

The EELA project: Biomedical Applications

Rafael Mayo CIEMAT NETTAB 2006 S. Margherita di Pula, 10-12.07.2006





www.eu-eela.org



Most of these slides have been made from previous ones presented by

Roberto Barbera, Ignacio Blanquer and Juan Luis Chaves

in different EGEE and EELA conferences



THE PROJECT

- The Goals
- The Consortium
- Budget and Human Resources
- The Structure
- Work Packages

THE BIOMED APPLICATIONS

- GATE
- WISDOM
- BiG Processing Service
- Phylogenetics

SUMMARY AND CONCLUSIONS

OUTLINE





E-infrastructure shared between Europe and Latin America

THE PROJECT



- Main purposes:
 - Build a bridge between consolidated e-Infrastructure initiatives in Europe and emerging ones in Latin America
 - Reinforce collaboration between Latin America and Europe

Objectives:

- Establish a human collaboration network between Europe and Latin America:
 - Setting up the structure of the collaboration network
 - Establishing adequate support mechanisms
 - Adopting policies regarding the shared use of e-Infrastructure
 - Evaluating new areas of collaboration and relevant partners, both in Europe and Latin America



- Build a pilot e-Infrastructure in Latin America:
 - Implementing basic mechanisms for an interoperable e-Infrastructure, adopting a security policy, establishing Certification Authorities and defining basic tools middleware
 - Setting up a Pilot Testbed, establishing Virtual Organizations and supporting application developers and users
 - Supporting advanced network services
- Promote a sustainable framework for e-Science:
 - Identifying research communities and applications
 - Supporting dissemination efforts
 - Coordinating participation in possible new projects
 - Defining a map for a future consolidated e-Infrastructure in LA



- EUROPE

- Italy: INFN
- Portugal: LIP
- Spain: CIEMAT(coordinator), CSIC, RED.ES, UC, UPV

– INTERNATIONAL ORGANIZATIONS

- CERN
- CLARA

– LATIN AMERICA

- Argentina: UNLP
- Brazil: CECIERJ/CEDERJ, RNP, UFF, UFRJ
- Chile: REUNA, UDEC, UTFSM
- Cuba: CUBAENERGIA
- Mexico: UNAM
- Peru: SENAMHI
- Venezuela: ULA

PARTNERS





E-infrastructure shared between Europe and Latin America

From 01.01.2006 to 31.12.2007

- Total Budget: 2568.32 K€
- EC contribution: 1700.00 K€
- Special CIEMAT funds for LA:
- Partners contribution: 468.32 K€

400.00 K€



HUMAN RESOURCES

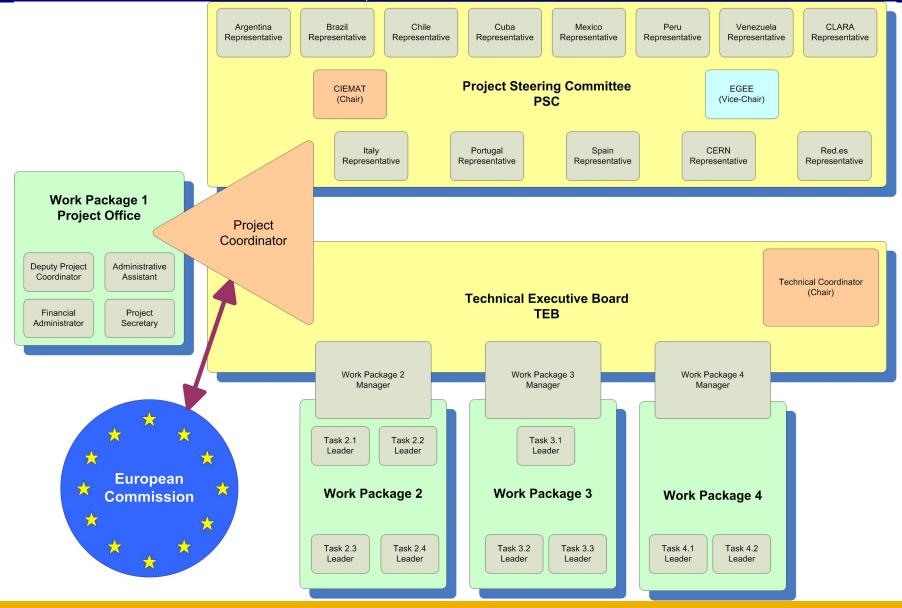
E-infrastructure shared between Europe and Latin America

WP No	Work package title	Lead contractor	Person- months	Deliverable No
1	Project administrative and technical management	CIEMAT	29	7
2	Pilot Testbed Operation and Support	UFRJ	297	12
3	Identification and support of grid enhanced applications	CIEMAT	576	8
4	Dissemination activities	INFN	207	11
	TOTAL		1109	



STRUCTURE

E-infrastructure shared between Europe and Latin America



IST-2006-026409



• WP1: Project administrative and technical management

- Manager: CIEMAT
- In charge of the financial and administrative parts of the project
- Assisted by the legal advisor of CIEMAT
- Elaborates technical documents, deliverables and reports
- Interacts with EC
- Takes care of the EELA private Web Site
- Distributes EC funds amongst the partners
- Controls budget and audits



E-infrastructure shared between Europe and Latin America

Two MoU's has been approved by the Project Managements and will be signed very soon by the PC's

- BELIEF (Bringing Europe's eLectronic Infrastructures to Expanding frontiers)
- SEE-GRID-2 (South Eastern European GRID)

