gLite grid enabled infrastructure

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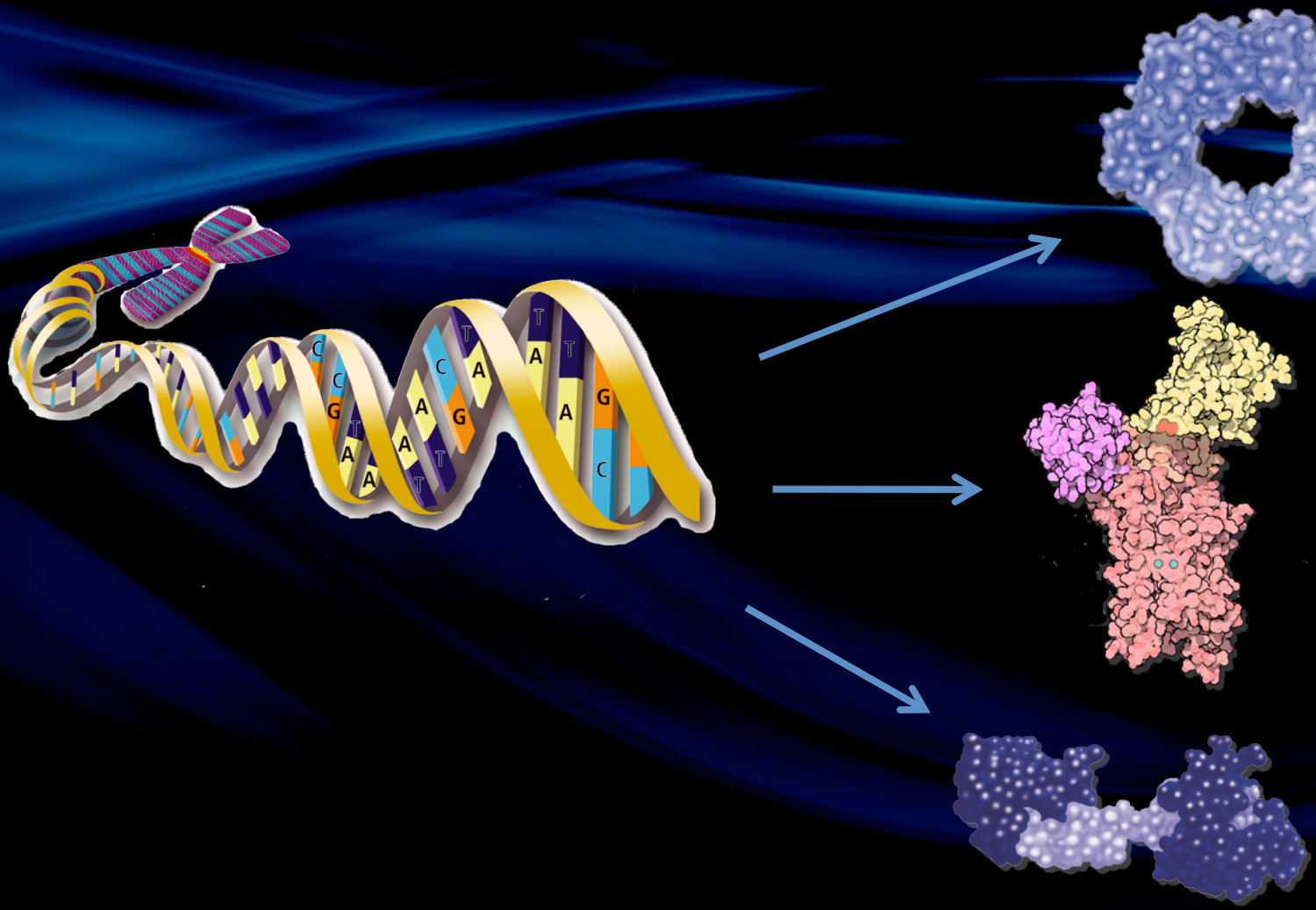
Outline

- Biological relevance of molecular machines
- Nuclear Magnetic Resonance
- enmr.eu virtual organization
- From Grid applications to web services
- enmr.eu VO status
- The future … we-NMR

