

DEISA

DEISA

Technological and user perspective

Andrea Vanni

CINECA, a.vanni@ Cineca.it

ISSGC'08

12/07/2008

www.deisa.eu



RI-222919



Agenda

- DEISA/eDEISA/DEISA2 projects
- DECI initiative

Vision & strategy for SuperComputing infrastructure in Europe

EU vision in FP6: enhance Europe's capability computing and science by the integration of Europe's most powerful supercomputing systems (Tier-1) in a European HPC e-infrastructure

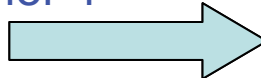


DEISA strategy: build a European Supercomputing Service on top of existing national services. This service is based on the deployment and operation of a persistent, production quality, distributed supercomputing environment with continental scope

Vision & strategy for SuperComputing infrastructure in Europe



EU vision in FP7: Establishing a future persistent European HPC ecosystem integrating national Tier-1 centres and the new European Tier-0 centres



DEISA2 strategy: Consolidate the existing DEISA HPC infrastructure and services and deliver a turnkey operational solution for the future persistent European HPC ecosystem

DEISA story

1° May
2004

1° June
2005

1° May
2008

1° June
2008

1° June
2009

30° April
2011

DEISA

eDEISA

DEISA2

eeDEISA

DEISA/DEISA2 HPC Centers



- DEISA
- eDEISA
- DEISA2 (associated partners)

DEISA2 HPC centers

BSC	Barcelona Supercomputing Centre	Spain
CINECA	Consortio Interuniversitario per il Calcolo Automatico	Italy
CSC	Finnish Information Technology Centre for Science	Finland
EPCC	University of Edinburgh and CCLRC	UK
ECMWF	European Centre for Medium-Range Weather Forecast	UK (int)
FZJ	Research Centre Juelich	Germany
HLRS	High Performance Computing Centre Stuttgart	Germany
IDRIS	Institut du Développement et des Ressources en Informatique Scientifique - CNRS	France
LRZ	Leibniz Rechenzentrum Munich	Germany
RZG	Rechenzentrum Garching of the Max Planck Society	Germany
SARA	Dutch National High Performance Computing	Netherlands
KTH	Kungliga Tekniska Högskolan	Sweden
CSCS	Swiss National Supercomputing Centre	Switzerland
JSCC	Joint Supercomputer Center of the Russian Academy of Sciences	Russia

DEISA/DEISA2 computing power

- DEISA 2004 ~ 30T/Flops
- DEISA2 2008 1P/Flops
- Dedicated 10 Gbit/s network connection
- Dedicated subset of computing resources for researchers

DEISA/DEISA2 HPC details

<i>DEISA Partner</i>	<i>Architecture</i>	<i>TF/s</i>	<i>#Cores</i>	<i>Memory in TB</i>
MPG-RZG	IBM BlueGene P	27.0	8,192	4.0
	IBM Power6	120.0	6,400	20.0
BAdW-LRZ	SGI-Altix Itanium	62.3	9,728	39.0
BSC	IBM PowerPC	94.2	10240	20.0
CINECA	IBM Blade Center	26.6	5120	10.0
	IBM Power5	3.9	512	1.0
CSC	Cray XT4 dc	10.1	2,024	2.0
	Cray XT4 qc	70.0	6,736	7.8
FZJ	IBM BlueGene P	223.0	65,536	32.0
	IBM Power4+	8.9	1,312	5.0
	IBM Power4+ successor	> 50	n/a	n/a
IDRIS-CNRS	IBM Power4+	6.7	1800	10
	IBM Power+ successor	> 40	n/a	n/a
SARA	IBM Power5+	14.6	1920	7.7
	IBM Power6	60.2	3328	15.6
UEdin-EPCC	Cray XT4	65.0	11,520	35.0
UStutt-HLRS	NEC SX-8	13.0	576	9.0

