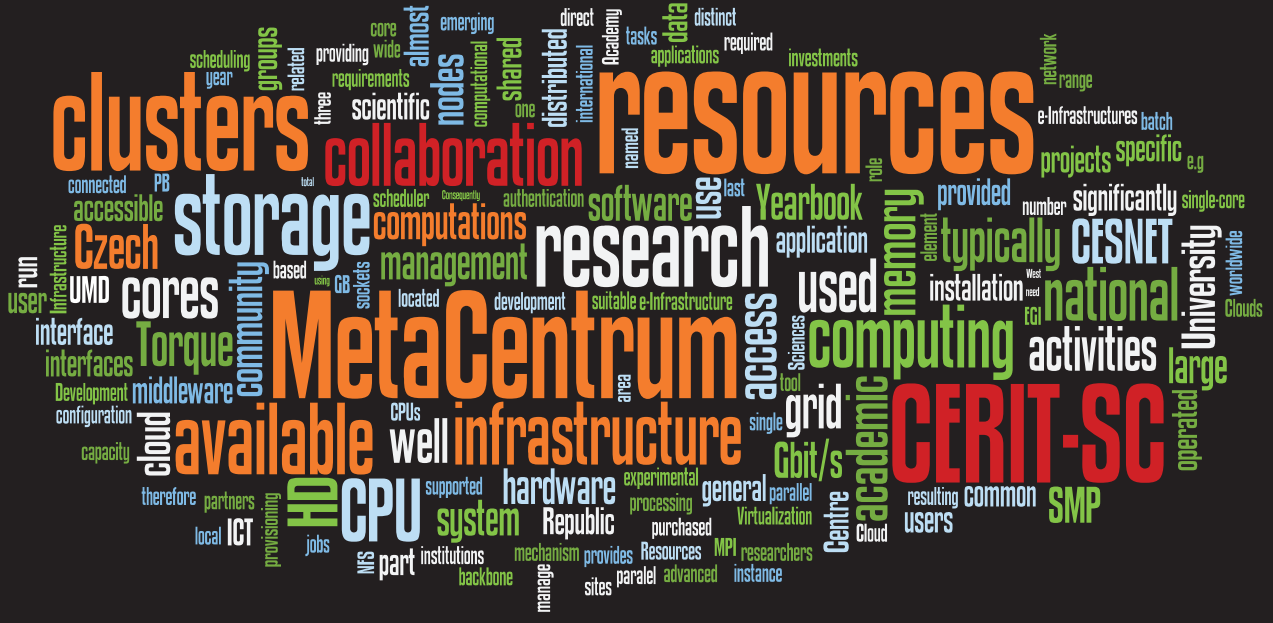
Yearbook 2011-12

National Grid Infrastructure Annual Report



MetaCentrum

cerit scientific cloud

Ivana Křenková, Tomáš Rebok, Aleš Křenek, Miroslav Ruda and Luděk Matyska (Eds.)

Yearbook 2011-12

National Grid Infrastructure Annual Report

MINISTERSTVO ŠKOLSTVÍ, MLÁDEŽE A TĚLOVÝCHOVY

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Preface

The need for advanced ICT resources has been recognised in virtually all scientific areas in the last decade, emerging into building *e-Infrastructures* for research and development worldwide. In the Czech Republic the trend is followed by significant investments into the national e-Infrastructure, as well as related changes in its organizational and funding schemes.

The foreseen Czech national e-Infrastructure is composed of three major parts, also identified as the only ICT projects of the *Roadmap for Large Research, Development and Innovation Infrastructures In the Czech Republic*[1], a strategic document approved by the national government. Those are:

CESNET provides the backbone of research and education network, system of large data storage facilities (tens of PB currently), and MetaCentrum—the national grid infrastructure (NGI). Specifically the MetaCentrum role is twofold—coordination of grid and non-commercial cloud activities at the national level as well as provisioning of non-trivial "seed" computing and storage resources for general use by the broad scientific community. Any member of the national academic community is eligible, however, the resources are available in non-exclusive, "best effort" mode. The resource provisioning is complemented with research and development activities in the area of e-Infrastructure technologies in particular.

CERIT Scientific Cloud continues the tradition of Supercomputing Centre Brno, providing resources of comparable size to MetaCentrum. However, the Centre is more focused on direct research collaboration with specific research groups. Joint research projects are run, targeted at ICT-assisted solution of specific scientific problem, as well as novel infrastructure architecture and its configuration, and resulting also in publications with both-sides authorship. The approach is also reflected in the resources operation, which run in a more experimental setup—as an experimental ICT facility—required for the collaboration, and giving higher priority to the joint research projects in general.

Centre of Excellence IT for Innovations builds computing facilities at least an order of magnitude larger than MetaCentrum and CERIT-SC, as appropriate for a supercomputing centre. As such, in a difference from resources provided by CESNET and CERIT-SC, the IT4I operation will follow the pattern of large supercomputing centres, access to resources will be assessed by a scientific committee, and once a project is approved, the allocated resources are guaranteed to the user. Hence the centre is more suitable for research project with massive needs for computing power, which are well understood in advance, rather than more experimental usage expected in CERIT-SC and MetaCentrum.

[1] `http://www.msmt.cz/vyzkum/ceska-roadmap`

All the three parts of the national e-Infrastructure signed a Memorandum of Understanding and they cooperate while approaching the scientific communities. However, due to the long history of collaboration, personal overlaps in the teams, and use of common technology, the collaboration between CERIT-SC and MetaCentrum is deeper, resulting also in this common Yearbook.

Altogether, as the e-Infrastructures mature worldwide, the focus gets shifted from the bare provision of hardware and software resources, when the users—the scientist's—stand in the role of *customers*, towards the relationship of *partners* in collaboration on definition and use of the resources for the purpose of specific research activities. This shift appears in the very mission of CERIT-SC, and it has been also driving the MetaCentrum activities since 2011, which puts significantly more human effort to user-support activities (training, custom software installation, ...). Consequently, it is also reflected in this Yearbook, which dedicates the largest part to the collaboration with the users.

Brno, January 2013

Miroslav Ruda
MetaCentrum Director

Luděk Matyska
CERIT-SC Director

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Foreword

This part of the Yearbook gives an overview of available hardware and software resources integrated into the operated infrastructure, developments in cluster operation, resulting in a significant resource utilisation increase in 2011–2012, and an overview of provided services and information resources available to the users (detailed statistics on the resources utilization is provided in Appendix A). User related activities (support, training, and dissemination), which are the other emphasis in the MetaCentrum activities in 2011–2012 are described here as well.

The MetaCentrum Infrastructure in 2011-2012

In the first part of this Yearbook, we describe the national grid infrastructure coordinated by CESNET (operated by its activity MetaCentrum), which is available for Czech academic community and researchers, and which is constituted by resources provided by various computing centers throughout the Czech Republic. The infrastructure, which is further integrated with the pan-European grid infrastructure of EGI project, comprises of a wide range of resources—computational and storage capacities, application programs, etc.—and services, providing its users with an environment for collaboration in the area of computations and data processing/management.

1 Hardware and Software Resources

The entire computing capacity, related storage space, and a wide range of application software and utilities are available to the students, academic workers and other researchers of the universities, Academy of Sciences institutes and other research organisations.

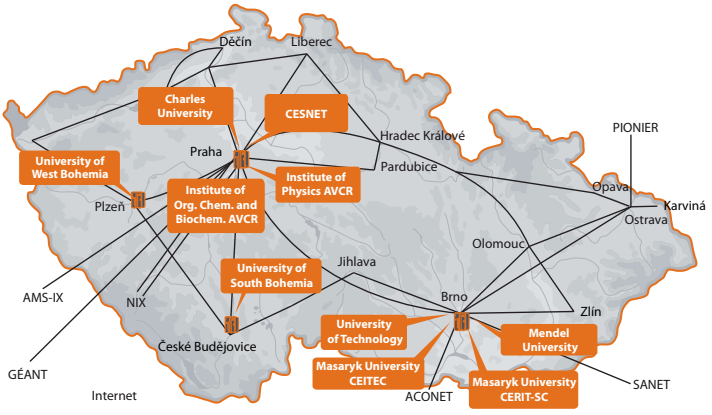

Fig. 1. MetaCentrum Resource Providers and Sites

The hardware resources consist of a combination of CESNET resources and computing systems provided by partners, notably CERIT-SC Centre[1] at the Masaryk University (transformed Supercomputing Centre Brno), Charles University in Prague, Bohemian University in České Budějovice, University of West

[1] `http://www.cerit-sc.cz/`

Bohemia in Pilsen, Institute of Physics AS CR in Prague, and other resources of local user groups from academic institutions. At the end of 2012, MetaCentrum and CERIT-SC manage 23 clusters, owned by 9 distinct academic institutions in 9 sites in 4 cities (Fig. 1). The total capacity is over 6000 CPU cores and almost 1 PB of online storage accessible through Torque and NFS (Sect. 1.1) and 2 sites with more than 4000 CPU cores and almost 2 PB storage accessible through UMD middleware.

To make the management of such distributed resources more convenient, a distributed configuration management tool named *Puppet*[2] has been employed during last year to automate the administrative tasks and basic software installations on the infrastructure nodes. On the other hand, to manage the user identities, accounts, as well as hardware overview of the operated infrastructure, we have developed our own management tool named *Perun*, which has been revised and significantly improved during 2011-2012 (see more details in the paper *Perun* in the following part (section "Identity Management, Operation and Tools Development") of this Yearbook).

