

METACentrum Czech National Grid Environment

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user support and application manager



- **Basic facts**
- **Infrastructure**
- **Hardware portfolio**
- **Application portfolio**
- **Additional services**
- **Summary & plans**

- **History**

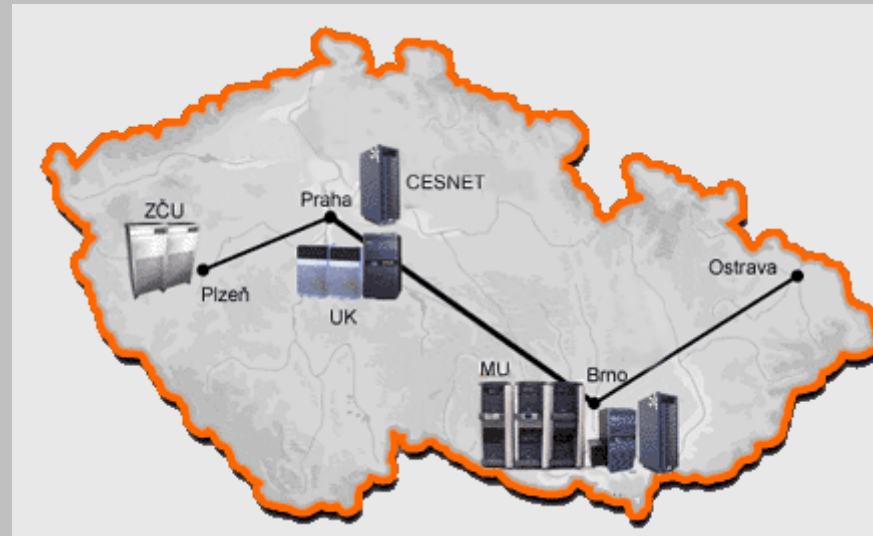
- one of the basic activities of CESNET (Czech NREN operator), started in 1996

- **Mission**

- cover majority of activities concerning Grids, super-, cluster- and grid computing and/or high performance computing
- main goal is to **provide users with an easy access to resources, hiding the complexity of the environment**
 - “Grid” (in current terminology), “Metacomputer” (cca ten years ago)
- maintain current computational resources and broaden available computational capacity

- **Structure**

- focus at development and production support of a distributed infrastructure that spans multiple independent organizations
 - nodes represent main academic supercomputing centers providing computing and storage resources
 - sites are connected with the CESNET backbone



- **Building blocks**

- unified authentication mechanism supporting single-sign on (SSO)

Kerberos

- shared disk space

AFS

- single batch queuing system

PBSPro

- user identity/accounts management system

Perun

- user support

- METAPortal
- RT system

<http://meta.cesnet.cz>

meta@cesnet.cz

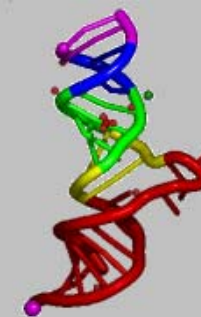
- **Computational resources**
 - clusters
 - based on various Intel Pentium CPUs cca **330 CPUs**
 - SMP machines
 - SGI and HP servers cca **100 CPUs**
 - small number of other architecture
 - IBM Power4+, AMD Opteron
 - currently about **200 active users**

- **Key application domains**
 - **computational chemistry / molecular modelling**
 - Amber, AutoDock, Gamess, Gaussian, Mopac, Spartan, Turbomole
 - **technical and material simulations**
 - ANSYS (with LS-DYNA module), Fluent, MSC.Marc, WIEN2k
 - **mathematical and statistical modelling**
 - Maple, Matlab, SNNS, gridMathematica, R, Vista
 - **development tools and environments**
 - PGI CDK, TotalView, Vampir, Paradise, SICStus Prolog