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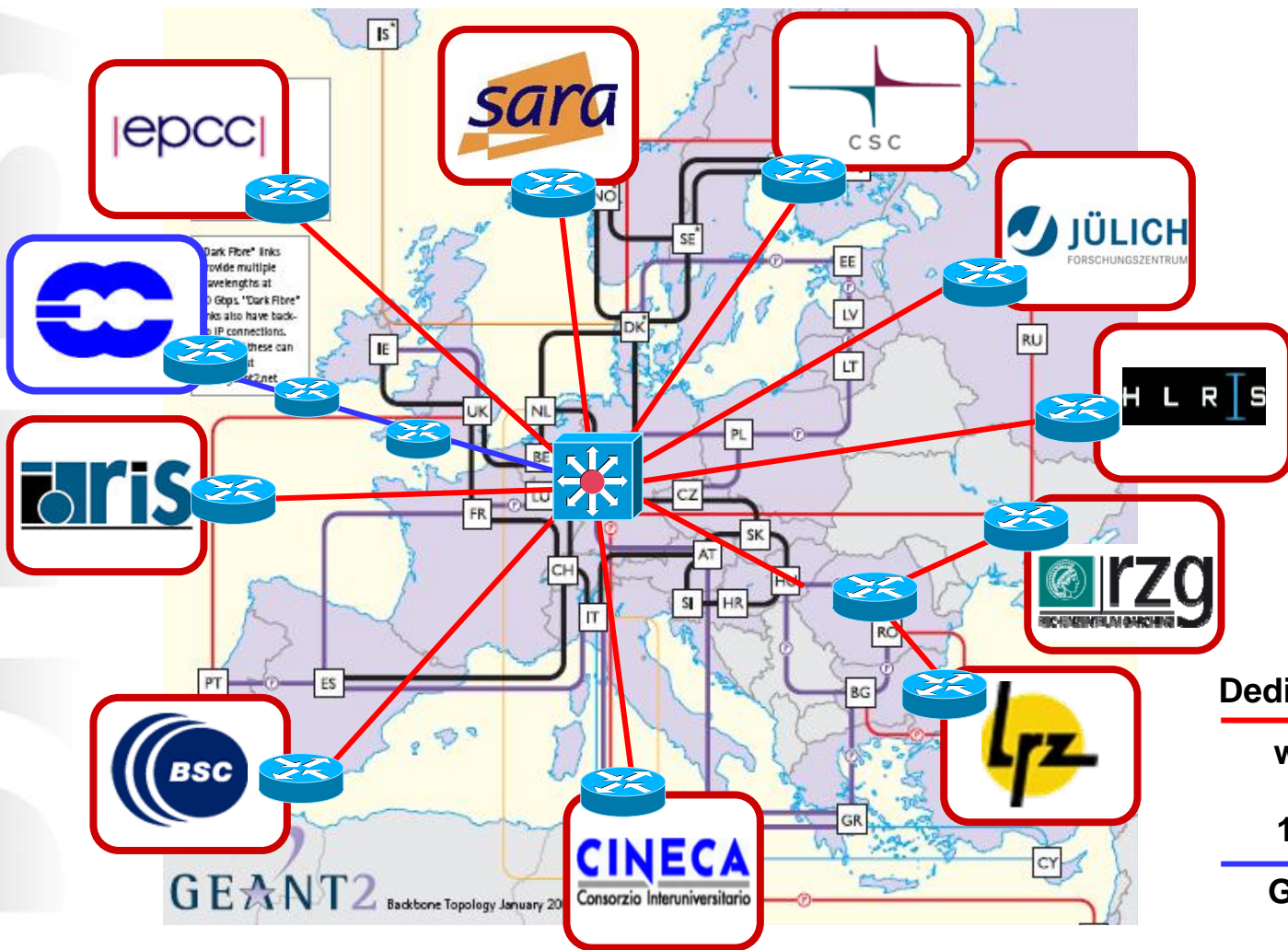
core infrastructure end services

- Dedicated high speed network
- Common AAA
 - Single sign on
 - Accounting/budgeting
- Global data management
 - High performance remote I/O and data sharing with global file systems
 - High performance transfers of large data sets (e.g. GridFTP)
- User Operational Services
 - Distributed Common Production Environment (DCPE)
 - Job management service
 - Common user support and help desk
- System Operational Services
 - Common monitoring and information systems
 - Common system operation
- Global Application Support

DEISA advanced services

- Supported Services
 - Workflow management and alternative access method
 - Grid middleware: UNICORE, DESHL
 - Science gateways to supercomputing resource, Portals
 - Job rerouting between identical architectures
- Additional Services
 - Co-Allocation
 - Other middleware components, e.g. from the Globus Toolkit

