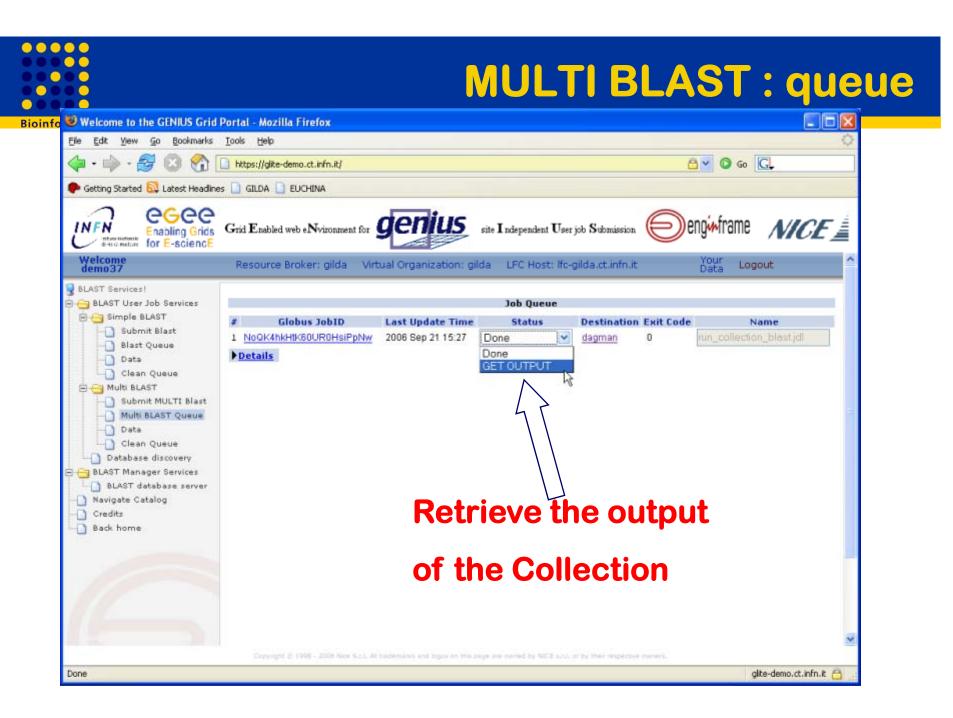
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Click <u>here</u> to inspect a typical output file produced by BLAST during the computation

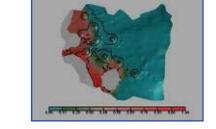
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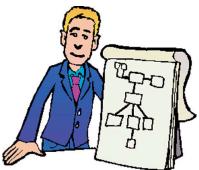
Presented at First view Presented at First Review Presented at First R **CODESA-3D**

This is a work supported in collaboration with Giuditta Lecca¹, Jawher Kerrou², Philippe Renard³ Giuseppe La Rocca⁴ and Roberto Barbera⁴

> 1 CRS4, Cagliari (Italy) 2 INAT, Tunis (Tunisia) 3 CHYN, University of Neuchatel (Switzerland) 4 INFN, Catania (Italy)