<u>File E</u> dit <u>V</u> iew <u>G</u> o <u>B</u> ookmarks	e shared between Europe and Latin America ::::::::::::::::::::::::::::::::::::	
	http://www.eu-eela.org/private/eela_new_communities_form.php	Go 🔍 Search
Home ⊟Bookmarks 🏷 We	bmail 🔗 FastWeb 🛇 FastWeb NA/RM 🛇 Missioni 🛇 Offerte 🛇 Ordini 🛇 GILDA 🛇 Mozilla.org	
	ICTURE SHARED BETWEEN	Contract no. 026409
WP 1	This assessment questionnaire should be filled by communities or individuals potentially interested aims to gather relevant information on the adoption of distributed and grid computing in Latina Amer	
WP 2	problems with the questionnaire, please contact Giuseppe Andronico and/or Maria Jose Lopez.	
WP 3		
WP 4		
» WP4 Leader (INFN)	Section A - GENERAL	
» Dissemination		
» Knowledge	1. Organisation/Institution	
» Presentations		
» Meetings	2. Dependment	
» Criteria for measuring the quality of WP4	2. Department	
» Questionnaire for new		
» Questionnaire for new Communities	3. Address	
» Questionnaire for new Communities » Training events	3. Address	
» Questionnaire for new Communities » Training events Documents		
» Questionnaire for new Communities » Training events Documents Structure	3. Address 4. Country	
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts	4. Country	
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts Dissemination		
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts Dissemination Official Documents	4. Country	
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts Dissemination Official Documents Collaborating Projects	4. Country	
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts Dissemination Official Documents Collaborating Projects News and Events	4. Country 5. Full Name (Title, Name, Surname) of the Person filling in this questionnaire	
» Questionnaire for new Communities » Training events Documents Structure Procedures & Drafts Dissemination Official Documents Collaborating Projects	4. Country 5. Full Name (Title, Name, Surname) of the Person filling in this questionnaire	

IST-2006-026409

è

S. Margherita di Pula, NETTAB 2006, 10-12.07.2006 13



• WP2: Pilot testbed operation and support

- Manager: UFRJ
- Establishes a common interoperable Pilot Grid Testbed between existing resources in Latin America and Europe
- GÉANT, RedCLARA and European and Latin American NRENs will provide the network infrastructure
- The grid infrastructure will be based on the EGEE middleware framework
- The EELA Pilot Testbed will support dissemination activities and application exploitation



The EELA e-Infrastructure

E-infrastructure shared between Europe and Latin America





• WP2 - Task 2.1 (Coordination of e-Infrastructure : Operation Management Team)

- Participants: UFRJ (Leader), CERN, CLARA, CIEMAT, CSIC, LIP, RED.ES, REUNA, UFF
- Provides a coherent coordination amongst all WP2 tasks
- Analyses prospective local Grid initiatives
- Coordinates other Grid initiatives



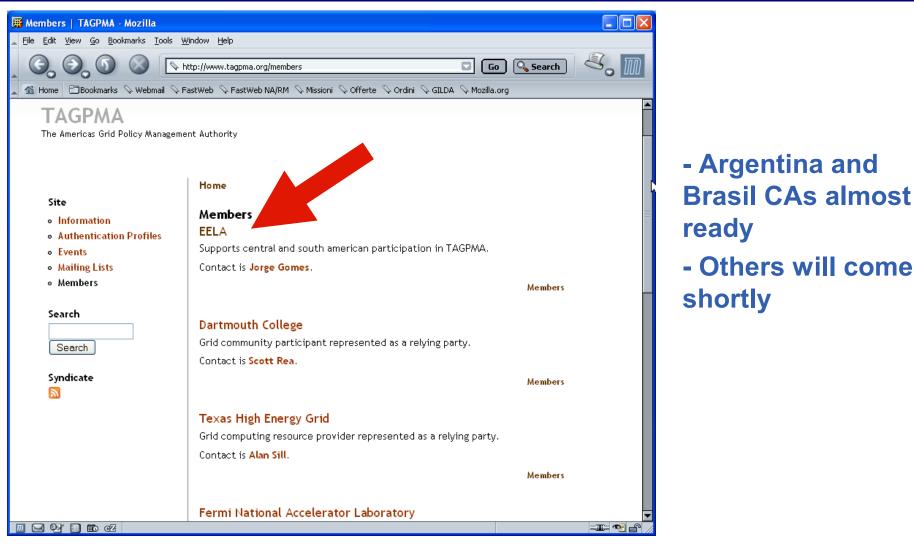
• WP2 - Task 2.2: Certification Authorities and Virtual Organizations

- Participants: LIP (Leader), CERN, CSIC, RED.ES, REUNA, UFF
- Deployment of Grid Certification Authorities in Latin America, accepted by the EUGridPMA
- Implementation of Virtual Organizations
- Support for dissemination and application users (HelpDesk, Portals,...)



EELA Certification Authorities

E-infrastructure shared between Europe and Latin America





EELA VOMS (managed by LIP) E-infrastructure shared between Europe and Latin America



m 🖂 🖓 🗐 🛍 oz

New registrations at: https://voms.lip.pt:8443/voms/EELA/webui/request/user/create

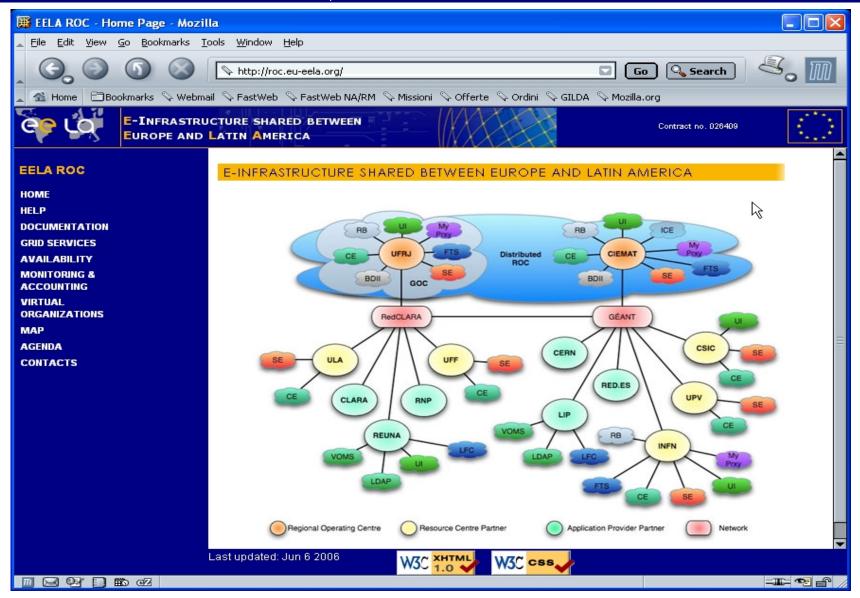


- WP2 Task 2.3: Pilot Testbed Operations
 - Participants: UFRJ (Leader), CERN, CIEMAT, CSIC, LIP, REUNA, UFF
 - Supports the integration of CIEMAT, UFF and UFRJ in a Pilot Testbed interoperable with EGEE
 - Identifies new sites for integration in the Testbed