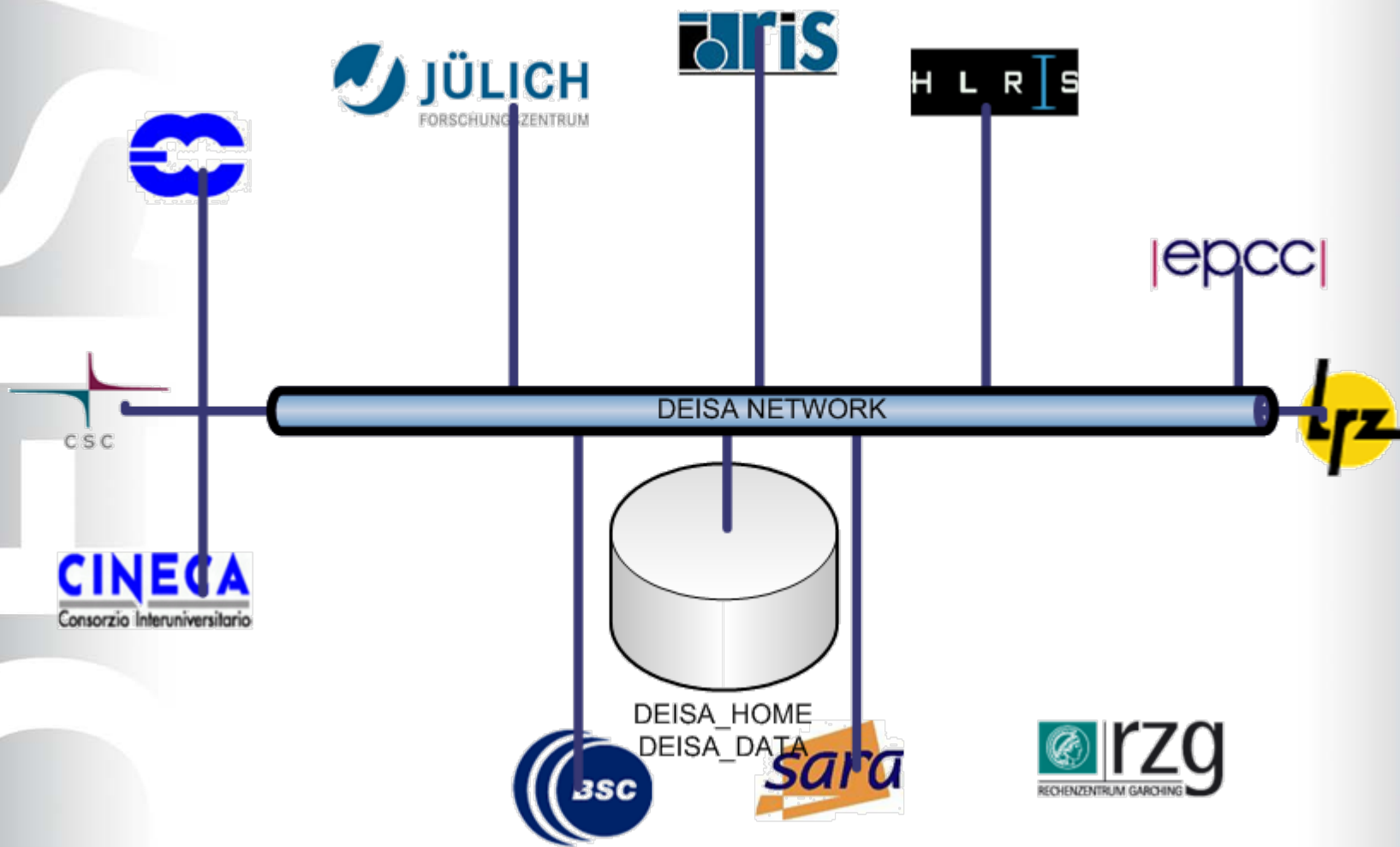
DEISA network connection



Dedicated 10 Gb/s
wavelength
1 Gb/s LSP
GRE-Tunnel

DEISA

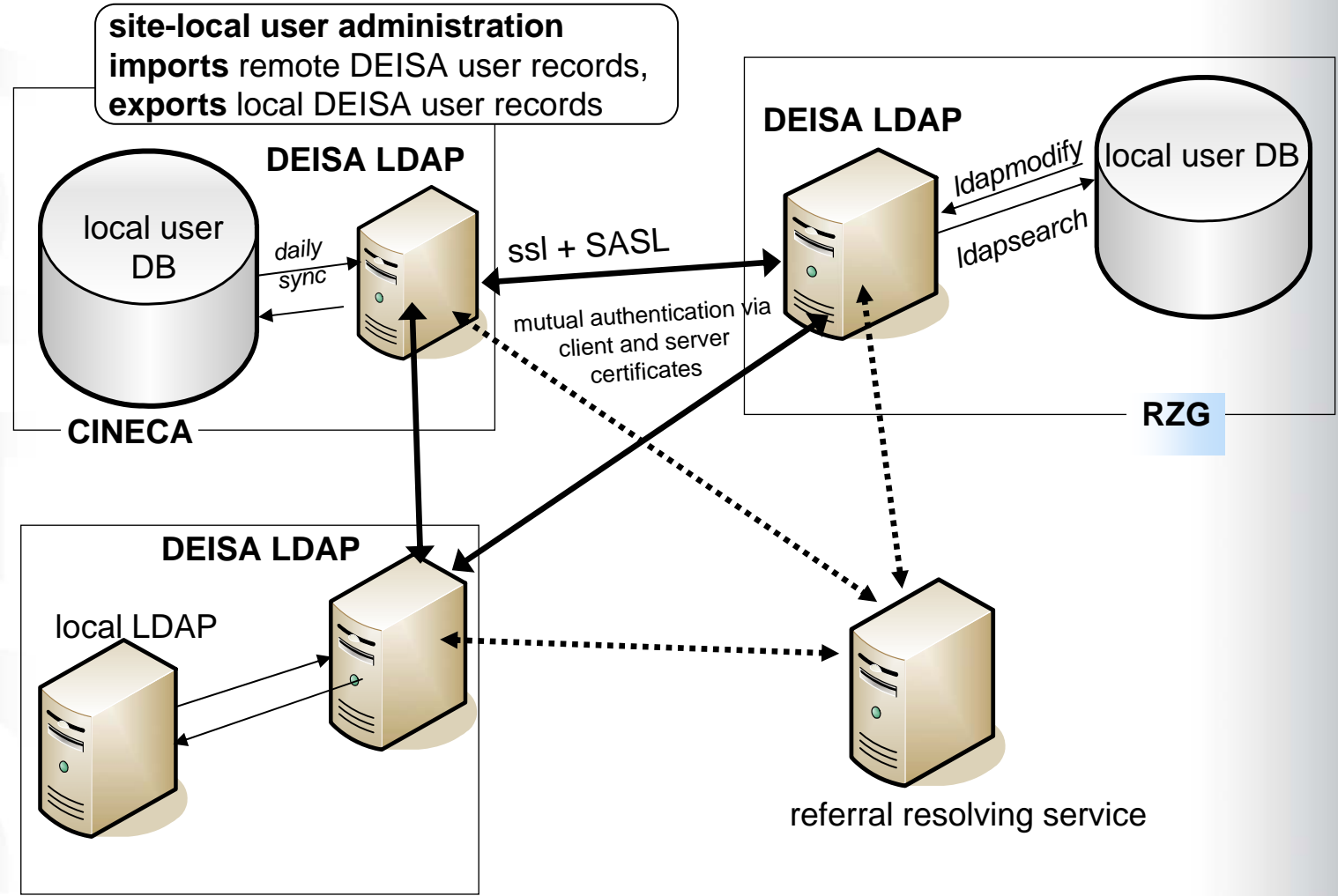
