

The key role of the UNICORE Technology in European Distributed Computing Infrastructures supporting e-Science Applications in the Decades to Come

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Outline





Outline

- e-Science with UNICORE
- UNICORE as part of EMI
- UNICORE & ESFRI Roadmap
- UNICORE & VPH Roadmap
- Summary
- References





'During the course of the talk we will create one potential roadmap of UNICOREs key role in the context of distributed computing infrastructures in the next decades...'



e-Science with UNICORE





Scientific Innovation with e-Science Infrastructures

'e-Science is about global collaboration in key areas of science and the **next generation infrastructure** that will enable it'

John Taylor (UK Research Council) in 2005





Different e-Science Infrastructures & Technologies





Approaches to conduct e-Science with UNICORE





European Commission Perspectives on e-Science

VRCs = Virtual Research Communities





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Sharing the best computational resources: e-Science grid, supercomputing

'...last call focused on distributed computing infrastructures (DCIs) and future proposal calls for European projects will be oriented towards virtual research communities...'

> Kostas Glinos (European Commission) at OGF28 Keynote in 2010

[3] Glinos, "The changing world of distributed computing and the role and contributions of the e-Infrastructure programme in this new environment, OGF28 Keynote, Munich, 2010



Roadmap Update: UNICORE, e-Science & VRCs





UNICORE as part of the **EMI**





European Middleware Initiative (EMI) in Context





UNICORE as one 'program' in a software suite...

- The EMI software suite might become similar to MS Office
 - Maybe not liked by everybody but widely used
 - Many complementary programs for dedicated purposes
 - 'One uses Outlook (e.g. UNICORE) for appointments'
 - 'One uses Powerpoint (e.g. gLite) for presentations'
 - 'One uses Word (e.g. ARC) for letters'
- UNICORE is one well-established 'program' in the EMI software suite among others
 - >10 years of experience in HPC with strong security, wide machine support & reliability
 - Easy installation significantly lowers the barrier for usage
 - The extensibility of the service environment provides excellent basis for further higher-level service 'developments/deployments' in Java







Large user community: Large Hadron Collider (LHC)





One EMI example: LHC data accessible via UNICORE





Roadmap Update: UNICORE, EMI, EGI & PRACE





UNICORE & ESFRI Roadmap





ESFRI List of Projects & Roadmap

- ESFRI = European Strategy Forum on Research Infrastructures
- A huge set of potential customers of infrastructures (and technologies)
- Costly resources for geographically dispersed user communities







ESFRI Projects – Number / Research Area Statistics



- Social Sciences and Humanities
- Environmental Sciences
- Energy
- Biological and Medical Sciences
- Materials and Analytical Facilities
- Physical Sciences and Engineering
- e-Infrastructures





ESFRI Projects – Evolution / Research Area Statistics





ESFRI Projects – Environmental Sciences



[6] ESFRI Website: http://ec.europa.eu/research/infrastructures/index_en.cfm?pg=esfri



ESFRI Projects – Biological and Medical Sciences



[6] ESFRI Website: http://ec.europa.eu/research/infrastructures/index_en.cfm?pg=esfri



ESFRI Projects – Costs and time-scale (1)

	PROJECTS	construction costs (M€)	Operations costs (M€/year)	first possible operations or upgrade
	(T(C))		2	2012
Social Sciences and Humanities	CESSDA	30	3	2013
	CLARIN	104	7.6	2014
	DARIAH	12	4	2013
	European Social Survey	54**	9**	2008
	SHARE	11.6	0.3	2008
			1	1
Environmental Sciences	AURORA BOREALIS	635	32.5	2014
	COPAL (ex EUFAR)	50	3 (+6000€/hour)	2012
	EISCAT_3D Upgrade	60-250	4-10	2015
	EMSO	160	32	2013
	EPOS	500	80	2018
	EURO-ARGO (GLOBAL)	80	7.3	2011
	IAGOS	15	0.5-1	2012
	ICOS	128	14	2012
	LIFEWATCH	370	71	2019
	SIAEOS	50	9.5	2012
Energy	ECCSEL	81	6	2011
	HiPER	800	under discussion	2020+
	IFMIF (GLOBAL)	1000	150-80	2020
	JHR	500	24-33	2014



ESFRI Projects – Costs and time-scale (2)

Biological and Medical Sciences	BBMRI	170	15	2013
	EATRIS	255	50	2013
	ECRIN	50	5	2014
	ELIXIR (GLOBAL)	470	100	2012
	EMBRC	100	60	2018
	EU-OPENSCREEN	40	40	2012
	EuroBioImaging	370	160	2012
	High Security BLS4 Laboratory	174	24	2018
	Infrafrontier	270	36	2010
	INSTRUCT	300	25	2012
Materials and Analytical Facilities	EMFL	120	8***	2015
	ESRF Upgrade	238	83	2009-2014
	EuroFel (ex-IRUV-FEL)	1200-1600	120-160	2007-2020
	European Spallation Source	1300	110	2019-2020
	European XFEL	1043	84	2014
	ILL20/20 Upgrade	171	5***	2007-2017
	CTA	150	10	2013
Physical Sciences and Engineering	E-ELT	950	30	2018
	ELI	400	50	2015
	FAIR	1187	120	2016
	KM3NeT	200	5	2016
	PRINS	1400	300	2009-2015
	SKA (GLOBAL)	1500	100-150	2016
	SPIRAL2	196	6.6	2014
e-Infrastructures	PRACE (ex EU-HPC)	200-400*	50-100	2009-2010
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ESFRI Projects – Application Enabling Work