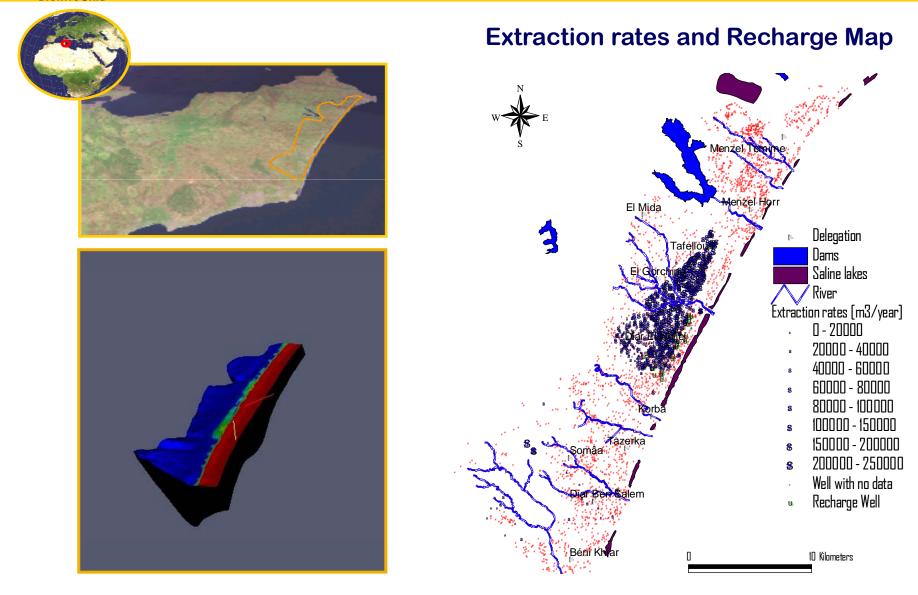
The CODESA-3D application

- CODESA-3D (COupled variable DEnsity and Saturation 3-Dimensional) is a software developed at CRS4 (Center for Advanced Studies, Research and Development in Sardinia - <u>http://www.crs4.it/</u>).
- Its aims to study, taking into account detailed mathematical representations of physical, chemical and biological processes that govern water flow, saltwater intrusion in freshwater coastal aquifers.

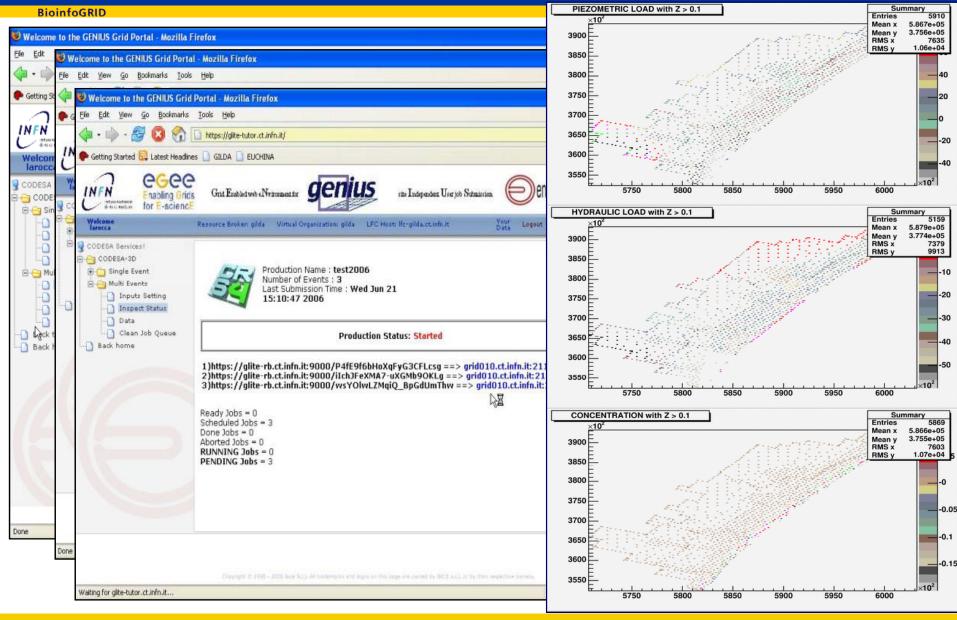




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Integration & results

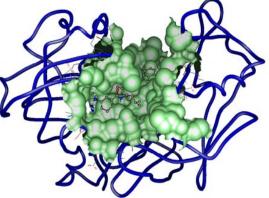


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- Internation Science Grid This Week (ISGTW)
 - <u>http://www.isgtw.org/?pid=1000341</u> March, 2007



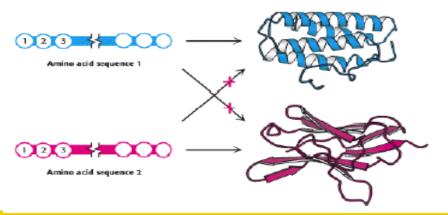


This is a work supported in collaboration with Fabio POLTICELLI (polticel@uniroma3.it) Pier Luigi LUISI (luisi@mat.ethz.ch) Giovanni MINERVINI (gminervini@uniroma3.it) Computational Biochemistry Lab. Department of Biology – Roma 3





- The protein folding "problem" and the structural genomics challenge
 - The combination of the 20 natural amino acids in a specific sequence dictates the three-dimensional structure of the protein.
 - Protein function is linked to the specific three-dimensional arrangement of amino acids functional groups.
 - With the advancement of molecular biology techniques a huge amount of information on *protein sequences* has been made available but less information is available on structure and function of these proteins.
 - The "ab initio" prediction of protein structure is a key instrument to better understand the protein folding principles and successfully exploit the information provided by the "genomic revolution".