DEISA GPFS



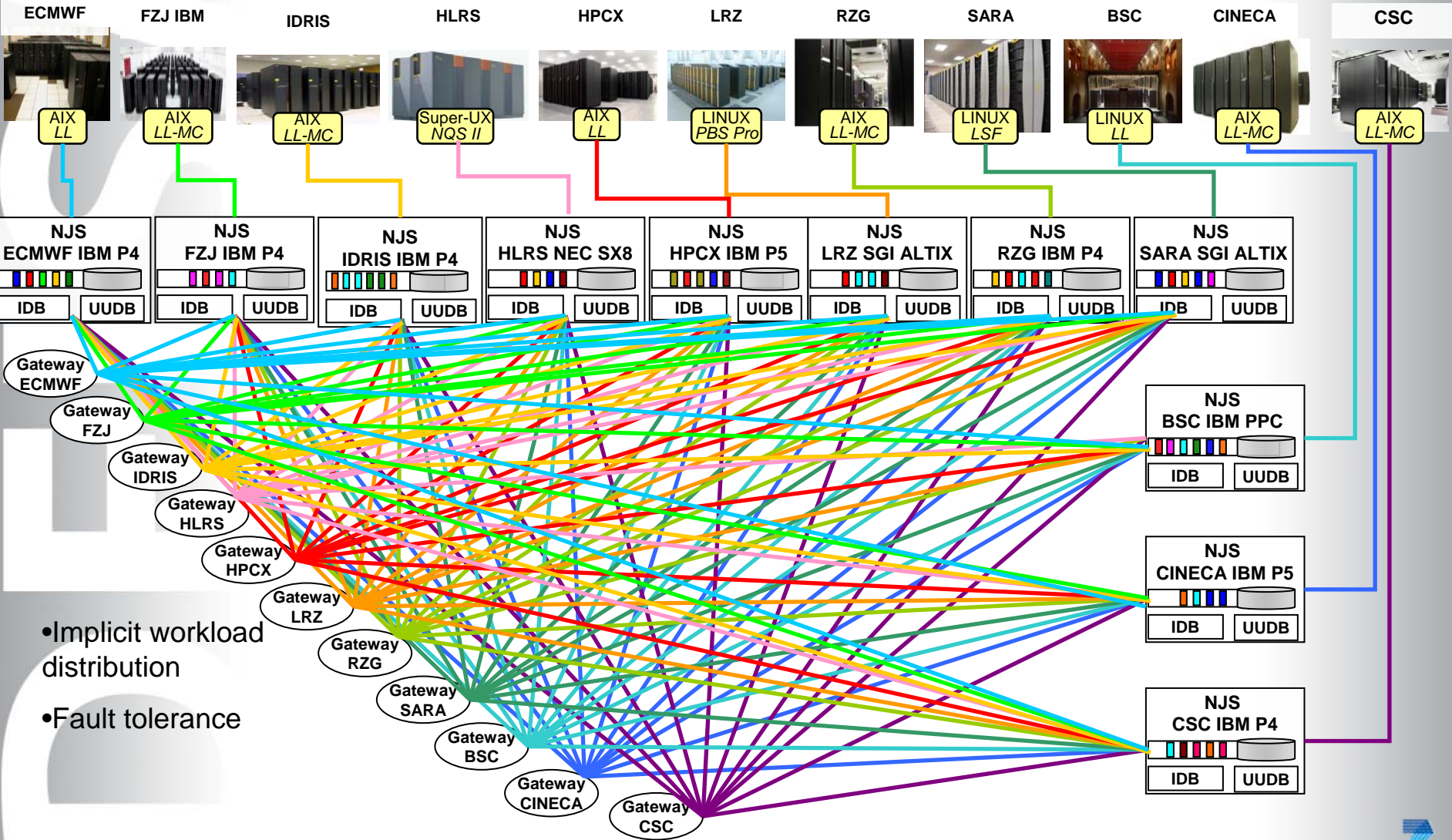
DEISA Data management

- Distributed filesystem accessible via DEISA_HOME DEISA_DATA environment
- Local GPFS (DEISA_SCRATCH) for computational temporary data
- Data staging scripts integrated into DEISA sites batch sub-systems