EELA ROC

(http://roc.eu-eela.org)

E-infrastructure shared between Europe and Latin America



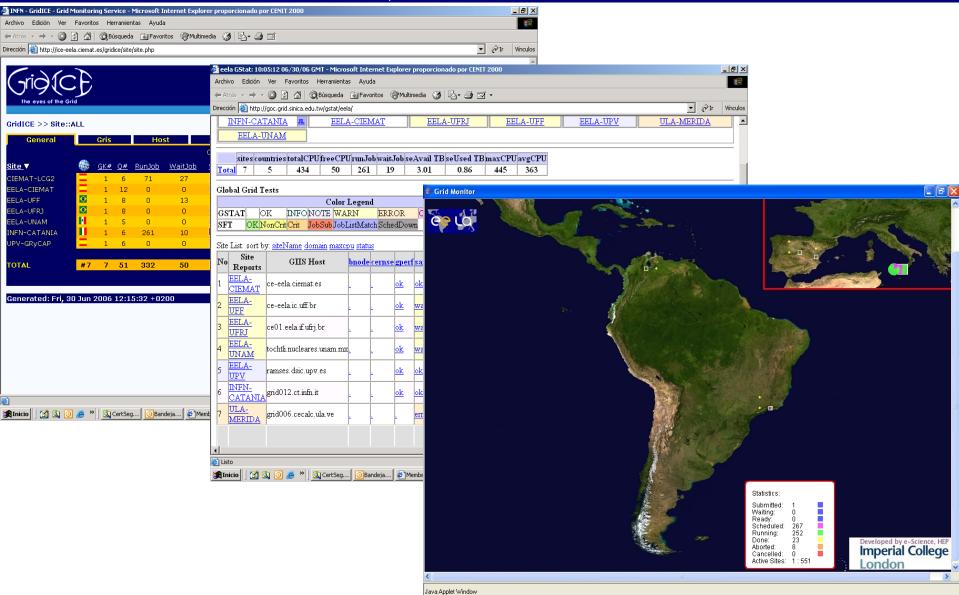
IST-2006-026409

S. Margherita di Pula, NETTAB 2006, 10-12.07.2006 21



EELA Monitoring Systems

E-infrastructure shared between Europe and Latin America



S. Margherita di Pula, NETTAB 2006, 10-12.07.2006 22



• WP2 - Task 2.4: Network Support and Operation

- Participants: CLARA, RED.ES, RNP (unfunded partner)
- Continuous surveying and upgrading of network service offerings by RedCLARA and LA-NRENs
- Definition of network services through standard modelling processes
- Study of operational procedures at Network Operation Centre in CLARA
- Introduction of the means for exercise of quality control of network services
- Interactions with EGEE activities SA2 and JRA4 and with the Joint Research Programme of GEANT2



• WP3: Identification and support of Grid enhanced applications

Manager: CIEMAT

- Identifies, selects and customizes relevant applications and tools suitable for the Grid dissemination process in Biomedical, High Energy Physics, Climate and e-Education
- Contributes to the definition of a common application interface with other research fields to encourage and help scientific and technology communities to easily migrate their applications to the EELA e-Infrastructure



• WP3 - Task 3.1: Biomedical Applications

- Participants: UPV (Leader), CUBAENERGIA, UFRJ, ULA
- Deployment of pre-existing EGEE biomedical applications:
 - GATE (GEANT4 Application to Tomographic Emission)
 - WISDOM (Wide In Silico Doking of Malaria)
- Support for identification and migration of two Latin American applications
- Integration of these new applications in the EGEE infrastructure
 - BLAST (Basic Local Alignment Searching Tool)
 - Phylogeny (MrBayes)
 - Bioinformatics portal of ULA



• WP3 - Task 3.2: High Energy Physics Applications

- Participants: UNAM (Leader), UFRJ, UNLP, UTFSM
- Running of Monte Carlo simulations for LHCb and ALICE experiments at LHC/CERN
- Interactive analysis with specific middleware deployed on the EELA infrastructure
- New applications
 - ATLAS
 - CMS
 - Pierre Auger Project



WP3 - Task 3.3: Additional Applications (Education in the Grid Environment)

- Participants: CEDERJ (Leader), CIEMAT, CUBAENERGIA, UNAM, UFRJ.
- Provide access to remote laboratory work, using communication and control technology
- Use of Grid Technology in the teaching process, including preparation of didactic material and digital libraries and repositories
- Teach GRID technology to students in mainstream courses
- Supply suitable applications to disseminate GRID technology in LA



• WP3 - Task 3.3: Additional Applications (Climate in the Grid Environment)

- Participants: CEDERJ (Leader), UC, UDEC, SENAMHI
- Migration of pre-existing data access/sharing tools appropriate to climate simulations and observations, focusing on El Niño phenomenon
- Migration to GRID of data mining clustering algorithms that relate both climate simulations and local observations



• WP4: Dissemination activities

- Manager: INFN
- INFN GILDA as strategic tool, already used in EGEE
- Introduce state of the art grid technologies and services to international community of users
- Bring more LA and EU groups into EELA



• WP4 - Task 4.1: Dissemination

- Participants: CLARA (Leader), CIEMAT, CEDERJ, CUBAENERGIA, CSIC, INFN, RED.ES, SENAMHI, UDEC, ULA, UNAM, UNLP, UPV, UFTSM
- Provide general picture of EELA
- Disseminate the purposes and benefits of Grid computing and of joining or using the EELA Grid infrastructure
- Define the dissemination methods and message content for reaching each community
- Provide dissemination materials adapted to the target audiences and make them available
- Inform the scientific communities on how to get involved in the project
- Direct potential users so that they may become EELA users
- Keep the communities informed of new improvements and functionalities



• WP4 - Task 4.2: Knowledge Dissemination

- Participants: INFN (Leader), CERN, CSIC, ULA
- Provide a deep technical information to potential users
- Allow potential users to learn, practice and experiment, using GILDA
- Permit potential users to assess the power of the grid
- Prepare the necessary knowledge to enable new users to start using the grid in the best possible way
- Keep the users aware of new improvements and functionalities by means of well-suited tutorials
- Provide advanced training to experienced users and administrators
- Supply special knowledge to site administrators, VO managers, security contacts, developers and other technical personnel