The protein sequences space

- The number of natural proteins, though apparently huge, represents just a tiny fraction of the theoretically possible protein sequences.
 - With 20 different co-monomers, a protein chain of just 60 amino acids can theoretically exist in 20⁶⁰ chemically and structurally unique combinations.
- Estimates of the number of proteins present in nature vary from a minimum of 10⁹ to a maximum of 10¹³, thus the ratio between the number of existing proteins and those theoretically possible is very small.
 - A particularly suggestive example is that this ratio correspond to that between the volume of the hydrogen atom and that of the entire universe.

The "Never Born Proteins"

- Rationale
 - There exist a huge number of protein sequences that have never been exploited by biological systems, in other words enormous number of "never born proteins" (NBP).
 - The NBP pose a series of interesting questions for the biology and basic science in general:
 - Which are the criteria with which the existing proteins have been selected?
 - Do natural proteins have peculiar properties in terms for example of thermal stability, solubility in water or amino acid composition?
 - Or else they represent just a subset of the possible protein sequences generated only by the contemporary action of contingency and physico-chemical forces?



- The Rosetta *ab initio* module (*developed by David Baker – University of Washington*) is a software application which <u>allows the prediction of the threedimensional structure of an amino acid sequences</u> starting from a secondary structure of the sequence itself and a set of fragments extracted from the *Protein Data Bank (PDB).*
- The Protein Data Bank (<u>http://www.wwpdb.org/</u>) is a repository of proteins and nucleic acids that can be accessed for free by biologists and biochemists from around the world.

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Rosetta: how it works !

- Module I Input generation
 - The query sequence is divided in fragments of 3 and 9 amino acids
 - The software extracts from the data base of protein structures the distribution of three-dimensional structures adopted by these fragments based on their specific sequence
 - For each query sequence is derived a fragments data base which contains all the possible local structures adopted by each fragment of the entire sequence.
- Module II Ab initio protein structure prediction
 - The sets of fragments are assembled in a high number of different combinations by a Monte Carlo procedure.
 - The resulting structures are subjected to a energy minimization procedure using a semi-empirical force field.
 - The principal non-local interactions considered are hydrophobic interactions, electrostatic interactions, main chain hydrogen bonds and excluded volume.
 - The compatible structures both with local biases and non-local interactions are ranked according to their total energy resulting from the minimization procedure.

- The procedure for input generation is rather complex but computationally inexpensive (10 min of CPU time on a Pentium IV 3,2 GHz).
- Due to the many dependencies of module I (*Blast* and *psipred*), the input generation is carried out locally with a script that automatizes the procedure for a large dataset of sequences.
- Approximately 500 input datasets are currently being generated daily.