DEISA user administration



DEISA Unicore infrastructure



- Implicit workload distribution
- Fault tolerance

DEISA Globus infrastructure

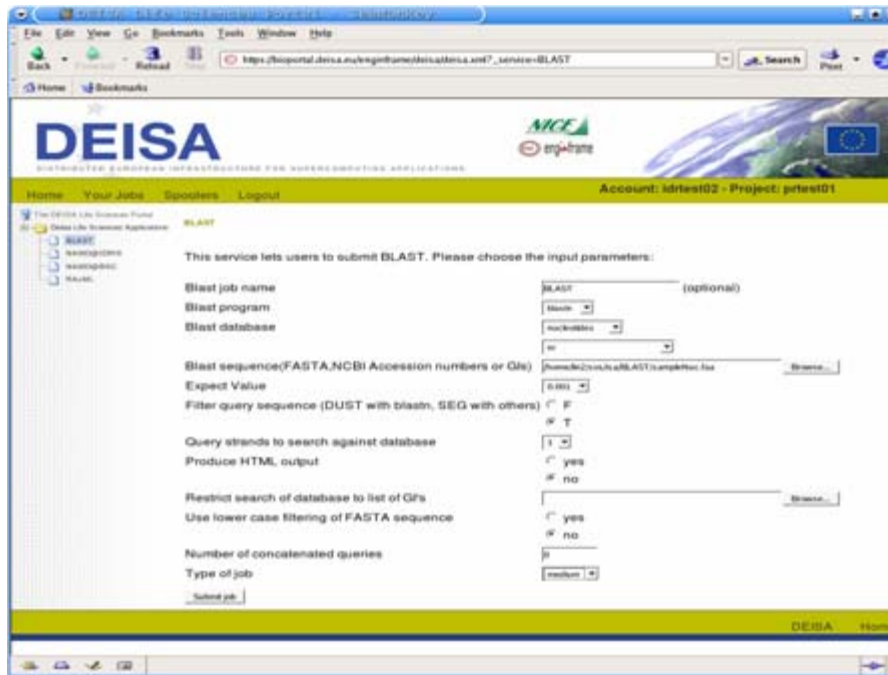


Internal and external interfaces for

- WS-GRAM
- GridFTP
- GSISSH

DEISA Disciplinary Web Portal

DEISA provides user with a Life science portal



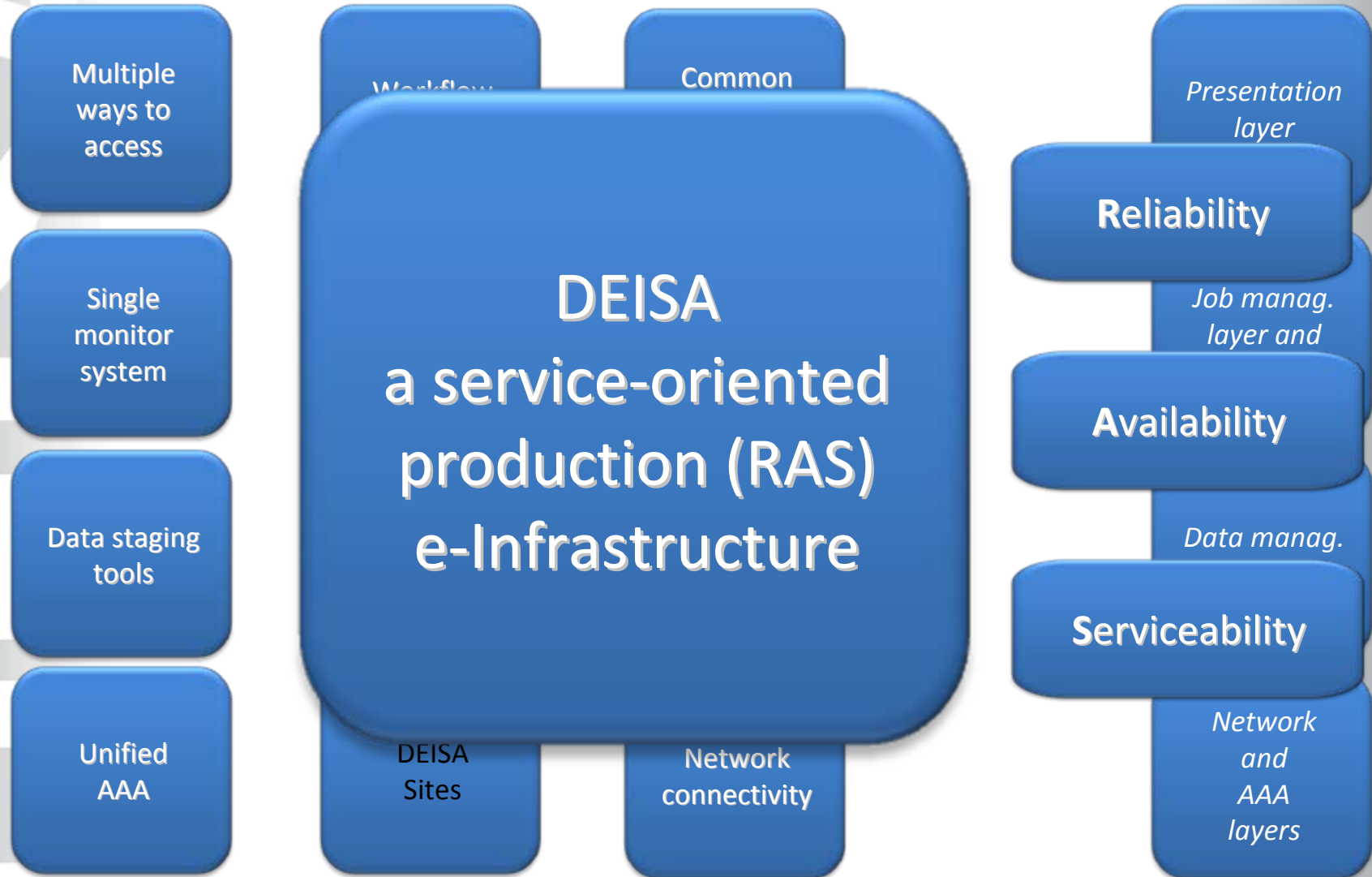
The screenshot shows a web browser window displaying the DEISA BLAST submission page. The browser's address bar shows the URL: `https://blastportal.deisa.eu/cgi-bin/blastdeisa.xml?_service=BLAST`. The page header includes the DEISA logo, the MICE logo, and the European Union flag. Below the header, there is a navigation menu with links for Home, Your Jobs, Spoolers, and Logout. The main content area is titled "BLAST" and contains a form for submitting a BLAST job. The form includes the following fields and options:

- Blast job name:** A text input field with the value "BLAST" and a "(optional)" label.
- Blast program:** A dropdown menu with "blast" selected.
- Blast database:** A dropdown menu with "nr" selected.
- Blast sequence(FASTA,NCBI Accession numbers or GIs):** A text input field with the value 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DEISA services