- Extensibility of UNICORE is very useful to support application enabling
 - E.g. Hosting of dedicated community services within the UNICORE container





ESFRI Projects – Social Sciences and Humanities



ESFRI Projects – CLARIN Application Enabling









Roadmap Update: UNICORE & ESFRI Projects





UNICORE & VPH Roadmap





UNICORE & VPH Roadmap

VPH = Virtual Physiological Human







UNICORE & VPH Roadmap





European Commission Projects in the context of VPH

The initial (Call 2) VPH projects are targeted as follows:

euHeart (IP) is a developing open source codes and multiscale/multi-physics models of heart electromechanics in clinical cardiac diagnostic and device development applications.

VPH2 (STREP) is developing decision support tools for heart disease.

preDiCT (STREP) is developing models of cardiac electrophysiology for drug design and toxicity testing.

ARTreat (IP) is developing an interventional decision support system for stenting procedures based on multiscale patient specific models of atherosclerotic disease.

ARCH (STREP) is developing clinical decision support tools based on patient-specific predictive modelling of vascular pathologies.

PASSPORT is developing an open source multiscale framework for diagnostics and surgical training in the liver, based on modelling liver cell regeneration.

IMPPACT (STREP) is developing minimally invasive, patient-specific treatment strategies for liver cancer based on bioengineering multiscale modelling principles.

PredictAD (STREP) is developing an evidence based statistical framework for diagnosis of Alzheimer's disease.

NeoMARK (STREP) is implementing collaborative research networks and tools for the early detection of oral squamous cell carcinoma.

CONTRACANCRUM (STREP) is using multiscale modelling techniques to simulate patient specific cancer treatment outcomes.

VPHOP (IP) is developing a patient-specific, multiscale modelling framework for predicting osteoporotic fracture in elderly patients.

HAMAM (STREP) is establishing a database of curated and annotated imaging data and software tools for breast cancer diagnosis.

ACTION-Grid (CA) is promoting collaboration in medical/biomedical Informatics and grid technologies to promote the interface between ICT and nanotechnology.

RADICAL (CA) is investigating security and privacy issues for VPH applications and best practices for medical and genetic data protection in distributed environments.



Further EU Calls planned...





The role of DEISA (and soon PRACE) for VPH





DEISA VPH virtual community

The NoE has also taken steps to build a relationship between the NoE and the VPH-I research projects through the development of a DEISA VPH Virtual Community. The Virtual Community, applied for and managed by the NoE on behalf of the VPH-I, provides access to high performance computing facilites for any VPH-I research project which requires such a facility; currently, over 50% of the projects are being supported in this manner. Moreover, additional EU funded projects working in e-Health related domains are also being supported.







Roadmap Update: UNICORE & VPH Vision





Summary





Roadmap Summary: UNICORE and its key role





Summary



- More details, facts, and figures in the full paper
- e-Science is accepted along the traditional scientific paradigms
 - Due to infrastructure & resource complexity middleware becomes necessary
- Application enabling work is necessary for many scientific approaches
 - EMI provides basic set of Grid services, but this might be not enough
 - The UNICORE environment provides a perfect basis for higher level services
 - ESFRI & VPH → require several specialized Web services for e-Research
 - Access to large-scale instruments and data demands need to be satisfied
- Demands for decades to come
 - ESFRI and VPH are strategic roadmaps with objectives for decades
 - Preparation, construction, and operation project phases will last for decades
 - The era of Grids does not 'end' the era of Grids is just about to 'begin'... (maybe under a 'new fancy cover name' while paradigms remain)
- UNICORE is well established in EU and other regions or e-Business?
- The only constant we have is continuous change it's e-Research...



References





References

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- [2] M. Riedel, A. Streit, F. Wolf, Th. Lippert, D. Kranzlmüller Classification of Different Approaches for e-Science Applications in Next Generation Computing Infrastructures, Proceedings of the 4th IEEE Conference on e-Science (e-Science) 2008, Indianapolis, Indiana, USA, pp. 198 – 205
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- [4] European Middleware Initiative Website: <u>http://www.eu-emi.eu/</u>
- [5] European Grid Initiative Website: <u>http://www.egi.eu/</u>
- [6] ESFRI Website: <u>http://ec.europa.eu/research/infrastructures/index_en.cfm?pg=esfri</u>
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