(http://www.eu-eela.org/private/eela_training_events.php)

EELA Tutorials

E-infrastructure shared between Europe and Latin America

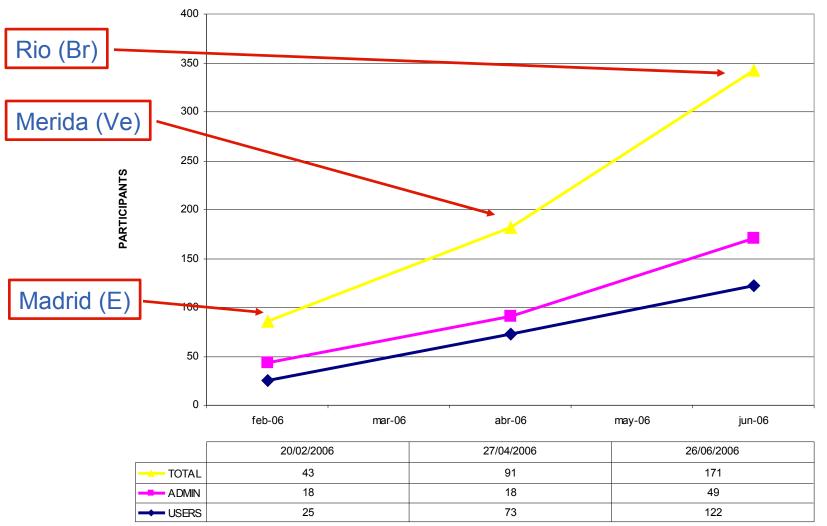
Where	Туре	When
Ciemat/Spain	Long/A+U	February, 20-24, 2006
ULA/Venezuela	Short/U	April, 24-28, 2006
Cederj/Brazil	Long/A+U	June, 26-30, 2006
UNAM/Mexico	Long/A+U	Aug, 28 – Sept, 1, 2006
Peru	Long/A+U	2006
Italy	Short/U	2007
Cuba	Short/U	2007
Portugal	Short/U	2007
Chile	Short/U	September, 6-7, 2006
Argentine	Short/U	2007

A = for Site Administrators U = for Users



EELA Training Statistics

E-infrastructure shared between Europe and Latin America



DATE

EELA Training Material

(http://documents.eu-eela.org/?c=Training+Material&as=0&In=en)

E-infrastructure shared between Europe and Latin America

🕱 <cdsnameintl>: Training Material - Mozilla</cdsnameintl>								
Eile Edit View Go Bookmarks Tools Window Help								
Co Co Search								
🔺 🐔 Home 🛛 Bookmarks 🛇 Webmail 🛇 FastWeb 🛇 FastWeb NA/RM 🛇 Missioni 🛇 Offerte 🛇 Ordini 🛇 GILDA 🛇 Mozilla.org								
Search Submit Personalize Help	' <u>baskets</u> :: <u>login</u>							
Home > Training Material								
Training Material								
Search records for:								
any field 🛛 Search Browse								
Search Tips :: Advanced Search								
Narrow by collection:								
Slides Grid tutorial for users and system administrators (Madrid 20-24 Feb 2006) (28) First Latin American EELA Tutorial								
(Mérida-Venezuela 24-29 April 2006) (12)								
Exercises								
Video Tutorials								
✓ User Guides								
	₣ॄ₽							





E-infrastructure shared between Europe and Latin America

Biomed Applications



E-infrastructure shared between Europe and Latin America

- To Present the Applications that Have Been Selected for Being Deployed in EELA in the Biomedical Area.
- To Present the Current Status of the Applications.
- To Present the Future Plans in the Frame of the Biomed Application Task.





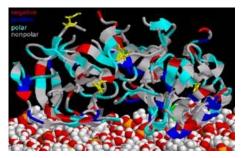
- Participants: UPV (Coordinator), CUBAENERGIA, UFRJ, ULA.
- Work in the Task
 - A3.1 Identification and selection of applications and tools. [COMPLETED]
 - A3.2 Customization of grid applications and tools. [IN PROGRESS]
 - A3.3 Evaluation of the impact on dissemination of the select applications and tools. [STARTED]
- Deliverables and Milestones (Biomed)
 - D3.1.1 Selection report, M2 [DONE]
 - D3.2.1 Application and tools customized, M6, M18 (Revised).
 - D3.3.1 Impact on dissemination report, M9, M23 (Revised).
 - M3.1 Successful use of the selected applications and tools, M9



- Grid Biomedical Applications Typically Fall into Four Categories
 - Bioinformatics Applications
 - Genomic, Genetic or Proteomic Analysis.
 - Computational Biochemical Processes
 - Molecular Biology and Chemical Interactions.
 - Medical Imaging
 - Image Posprocessing and Sharing.
 - Biomodels Simulation
 - Simulation of Structural, Flow, Electrical, etc. Biomodels.









Selection of Applications

- Types of Applications
 - Mature Applications (Applications from EGEE).
 - Applications Already Deployed in EGEE.
 - Applications Selected: GATE and WISDOM.

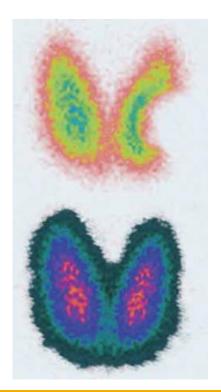


- Low Effort on Porting and Configuring those Applications: Ready at the Beginning of the Project.
- Success Stories Already Available.
- To be Customised for the Specific Needs of the LA Community.
- Selected by the User Community and With a Clear Usage Plan.
- New Applications
 - Applications Proposed by the EELA Consortium.
 - Applications Proposed: BiG and Phylogenesis.
 - Answering to Real Needs of the LA Community.
 - Supported by a Reasonably Large User Community.
 - Feasible to be Migrated and Deployed in a Reasonable Time.
 - Effective on the Grid.





