EGI-InSPIRE



Virtual Research Communities: EGI's model for supporting the Life Sciences Grid Community

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Supporting the LSGC

1. Managing a sustainable infrastructure

- 2. Building sustainable user services
- 3. Cultivating sustainable communities



Resource Infrastructure (Showing yearly increase)

338 Resource Centres → +6.8%
Europe, Asia Pacific, North and South America 96 supporting MPI → +31.5%
51 Countries (57 with integrated RPs) →+18.75%
Capacity 240,000 CPU cores

(339,00 with integrated and peer RPs) → 24.9% 1.89 Million HEP-SPEC 06* 102 PB disk, 89 PB tape

* Million HEP-SPEC 06 Normalised CPU time to a reference value of Mega HEP-SPEC



What is a Grid?

- A grid consists of distributed resources controlled by separate organisations that be systematically used securely by users external to that organisation
- Resources can include:
 - Commodity or HPC clusters
 - Disk or tape storage
 - Instruments
 - Data Archives or Digital Libraries



Infrastructure is the basic physical and organisational structures needed for the operation of a society or enterprise, or the services and facilities necessary for an economy to function

The Enterprise is the European Research Area

EGI provides a service infrastructure that exposes and helps coordinate a resource infrastructure



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EGI Resource Infrastructure



Integrated: infrastructure operated by a non-EGI-InSPIRE partner but relying on EGI operational services (MoU) **Peer**: infrastructure accessible to EGI users, but relying on own operational services

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- Coordination for European Grid resources
 - Established February 8th 2010
 - Central policy & services needed to run a grid
 - Sustainable small coordinating organisation
- Based in Amsterdam
 - Coordinating core (~20 people) in Amsterdam
 - Technical services from partners (~20 people)

EGI and EGI.eu supported by EGI-InSPIRE project



EGI-InSPIRE Project

Integrated Sustainable Pan-European Infrastructure for Researchers in Europe

A 4 year project with €25M EC contribution

- Project cost €72M
- Total Effort ~€330M
- Effort: 9261PMs

Project Partners (50) EGI.eu, 38 NGIs, 2 EIROs Asia Pacific (9 partners)





- A sustainable production infrastructure
 - Resource providers in Europe and worldwide
 - With new technologies as they mature
- Support structured international research
 - Sustain current domain specific services
 - Attract new user communities (e.g. ESFRI)

A Virtuous Service Cycle



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EGI: coordinating the user experience





Integrate current and future use





UCB and the Virtual Research Community model: purpose and benefits



Benefits:

- 1. Defined communication channels: named contact points between communities & EGI
- 2. Application integration
- 3. Policy and procedures: define interaction between EGI and users
- 4. Requirements gathering: solutions and influence
- 5. Dissemination: sharing of news, breakthroughs, best practice and innovation

User Community Board

with representation from: Life Sciences, WLCG, WeNMR, Astronomy & Astrophysics, Earth Sciences, Computational Chemistry, Arts & Humanities, Hydrometeorology

NGI User Support Teams

					Training marketplace			
	Application Det	tails - SIMAP			Home * User Suggert * Trening	metalplace		
	Information	Publications						
		ID: Type:	555 (Permalink) Application		The EGI Training Marketplace exists as a service to coordinate training across communities, projects and national teams. The new Training Marketplace enables trainers to advertise events and resources, and users to locate, comment on and suggest training material and events that meet their needs.			
		Name:	SIMAP					
На		Description:	Simulating and analys models	sing the dynai	EGI Hands	On Training for AEGIS Users		
		Discipline: Subdiscipline:	Computational Chemi Biochemistry	istry	Friday 25 March 2 at Institute of Phy	2011 from 10:00 to 17:25 (Europe/Belgrade) ysics Belgrade (Library)		
		Website			Support	slavnic@lpb.ac.rs		
	The S	IMAP Utility is a	a platform-independer	nt environme	Friday 25 March 2011			
Document	network models	ks, and also for s. The SIMAP utility	simulating and analys provides a Graphical	sing the dyn: User Interface	10:00 - 10:05	Opening 05' Speakers: Antun Balaz (Institute of Physics Belgrade)		
Processes	import, The co	create, edit, and	export the biochemica	al models con E Solver Libra	10:05 - 10:10	Overview of the training 05' Scenkers: Actus Balay (Institute of Physics Belorede)		
& apps.	Abstract: of com	nputational modu	iles for simulating ai quations-based simul	nd analysing	10:10 - 10:40	Introduction to Grid Technology 30' Speakers: Antun Balaz (Institute of Physics Belgrade)		
SIMAP added	scanne	er, a model fitting i	module, a gene knockd	lown analyse		Material: Sildes 📾		
4 March	The ap	plication was port	ed within the framewor	rk of the FP7 E	10:40 - 11:40	Hands-On Session: Linux shell environment 1100' - Navigating the file system - Standard Linux commands		
2011, (Comp.	Related Country:	United Kingdom/	ireland 🗮 🚺			- Archive tools - Data management - Script Januara		
	VOS: Middlewares: BO	INC				Speakers: Nikola Grkic (Institute of Physics Belgrade)		
Fe	Status: Ready for	standalone use/	running on a local clus	ter		Material: Sildes 📆		
	Added on 2011-03-04, by Noam Weingarten				11:40 - 11:55	Coffee break Hands-On Session: Setting up the user account %		
		Scientific Contacts		ontacts	11.00 - 12.20	- User Interface (UI)		
	V	Veingarten Noam	n 🕋	Kiss Tamas		- Grid Security Infrastructure (GSI) - Obtaining certificate		
	T o	Other		Scientific Coo		- How to use certificate - Proxies		
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						Material: Sildes 📆		