1.1 Interfaces to resources

Due to divergent needs of different user groups, three distinct interfaces to the hardware resources are currently available:

Torque batch system and NFS. MetaCentrum used the PBS batch system, predecessor of Torque, since the introduction of x86 based clusters in 2000. Mostly because of the ease of use this is still the primary access interface to the computing resources. MetaCentrum runs one "catch-all" instance of Torque serving most of the clusters, CERIT-SC provides another one on its clusters (while both the instances have operated independently so far, our goal for 2013 is to ensure an interoperability between both of them so that it won't be required to explicitly specify the scheduling server for submitted jobs—the jobs will be automatically exchanged between the servers based on their resource requirements and resources available). Similarly, shared storage resources are available as NFSv4 filesystems. Kerberos is used as the common authentication mechanism.

UMD middleware. Resources available to the international community are accessible with EGI-compliant interfaces, provided by UMD middleware components, specifically the ex-gLite ones, e.g. CREAM computing element, WMS metascheduler, and DPM storage element. X.509 certificates and virtual organization management by VOMS are used as the authentication and authorization mechanism.

Cloud interfaces. The emerging cloud paradigm installation is available for early adopters[3]. The resources are managed by a single OpenNebula instance to access the Dukan (MetaCentrum) and part of Zegox (CERIT-SC) clusters.

[2] `https://puppetlabs.com`

[3] `http://meta.cesnet.cz/wiki/Kategorie:Clouds`

The EGI *FedCloud* testbed[4] is also supported by this installation. Further details about the cloud interface are described in the paper *HPC Clouds* located in the Part II. (section "Clouds and Scheduling Development") of this Yearbook.

1.2 Computational clusters

The computational resources are clusters of nodes (computers) of two main classes:

High density (HD) have up to 2 CPU sockets, hence 4–24 CPU cores only, and 8–128 GB memory (mostly depending on the year of purchase). In the same generation, cores of HD cluster are faster than SMP ones typically, and they are purchased for much lower price per core. The clusters are suitable for single-core or limited-parallelism computations (or those leveraging explicit distributed computing model eventually), and high-throughput computations (i.e. large collections of single-core tasks). Virtualization of HD clusters imposes negligible overhead therefore they are suitable for the cloud or the advanced features of job scheduling (see the paper *Virtualization & Magrathea* located in the Part II., section "Clouds and Scheduling Development").

Symmetric MultiProcessing (SMP) have 4–8 CPU sockets, hence upto 80 CPU cores in shared memory (at least 256 GB). A single CPU core in the SMP system is typically slower than in HD, however, fine grain parallelism using access to the shared memory can be leveraged. The machines also can host computations with enormous requirements on memory (regardless the number of cores used). Due to non-uniform speed of access to memory, performance penalty would be high therefore virtualization is not used in general.

All clusters purchased recently are connected with the InfiniBand network (40 Gbit/s with very low latency). IB is used to run MPI applications as well as to access local disk storage typically. HD nodes are connected with 1 Gbit/s Ethernet typically, having 10 Gbit/s uplink to the CESNET backbone. SMP nodes have direct 10 Gbit/s interface typically.

Some of the HD clusters also provide GP-GPU accelerators for specific applications (e.g. image processing, molecular dynamics, ...), whose highly parallel structure makes them significantly more effective than general-purpose CPUs for algorithms where processing of large blocks of data can be done in parallel.

In 2011 and 2012 the number of CPUs almost tripled w. r. t. the preceding period. The rapid grow is due to the large investments supported by the CESNET's eIGeR and MU's CERIT-SC projects in the Research and Development for Innovations Operational Programm[5]. In these years the following clusters were purchased:

[4] `https://wiki.egi.eu/wiki/Fedcloud-tf:Testbed`
[5] `http://www.msmt.cz/european-union/erdf`

- **Zewura:** CERIT-SC, 1600 cores, 12/2011. This is the first SMP cluster with Intel Xeon E7-2860 CPUs (80 cores per node).
- **Dukan:** CESNET, 240 cores, 2/2012, Intel Xeon E5649. The cluster is dedicated to the OpenNebula cloud (Sect. 1.1).
- **Mandos:** CESNET, 896 cores, 3/2012. SMP cluster with AMD Opteron 6274 CPUs. In addition to node-local "scratch" disks also significantly faster shared scratch (27 TB) filesystem is available.
- **Minos:** CESNET, 600 cores, 3/2012, Intel Xeon E5645.
- **Zegox:** CERIT-SC, 576 cores, 7/2012. Intel Xeon E5-2620 CPUs. All nodes of the cluster are included in the OpenNebula cloud, thus being available to run user images of operating system when required. Complementarily, the nodes of the cluster which are not utilized by the cloud users run "CERIT-SC standard" OS image which is a worker node of the Torque batch system. Hence the nodes become available in the batch system transparently.
- **Gram:** CESNET, 160 cores, 12/2012, Intel Xeon E5-2670. This cluster consists of 10 nodes, each of which having 4 nVidia Tesla M2090 6GB GPU processing units.
- **Hildor:** CESNET, 416 cores, 12/2012, Intel Xeon E5-2665.
- **Ramdal:** CESNET, 32 cores, 12/2012, Intel Xeon E5-4650. This is a specific single node providing powerful CPUs and large (1 TB) RAM for memory-demanding computations.

Figure 2 shows the number of CPU cores in MetaCentrum during the past years. Up-to-date number of machines, CPUs and their utilisation is displayed on the MetaCentrum portal[6].

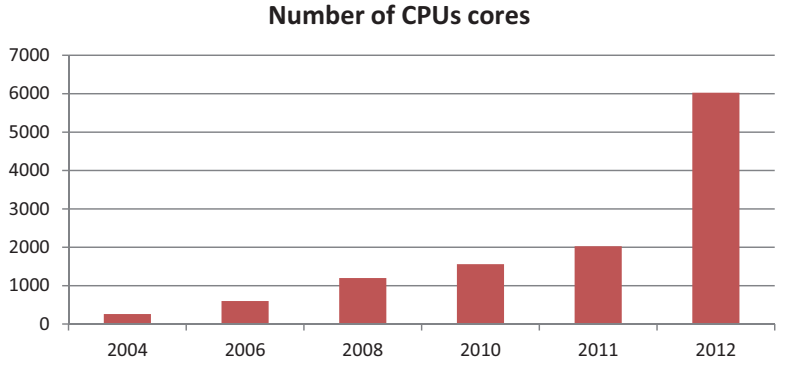

Fig. 2. Numbers of CPU cores operated by MetaCentrum in recent years

[6] `http://metavo.metacentrum.cz/`

Name	nodes x cores	description	memory per node	owner
Ajax	1x8	SGI Altix 350	72 GB	ZČU
Alela	8x12	PC Cluster	8 to 32 GB	VUT
Dukan	10 x16	PC Cluster Xeon	96 GB	CESNET
Elixir	1x48	PC Cluster AMD	512 GB	CESNET
Eru	2x32	Cluster SUN	132 to 256 GB	CESNET
Gram	2x8	PC Cluster Xeon	64 GB	CESNET
Hermes	12x8	PC Cluster Xeon	16 GB	JČU
Hildor	16x16	PC Cluster Xeon	64 GB	CESNET
Konos	11x12	PC Cluster AMD GPU	24 GB	KMA/ZČU
Kudu	1x8	Intel Xeon GPU node	48 GB	CERIT-SC
Losgar	2x48	Cluster AMD	64 GB	LL/MU
Loslab	14x12	PC Cluster Intel	12 GB	LL/MU
Luna	5x32	PC Cluster AMD	4 to 256 GB	FZU AV
Manwe	7x16	Cluster SUN X4600	32 to 128 GB	MU, CESNET
Mandos	14x64	Cluster AMD (SMP)	256 GB	CESNET
Minos	50x12	PC Cluster Intel	24 GB	CESNET
Nympha	20x8	PC Cluster HP	16 GB	CESNET
Orca	18x4	PC Cluster AMD	8 GB	NCBR/MU
Perian	40x8+16x12	PC Cluster Xeon	8 to 48 GB	NCBR/MU
Quark	16x4	PC Cluster Xeon	2 to 18 GB	MU
Ramdal	1x32	Intel Xeon node	1 TB	CESNET
Skirit	31x4	PC Cluster Xeon	4 GB	CESNET
Tarkil	24x8	PC Cluster SGI Altix	24 GB	CESNET
Zegox	48x12	PC Cluster Intel	90 GB	CERIT-SC
Zewura	20x80	Cluster Intel Xeon (SMP)	512 GB	CERIT-SC

Table 1. Currently available clusters and machines (the ones purchased in 2011-2012 are denoted in bold)

Major owners are CERIT-SC and CESNET (approx. 80 % CPU cores together), the remaining resources are owned by other institutions, however, management of the clusters is done by MetaCentrum. Details are shown in Tab. 1.2.

Figure 3 shows utilization of all clusters (with the exception of those included in the experimental cloud environment, i.e. Dukan and some nodes of Zegox). Utilization above 60% is considered as optimal; on the other hand utilization higher as 90% means that cluster is fully saturated and users have to wait long time before their jobs are executed. The main part of clusters are in the range 60% to 90%, thus they are in the optimal range. In general, the demand on newer (hence faster) CPUs is higher, yielding higher utilization as well. On the other hand, scheduling many-cores or huge-memory computations is more difficult (machines must be drained off smaller computations first), therefore utilization of SMP clusters is slightly lower.

Clusters with lower utilization (e.g. Loslab, Quark, and Orca) run in a restricted mode with significant capacity dedicated to their owners, therefore the total utilization is lower. On the contrary, Perian is owned by the group (NCBR) which generates the largest fraction of the whole MetaCentrum load, therefore it is well utilized too. Moreover, the jobs run there are specifically crafted to match number of CPU cores per node and available memory, hence using the resources optimally.