Rosetta: module II



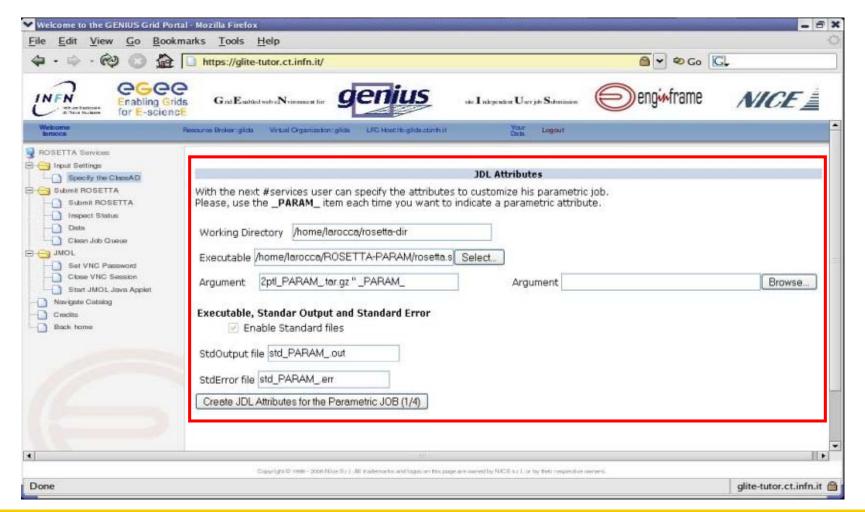
- Input
 - fragment files generated by module 1
 - secondary structure prediction using psipred
- In output the user obtains a number of structural models of the query sequence ranked by total energy
- A single run with just the lowest energy structure as output takes approx. 10-40 min of CPU time depending on the degree of refinement of the structure
- The Module II has been implemented in GRID through the use of the GENIUS Grid Portal (<u>https://glite-tutor.ct.infn.it</u>)
 - From this portal, exploiting the last feature of the gLite middleware, (<u>www.glite.web.cern.ch/glite</u>) it's possible submitting parametric jobs and run, in one shot, a large number of jobs (structure predictions).

Step 1. After MyProxy initialization the user connects to the GENIUS portal to set up the parametric JDL, specifying the number of runs (equivalent to the number of amino acid sequences to be simulated) to be carried out.

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Step 2. The user specifies the working directory and the name of the shell script.

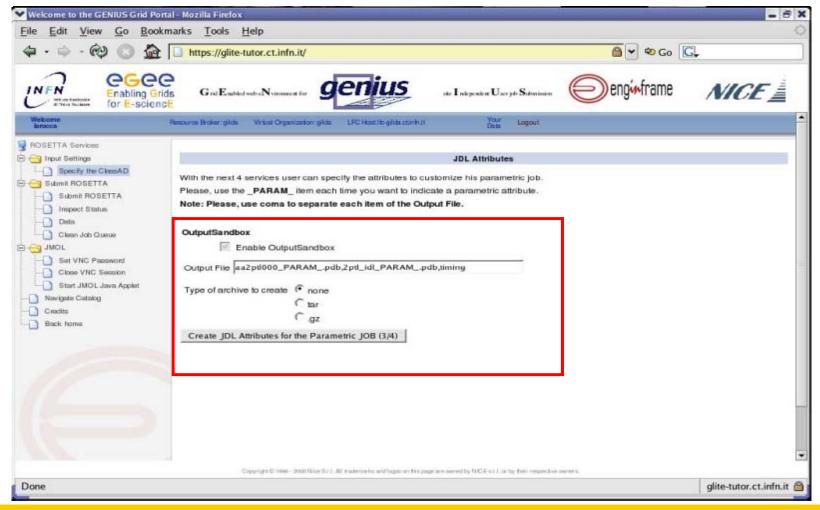


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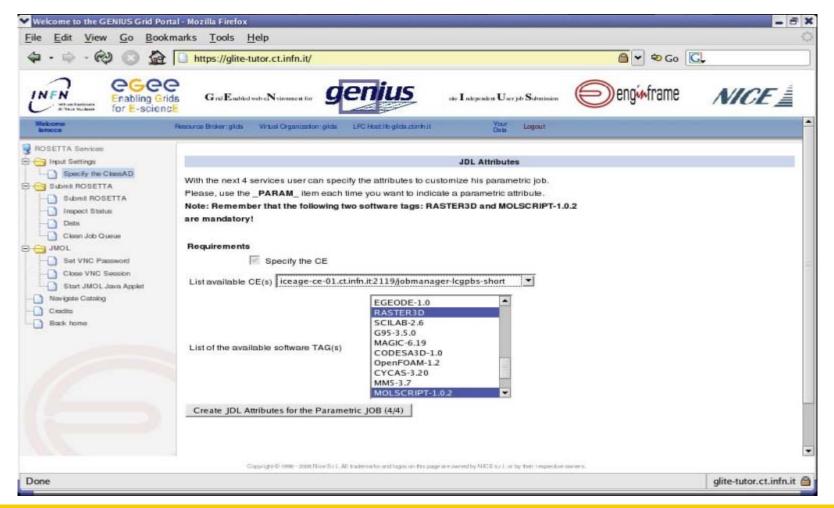
Step 3. Input files (fragment libraries) are loaded as a single .tar.gz folder per amino acid sequence.