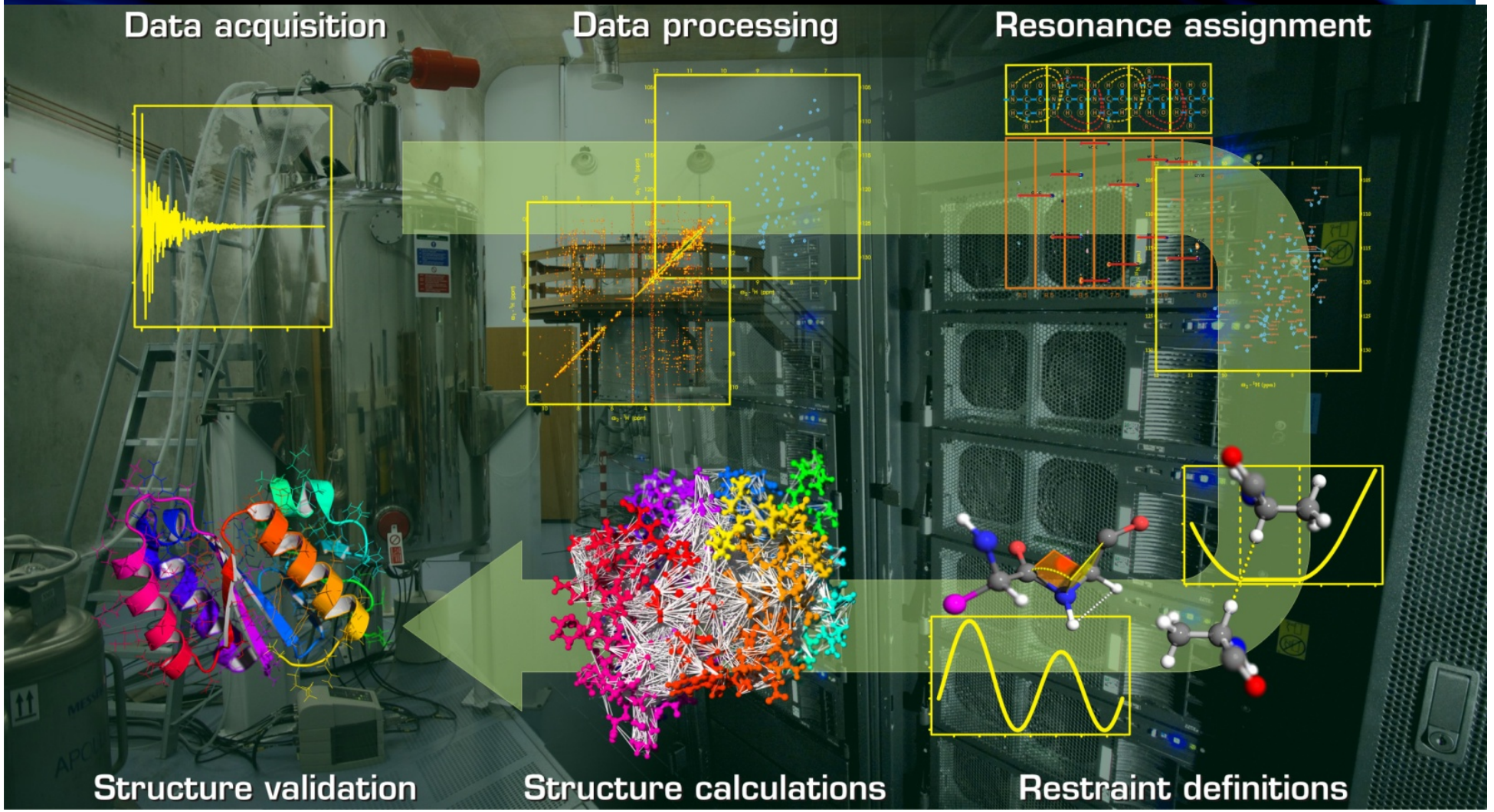
Biological background



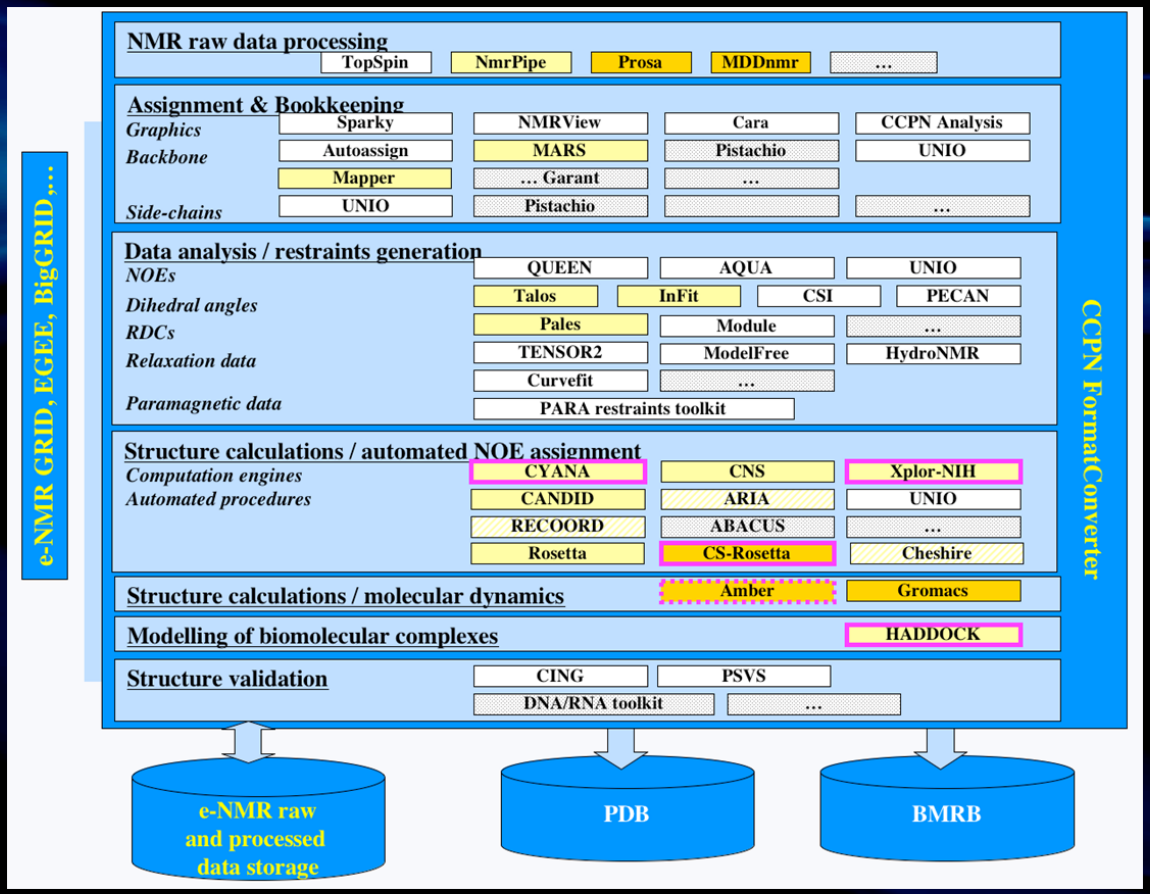
Structure of biomolecules. Why?