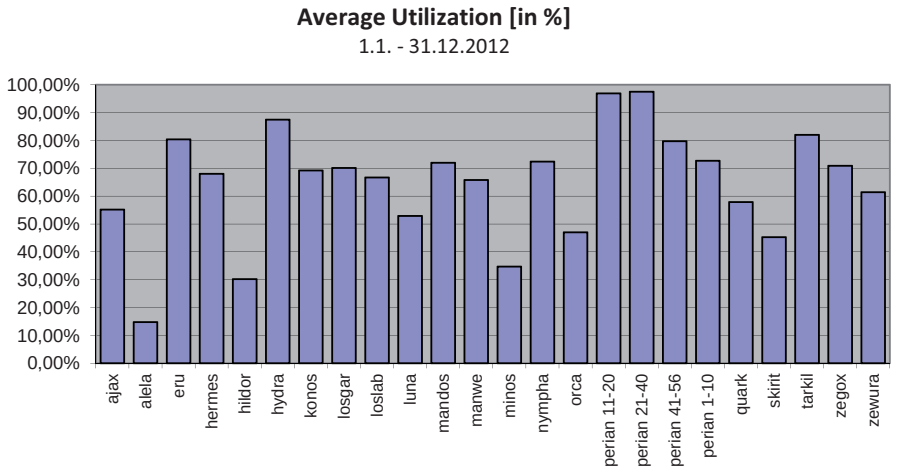

Fig. 3. Average utilization of MetaCentrum clusters

By the end of 2012, MetaCentrum registers 613 active users. Out of this number 301 accounts were extended and we gained 312 new users in 2012.

In 2012, the users and their jobs utilized 22 millions CPU hours (58 thousands CPU years) via Torque. Comparing to 2011, both the number of CPU cores and the total CPU time increase by approximately the same factor of three. This is a strong confirmation that the massive investments to the infrastructure are appropriate because there is a matching user demand. At the same time, the MetaCentrum services and organization were clearly able to handle this growth.

Beside the above mentioned resources available at the national level in MetaCentrum via Torque batch system, there are additional resources available to the international community accessible with EGI-compliant interfaces. Czech Republic provides almost 4000 CPU through two centres – 80 CPU in CESNET and rest in Institute of Physics ASCR. These resources are used by international VOs registered in EGI. We support two international VOs managed by MetaCentrum (auger and voce) and number of other VOs cooperated with users from the Czech Republic (belle, supernemo, euasia, alice, voce,...). Users from all these VOs used almost 40 million CPU hours in 6 million jobs. The proportion of computed CPU time in the largest VOs shows Fig. 4.

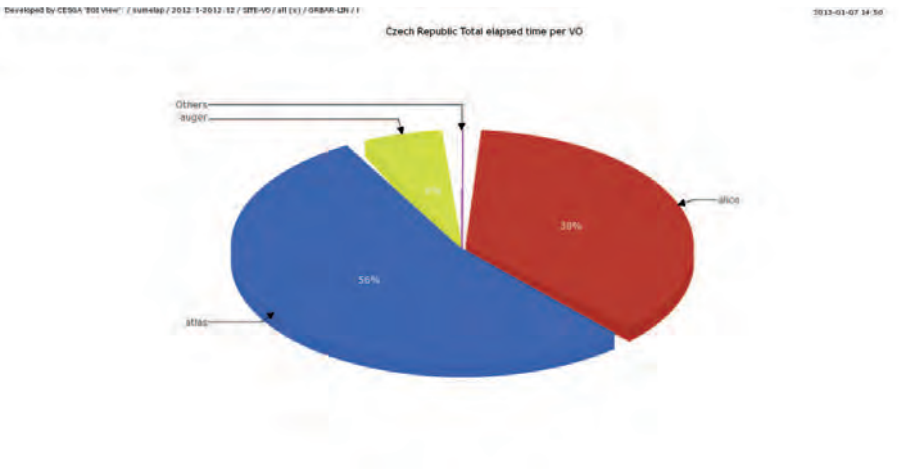

Fig. 4. Total elapsed time per VO in the Czech Republic.

1.3 Data Storage

During the recent years, we decided to review the way of providing storage resources for temporary and semi-permanent data to the users of our infrastructure, including an integration of relevant storage services provided by the operated e-Infrastructure.

In terms of semi-permanent data storages (the main storages for storing user data), the goal we agreed on was to abandon from the previous idea of computing clusters providing their own local storages (i.e., "storage per cluster"), and to make these storage resources more global, i.e. centralized and shared by multiple clusters within a specific location (the clusters "close" to the particular storage). Thus, after a successfull pilot deployment of the first centralized 100 TB storage server (located in Brno), which was made available via the NFSv4 protocol, we continued with these efforts in the late of 2011—in December, two additional storage servers were purchased by CESNET (each with the storage capacity of 100 TB)—as well as in 2012, when three other storage servers (two in Brno and one in Pilsen) were purchased by both CESNET and CERIT-SC. Thus, the total storage capacity of ca 600 TB became available to the users (currently, roughly 350 TB is occupied by user data). However, it is necessary to point out, that besides the space for user data, these storages further provide storage capacities for overheads and services needed for proper management of the clusters and the virtualized cloud environment (including development and application software).

The temporary data storages—also known as "scratches"—which are used to store the temporary data of running jobs, were (till the end of 2011) just the storages locally present within each node of a cluster (thus providing the fastest data storage for storing running jobs' data available within the infrastructure). However, this approach results in several drawbacks: first, these storages provide rather limited capacity (up to 1TB), which makes some jobs impossible to make

use of them. Second, because of not being shared by nodes of (at least) a cluster, some jobs requiring a shared high-performance data storage are unable to use them as well. To cope with these limitations, we introduced a first shared scratch (located in Brno) with the capacity of 27 TB, which is available from all the nodes of the *mandos* cluster. The scratch is available via Infiniband interconnection from the cluster nodes, thus aiming to provide as high performance as possible.

Storage	Capacity	Location	Owner
`/storage/brno1`	100 TB	Botanická 68a, Brno	CESNET
`/storage/brno2`	120 TB	Botanická 68a, Brno	CESNET
`/storage/brno3-cerit`	260 TB	Botanická 68a, Brno	CERIT-SC
`/storage/plzen1`	80 TB	Univerzitní 20, Pilsen	CESNET

Table 2. Currently available storage volumes

CERIT-SC and CESNET also operates a high-capacity data storage (Hierarchical Storage Management, HSM) directly connected to the grid and cloud computing infrastructure at the national and international levels, which serve as guaranteed data depots for storing and sharing semipermanent and permanent scientific data, results of computer simulations, or data provided directly from experiments and measurements (sensors). To provide our users with a high-capacity data storage dedicated for storing permanent data as well as archival purposes, we plan to integrate a dedicated part of the HSM data storage located in Pilsen into the operated grid infrastructure during 2013, thus allowing the users to directly access and conveniently use it without any needs for additional registrations or complex access methods.

1.4 Application Programs

In order to make the usage of the provided infrastructure more convenient for the users, it is necessary to provide them with a pre-configured and ready-to-use software portfolio they can use for their scientific computations. The MetaCentrum's software portfolio covers a wide range of application programs (around 160 distinct application programs—including the commercial as well as free ones—are currently provided to the users), which could be roughly divided into the following research areas (we present just the selected ones—the comprehensive and up-to-date list of all the available applications is available on the MetaCentrum wiki[7]):

[7] `http://meta.cesnet.cz/wiki/Kategorie:Aplikace`

– *Mathematical and Statistical Modelling software*—e.g., Matlab, Maple, gridMathematica, R, etc.
– *Computational Chemistry & Molecular Modelling software*—e.g., Amber, Gaussian/GaussView, Gromacs, MolPro, etc.
– *Structural Biology and Bioinformatics*—e.g., QUEEN, MrBayes, CS-Rosetta, etc.
– *Technical and Material Simulations*—e.g., Ansys CFD (Fluent + CFX), Open Foam, etc.
– *Development Tools and Environments*—e.g., Intel CDK, PGI CDK, TotalView, Allinea DDT, Vampir, Numpy, Scipy, etc.

It is necessary to point out, that the provided software portfolio continuously extends in time—we are continuously looking for software proposals from our users/partners, in order to reasonably extend the portfolio by both free/open-source as well as commercial applications. To illustrate these efforts during 2011-2012, during which period the MetaCentrum became more active in providing commercial applications to the scientific community, let us present a selected set of purchased/upgraded commercial as well as free/open-source applications, which have been installed into the infrastructure, and which are ready to be used by the users.

Last, but not least, it should be mentioned that the commercial applications are purchased either directly by the MetaCentrum itself (via its research projects), or in cooperation with the integrated HW centres (e.g., the CERIT-SC Centre).