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Step 4. Output files (initial and refined model coordinates) are specified in parametric form.



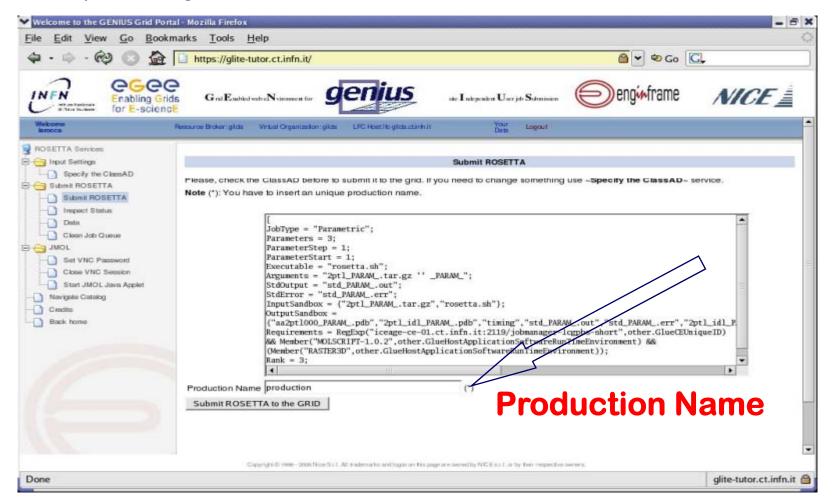
Step 5. The software requirements are specified in order to properly run ROSETTA.



Submit ROSETTA to the Grid /1

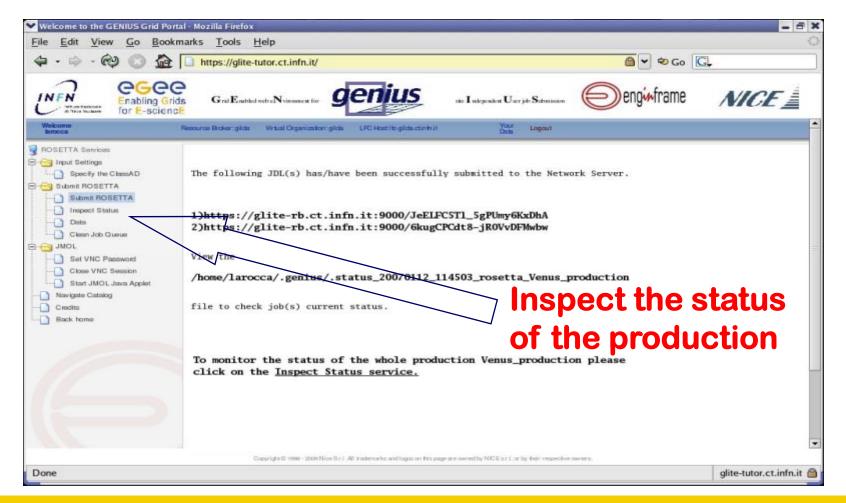
BioinfoGRID

Step 6. The parametric JDL file is generated and visualized to be inspected by the user.