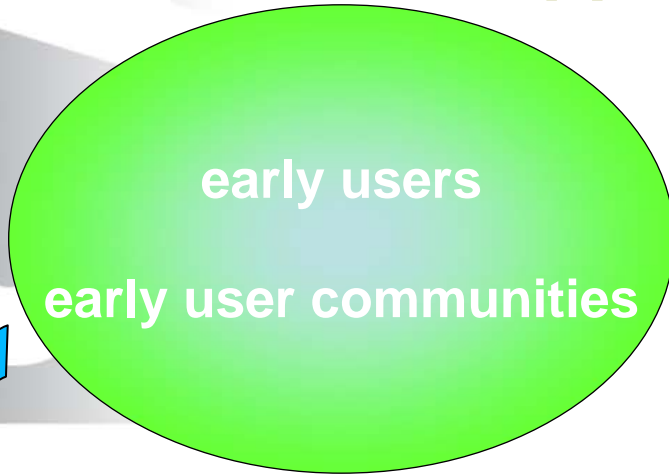


DEISA services

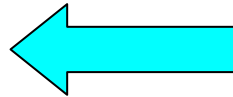


DEISA

user application & support



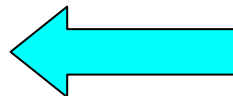
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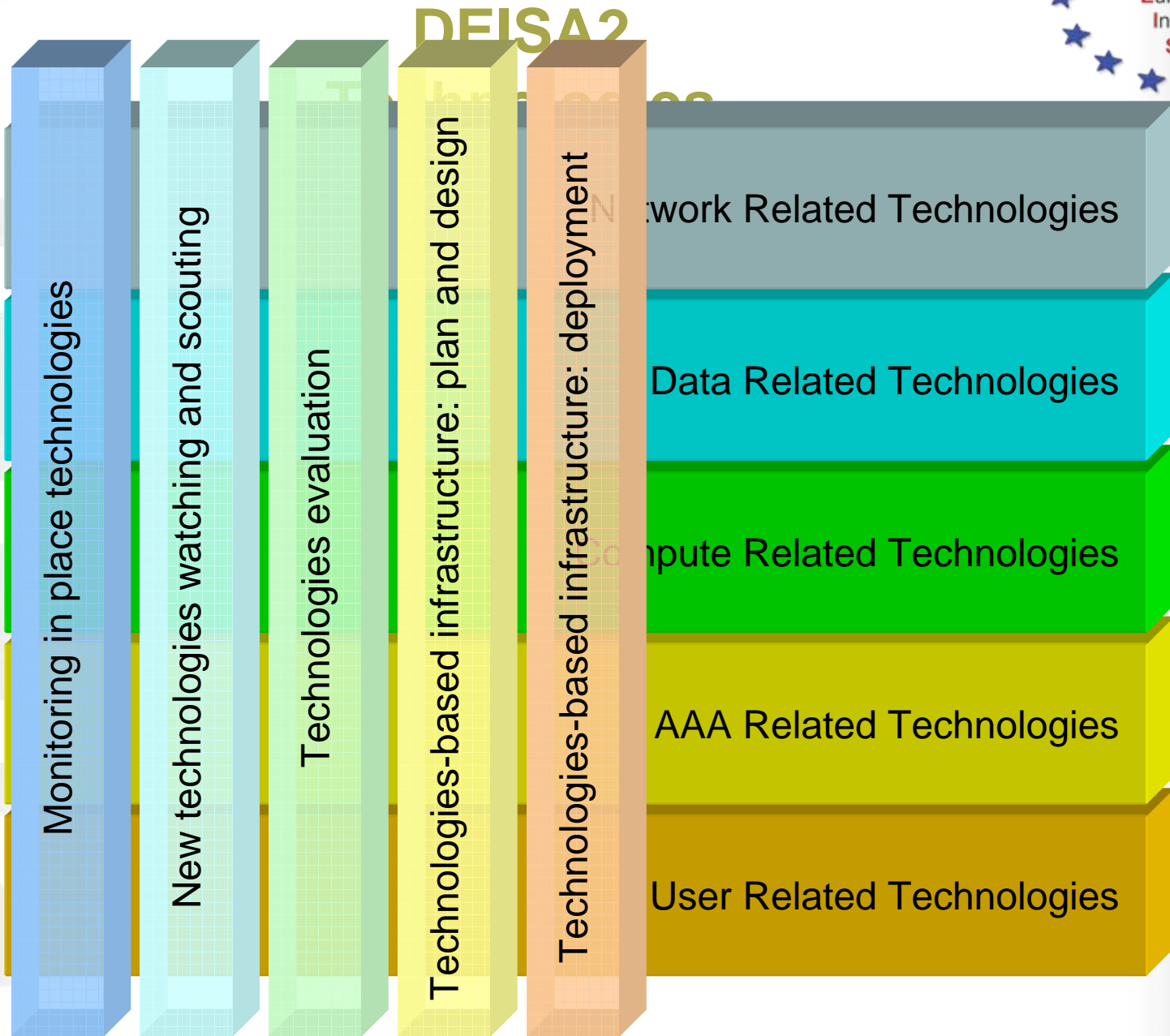
DEISA2