- Function and Mechanism of Action
- Design of Experiments
- Understand Effects of Mutations
- Drug Design

Nuclear Magnetic Resonance



Pratical issues …



- # programs
- Expertise
- CPU/storage space

e-NMR Objectives

- Integrated protocols of NMR applications
- Easy access to web interfaces
- Exploit GRID technology
- Lower the access level to GRID technology in life sciences

e-NMR : Integrated Infrastructure Initiative

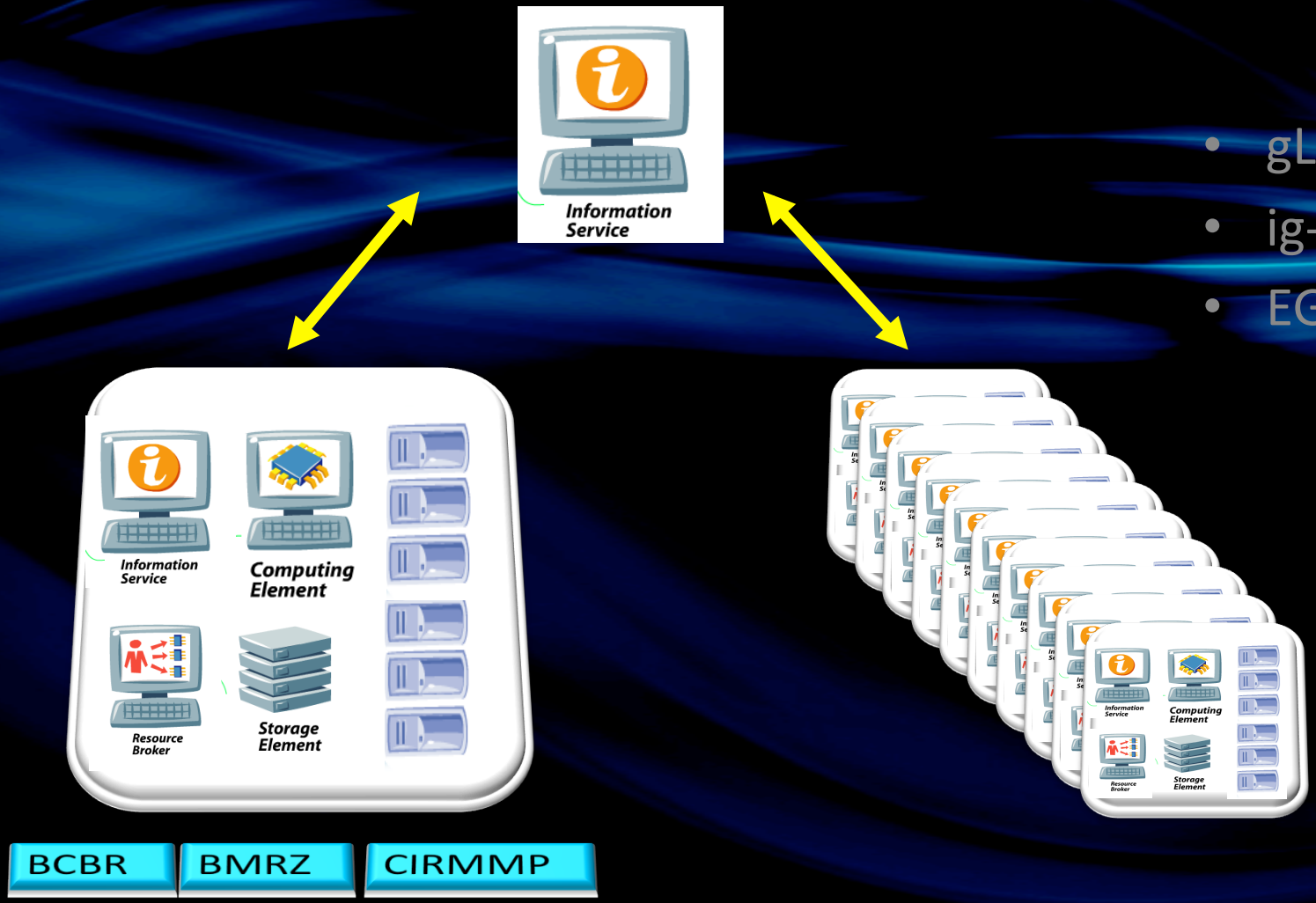
I3 initiatives

- EU-NMR
- EAST-NMR

Coordination action

- NMR-Life

enmr.eu VO grid architecture



- gLite 3.x
- ig-release
- EGEE release

e-NMR portal @ www.enmr.eu

e-NMR

NMR computational infrastructure

WELCOME TO THE E-NMR WEB PORTAL >>

e-NMR aims at deploying and unifying the NMR computational infrastructure in system biology, a project funded under the 7th framework program of the European Union (Contract no. 213010 - e-NMR).

NMR plays an important role in life sciences (biomolecular NMR), and structural biology in particular, at both European and international levels. Our main objective is to optimize and extend the use of the NMR Research Infrastructures of EU-NMR through the implementation of an e-Infrastructure in order to provide the biomolecular NMR user community with a platform integrating and streamlining the computational approaches necessary for NMR data analysis and structural modelling (e-NMR).