- Geant4 Application for 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://wwwlphe.epfl.ch/GATE).
- The Interest of the LA Community is Leaded by CUBAENERGÍA
 - It is Focused Towards Two Main Oncological Problems:
 - Thyroid Cancer.
 - Treatment of Metastasis with P³².
 - 9 centers in Cuba are Interested (5 Hospitals and 4 Oncological Centers and Institutions)



GATE





- Resources Available
 - CIEMAT (ce-eela.ciemat.es; GATE-2.1.0)
 - UFF (ce-eela.ic.uff.br; GATE-1.0.0-3)
 - UFRJ (ce-eela.uf.ufrj.br; GATE-1.0.0-3)
 - UPV (ramses.dsic.upv.es; GATE-1.0.2-3)
- Expected Demand
 - They Plan to Submit Around 90 Cases per Month.
 - Cases Data Size will be in the Range of 0.5-1 Gbyte Each, and Total Computing will be on the Order of 600 CPU-hours per Month.

Technological Barrier

- Network Bandwidth Requirements are High for Cuban Centres
 - Install a Local Environment for Short Cases and Learning.
 - Send Physically Large Cases to EELA Operators.
- Contact New LA Users Through the OpenGate Collaboration
 - USACH





- 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 to the 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.
- However is Being Applied to Other Diseases, such as H5N1 (Avian Flu).







- Each Target Implies Around 7000 Jobs and Input Data Files. Results are on the Order of Tens of GBytes per Target.
- Interests Raised from the LA Community.
 - ULA is Leading the Interest in the LA.
 - Collaboration is Started in Two Main Lines
 - Analysis of New Targets: Malaria, Influenza and Human Papillomavirus (HPV). ULA will Select New Targets which will be Included in Large-Scale Docking Experiments
 - Collaboration on the Data Challenges to Reach a Larger Number of Results and to Gain Practice for Own Targets.





- WISDOM Activity was Delayed Until the Availability of a Newer Version (Released on May).
- UPV Participated in the Last H5N1 Docking Data Challenge.
- Testing Package of WISDOM has Been Prepared, but Starting has Been Delayed Due to Issues Regarding Certificates.
 - Finally, users from ULA have Accessed to Certificates and a UI in the UPV with WISDOM Scripts Installed. CIEMAT also Installed the WISDOM Package.
 - Initial Tests have Started.
- Next Steps will be:
 - Set ULA as Docking Data Challenge Operator.
 - Inclusion of Targets in New Data Challenges.
 - Plan EELA Data Challenges.





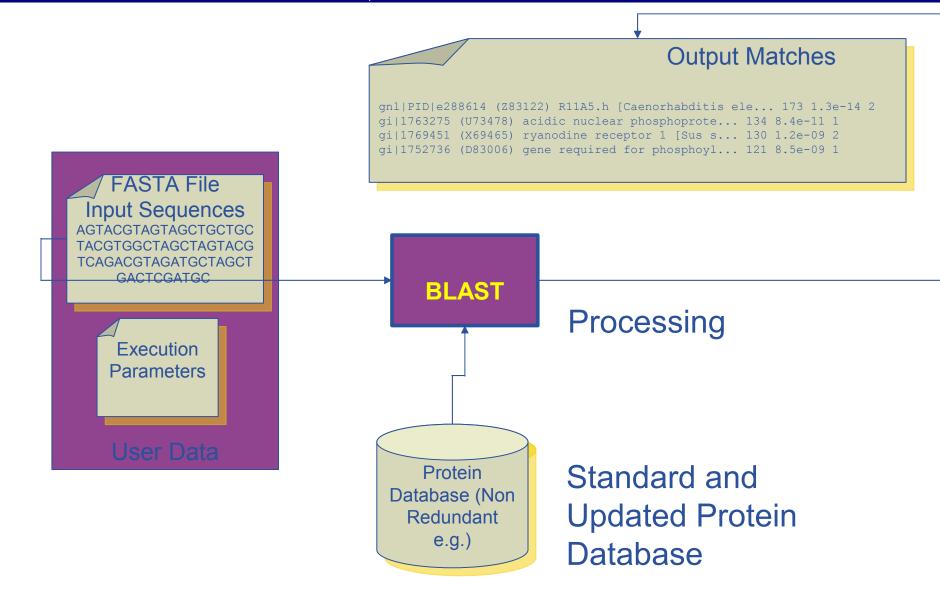
- BiG: BLAST in Grid is a Grid-enabled BLAST Interface.
- BLAST (Basic Local Alignment Search Tool) is a Bioinformatics Procedure Applied to Identify Compatible Protein and Nucleotids Sequences in Protein and DNA Databases.
- BLAST can be Applied, Among Other Uses, to Annotate the Estimated Function of Unknown Sequences.
- BLAST is Computationally Intensive.





BLAST Workflow

E-infrastructure shared between Europe and Latin America

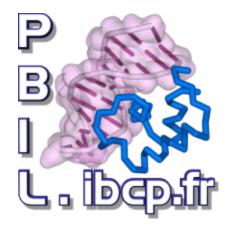


IST-2006-026409

S. Margherita di Pula, NETTAB 2006, 10-12.07.2006 46



- Local Executions
 - BLAST
 - High Computational Cost: 1 User with 1 Medium Input Database (5K Sequences) Would Require More than 4 CPU Days.
 - MPIBLAST
 - Requires a Computing Cluster (MPI-Based).
 - Reasonable Speed-ups, Still High Computational Cost for a Multiuser Production Service.





- Remote Processing Services
 - NCBI (National Center for Biotechnology Information) Web-Based BLAST Service (http://www.ncbi.nlm.nih.gov/BLAST/)
 - 1 Sequence with One Database.
 - Public Resource with Intense Use at International Level.
 - (GPS@) Grid Protein Sequence Analysis Web-Based BLAST Service (http://gpsa.ibcp.fr)
 - I Sequence with One Database.
 - Public Resource With Intense Use From the Biomedical French Community (5K Analysis per Day).



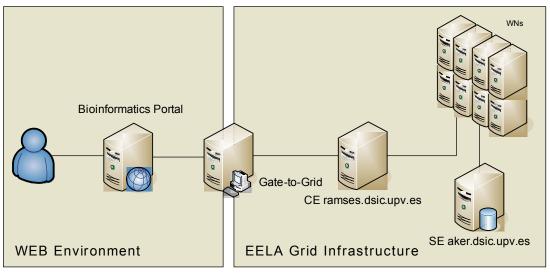


BiG Design Objectives

- Easy Interface with High Compatibility (Web Service + NCBI Based)
 - Same Parameters as BLAST.
 - User-friendly and Intuitive.
- Support to Searching Simultaneously on Multiple Databases
 - Parallel Process on Multiple Database Queries.
- Exportable Architecture to Other Common Problems
 - Fast Capability to Migrate to Other Problems Because of the Structure in Modules and Independence of the System Components.
- Scalability
 - Data Partition in Grid Approach Gives Scalability with Huge Quantities of Data.
- High Performance
 - Grid Computing + MPI Parallel Jobs in Dedicated Clusters.
- Robust
 - Fault Tolerance on Server and Client.