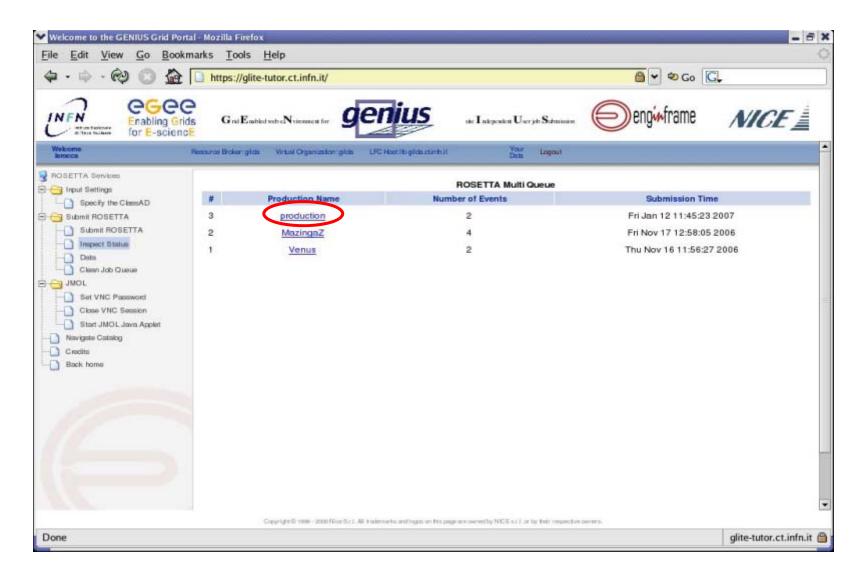
Submit ROSETTA to the Grid /2

Step 7. The parametric job is submitted and its status as well as the status of individual runs of the same job can be checked.



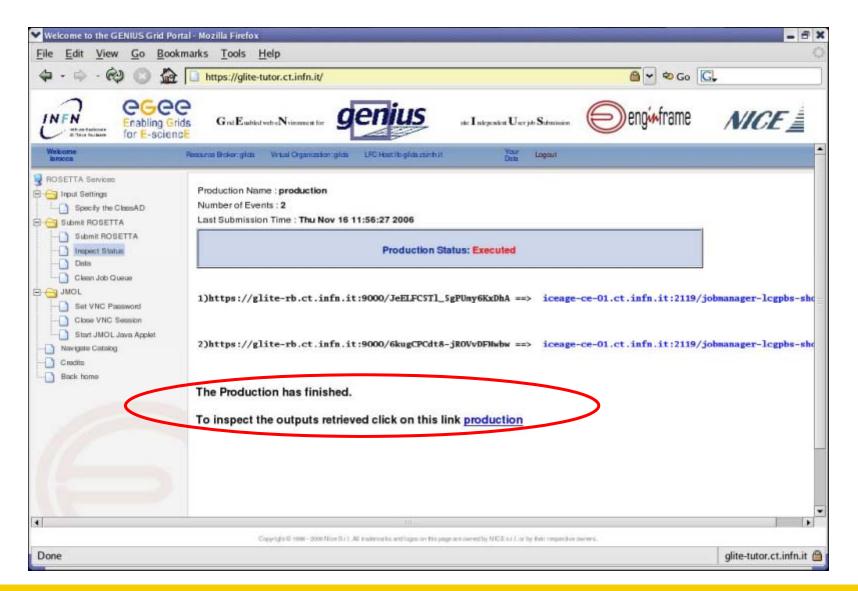


Inspect Status /1





Inspect Status /2

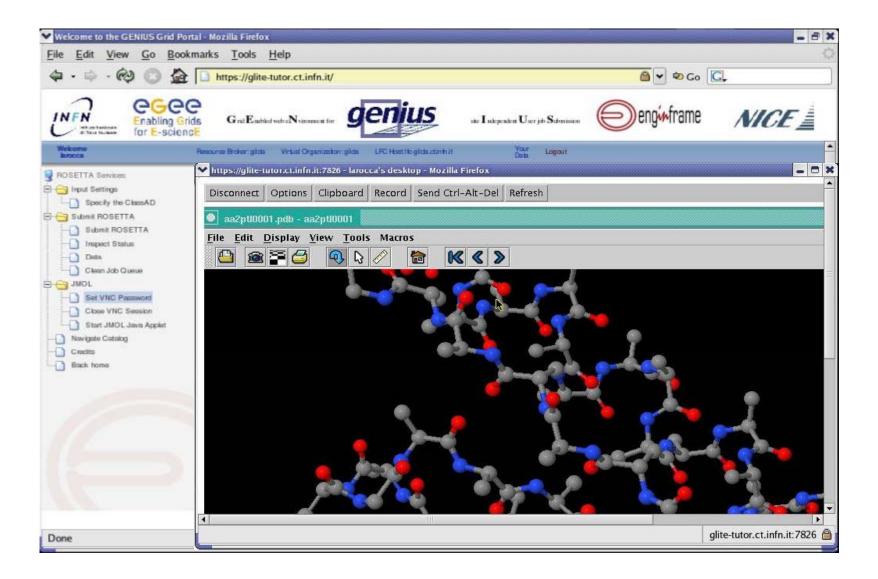




Click <u>here</u> to inspect the typical output files produced by ROSETTA at the end of the prediction process