HADDOCK Biomolecular Docking

HADDOCK (High Ambiguity Driven protein-protein DOCKing) is an information-driven flexible docking approach for the modeling of biomolecular complexes. HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. HADDOCK can deal with a large class of modelling problems including protein-protein, protein-nucleic acids and protein-ligand complexes. | GO TO SERVICE >>

PROFILE >>

e-nmr

e-infrastructure

Services

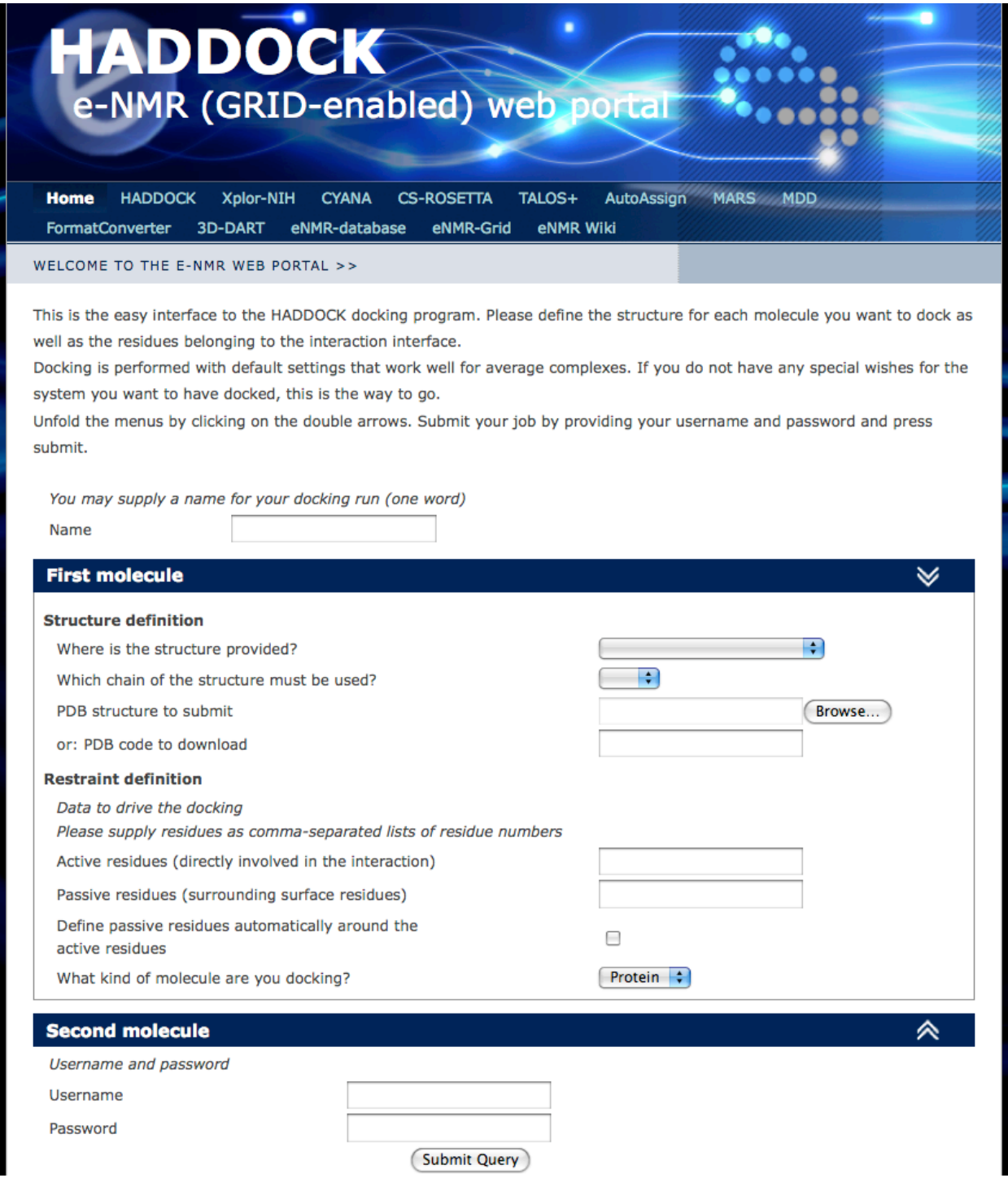
The e-NMR web portal is an easy gateway for you to use many of the powerful software packages ported by the e-NMR consortium to the GRID.

LEARN MORE >>

Links:

NMR SPECTROSCOPY >>
NMR Research Group, Bijvoet Center for Biomolecular Research, Utrecht University