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Services provided by a few NGIs for the whole community

- To support the Virtual Research Communities
- To facilitate the work of NGI support teams
- To improve communication among NGIs, among users and with users
- Bring in expertise and services from Heavy User Communities (HUCs)

Tools and services (current list – will be expanded):

- 1. EGI Application Database (Marios Chatziangelou, GRNET)
- 2. Services for VOs (Ignacio Blanquer Espert, UPV; Gonçalo Borges, LIP)
- 3. Training Marketplace (Claire Devereux, STFC)
- 4. Requirement Tracker (EGI.eu with help from CESNET)

EGI Application Database

Benefits of AppDB:

- gives recognition to reusable applications and tools
- gives recognition to application developers

Use of AppDB

- Register applications/tools
- Reuse of applications/tools
- Map of application landscape
- AppDB gadget has been instantiated by:
 - WeNMR, LSGC, GridPP,
 Serbian, UK and Hungarian NGIs

AppDB: PY1 statistics

111 new applications per country

- United Kingdom/Ireland
- Spain
- Brazil
- Poland
- Netherlands
- Portugal
- Finland
- Mexico
- Argentina
- Colombia
- Cuba
- Egypt
- Germany/Switzerland
- Italy
- Taiwan
- Others

New additions to the **Applications Database** during Project Year 1 (Data: largest to smallest)

93 new applications by discipline

- Life Sciences
- Computer Science and Mathematics
- Others
- Computational Chemistry
- Earth Sciences
- Fusion
- Multidisciplinary
- Astronomy, Astrophysics, and Astro-Particle Physics
 High-Energy Physics

Note: Apps. Can be associated with > 1 country

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Training marketplace

- Integration of:
 - Training event calendar
 - Digital library (of training materials)
 - Service offering & requesting form
- Purpose of Training Marketplace:
 - Register training events
 - Use, reuse and share training materials
 - Offer training-related services (infrastructure, VO, CA, ...)
 - Feed training-requirements
 - Delegate representative to EGI Training Working Group
- Results:
 - Approximately 60 training events were added during Project Year 1.

Coordination of services for VOs

- VO-specific testing of sites is required by VO managers within VRCs
- basic services are available from within the infrastructure
- typically delivered through the operations teams and NGIs

Coordination consists of:

- Reviewing available services: management, monitor & accounting tools (NAGIOS SAM, GANGA, DIANE, CERN dashboard & mini dashboard)
- Consultancy/help for VO managers*
- Specification of requirements for improving operational tools to simplify VO management
- Provisioning basic services for new VOs
- Developing dashboard infrastructure
- * Further consultancy is provided by NGIs

- VRCs contain one or more VO.
- Each VO needs to monitor many resources

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VO Services: NAGIOS SAM

Provision of VO support software for VRCs & VOs (e.g.WeNMR, BioMed)

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NAGIOS SAM triggers the executions of probes in grid sites

- Tests to the Storage resources
- Tests to the Computing Resources
- Summary views of successful and unsuccessful services
- Sends emails to the site admins in case of failures

Sites from a VO are tested (infrastructure tests run probes on NGIs)

- Ability to develop and integrate VO's own probes
- A VO can use the central installation from LIP/UPV, or can install its own

Service Status Details for: **phys.vo.ibergrid.eu**

Scheduling Oueu

Processing EGI requirements; implementing solutions

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www.egi.eu/user-support

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- Motivation for workshops (from EGI Forums):
 - Users indicated need for collaboration & exploration
 - More smaller and focused meetings needed
 - Bring specialists together
- Purpose:
 - Inform and educate, clarify and specify
- Emerging themes (from requirements):
 - portals, visualisation, data management, scalability, workflow, supporting users, planning training events, developing and provisioning sustainable apps.