- **Studied topics**

- **computational chemistry / molecular modelling**

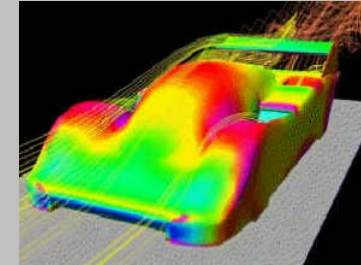
- quantum chemical calculations of biomolecules and supramolecules
- protein engineering of enzymes reactions
- Monte Carlo simulations of water radiolysis
- simulation of chemically modified DNA / RNA molecules
- physical chemistry of polymers, quantum anorganic chemistry
- study of conformational behaviour of biomolecules, bioinformatics
- simulation for ultrasound tomography
- quantum chemical calculations of NMR parameters
- study of ion behavior at phase interfaces



- **Studied topics**

- **technical and material simulations**

- thermodynamics and phase diagrams in advanced metallic materials, behaviour at extreme volume and shape deformation
- study of plasma generators
- *ab-initio* studies of alloys
- thermomechanical numerical simulations
- hydrology simulations
- numerical modelling of fluids flow
- periodical, quaziperiodical and chaotic behaviour of electrical system
- study of physical characteristic of asteroids



- **Planned application extensions**
 - planned support for following applications
 - Abinit electronic structure program for molecules and periodic solids
 - ADF Amsterdam Density Functional (ADF) package
 - CPMD Car-Parrinello molecular dynamics suite
 - Dalton quantum chemistry program
 - Linda environment for parallel execution of Gaussian

- PBSPro monitor**

PBSPro monitor (skirit-f.ics.muni.cz/PBSPro_7.0.0.51060)
 Saturday, January 14, 2006 1:39:48 PM CET
 total jobs: 276

Nodes

More detailed list from Ganglia

job busy	partially free	free	down	state unknown	total
115	21	64	3	10	213

glamdring	minos	narsil	nympha	perian	puu	skirit	skirit-f	skurut
minos1	minos2	minos3	minos4	minos5	minos6	minos7	minos8	
minos9	minos10	minos11	minos12	minos13	minos14	minos15	minos16	
nympha1	nympha2	nympha3	nympha4	nympha5	nympha6	nympha7	nympha8	
nympha9	nympha10	nympha11	nympha12	nympha13	nympha14	nympha15	nympha16	
perian1	perian4	perian5	perian6	perian7	perian8	perian9	perian10	
perian11	perian12	perian13	perian14	perian15	perian16	perian17	perian18	
perian19	perian20	perian21	perian22	perian23	perian24	perian25	perian26	
perian27	perian28	perian29	perian30	perian31	perian32	perian33	perian34	
perian35	perian36	perian37	perian38	perian39	perian40	perian41	perian42	
perian43	perian44	perian45	perian46	perian47	perian48	perian49	perian50	
perian51	perian52	perian53	perian54	perian55	perian56	perian57	perian58	
perian59	perian60	perian61	perian62	perian63	perian64	perian65	perian66	
perian67	perian68	perian69	perian70	perian71	perian72	perian73	perian74	
perian75	perian76							

- **PBSPro monitor**

PBSPro monitor (skirit-f.ics.muni.cz/PBSPro_7.0.0.51060)
 Saturday, January 14, 2006 1:33:09 PM CET
 total jobs: 276