- Consolidation of the existing DEISA infrastructure
 - ⇒ **develop and provide a reliable turnkey operational solution for a persistent European HPC ecosystem**
- Evolvement of this European infrastructure towards a robust and persistent European HPC ecosystem
 - Enhancing the existing services, by deploying new services including support for European Virtual Communities, and by cooperating and collaborating with new European initiatives, especially PRACE that will enable shared European PetaFlop/s supercomputer systems
 - ⇒ **DEISA2 as the vector for the integration of Tier-0 and Tier-1 systems in Europe**

DEISA2

- **DEISA2 advancing computational sciences in Europe**
 - DEISA2 will provide a consistent infrastructure for virtual organisations as the European Fusion Development Agreement (EFDA) supporting ITER, the Climate Modelling Community, the Cosmology Consortium VIRGO, Material Sciences projects/communities, Life Science projects/communities
- **DEISA2 as an extended partnership**
 - DEISA2 targets the integration of further national Tier-1 partners
- **DEISA2 bridging worldwide HPC projects**
 - Interoperation in a Grid context worldwide is seen as an important step for supporting international science communities which acquire computing time traversing existing political boundaries

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Actions on Technologies

- Evaluation of network security issues
- Enhancement of DEISA2 network monitoring
- Evaluation of file system technologies
- Evaluation of generic multi-disciplinary data access and discovery services
- Evaluation of UNICORE 6 and GT4.2 and deployment
- Evaluation of monitoring tools
- Evaluation of shibboleth for web SSO and other AAA aspects and Evaluation of GSI-SSH for user logins
- Comprehensive system accounting to be integrated in batch schedulers
- Evaluation of JSR-168, JSF and technology neutral portal targeted to the design of a DEISA2 horizontal portal
- Introduction of a "remote visualisation" service

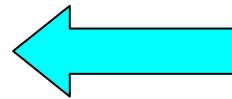
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Extreme computing
projects from
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- WP5: Applications enabling
- WP6: Environment- and User-related Application Services
- WP7: Extreme Computing Projects and Benchmarking

DEISA Extreme Computing Initiative (DECI)



The basic service providing model for scientific users is currently the Extreme Computing Initiative

- DECI launched in early 2005 to enhance DEISA's impact on science and research
- European Call for proposals in May-June every year. Multi-national proposals strongly encouraged
- Identification, enabling, deploying and operation of "flagship" applications in selected areas of science and technology
- Complex, demanding, innovative simulations that require the capabilities of DEISA compute resources
- Proposals reviewed by national evaluation committees
- Applications are selected on the basis of scientific excellence, innovation potential and relevance criteria – and national priorities
- Once approved, the most powerful HPC architectures in Europe assigned to the most challenging projects, and the most appropriate supercomputer architecture selected for each project

DEISA Extreme Computing Initiative (DECI)



Supporting environment

- Application enabling by Applications Task Force (ATASKF), team of leading experts in high performance and grid computing
- DEISA Common Production Environment (DCPE): homogenising the heterogeneous DEISA software environments
- General environment and user related application support
- European team of system operation specialists handling coordination and synchronisation of system services, maintenance measures and failure situations
- Training sessions

DEISA Extreme Computing Initiative (DECI)

DECI call 2005

- 51 proposals, 12 European countries involved
- 30 mio cpu-h requested
- 29 proposals accepted, 12 mio cpu-h awarded (normalized to IBM P4+)

DECI call 2006

- 41 proposals, 12 European countries involved
- 28 mio cpu-h requested
- 23 proposals accepted, 12 mio cpu-h awarded

DECI call 2007

- 63 proposals, 14 European countries involved
- 70 mio cpu-h requested
- 45 proposals accepted, ~30 mio cpu-h awarded

DECI call 2008

- 4th call for proposals currently open until June 30th, 2008
<http://www.deisa.eu/science/deci/projects2008-2009/deci-call-for-proposals>

DECI Projects – Publications

Cover story of Nature May 24, 2007 DECI project POLYRES

Benedict J. Reynwar, Gregoria Illya, Vagelis A. Harmandaris,
Martin M. Müller, Kurt Kremer & Markus Deserno:
***Aggregation and vesiculation of membrane proteins
by curvature mediated interactions,***
NATURE Vol 447|24 May 2007| doi:10.1038/nature05840



Dozens of publications so far, among them
NATURE, Phys Rev B, Phys Rev Lett, PNAS

Further information see <http://www.deisa.eu/about/results>

DEISA Technological and user prospective



QUESTIONS