HADDOCK web portal



e-NMR grid status

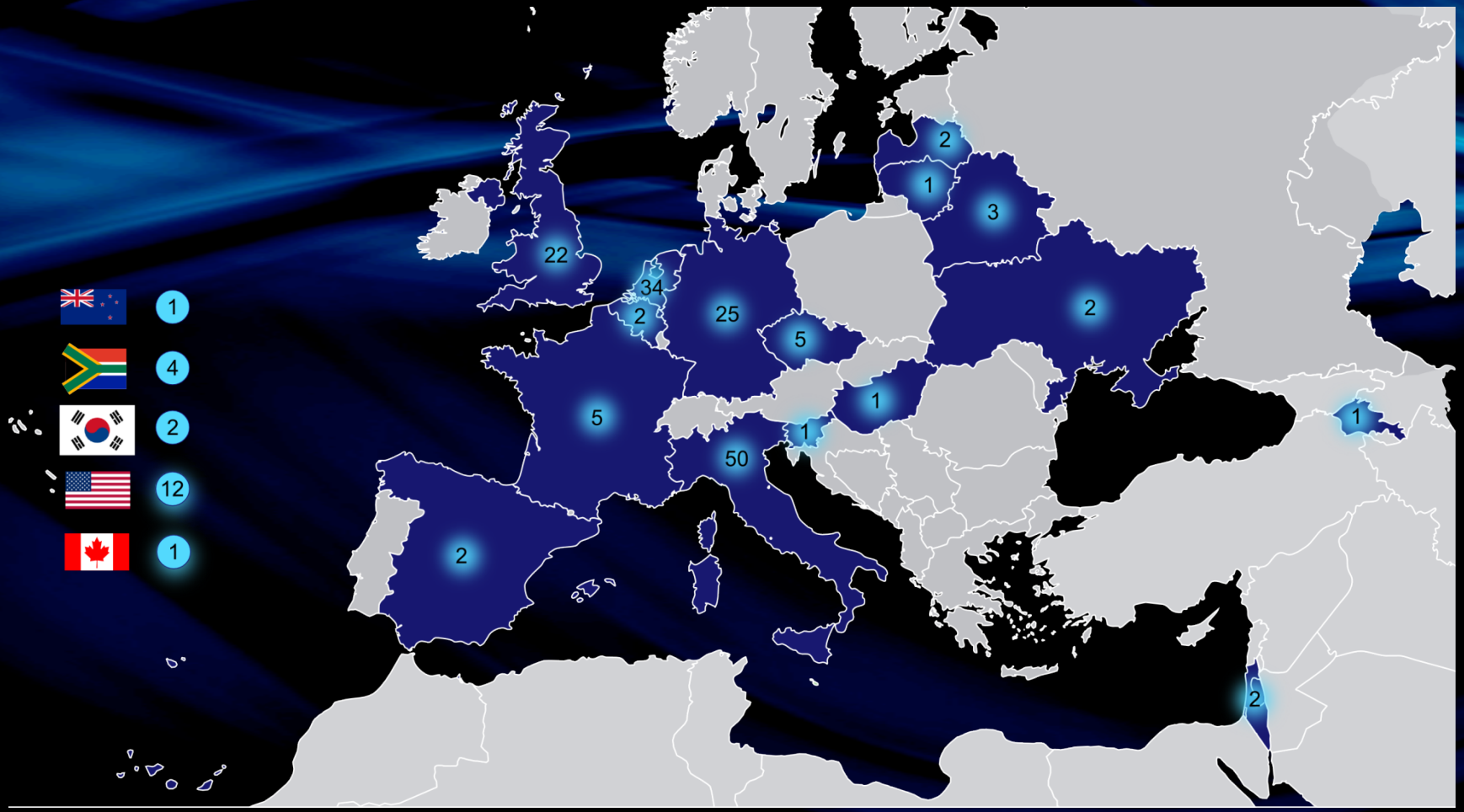
- 2nd largest VO in life sciences with 178 users registered (May 2010)
- 25% of life-science calculations done on the GRID
- 15 grid-sites in 5 countries with ~ 10K CPUs / 150 TB storage
- 9 web portals, ~ 20 applications ported to the grid
- ~ 200 CPU years over last year

GSTAT	.	OK	INFO	NOTE	WARN	ERROR	CRIT	MAINT	OFF
SFT	.	OK	.	.	WARN	ERROR	CRIT	SchedDown	

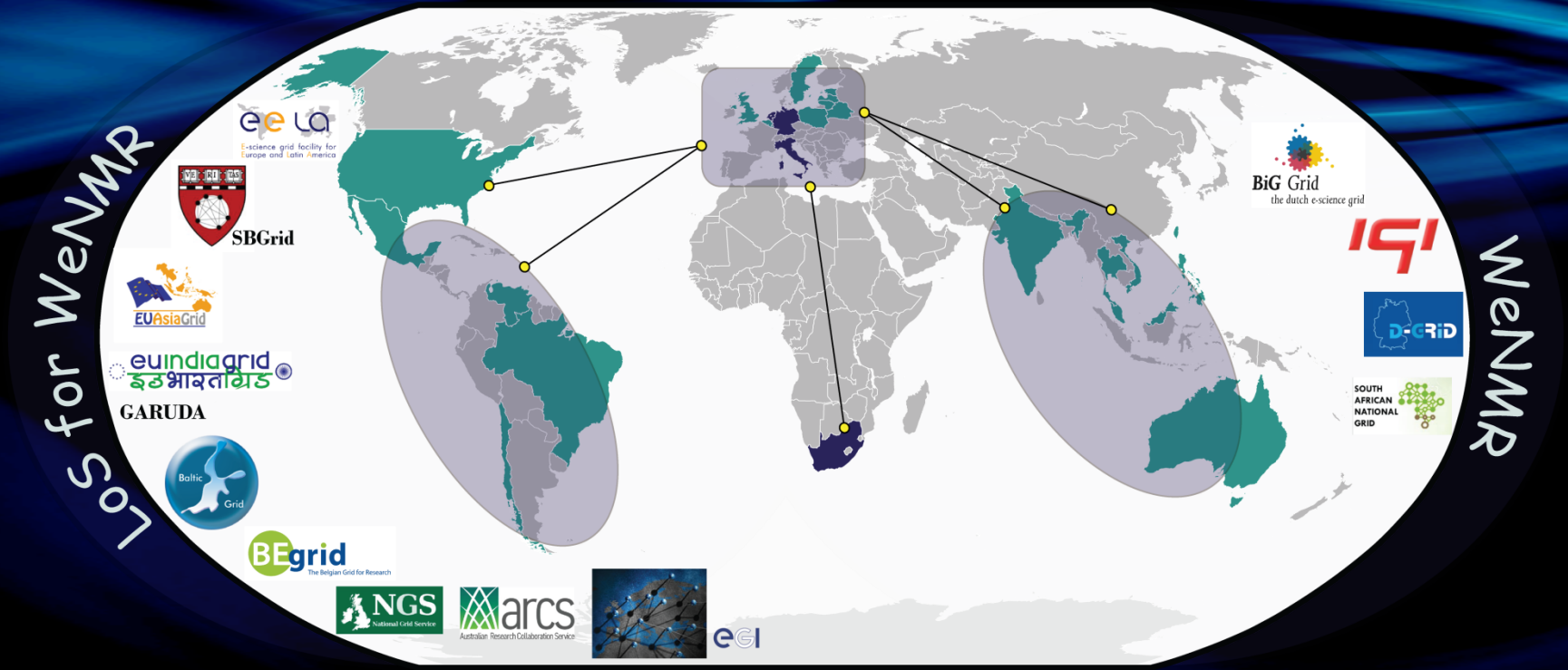
Site List. sort by: siteName domain maxcpu status