- Users Access the Service Through a Web Portal.
- Access to the EELA Grid is Performed Through the Gate-to-Grid.
- Gate-to-Grid is an EELA Grid Node Which Provides a WSRF-Based Web Interface.
- BiG divides sequences into blocks.
- A block will be assigned to an EELA Grid job.
- A single block will generate as many output files as databases used.





Technologies

- Secure Connection HTTPs for Remote Calls (Based on SSL)
- GRIDftp for File Transferring (Based on SSL)
- Needed X509 Certificates to Guarantee System Security (Privacy and Users Authentication)
- Two Levels of Certificates
- Authentication Procedure Alternatives
 - Usage of EELA Certificates for All Users.
 - Access Rights to the Whole EELA Infrastructure Granted to All Users.
 - More Complex Certification Issuing Process.
 - Usage of non-EELA Certificates for Portal Users and Mapping on a Portal Certificate.
 - Restricted Access to the Portal Users.
 - Currently not Officially Supported.
 - Local Management of the Certificates.





Current Tests on EELA

E-infrastructure shared between Europe and Latin America

Application has Been Installed on UPV, ULA and CIEMAT **Computers.**

Menu Prin

Mis Datos

Inicio

Salir BLAST

Noticias

Diario

Enlaces

Gooale

- **Tests Have Been Performed Suc** ۲ 3000 Sequences of the Plasmod
- Integration in the Bioinf

Portal is (Nearly) Finished.





- Web-based site that offers users an organized and easy single access point to reach resources and users communities related with the bioinformatics (Genomic, Genetic or Proteomic).
- Installed at the National Centre for Scientific Computation of the Universidad de Los Andes in Mérida-Venezuela



Initiative for:

- spreading of findings in Bioinformatics in Venezuela and other Ibero-American Countries
- consolidate on-line academic and research communities

From this portal users can:

- Locate Resources/Documentation
- Organize/Affiliate to group/list of users
- Access various Bioinformatics on-line Applications/Systems (only for registered users)
- To also Foster the Use of Grids and the Take off of New Applications
- Security in process (trace / my proxy server)



The Bioinformatics Portal

E-infrastructure shared between Europe and Latin America

http://portal-bio.ula.ve

	BioInformática MetaPortal					
Create an account	<u>Principal</u> · <u>_TOPICS</u> · <u>Members Area</u>	June 20, 2006				
Menu Principal • <u>Inicio</u> • <u>Mis Datos</u> • <u>Administracion</u> • <u>Direccion de Contacto</u> • <u>Salir</u>	Portal de Bioinformática El Portal Iberoamericano de Bioinformática nace como iniciativa para divulgar la bioinformática en los países de habla española y portuguesa. El Portal se publica en forma electrónica y la misma se puede consultar gratuitamente para quienes deseen consultar las diversas publicaciones, noticias, eventos, talleres y/o cualquier información en el área de bioinformática. Por otra parte, permite publicar en forma gratuita dicha información, asi	estadisticas TOP Paises 1.≝ Australia 2.≝ USA 3.≝ Uruguay 4.≡ Holanda 5.≝ Venezuela				
Alineamiento con BLAST • Alineamiento con BLAST • Proyecto EELA EMBOSS	Segundas Jornadas Iberoamericanas de Bioinformática, Sedundas Jornadas Iberoamericanas de Bioinformática, Sedundas Jornadas Iberoamericanas de Bioinformática, Sedundas Jornadas Iberoamericanas de Bioinformática, Segundas Jornadas Iberoamericanas de Bioinform	5. Solution 6. III <u>Mexico</u> 7. <u>España</u> 8. <u>Chile</u> 9. <u>Argentina</u> 10. <u>Colombia</u> <u>Vea todos los países</u>				
• <u>EMBOSS</u> Noticias • <u>Noticias - enviar</u>	las segundas jornadas en coincidencia con la reunión de FIBECYT (Foro Iberoamericano de Ciencia y Tecnología) Participarán destacados investigadores latinoamericanos e ibéricos en un	Enlaces • <u>Biotutor</u> • <u>Curso BioInfo</u>				
Recursos del Portal Recomendar Libros Libreta de direcciones Estadisticas Diario Enlaces	programa que cubrirá bases de datos y herramientas para el estudio de proteínas y ácidos nucleicos, su estructura y función, comparación de genomas, metabolómica, etc El programa detallado puede consultarse en: http://www.cyted.org/Fibecyt/documentacion/II%20Jornadas%20Iberoamericanas .pdf	Usuarios Bienvenido Invitado Nick Pass Recordarme				
Red Iberoamericana de Bioinformática (RIB) • Páqina principal • Acerca de la Red • Participantes	Enviado por risea el Lunes, 12 de Junio de 2006 - 11:47 AM AST (54 lecturas) Leer más (1553 bytes más) ¿comentarios? 🖾 🖻 Curso Teórico Práctico : "Bioinformática estructural Curso de Postgrado Teórico Práctico : "Bioinformática estructural"	Miembros Vitimo: danieldr Total: 647				