Commercial Applications
Regarding the commercial applications, the software portfolio of the provided infrastructure has been extended by the following set of applications during 2011-2012:

– **Gaussian/Gaussview** – a package of programs based on basics of quantum mechanics—it serves to predict energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types.
  • the newest Gaussian revision C.01 was purchased
– **Matlab** – integrated system comprising of tools for symbolic and numeric computations, analyses and data visualizations, modeling and simulations of real processes, etc.
  • continuous upgrades—version 7.12, 7.13, 7.14, and 8.0
  • the number of core Matlab licences increased by 100 (current status: 350 core licences)
  • several new toolboxes were purchased or were increased in terms of available number of licences:
    Matlab Compiler – 5 lic. purchased (7 lic. available in total)
    Matlab Coder – 5 lic. purchased (7 lic. in total)
    Java Builder – 5 lic. purchased

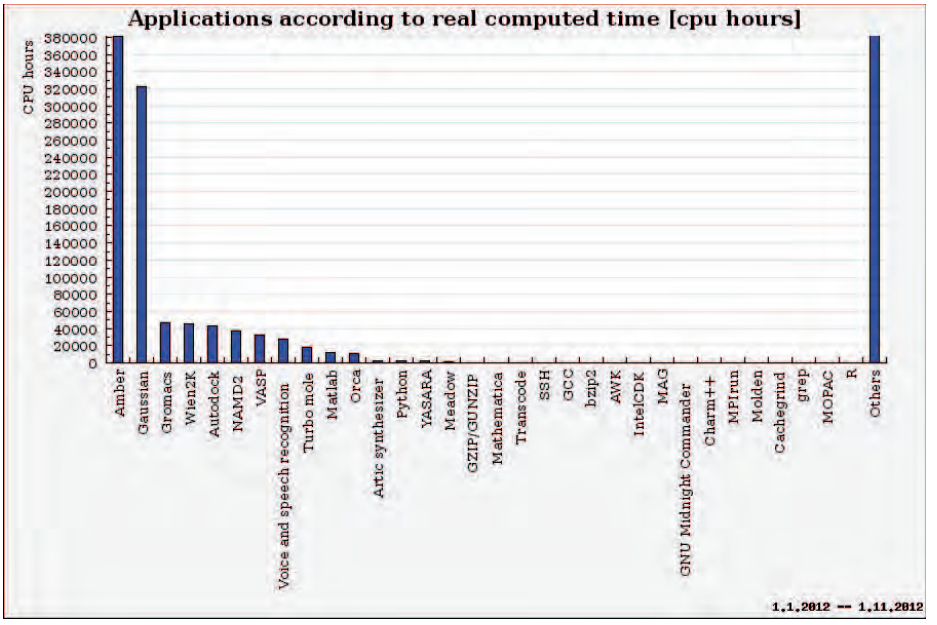

Fig. 5. An illustration of the most frequently used applications (year 2012).

Bioinformatics Toolbox – 10 lic. purchased
Database Toolbox – 5 lic. purchased (9 lic. in total)
Parallel Computing Toolbox – 10 lic. purchased (15 lic. in total)
Distributed Computing Engine – 128 lic. purchased by CERIT-SC (160 lic. in total)

- **Maple** – an environment for sympolic computations, solving scientific and engeneering problems, mathematic research, and/or data visualizations
  - the Maple version 15 was purchased in the number of 30 licences
  - later upgraded to version 16
- **gridMathematica** – integrated extension system for increasing the power of Mathematica licenses (network-enabled Mathematica computation kernels for running distributed parallel computations over multiple CPUs)
  - 15 licenses of gridMathematica version 8 purchased for the academic owners of the Mathematica SW (thus allowing to use up to 240 CPUs for Mathematica computations)
- **Ansys CFD (Fluent + CFX)** and **Ansys HPC** – a comprehensive suite of computational fluid dynamics software for modeling fluid flow and other related physical phenomena; the Ansys HPC further enables parallel processing for solution of the toughest, higher-fidelity models
  - the Ansys CFD version 14.5 purchased in the number of 25 licences
  - the Ansys HPC purchased in the number of 60 licences (thus allowing to run parallel computations using up to 60 additional cores)

– **Intel Composer XE** and **PGI Accelerator CDK** – tools for development of parallel as well as serial programs programmed in various programming languages (includes compilers, support libraries, and further tools)
  - the Intel Composer XE version 12 purchased in the number of 2 licences
  - the licences for Intel C/C++ compilers further increased by 2 (by the purchase of *Intel C++ Composer XE*)
  - the PGI Accelerator CDK version 12.4 purchased by CERIT-SC in the number of 2 licences
– **TotalView** and **Allinea DDT** debuggers – debugging tools providing an interactive graphical user interfaces for debugging both single-threaded and parallel/distributed applications
  - 64 licences of TotalView version 8.10 purchased (allowing to debug up to 64 simultaneous processes), including the CUDA debugging support
  - 32 licences of Allinea DDT version 3.2 purchased (allowing to debug up to 32 simultaneous processes)

Free/Open-source Applications
The major part of the provided software portfolio is represented by free/open source applications. The proposals, which applications to install/upgrade, are continuously provided by our users—the applications are either installed by us or prepared by the users themselves (see the following subsection for details).

During 2011-2012, roughly 130 distinct free/open-source applications were installed or upgraded (ca 40 in 2011, ca 90 in 2012); the upgrades comprise both from version upgrades as well as from upgrades targeting to improve the applications' performance (e.g., linking with powerful Intel MKL libraries in the case of Numpy/Scipy). Let us present a list of selected installed/upgraded ones in the following table:

abyss	espresso	namd
amber	freesurfer	novoalign
amos	fsl	numpy
artemis	gamess	NWChem
autodock	garli	oases
beast	gromacs	openfst
BLUPF90	idv	phylobayes
bowtie	lucida	phyml
bwa	metabase	picard
clustal	migrate	R
cmaq	mira	ray
cufflinks	mono	repeatmasker
dataanalysis	mosaik	samtools
dmu	moses	scientificpython
edena	mrbayes	scilab
elk	mummer	scipy
emboss	muscle	sklearn

SOAPdenovo	tophat	wgs
spades	trinity	wien2k
srilm	unafold	wrf
structure	vce	
survivalkit	velvet	
tnt	vina	

Additional Efforts
As briefly mentioned in the previous subsection, we have started to support the users' installations of application programs into the infrastructure's software portfolio—the goal is to let the users prepare (set-up, compile, etc.) the applications on their own, i.e., to allow them to tune (even continuously) the applications based on their needs. From the users point of view, such a (tuned) application becomes easily available for all the users (i.e., for the whole user group they collaborate with), which is the key benefit against compiling such applications in users' home directories.

Moreover, during 2012 we started to perform significant improvements in the applications' documentation (available on the MetaCentrum wiki[8]), aiming to provide the users with all the necessary information regarding the particular applications—except the base information their step-by-step batch/interactive use within the provided infrastructure, parallel/distributed computation possibilities, licence policies, etc.

2 User Support, Training, and Dissemination

The user support, provided by MetaCentrum, encompasses wide range of related tasks, whose common point is to make users informed and able to use the provided infrastructure. Based on this idea, the MetaCentrum activities related to users could be divided into *direct user support* (i.e., training the existing/new users, making them informed about both the current state as well as news of the centre, addressing their computational problems, providing evaluated feedback to the operation activities, maintaining the MetaCentrum web pages and infrastructure documentation, etc.), *collaboration support* (i.e., starting and maintaining collaborations with involved user communities, writing colaborative scientific papers, etc.), as well as *dissemination activities* (i.e., presentations on seminars or workshops, meetings with prospective new users or user groups, etc.).

Since the collaboration support is addressed in detail in the following part of this Yearbook, this section focuses mainly on the dissemination and newly provided training activites.

2.1 Dissemination activites

In 2011, our dissemination activities focused mainly on mass user forums (i.e., events for general audience), where the MetaCentrum activities as well as our research results were presented:

[8] `http://meta.cesnet.cz/wiki/Kategorie:Aplikace`

- *April, 11th-14th:* **EGI User Forum 2011**, held in Vilnius, Lithuania. The EGI User Forum aims to help all members of the EGI community, from end-users to application developers, operations staff and technology providers, to share their knowledge and build collaborations. The programme also included numerous networking and social events and opportunities to "meet the experts".
- *September, 19th-23th:* **EGI Technical Forum 2011**, held in Lyon, France. The EGI TF is a major event within the EGI community (EGI InSPIRE project). It brings together European distributed computing projects and their collaborators in academia and businesses, from around Europe and around the world. The major theme of the meeting, achieved through technical sessions, a demonstration and exhibition area, networking space and events, is to establish collaborations between the new and the current European Distributed Computing Infrastructure projects to meet the needs and requirements of the research community. The European Grid Infrastructure today supports thousands of researchers and scientists around the world, helping them to meet their daily e-science challenges
- *November, 7th:* one day's **Grid Computing Seminar 2011**, held in Brno. The seminar was devoted to an overview of the Czech national grid environment coordinated by MetaCentrum, describing its current status and implementation of new services in particular. The main goal of the meeting, which was attended by roughly sixty experts, was to inform current and potential users of high-performance/high-throughput computing about the possibilities available for solving research problems at national as well as international level.
  The seminar included a keynote lecture covering current and future CPU architecture, GPU architecture, power saving mechanisms explanations and benefits (new ways of GPU deployment in HPC environment—*Open CL*—were also addressed). The keynote was given by Andre Heidekrueger from AMD, which co-organised the event.