No	Site Reports	GIIS Host	bnode	cernse	qperf	sanity	serv	serEntry	version	sclust	totalCPU	freeCPU	runJob	waitJob	seAvail TB	seUsed TB	maxCPU	avgCPU	gice
1	BCBR	bdii1-enmr.chem.uu.nl	ok	note	ok	ok	ok	ok	GLITE-3_2_0	ScientificSL 5.4	44	0	16	37	1.81	0.10	44	43	.
2	BMRZ-FRANKFURT	ce-enmr.chemie.uni-frankfurt.de	.	.	ok	ok	ok	ok	GLITE-3_1_0	ScientificSL 4.8	11	34	6	14	0.86	0.07	11	10	ok
3	CIRMMP	ce-enmr.cerm.unifi.it	ok	note	ok	ok	ok	ok	GLITE-3_1_0	ScientificSL 4.5	8	12	0	0	0.48	0.03	8	7	ok
4	CNR-ILC-PISA	gridce.ilc.cnr.it	.	.	ok	ok	ok	ok	GLITE-3_2_0	ScientificSL 5.4	2	2	2	0	0.23	0.18	2	1	ok
5	HTC-BIGGRID	deimos.htc.biggrid.nl	.	.	ok	ok	ok	ok	GLITE-3_1_0	ScientificSL 4.6	412	1111	126	3	6.02	0.41	412	411	ok
6	INFN-BARI	gridba2.ba.infn.it	.	.	.	error	error	.		na							757	264	sd
7	INFN-CATANIA	grid005.ct.infn.it	.	.	ok	ok	ok	ok	GLITE-3_2_0	ScientificSL 4.5	440	76	358	444	5.44	34.07	440	217	ok
8	INFN-LNL-2	t2-ce-03.lnl.infn.it	.	.	ok	ok	ok	ok	GLITE-3_1_0	ScientificSL 5.3	136	0	484	135	66.47	172.66	136	132	ok
9	INFN-PADOVA	prod-bdii-02.pd.infn.it	ok	note	ok	ok	warn	ok	GLITE-3_1_0	ScientificSL 4.6	54	4	65	119	28.07	1.55	54	54	ok
10	INFN-TRIESTE	grid001.ts.infn.it	.	.	ok	warn	error	ok		na							136	135	sd
11	NIKHEF-ELPROD	siteinfo03.nikhef.nl	ok	ok	ok	ok	info	ok	GLITE-3_1_0	CentOS 5.4	1376	76	4898	0	0	3862.77	1376	1320	ok
12	UKI-SCOTGRID-DURHAM	bdii.dur.scotgrid.ac.uk	.	.	ok	ok	ok	ok	GLITE-3_2_0	ScientificSL 5.3	168	0	664	185	26.85	7.30	168	167	ok
13	ZA-NWU	ce-lnx1.nwu.ac.za	.	.	ok	warn	.	ok	GLITE-3_1_0	ScientificSL 4.7	24	16	0	0			24	23	.
14	ZA-UCT-ICTS	za-uct-ce.uct.ac.za	.	.	ok	ok	.	ok	GLITE-3_1_0	ScientificSL 4.8	16	14	0	0	0.29	0.09	16	11	.
15	ZA-UJ	glite-ce.grid.uj.ac.za	.	.	.	error	.	.		na							2	0	.
							sites	countries	totalCPU	freeCPU	runJob	waitJob	seAvail TB	seUsed TB	maxCPU	avgCPU			
						Total	15	5	2691	1345	6619	937	0	4079.28	3586	2795			

VO users



The future …



"Bridging the gap between European e-Science and Iberian America"

In brief

- e-NMR is a new GRID initiative in life sciences
- The e-NMR grid is operational at the various partner sites
- A variety of NMR applications have been successfully ported to the grid
- Several user-friendly web portals are operational
- Use-case examples and tutorials are available online
- Check the current status at www.enmr.eu

Acknowlegments

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gLite grid enabled infrastructure

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/O=universiteit-utrecht
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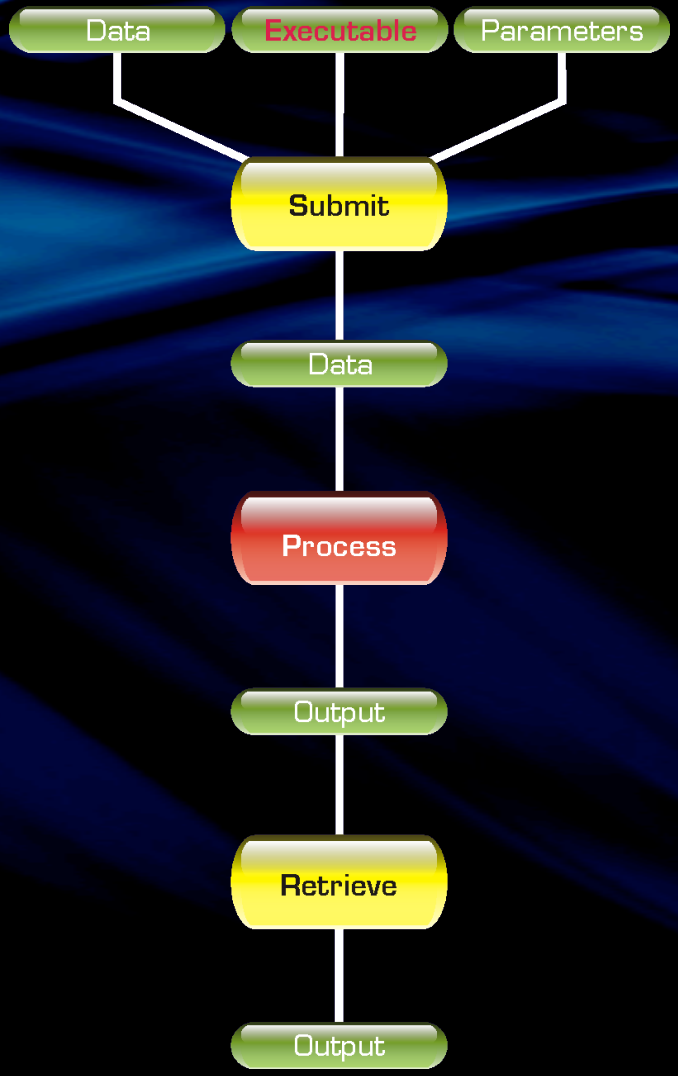
Running Applications on the GRID