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New user communities: gathering new requirements

Design

What makes up a Virtual Research Community?

Virtual Organisations

VRCs provide EGI with:

- Requirements
- Applications and tools
- Data collections
- Training modules
- Success stories
- Experts
- Users

EGI offers VRCs:

- Easy to use infrastructure
- Grid-ready applications
- Training resources
- Help and support
- Involvement in open development processes
- Workshops and forums

Integrated Services

- Human
- Technical
- Infrastructure

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Deliver

Discover

- Shared stories

Mailing lists

Workshops

Forums Blogs

Projects

- Best practices
- Collaborations
- Laboratories
- Partnerships

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LSGC has just signed an MoU with EGI: http://www.egi.eu/collaboration/LSGC.html

- Application developers will be major element
- Portal and gateway developers too
- Developers are the bridge between research and the infrastructure
- Event such as IWSG-Life2011 and the HealthGrid conference bring such people together

MoU – Memorandum of Understanding

The Life Sciences community:

- Clearly well established, however...
- Many new requirements to be satisfied
- Especially to increase researcher numbers
- How will this be achieved?
- Use of the existing EGI support services
- Participation in UCB
- Workshops, forums and road-shows

• Timeline

- June 2010: open workshop at the HealthGrid conference
- Agreed on a statement of goals and missions
- Monthly phone meetings

Participating user groups

- VOs: biomed (catch-all), vlemed, lsgrid
- German life-science user community
- Lifewatch

Supporting NGIs

Dutch, French, Italian, Spanish and Swiss

Hosting body

HealthGrid, a non-profit association

Purposes and goals (1)

• Represent the LS grid users, in particular to

- Negotiate resources
- Promote their requirements
- Liaise with the European Grid Infrastructure

Coordinate actions

- Serve as a contact point for new users
- Share expertise in the community
- Avoid replication of efforts
- Define common requirements
- Encourage sharing of resources, data and tools

Purposes and goals (2)

Provide technical services

- Operate and support common VOs
- Operate shared services
- Provide targeted user support and application porting

Training and induction

- Organize community-specific training events
- Smooth the learning curve, lower the start-up cost

Dissemination

- Transfer knowledge among VRC partners
- Advertise actions
- Liaise with other groups of interest

d Infrastructure

UICOI

e grid infrastructure

Applications Database

1 11101

2d-ANACONDA 2d-ANAlysis of COpy Number DAta

Amplitudes.

BIG (GISELA)

Blast in Grids

BLAST_in_JST

Comparison

Portal

CLUSTER

Large Scale Proteome

Laboratory for Complex

Chaotic map clustering

Systems (LSC) Cardiology

ALMOST almost - all atom molecular simulation toolkit

4 >

AMBER The AMBER molecular dynamics workpackage

AMCBI

AMC e-Bioscience Infrastructure

AMIAS A Model Independent Analysis Scheme (AMIAS)

for Extracting Multipole

AquaMaps AquaMaps

ARCEM

Grid Computing Technology and the Recurrence Quantification Analysis to Predict

AutoDock (EUAsiaGrid)

Biomedicine / Molecular Biology - using Molecular dynamics

To draw a comparison by BLAST between all sequences of prokaryotes, fungi, plant...

Combinatorial Association Logic Networks Inference

CLUSTALW ClustaW

NMR chemical shift-based structure prediction

BioMD (EPIKH) Life Sciences / Drug discovery - using Molecular dynamics

Basic Local Alignment Search Tool

BTR

BIOTREE

EO.B

CNS1.2-para

Crystallography and NMR system - structure

ClustalW ClustalW

CNS1.2

BM Portal **Bio Medical Portal**

2 3

1

More information

- Contact
 - Wiki page: http://wiki.healthgrid.org/LSVRC:Index
 - Mailing list: lsvrc@healthgrid.org

How to benefit from the LSGC?

- Established VOs
 - Discuss technical issues with other VOs
 - Submit requirements to the EGI
 - Advertise your services ; use others'
- New communities
 - Join an existing VO and benefit from its expertise
 - Get information on related applications and porting efforts
 - Get application porting support
 - Browse training material and events

Summary

- EGI Virtual Research Community (VRC) model available and LSGC VRC created
 - LSGC participating in User Community Board
 - LSGC contributing to Requirements Tracker process
 - EGI supporting NGIs who support LSGC
- Technical Support Services:
 - User requirement-driven process established
 - AppDB gadget: being used by LSGC and NGIs
 - User Support Platform based around EGI gadgets
- Community Support Workshops:
 - Life Sciences themes will be investigated and acted upon; your themes

Thanks for your time! steve.brewer@egi.eu