During 2012, besides the mass events (EGI Technical and Community forums), we decided to further address new users at smaller, local events—we presented the MetaCentrum and CERIT-SC services and/or research results on various workshops/seminars/user meetings, trying to address promising users and user groups interested in high-performance computing. Since the comprehensive list of all the presentations given is out of the scope of this Yearbook, we present just the selected ones (many presentations were further given to the grid development communities at various international and national conferences):

- *February, 10th:* Mathematica/gridMathematica Users Workshop: Institute of Chemical Technology, Prague
- *March, 8th:* Institute of Animal Science, Praha-Uhříněves
- *March, 13th:* Matlab and Simulink workshop: Model-based Design, Humusoft Company, Prague
- *March, 26th-30th:* EGI Community Forum 2012, Garching near Munich, Germany

- *April, 2nd:* Institute of Experimental Botany, Academy of Sciences of the Czech Republic, Olomouc
- *April, 2nd:* Institute of Biophysics, Academy of Sciences of the Czech Republic, Brno
- *April, 5th:* PRACE and IT4Innovations Workshop: HPC Users Access, Ostrava
- *April, 13th:* Matlab Users Workshop: Faculty of Mechanical Engineering, Brno University of Technology
- *September, 17th-21st:* EGI Technical Forum 2012, Prague, Czech Republic
- *November, 11th:* PRACE and IT4Innovations Workshop: HPC Users Access, Ostrava
- *November, 28th:* Ceremonial opening of the Institute of Molecular and Translational Medicine and the New Facilities of the Faculty of Medicine and Dentistry, Palacký University in Olomouc – informal meeting with prospective users/partners
- *December, 6th:* Workshop with Industrial Partners: Faculty of Informatics, Masaryk University, Brno
- *December, 14th:* Meeting with CEZ Group Partner: Institute of Computer Science, Masaryk University, Brno

One might notice, that the EGI Technical Forum 2012 was held in Prague—the event was organized by the Cesnet/MetaCentrum NGI together with the Czech Academy of Sciences, that represents the Czech Republic in the EGI Council. The forum provided an opportunity for the EGI community to showcase its achievements and common issues through several talks, workshops, tutorials, posters, and sessions. The exhibition area further featured a range of supporting posters, demonstrations, and booths available to projects, academic institutions as well as business companies.

2.2 User-training activites

Since the MetaCentrum services are continuously developed (the current ones are changed/updated, the new ones are installed), the efficient use of the MetaCentrum infrastructure may change in time. However, even though these updates are distributed among the users, we have noticed that these are usually not sufficiently reflected by the users that are used to use the infrastructure in a time-proven way. To distribute such a knowledge among the users (current as well as new ones) more efficiently, we have decided during 2012 to organize hand-on training seminars—during a 4-hours seminar, a selected group of users is informed about infrastructure updates/news, as well as practically trained to be able to use the MetaCentrum services in an efficient way (focusing on their common activities). After the seminar, the users are asked to provide us with an anonymous feedback, which is (together with the feedback provided during the seminar) further discussed and reflected by us in order to make the provided infrastructure more user-friendly.

In 2012, there were seven hands-on seminars organized:

- *April, 11th:* Masaryk University in Brno (RECETOX, Institute of Scientific Instruments and Institute of Biophysics of the ASCR)
- *June, 7th:* University of South Bohemia in České Budějovice
- *June, 15th:* University of South Bohemia in České Budějovice
- *November, 14th:* Institute of Experimental Botany, Academy of Sciences of the Czech Republic, Olomouc
- *November, 15th:* Institute of Experimental Botany, Academy of Sciences of the Czech Republic, Olomouc
- *December, 7th:* Centre for Structural Biology, Central-European Technology Institute, Masaryk University, Brno
- *December, 13th:* Institute of Biostatistics and Analyses at the Faculty of Medicine, Masaryk University, Brno

The seminars are intended for small-groups of participants (up to 10 participants within each group), since the goal is to make the seminar as interactive as possible (including online practical examples). Thus, the mentioned seminars covered "just" roughly 50 users in 2012. Since the collected feedback was highly positive (indicating both very high interest within the users, as well as positive in terms of provided information), we suppose to cover much higher number of users in the future—during 2013, we plan to announce and organize such seminars in all the important cities within the Czech Republic.

Fig. 6. MetaCentrum Hands-on Seminar at Institute of Experimental Botany, Academy of Sciences of the Czech Republic, Olomouc.

3 Operation, Tools and Security

In this section, we present some operational information about the maintained infrastructure. First, we present a list of new services which the infrastructure was enriched with during 2011-2012; later, the current state of the Request Tracking system (RT) as well as operational security services are presented. At the end of this section, the organized user training courses, workshops, and disseminations activities are discussed.

3.1 Integration of CERIT-SC

Before integration of CERIT-SC the Metacentrum resources were managed in very homogeneous way. Even the resources owned by 3rd parties are managed, apart of hardware maintenance, by the single Metacentrum team, using the same operating system image, management tools, batch system etc. Similarly, policies of resource access are homogeneous as well, with the possible exceptions of prioritized access of the resource owners (however, implemented using homogeneous methods again).

On the contrary, CERIT-SC is a centre of competitive size, and we take the opportunity to implement the integration in a way as seamless as possible for the users, however, allowing the centre to implement policies on its own.

First, the set of users is the same. After passing the registration process in Metacentrum, the user becomes a user of CERIT-SC automatically. The primary authentication mechanism, Kerberos, is shared as well.

Access to computing resources is handled by a separate instance of Torque batch system, its versions are synchronized with Metacentrum. Hence the users use the same tools (both command-line and web) but they interact with another server. This approach keeps the user barrier minimal while allowing different policies to be implemented. Unlike default Metacentrum Torque with *short, normal,* and *long* job queues with predefined limits on job duration, there is a single queue in CERIT-SC Torque, but the users are requested to provide an explicit estimation of job duration. Internally, the jobs are reassigned to several queues in order to keep rather complex balance among resource allocation, job slowdown etc. Altogether, the model is more flexible, it allows resource allocations for prioritized experiment with less impact on the other users, and it is believed to be more fair and more predictable.

The data storage, including foreseen aceess to the CERIT-SC HSM, appears homogeneously to the users, as filesystems in the `/storage` tree mounted on all Metacentrum machines over NFSv4, using Kerberos to authenticate. On the other hand, the filesystems *are not* backed up regularly to external storage. Instead, data are protected against hardware failure by internal redundancy of the disk arrays, and against accidental removal by daily snaphosts. Technically, there are also several performance-boosting shortcuts between the filesystems and CERIT-SC clusters – using InfiniBand, bypassing Kerberos where it is not a security problem, and mounting via native GPFS to SMP clusters.

3.2 RT and RT/GGUS Interface

RT Status

Metacentrum continues to maintain the RT request tracking system[9] to interact with the users and solve their problems. In the year 2012 we have been still maintaining the 3.7 branch of the RT by Bestpractical together with all our modifications and enhancements including the RT/GGUS interface. Among the last modifications and improvements we have namely redefined the semantics of the queues and the system of emails notifications in order to eliminate especially email duplicities for users having multiple user roles for some tickets or queues. During the year 2012 the users have filed in 3281 tickets in 25 queues including 541 tickets in the Metacentrum first level user support queue and 183 tickets concerning involvement in the international Grid environment. The usage of the RT ticketing system for the Metacentrum grew considerably in comparison with 2100 tickets filed in the year 2011.

We also keep maintaining a separate RT instance for the EGI community which grew over the course of the project into a tool supporting wide spectrum of groups and communities. As for the EGI RT development this year we have especially redefined the whole user/groups based access rights system to allow for partial guest access to the RT. We are still developing the software release workflow for UMD middleware deployment and provisioning to match current needs and development byt EGI Technology Providers. During this year we had 1416 tickets filed in 47 queues. The raw usage of the EGI RT system is lower then last year with almost 2000 tickets filed in. Namely the number of internal requests dropped significantly, while the EGI RT usage for e.g., the software release workflow or security incidents handling keeps at the same levels as last year.

3.3 Operational Security

MetaCentrum operates a large infrastructure where security incidents might be of huge impact. In order to handle security issues in a controlled manner, MetaCentrum runs a security team that is responsible for its operational security. The team is closely coupled with the CESNET Computer Security Incident Response Team that is responsible for incident handling in the CESNET2 network. As part of national and international collaborations, the team is also personaly linked with the security team of the European Grid Infrastructure (EGI CSIRT) as well as teams at two universities in the country.

We heavily leverage the connections to other teams since they make it easier to follow various sources of information on current security incidents and vulnerabilities and also to assess emerging risks properly. The security team also develops tools to ease the management of the infrastructure and its monitoring, more details on these activities are available in the section “Security Monitoring” in Part II of this Yearbook (e-Infrastrucure Research and Development).

[9] `http://bestpractical.com/rt/`

Security Assessment

The infrastructure of MetaCentrum is quite complex and evolves gradually. In order to keep the infrastucture secure, we run internal security assessments, which consist of detailed penetration tests. The results reveal both technical issues and also more general areas opening weak spots in the environment. The assessment is performed by the security team and it starts with a detailed reconnaissance of the networks hosting MetaCentrum resources. For that step we used the Nessus Professional tool that was suplemented with custom scanner Sner. Sner was developed by the security team and utilizes the usual job management of MetaCentrum to run bunch of partial scanners that collect information about the computers and networks on which they get launched.

Collected results were processed by the Metasploit framework, which makes it easier to find exploitable services in the huge number of data. Selected vulnerabilities were additionaly checked with other tools.

The run of the assessment identified several weaknesses in the infrastructure with different level of severity. The issues are followed up in the ticketing systems and are being addressed gradually. In addition, the assessment pointed to few broader areas that will require attention in terms of security. One example of such a discovery is a minor flaw in the design of the new identity management mechanisms that were launched in 2012. Based on results of the assessment we were able to strengthen the system for creating of new accounts.

4 International Projects

MetaCentrum is fully integrated into international activities and related projects.

The projects focused on development of tools, procedures and environments for effective utilization of distributed infrastructure. We used the openings of new projects for acceleration of connections among MetaCentrum activities and those international subjects to take profit from synergies that follow on national and international operations. MetaCentrum connected the CESNET association with the main international activities at the European level so the association holds its position as an important partner on the field of distributed computing infrastructures. Besides preparation of new projects, MetaCentrum has been participating in the whole range of national and international projects in the area of grid infrastructure development.