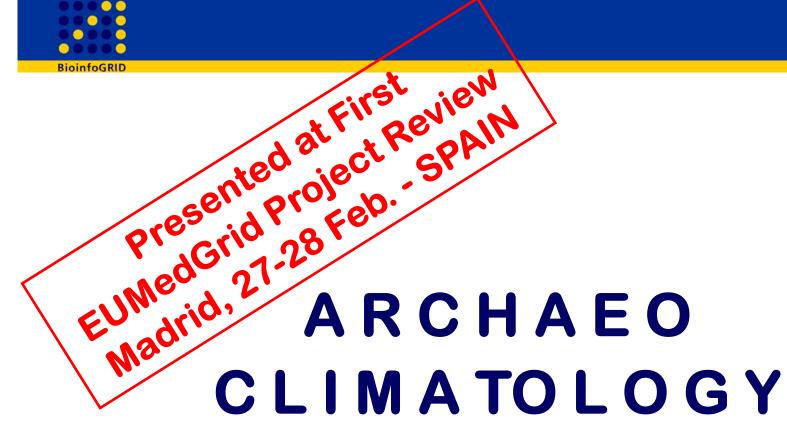






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This is a work supported in collaboration with Pier Giovanni PELFER (pelfer@fi.infn.it) University of Florence - ITALY

The Mediterranean Region at the end of the urban revolution



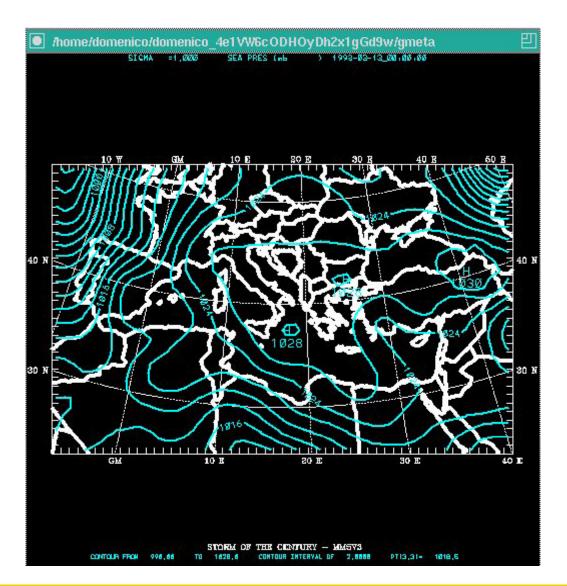


ArchaeoGrid aims to investigate the paleoclimate situation in the Mediterranean Area between XVIII centuries B.C.

This kind of studies are made available, within EUMEDGRID, using a metereological modelling software called MM5. It allows to create complex atmospheric simulations and simulate weather evolution.

The result

The MM5 program, thanks to the description of the environment, elaborates the meteorological data and generate the forecast



References

 "Archaeological Applications on e-Infrastructures by ArchaeoGRID"

BioinfoGRID

Dr. PELFER, Giuliano – Dr. CECCHINI, Roberto – Prof.
 PELFER, Pier Giovanni, Dr. POLITI, Antonio – EGEE User
 Forum 09-11 May 2007.



- Grid Portals technology
- EnginFrame Framework
- The GENIUS Grid Portal
- Some Integrated Applications
- References

References

- NICE web-site <u>http://www.nice-italy.com</u>
- EnginFrame Framework <u>http://www.enginframe.com</u>
- GENIUS Portal <u>https://genius.ct.infn.it</u>
- GENIUS Repository at https://geniuscvs.ct.infn.it

GENIUS Installation

- GENIUS Repository at https://geniuscvs.ct.infn.it
- Write an email message to <u>alberto.falzone@nice-italy.com</u> or <u>nicola.venuti@nice-italy.com</u> for an account request to download the GENIUS package