Hits: 547.116



Plasmodium falciparum Genome

E-infrastructure shared between Europe and Latin America

The *Plasmodium Falciparum* genome takes 23 Mb, organized in 14 chromosomes

S NCBI			and a state		N	СВ	Ma	p Vi	iewer 。							
PubMed	Nucleotide	_	Protein	n i		Genome	•		Gene	Structure		PopSet		íaxonomy		Help
Search for		or	1 chror	nosom	11 - 11 - 11 - 13				Find						Advance	ed Search
Show related entries				V	Aap Vie	wer ho	me									
Entrez Genomes	Plasmoo	lium	falc	ipan	ım a	enor	ne v	iew					BLAST s	earch th	e Proto	zoa genome
Map∨iewer Home)	Build 1.1 sta															
FTP SITE		1	1	l	I]			I							
Sequencing		1	2	3	4	5	6	Z	8							
Centers: STANFORD																
The Sanger Centre TIGR						1										
			6	1												
Other Apicomplexa Sequencing																
Projects: Babesia bovis		J.	ų	J.	ų	U.	ų	0.91								
Cryptosporidium		2	<u>10</u>	11	<u>12</u>	<u>13</u>	<u>14</u>	MT								
parvum Eimeria tenella	Linea	ge: E	ukarvo	ota: Al	veolata	a: Api	compl	exa: H	laemosporid	a; Plasmodium	n: Plasmo	dium falci	parum 31	07		
Plasmodium berghei Plasmodium chabaudi		-														
Plasmodium										e genome of t						
falciparum Plasmodium knowlesi										: <u>The Institute</u> and the <u>Stanfo</u>						
Plasmodium vivax Plasmodium voelii										ortium establis						oniversity.
Theileria annulata			Ψ			0.00000		an of the	1999-1999 - 1997-1997							

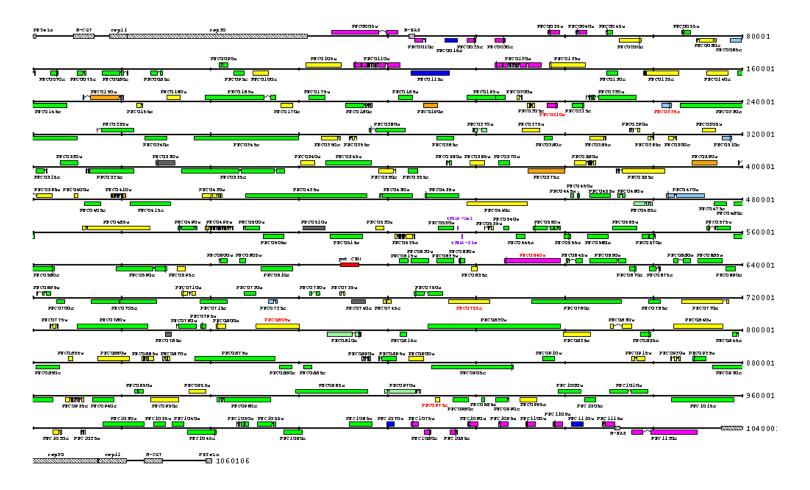
The protozoan parasite *Plasmodium Falciparum* is the agent that causes human malaria. Remember that Malaria is a devastating parasitic disease; it infects 300 million people and kills up to three million people per year



Chromosome 3 with 247 proteins

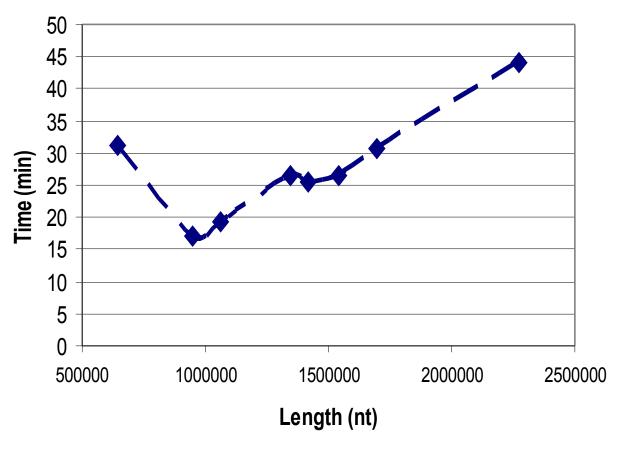
E-infrastructure shared between Europe and Latin America

247 protein Length: 1,060,087 nt Input File Size: 0.203 Mb



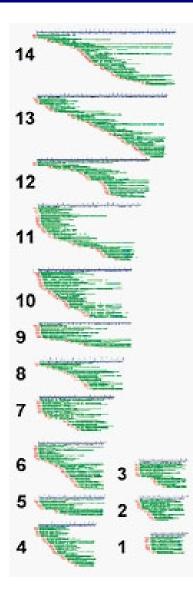


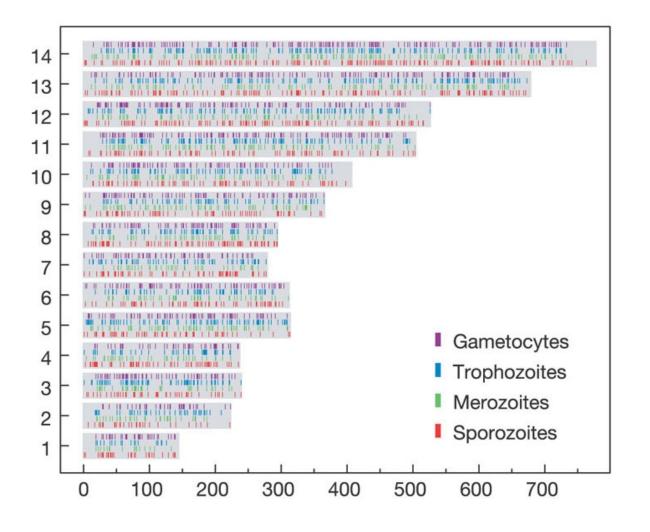
- Chromosome 1 Length: 643,292 nt 140 protein, Time: 31m 59s
- Chromosome 2 223 protein, Length: 947,102 nt Time: 17m 14s
- Chromosome 3 Length: 1,060,087 nt 247 protein, Time: 19m 3s
- Chromosome 5 312 protein, Length: 1,343,552 nt Time: 26m 58s
- Chromosome 6 Length: 1,418,244 nt 307 protein, Time: 25m 46s
- Chromosome 9 355 protein,Length: 1,541,723 nt Time: 26m 43s
- Chromosome 10 403 protein, Length: 1,694,445 nt Time: 30m 58s
- Chromosome 12
 526 protein, Length: 2,271,477 nt Time: 44m 12s





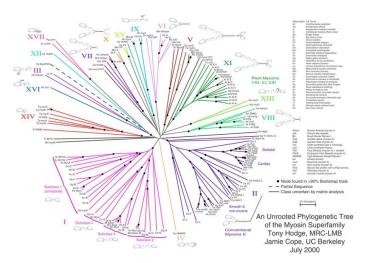
Future work!