EGI InSpire European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe (5/2010–4/2014)

http://www.egi.eu/

Project continues the transition towards the sustainable pan-European e-Infrastrusture initiated within series of EGEE projects through support of Grids of high-performance and high-throughput computing. The primary partners for EGI-InSPIRE

are the national grid infrastructures from practically all European countries, Russia, Southeast Asian countries and the US. Primary goal of MetaCentrum is to provide all required services as grid operations, monitoring, and helpdesk system at the national level thus allowing incorporation of Czech grid environment into EGI ecosystem and simultaneously enable Czech researchers to become users of the European wide EGI infrastructure. The project co-ordinator is EGI.eu, an organization established in Amsterdam in February 2010 and controlled by a consortium of NGIs. The Czech Republic is part of the Central European group. Association representative prof. Luděk Matyska has been elected Chairman of the Project Management Board in 2011 and the chairman of the EGI Council in 2012.

EMI – The European Middleware Initiative (5/2010–4/2013)

http://www.eu-emi.eu/

Under the closely related EMI project, the Association continues developing grid middleware, specifically the Logging and Bookkeeping service, as well as certain components associated with operational security. It associates representatives of three most important grid middleware systems being developed in Europe—ARC, gLite and UNICORE. The aim of the project is to make and further develop a consolidated set of middleware components designed for the EGI grid, PRACE and possibly also other DCI (Distributed Computing Infrastructures).

CHAIN – Co-ordination and Harmonisation of Advanced e-INfrastructures (12/2010–11/2012)

http://www.chain-project.eu/

The objective is to connect regional grid infrastructures with the EGI grid. Here, regions refer to areas outside Europe, such as Asia, Latin America and Africa. The EU has supported the development of EGI-compatible infrastructures in all those regions as separate projects (including the EUAsiaGrid, for instance). Under the CHAIN project, the activities will be integrated and co-ordinated at a higher level in order to ensure truly global, boundary-free cooperation of scientific teams making use of distributed computing infrastructure.

EPIKH – Exchange Programme to advance e-Infrastructure Know-How (3/2009–3/2013)

http://www.epikh.eu/

The main aim of the project is to reinforce the impact of e-infrastructure in scientific research defining and delivering stimulating programme of educational events, including Grid School and High Performance Computing courses. Broaden the engagement in e-Science activities and collaborations both geographically and across disciplines.

Moonshot

http://www.project-moonshot.org/
Project Moonshot in partnership with the GÉANT project and others develops a single unifying technology for extending the benefits of federated identity to a broad range of non-Web services, including Cloud infrastructures, High Performance Computing&Grid infrastructures and other commonly deployed services including mail, file store, remote access and instant messaging. CESNET participates in the project mainly on integrating the technology with Grid tools (e.g. for on-line CAs) and with distributed file systems.

Part II

e-Infrastructure Research and Development

Foreword

Besides operating the infrastructure and providing it to researchers from various scientific areas, there is also a need to maintain and develop its "background" services—the services, which (from one point of view) serve the infrastructure administrators to cope with various infrastructure-related issues (e.g., scheduling subsystem, clouds and virtualization mechanisms, security and monitoring, etc.), as well as the services, which (from the other point of view) serve the infrastructure users (e.g., PBSMon, Perun, etc.). Since these issues often lead to new research challenges, this part of the Yearbook describes the internal infrastructure-related research, performed by MetaCentrum/CERIT-SC staff.

e-Infrastructure Research and Development:

Clouds and Scheduling Development

HPC Clouds

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Abstract. Virtualization of computational resources is used heavily in MetaCentrum. With growing demand on cloud approach and with availability of free cloud middleware, we have also investigated possibility to provide cloud services for HPC [1]. In 2011, we did extensive evaluation of several cloud implementations and we have chosen OpenNebula[1] as foundation for MetaCloud[2]. Current state of the cloud service, together with a description of use cases already supported by the cloud group, is given in this paper.

1 Introduction

In the last few years, there has been a rising demand for flexible computing resources in the grid environment. Existing grid users are becoming interested in on-demand resource provisioning, extensive customization possibilities and deployment across multiple resource providers. This lead to the proliferation of High-Performance Computing clouds – cloud environment tailored to HPC needs [1].

In 2011, we evaluated four major cloud middleware implementations—OpenStack, OpenNebula, Nimbus and Eucalyptus. All four implementations were installed in our laboratory and tested for compatibility with existing cloud protocols, stability of implementation, possibility of integration with MetaCentrum and EGI services and extensibility. At the same time we have joined the EGI FedCloud Task Force[3], which is oriented to providing cloud services integrated into the European Grid Infrastructure (EGI). In both activities, OpenNebula and OpenStack were identified as leading solutions, providing comprehensive set of services and promising further development of their implementation. We have chosen OpenNebula for better support of required protocols and its extensibility. We agreed to provide cloud service as joint project of MetaCentrum and CERIT-SC[4].

We deployed experimental HPC cloud service, *MetaCloud*, based on an open source cloud middleware OpenNebula back in November 2011. We have spent the past year improving the user experience and adding new features requested by the users.

[1] The OpenNebula Project, http://opennebula.org/
[2] MetaCloud Wiki, https://wiki.metacentrum.cz/wiki/Kategorie:Clouds
[3] EGI FedCloud Task Force, http://www.egi.eu/infrastructure/cloud/
[4] CERIT Scientific Cloud, http://www.cerit-sc.cz/en/

2 Infrastructure

An HPC cloud infrastructure is a combination of a virtualization platform and a cloud middleware (otherwise known as a cloud platform) which exposes virtualized resources to end users.

MetaCloud currently uses KVM (Kernel-based Virtual Machine) and the XEN hypervisor as its virtualization platforms. KVM offers support for copy-on-write image formats and full hardware virtualization, XEN offers support for paravirtualization alongside full hardware virtualization and provides compatibility with virtual machine images currently deployed in the MetaCentrum environment.

The cloud middleware part of our infrastructure is provided by OpenNebula, a mature open source project, currently deployed in version 3.8 with a graphical user interface Sunstone. OpenNebula controls the deployment of virtual machines including a basic form of scheduling, resource management and network configuration (VLANs, firewalling etc.).

2.1 Hardware

Our HPC cloud infrastructure uses three basic types of servers:

- **Virtualization servers** - a clustered set of virtual machine hosts running KVM or XEN as the virtualization platform. Since MetaCloud is a joint project of MetaCentrum and CERIT-SC, both participants provide hardware resources.
- **Storage servers** - large storage array for virtual machine images and user data. Currently 44 TB of storage provided as the GPFS shared file system to virtualization and application servers.
- **Application servers** - virtual machines running cloud middleware and other necessary services provided to end users. Application server are running in a HA (High Availability) mode to minimize downtime.

The list of hardware resources also includes on-site networking devices such as infiniband switches, ethernet switches and routers. These have been omitted for simplicity.

3 Services

MetaCloud gives users the ability to control the life cycle of virtual machines using a standardized API. It also provides an object-based storage API for arbitrary user data, e.g. large data sets. Services are provided by the cloud middleware, in our case OpenNebula, and an S3-compatible storage element, Cumulus.

3.1 Virtual Machine Management

Virtual machine management includes, but it is not limited to, management of virtual resources, instantiation (the act of creating a new instance of a virtual machine), restarting, shutting down and basic monitoring of virtual machines. This functionality is exposed to end-users through a set of comprehensive user interfaces.

Virtual Resources Virtual machine (in the cloud environment) is a collection of virtual resources. Virtual resources chosen for a particular virtual machine will determine its properties such as the number of CPU cores, amount of RAM, networking capabilities or the type and number of attached images (hard disks, CD-ROMs, swap partitions, etc.).

OpenNebula defines the following virtual resources:

- **Virtual Network** - adds network connectivity to the virtual machine using a specific IP address (a lease).
- **Image** - adds a hard drive (or a CD-ROM) to the virtual machine, e.g. a partition with an operating system.
- **Virtual Machine** - collection of virtual resources, here the user can specify HW requirements for the virtual machine, add network interfaces and images.

User Interfaces OpenNebula provides two types of interfaces, Graphical User Interfaces (GUIs) and Application Programming Interfaces (APIs). This allows users to interact with MetaCloud using web browsers, shell utilities and their own applications.

- **Sunstone** - GUI implemented as a web application, provides a user-friendly access to the cloud.
- **OCA** - native OpenNebula API accessible via shell utilities written in Ruby.
- **OCCI** - Open Cloud Computing Interface, uses a standardized protocol to facilitate compatibility across multiple cloud providers and middleware.

3.2 Data Storage

MetaCloud allows users to access its storage elements using the following well-known protocols:

- **GridFTP** - file transfer suite used in the grid environment, requires an X.509 certificate and can be used when uploading large virtual machine images to OpenNebula. These can be subsequently registered and used in virtual machines.
- **S3** - object-base storage interface compatible with Amazon's S3, can be used for file transfers between running virtual machines or as a permanent storage for computation results.

3.3 User Images

MetaCloud offers users the possibility to run their own images on our infrastructure. Users are encouraged to provide us with images created in VirtualBox, VMWare or other commonly used end user virtualization tools. As part of the service, we will convert these images and make any other modifications necessary to make them cloud-compatible and ready for deployment within OpenNebula. This gives users a chance to install any software in the comfort of their own home and subsequently move to a large-scale deployment in our infrastructure with ease.