Jobs

job	used CPU ↓	name	user	CPU time	Wall time	state	queue	time created
76155.skirit-f.ics.muni.cz	16	S007	matousek			Q - queued	cpmd	1/12/06 3:48 PM
74139.skirit-f.ics.muni.cz	12	s2_250_05.run	vrba	4572:57:20	381:13:43	R - running	parallel	12/29/05 4:18 PM
74086.skirit-f.ics.muni.cz	8	250_01.run	vrba	3066:07:50	384:02:23	R - running	parallel	12/29/05 1:29 PM
76293.skirit-f.ics.muni.cz	8	trubka.run	vadamek	22:30:59	23:18:01	R - running	normal	1/13/06 2:14 PM
76297.skirit-f.ics.muni.cz	8	trubka1.run	vadamek	22:22:02	23:14:58	R - running	normal	1/13/06 2:16 PM
72179.skirit-f.ics.muni.cz	2	QUI-kt42-k	filip	555:32:09	462:15:45	R - running	ncbr	12/19/05 1:52 PM
72944.skirit-f.ics.muni.cz	2	dbja-m348s-hal	rowan	08:44:06	516:18:05	R - running	long	12/21/05 6:15 PM
72945.skirit-f.ics.muni.cz	2	dbja_free_md6	rowan	00:00:05	507:59:29	R - running	long	12/21/05 6:16 PM
74471.skirit-f.ics.muni.cz	2	jedu	filip	172:49:17	196:06:58	R - running	ncbr	1/2/06 11:53 AM
74487.skirit-f.ics.muni.cz	2	jedu	filip	263:31:22	286:21:01	R - running	ncbr	1/2/06 3:11 PM

- **PBSPro monitor**

PBSPro monitor (skirit-f.ics.muni.cz/PBSPro_7.0.0.51060)
 Saturday, January 14, 2006 1:35:07 PM CET
 total jobs: 276

Queues

queue	Priority	time limits	required property	jobs				
				queued	running /max	completed	total	max jobs per user
preempt	110	0 - 0		0	0 /	0	0	
maintenance	99	0 - 0		0	0 /	0	0	
priority	80	0 - 720:00:00		0	0 / 16	0	0	16
gridlab	80	0 - 720:00:00	globus	0	2 / 4	0	2	4
test	80	0 - 0		0	0 / 300	0	0	300
interactive	70	0 - 04:00:00	linux	0	0 / 6	0	0	6
short	60	0 - 02:00:00	linux	0	0 / 12	1	3	8
iti	55	0 - 720:00:00	iti	0	0 / 32	0	0	32
normal	50	02:00:01 - 24:00:00	linux	0	8 / 64	2	10	32
quark	45	0 - 720:00:00	quark	0	0 / 10	0	0	10
ncbr	45	0 - 720:00:00	per	0	46 / 120	1	47	16
cpmd	45	0 - 0	onlycpmd	54	27 / 120	27	108	32
parallel	40	0 - 720:00:00	linux	14	16 / 16	0	30	16
long	40	24:00:01 - 720:00:00	long	3	71 / 96	2	76	32
default		0 - 0		0	0 /	0	0	

- **Storage services**
 - **regular backups** of /home directories on tapes
 - offer of **disc capacities** of tenths of TBs
 - based on agreement according to user's needs and our possibilities
 - authorized requests (real research needs with corresponding publication outputs) are going to be fulfilled
 - current work on starting operation of two **tape libraries**
 - each with capacity of 200 TBs of on-line accessible data
 - possible help to user communities encountering problems with their local data/storage capacity

- **Support for PKI infrastructure**

- interest in PKI support requested for interaction with Grids
- some applications support PKI better than Kerberos (email signing, web authentication)
- private key management too weak

- project „Hardware tokens for METACentrum“



- **token** – device that allows to store private keys and perform basic cryptographic operations (smart card or USB token)
- funds to equip METACentrum users with USB tokens
- adaptation current infrastructure to **support PKI and HW tokens**
- distribution to the end users

- **CHARON system – application framework**
 - **single job management**
 - encapsulation of a single computational job
 - minimization of overhead resulting from direct batch system and/or middleware usage
 - easy submission and navigation during job lifetime
 - **application programs management**
 - comfortable application software management and administration
 - current ways of utilization
 - **METACentrum** experimental utilization, best effort support
 - **EGEE / VOCE** prototype utilization, guaranteed support

- **Summary**

- METACentrum built on „Grid“ roots already in pre-Grid era
- relatively „simple“ infrastructure but suits perfectly for solving real research day-to-day problems
- provides support for broad range of application areas

- **Plans**

- integration with European-wide scale productional grid environment (EGEE/VOCE)
- further expansion of cluster resources
- extension of available application portfolio based on users requests / feedback