- A Phylogeny is a Reconstruction of the Evolutionary History of a Group of Organisms.
- The Inference of Phylogenies with Computational Methods is Widely Used in Medical and Biological Research and has Many Important Applications, Such as Gene Function Prediction, Drug Discovery and Conservation Biology.
- Most Approaches Depend Upon a Mathematical Model Describing the Evolution of Characters Observed in the Species Included, and are Usually Used for Molecular Phylogeny Where the Characters are Aligned Nucleotide or Amino Acid Sequences.
- Interest of the LA Community
 - ULA is Leading the Interest in the LA.
 - A Grid Service Will be Developed to Run a Parallel Version of MrBayes from the Bioinformatics Portal.
- Analisys of the Application has Started.





- A new application proposed by UFRJ
- An academic program for molecular dynamics simulations that we are trying to use in Grid
- User Community
 - Number of potential users and names of the centres that will be involved.
 - Number of potential simultaneous users.
 - Specific target that is going to be addressed (disease, drug, etc.)
 - Estimated benefits (throughput, quality, new targets)
- Application Usage
 - Estimated individual cost for each study.
 - Estimated number of studies to be analysed.
 - Estimated individual data size



- Deployment of Mature Applications
 - GATE
 - At Least 62 Computing Resources have GATE Available
 - Network Restriction will Force to Have a Cuban Installation for Short Cases and Training.
 - New partners (USACH)
 - WISDOM
 - Last Version (Released on May) is Installed in UPV and CIEMAT and Tests Have Been Started.
 - UPV's UI has been Opened to EELA Users for this Application, and both UPV and ULA will act as Docking Experiment Operators in Next Experiment.

Development of New Applications

- BiG
 - First Prototype Available.
 - Early Runs from ULA have Been Made. Installed in UPV and CIEMAT
 - Integration in the Portal is (Nearly) Finished.
- Phylogenetics
 - Analysis of the MrBayes Application has Started.
 - Migration is Expected to Start After the Deployment of BiG.



- Several Actions Already Performed.
 - Mérida and Rio EELA Workshops: An Outline of the Applications and the Technical Details of BiG.
 - HealthGrid 2006 Conference
 - Participation in the WISDOM Workshop.
 - Poster with All the Applications.
 - Talk about Technical Details of BiG.
 - Stand of the UPV with a Demo on BiG and a Poster and Shared Flyer.
 - ICT for Bio 2006
 - Presentation of the Project
 - Discussion with the Responsible of the

Iberoamerican Network of Bioinformatics.

Information sheet



- Expected results
 - The Running of at Least 2 EGEE Biomedical Applications in the EELA Pilot Testbed.
 - The Processes of Identification of, at least two, new Applications that Could Provide Solutions to Problems, Which are More Relevant to Local LA Partners and use them on Dissemination Activities.
 - To Achieve at Least 3000 Executions of the Biomedical Applications From at Least 50 Users.
 - To Transfer at Least 1 of the New EELA Applications to EGEE Infrastructure.
 - To Reach at Least Impact on 4 Different Countries (European + Latin American).



Status of Applications

- Three Applications are Effectively Installed: GATE, WISDOM and BiG. GATE Needs to Increase the User Community.
- Two New Applications were Identified, and One is Already Deployed on the Grid.
- The Number of Users is Small Yet, But the Expectances of Growing are Promising since the Bioinformatics Portal has 1000 Users from Almost all the Countries in EELA.
- BiG has Been Proposed to EGEE for their Adoption
- Phylogenetic Application has Also Raised the Interest.





- EELA is a concrete reality and represents the first step to bridge EU and LA in e-Science exploiting GEANT2 and RedCLARA networks and following the EGEE policies.
- The EELA workplan is very challenging but holds the promise to alleviate the digital divide in Latin America



UPV:

Vicente Hernández, Ignacio Blanquer, Gabriel García, Gabriel Aparicio

ULA:

- Raúl Ísea, Juan Luis Chaves, Luis Núñez CUBAENERGÍA:
- Henry Mora, Manuel Fernández
- **UFRJ:**
- Paulo Bisch
- CIEMAT:

Javier Pérez-Griffo, Esther Montes, Alicia Acero, Rafael Mayo



Project Coordinator: Jesús Casado – CIEMAT jesus.casado@ciemat.es **Deputy Project Coordinator: Bernard Marechal – UFRJ** marechal@if.ufrj.br **Technical Coordinator: Roberto Barbera – INFN** roberto.barbera@ct.infn.it Work Package Manager: Rafael Mayo – CIEMAT rafael.mayo@ciemat.es Task Leader: Vicente Hernández – UPV vhernand@dsic.upv.es

http://www.eu-eela.org



Future Collaborations

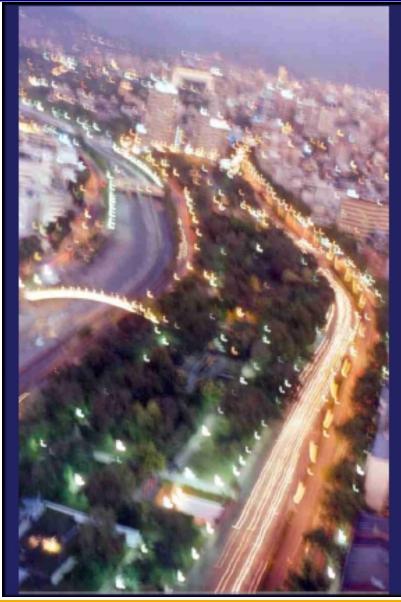
E-infrastructure shared between Europe and Latin America

EELA is open to all interested people/Institutes willing to collaborate.



The First EELA Conference

E-infrastructure shared between Europe and Latin America





First EELA Conference Date: September 4 - 5



Venue: Úniversidad Técnica Federico Santa María (Sede Santiago, Av. Santa María 6400, Vitacura)

EELA Tutorial Date: September 6 – 7 Venue: NH Hotel (Av. Condell nº40, Providencia)

The EELA Conference will be followed by the EELA Tutorial and the First National e-Science Congress that will be hosted by REUNA (Chilean NREN) during September 6 and 7 (special price for EELA members).

The partners of the EELA project, will stay at the NH Hotel – Santiago. For reservations and more information, please contact Maria José López: milopez@reuna.cl

Registration at: http://www.eu-eela.org/private/eela.chile.conference.registration.php



Thanks for your attention!