At the moment, we support following image formats and layouts:

- **Raw Disk Image** - an image containing the whole disk layout, including MBR and partition tables. Without additional formatting.
- **QCOW(2) Disk Image** - an image containing the whole disk layout, including MBR and partition tables. Formatted as a copy-on-write image.
- **VMDK Disk Image** - an image containing the whole disk layout, including MBR and partition tables. Format used by the VMWare virtualization platform.
- **VHD Disk Image** - an image containing the whole disk layout, including MBR and partition tables. Format used by the VirtualBox virtualization platform.
- **Raw Partition Image** - an image containing a single partition (a file system). Without additional formatting, commonly used by the XEN virtualization platform.

3.4 Notifications

Since MetaCloud gives users full control over virtual machines, it is important to keep them well-informed about their state. For example, users should know when a virtual machine comes online and it is ready to accept jobs.

Notification in MetaCloud is handled by the Logging & Bookkeeping service developed as a part of the EMI project [2]. Users can use LB's RSS feeds to receive real-time updates.

4 Use Cases

The following users and user communities with their use cases were active in our cloud environment in the past year. This summary includes internal/experimental users and everyday users as well as user communities coming from the EGI FedCloud Task Force.

4.1 MetaCloud

MetaCentrum staff performed several experiments with providing grid worker nodes on a cloud platform. Standard EGI worker nodes equipped with a standard

CREAM interface were experimentally provided for Auger VO during the EGI Technical Forum 2012.

Internally, CERIT-SC is using OpenNebula as the main tool for management of its HPC clusters where certain CERIT-SC projects can run their own virtual machines on selected cluster nodes, the remaining nodes are running standard worker nodes for MetaCentrum. MetaCentrum staff is using MetaCloud as its development and testing platform. Including the groups working on Perun, RT or day-to-day maintenance of MetaCentrum's computing clusters.

4.2 EGI FedCloud

The following user communities performed tests or pilot computations on our cloud infrastructure and provided feedback.

- **WeNMR** - an extension of the NMR and SAXS research infrastructures through the implementation of an e-infrastructure in order to provide the user community with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling.
- **BNCWeb** - a powerful search and analysis platform for searching the text and exploiting the detailed textual metadata. It is an open source project, and the BNC is freely available for educational and research purposes.
- **WS-PGRADE** - a portal environment for the development, execution and monitoring of workflows and workflow based parameter studies on different Distributed Computing Infrastructures (DCI).
- **DIRAC** - an interware project provides a framework for building ready to use distributed computing systems.
- **BioVel/OpenModeller** - a generic framework that includes various modelling algorithms and which is compatible with different data formats.

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Torque Batch System

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Abstract. The core component of a grid system is usually a batch system, which is responsible for managing the life time of computational jobs and the management of resources. This covers everything from user job submition, through resource scheduling and allocation, job execution and monitoring, up to collection of results and accounting.
MetaCentrum, the maintainer of the Czech National Grid, is actively developing a fork of the Torque Batch System. While Torque itself is a very competent batch system, we have further enhanced it with many stability and performance improvements as well as significant changes in the core functionality.
Bundled with a fork is a custom, queue based, high performance scheduler which is also being continuously improved to properly support all features provided by the grid infrastructure.
We have detailed our transition towards Torque in the previously published papers. In this article we will provide an overview of the most notable changes implemented into our Torque fork. These changes will be presented in contrast with the unmodified Torque functionality.

Three years ago, MetaCentrum made a big switch from the commercial PBSPro [1] to the open source Torque [2]. Torque was chosen mainly because it shares a common ancestor with PBSPro in the OpenPBS [3] system. This was an important factor as we did not have to change the command line tools users were comfortable with and also we could easily transition custom features from PBSPro to Torque.

Since the switch, we have been developing our custom fork of the Torque Batch System. This fork concentrates mainly on stability of the solution, but we also implemented significant new features that mirror new development in our grid infrastructure.

In this paper we will provide an overview of the most important features provided by our grid infrastructure and fully supported by our Torque fork.

1 Security

When it comes to security, Torque supported only very basic features. While the situation did improve since we started using Torque the main security features still rely on privileged ports. This effectively grants any root user on any of the trusted machines full access to the system.

This problem requires the system to be configured with a very restrictive configuration, only allowing access to the server from machines that are under full control.

Second aspect of this issue relates to users in the system. Grids provide a complex set of services, from access to network file systems to software licenses. This access is usually managed using grid certificates. This approach can be problematic especially when it comes to key distribution, managing multiple identities and key expiration.

1.1 Kerberos

These issues lead to the use of Kerberos [6] inside the Czech National Grid, which we back up with complex support inside the Torque batch system.

Users are required to have a valid Kerberos ticket when submitting into Torque (this can be achieved either manually, or by logging to a trusted front-end machine). Torque will then take care of generating and renewing the Kerberos ticket during the execution of the users job. This provides identical access rights for the user, both from outside and inside of the jobs environment.

Administrators can easily configure which Kerberos realms and even specific Kerberos principals can access various parts of Torque.

2 Resource semantics

Original Torque did not support resource semantics apart from managing processor cores. Such logic was left to be implemented in the scheduler, which would work directly with the state reported by the computational nodes.

This approach did cause scaling issues as it would require the scheduler to directly communicate with each of the nodes (see Fig. 1). This would cause scheduler lockups during any outage in the system.

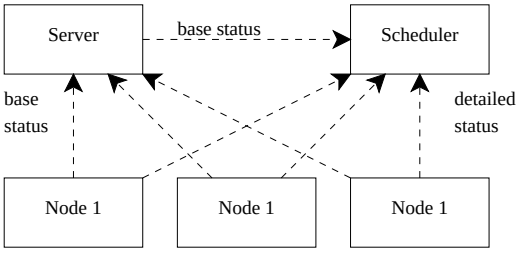

Fig. 1. Original Torque communication scheme

To provide better scalability, improved tolerance of node outages and to support our new distributed architecture, in which a scheduler needs to access

state from multiple servers, we re-implemented full generic resource support inside the server. The scheduling logic still remains in the scheduler, but server now acts as a gatekeeper, verifying every resource request. Since a full resource state is now maintained inside the server, the scheduler only needs to read the state from the server (see Fig. 2).

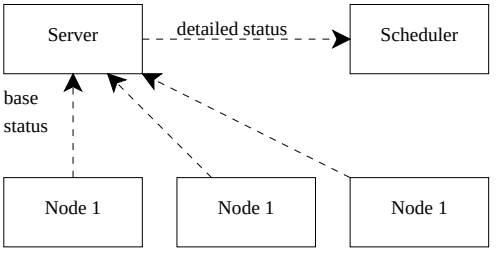

Fig. 2. New Torque communication scheme

With full resource semantics inside the server, access to queues can be easily limited using any of the supported resources. For example access to GPU cards can be limited to a specific queue.

2.1 GPU cards

GPU cards are a complicated type of resource. First complication comes with different modes in which GPU cards can operate. GPU cards can be exclusively assigned to one thread, one process, or even shared between processes. The optimal mode usually depends on the application used and therefore we had to provide users with the option to manipulate the mode of the GPU card.

Such model requires that access to GPU cards is controlled outside of the GPU exclusivity configuration. Our implementation is using UNIX access rights to allow access to GPU cards only to jobs that have requested a GPU card. This coupled with GPU allocation information available in the job environment is enough for all current use cases.

2.2 Licenses

Software licenses are another problematic resource.

First complication we have to deal with is that the license pool used in the Czech National Grid is shared between users both inside and outside of the grid. This combined with the fact, that software licenses cannot be easily reserved, leads to race-condition issues when scheduling jobs requiring software licenses.

Second complication comes from the way software licenses are consumed. Licenses can be allocated and released multiple times during a single jobs runtime.

To deal with these issues, we are employing a simulated reservation engine that is implemented inside the scheduler. Scheduler treats each previously assigned license as a reservation and is therefore capable of tracking the number of unassigned licenses. This allows us to avoid race-condition inside the system.

It is impossible to fully avoid race condition between the grid and outside users, but with conservative scheduling (ignoring small amounts of highly fluctuating licenses) we were able to limit these race conditions to a minimum.

2.3 Resource requests, information and accounting

Support for generic counted resources has to be coupled with support for resource requests from users. We have extended the node specification syntax of Torque to provide multiple enhancements, from simple heterogeneous requests, to support for negative properties (requesting nodes that do not have a specified property).

This is coupled with an overview property specifying the total of requested resources. These values are required to provide proper accounting.

Users using heterogeneous requests (for example one node with 2GB memory and two nodes with 1GB memory) need information to distinguish between these nodes. For this purpose we are providing full resource information inside the job environment. This includes both the resource values specific to the current node as well as total resource values.

To avoid conflicts between different jobs running on the same node we are also providing full resource enforcement on the node level.

3 Distributed Torque

Our work on a distributed version of the Torque batch system was originally [5] motivated by stability and performance issues of the single server configuration [7][10]. In a centralised configuration, localised network outages can easily cause global inaccessibility of the grid.

While this is still a concern, we improved the stability and performance of Torque so dramatically, that this ceased to be our primary motivation.

Instead we have shifted the focus of the distributed Torque architecture towards the connection of multiple organisations with separate Torque installations into a single grid. This still requires these organisations to use similar version of Torque, but allows them to setup local policies to their liking and define the semantics of the cross-realm connection.

The main tool we are using to express the distributed system is the notion of global queues (see Fig. 3). These queues can span across multiple servers and while each server sees this queue as a fully local, schedulers maintain the illusion of a global queue by merging jobs across all servers.