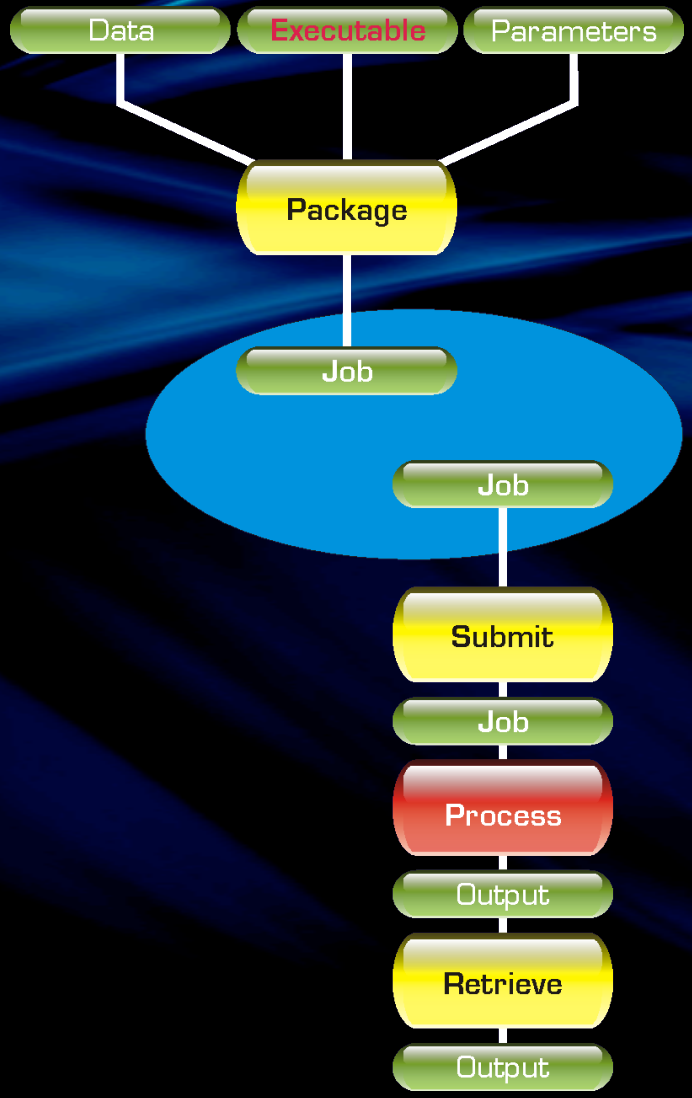


Job consisting of
- JDL
- Data
- Executable
- Program dependencies

Submission through WMS

Retrieval through WMS

Running Applications on the GRID

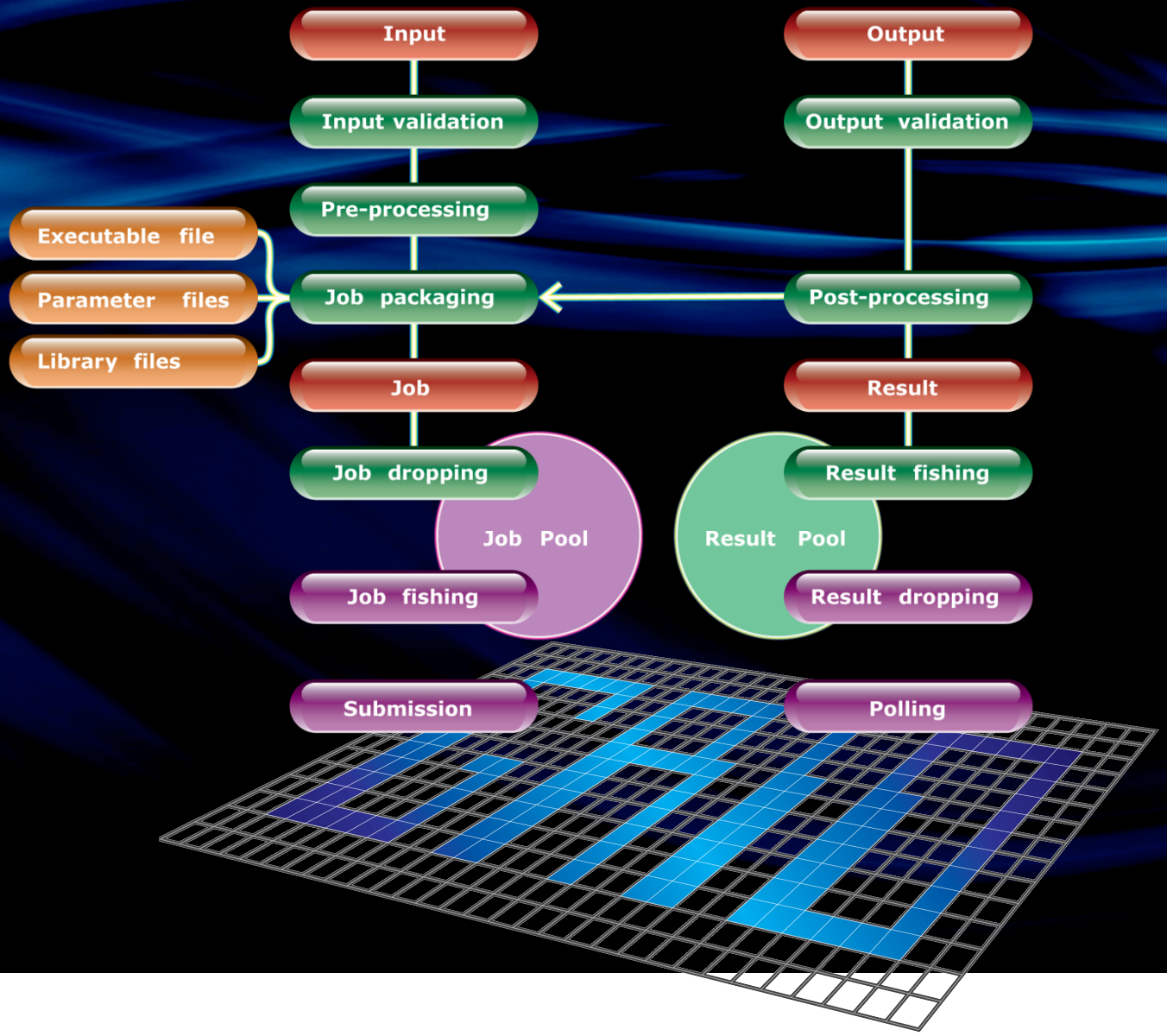


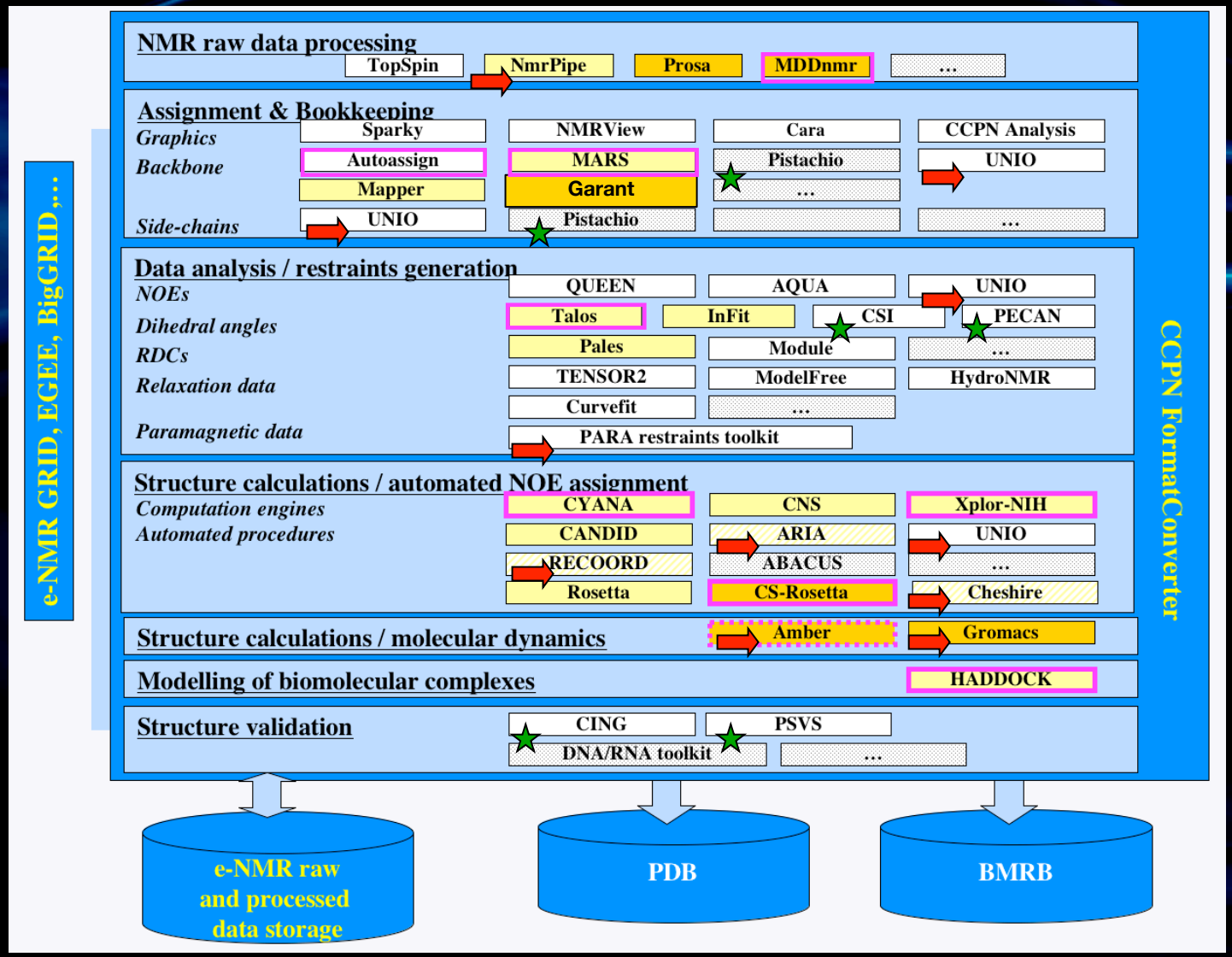
Jobs are packaged and deposited in a pool

Submission Daemon takes jobs from pool

Polling Daemon checks status for submitted jobs and retrieves data

From GRID application to Web service





In progress

GRID enabled

GRID enabled (T3.4)

web portal

Portal development

★ Existing external web portals