Jobs in remote parts of the queue (submitted on a remote server) are treated identically to jobs submited locally. Since the queue is still subject to all local policies, administrators can easily control the influx of jobs from remote servers.

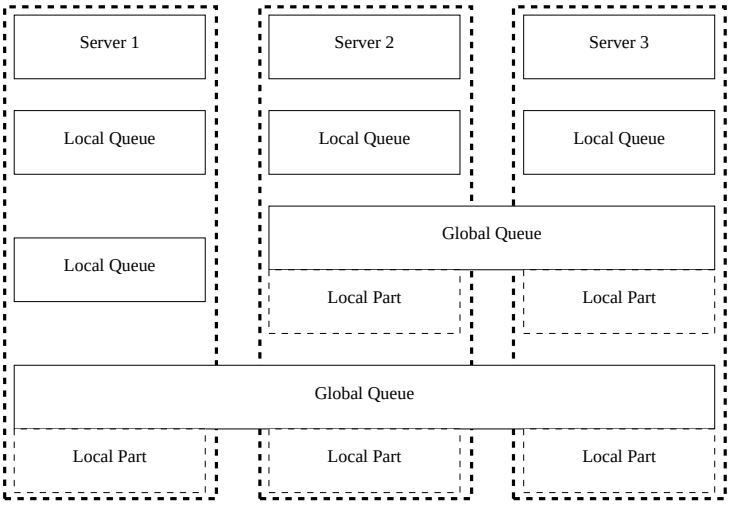

Fig. 3. Global queues

4 Virtualization

Virtualization is an important part of our grid infrastructure [9]. Torque is being continuously enhanced to support more and more complex use cases on top of our virtualized infrastructure.

4.1 Preemption

The initial support was mainly concerned with full machine preemption (see Fig. 4). This use case was required for machines whose owners required high-priority access. Without full-machine preemption we wouldn't be able to utilise these machines at all [4].

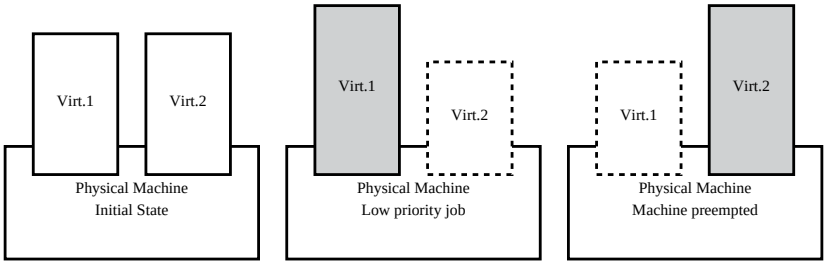

Fig. 4. Preemption on top of virtualized infrastructure

Each physical machine is split into two virtual machines that both represent the entire physical machine and can switch the resources of the physical machine between them. In the initial state, both virtual machines can accept a job. Once a low priority job is run, the low priority virtual machine overtakes all of the resources. This still allows a high priority job to run on the system, in which case, the system will be preempted and the high priority virtual machine will overtake all of the resources.

4.2 Virtual Clusters

Virtual clusters (see Fig. 5) allow users to request dedicated clusters of virtual machines with specific system images. These virtual machines can be further connected using a VLAN [8].

Using this feature we are able to cover even extreme user requirements without permanently allocating machines for these users. This includes the support for Windows based virtual machines.

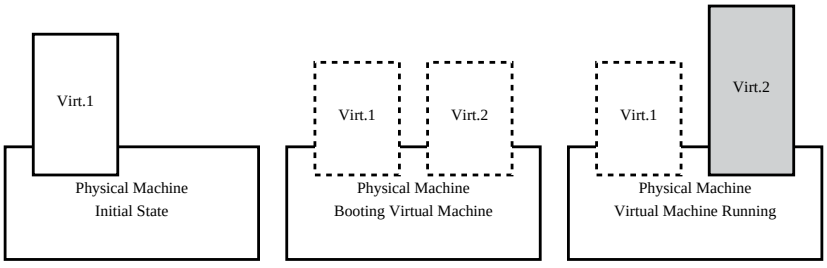

Fig. 5. Virtual cluster support

In this scenario one of the machines is kept offline and is only installed and started when requested. Once the virtual cluster ends, the machine is returned back to its offline state.

4.3 On-demand virtual clusters

On-demand virtual cluster are a very natural extensions of virtual clusters. Virtual clusters are only constructed when explicitly requested by the user, but booting a specific system image is useful for other cases as well. If this process would be automated for normal jobs, we could easily scale the amounts of different software images supported in the system.

This is exactly what on-demand virtual clusters are. Virtual clusters are constructed as required and this feature is used for balancing the amounts of installed system images. For example if one user suddenly requests large amounts

of Scientific Linux instances we can now easily satisfy such request even though Scientific Linux is not pre-installed on any of the machines.

5 Torque fork

If you are interested in trying out our fork of the Torque Batch System, you can check it out at `https://github.com/CESNET/torque`.

The repository is the representation of the version currently deployed in the Czech National Grid. The last git tag represents the last package version that is used by external centers like CERIT.

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Virtualization & Magrathea

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Abstract. Virtualization of computational nodes is technique which becomes very popular with wider adoption of cloud computing. In MetaCentrum, virtualization is studied and used in production already for five years. Primordial idea that each computation is encapsulated in virtual machine, together with complete environment, is still driving idea not only for cloud computing, but also for MetaCentrum' usage. Computational resources like CPU or memory can be assigned to virtual machines dynamically and just allow features like preemption of jobs by highly privileged jobs, migration of jobs to less used resources and other scheduling techniques. Moreover, encapsulation into virtual machines allows running each job is it's specialised environment, starting from choice of operations system or at least Linux flavor and continuing to Linux installations with changed specific libraries or versions of scripting languages. In MetaCentrum, virtualized resources can be not only CPU and memory, but also network – virtual machines can be bound in private network etc.

1 Introduction

Application of virtualization techniques in MetaCentrum was driven by several use-cases, which are summarized in this article. For more precise description see technical reports [1, 3, 4]. Implementation of these use-cases allows several unique features provided by MetaCentrum grid environment such as preemption of standard workload by jobs submitted by cluster owners, possibility to run jobs in various Linux distributions or MS Windows and possibility to provide semipermanent cluster of virtual machines, built from user-supplied images and hidden in VPN.

Batch scheduling system Torque is used in MetaCentrum. While we have modified this system to utilize possibilities of virtual machines, we had also developed system *Magrathea*, which provides abstraction layer on top of virtual machines and makes Torque modifications less complicated.

2 Magrathea

In order to support scheduling of virtual machines on MetaCentrum clusters, we have developed system Magrathea, which allows scheduling systems to deal with several virtual machines deployed on a physical cluster node, build them

according to user or system requirements and schedule jobs to such virtual machines with minimal requirements on modification of batch systems. The original architecture of the system is described in [1, 2]. We have extended the system to support management of virtual clusters—groups of virtual machines ([3, 6]) and this year we did several extensions too—job can specify that it must be started in temporary instantiation of specific type of virtual environment, which will be destroyed after job is finished and arbitrary number of virtual machines can be started on physical one.

Together with Magrathea, caching information service called `pbs_cache` was developed too. In current setup, it stores not only information about state of virtual machines, but also other dynamic information used by scheduling system like availability of dynamically allocated software licenses or disk space on scratch filesystem. This service is used not only by Torque scheduler but also by other services providing MetaCentrum user interface etc.

3 Supported use-cases

Two static domains. Two virtual machines run on a physical one, just one virtual machine is allowed to run a user job. The active domain is given most of available hardware resources (CPUs, memory), while the other domain runs with minimal resources, just to stay visible for the scheduling system. This setup can be used for dynamic switching between two different Linux flavours, with minimal requirements on batch system modification. The batch system must only handle both of the virtual machines running on a single physical one as occupied.

The virtual machines can be statically installed on the physical substrate. Moreover, current Magrathea versions are capable of installing virtual machines on-the-fly, therefore the virtual machine images can be also injected to the physical resources on demand.

Preemption. Preemption is an extension to the first scenario. One domain is set as "privileged" and can preempt job running in the second, "ordinary" domain. This setup is used in MetaCentrum when providing privileged access for cluster owners. Many cluster owners allow the cluster to be used by other infrastructure users on the condition that the owners have priority to run their jobs on the hardware.

In this setup, jobs submitted by the cluster owners can be started in this privileged domain on the cluster, waiting only a negligible penalty until the domains are rescheduled. Jobs in the ordinary domain are suspended while the owners' jobs run and are resumed after the privileged job is finished.

Virtual cluster. Cluster containing nodes on virtual machines, built from node images stored in a central image repository. The cluster is built using standard batch system interface, with very minimal difference to standard job submission—the cluster is an ordinary job from scheduling point of view. Virtual cluster nodes

are built on request, according user requirements on node properties (which may include, e.g., Linux flavor). Various usage scenarios are supported, starting from cluster nodes based on standard MetaCentrum node image—in such case, cluster serves as reservation of nodes for user or user group, jobs submitted later to the cluster are managed by the central batch system. In second scenario, cluster nodes are built from non-default images (nevertheless images supported by MetaCentrum) providing just the possibility to run sets of jobs or parallel job on different cluster image. In the last scenario, the node image is supplied by users, OS installed on cluster nodes is independent on management tools provided by MetaCentrum and also job management on these nodes in completely under user control.

Private cluster. Virtual cluster encapsulated in private VLAN. Two basic motivations were identified in [3, 5, 4]: (1) separation of user supplied images from CESNET IP network for the purpose of not taking responsibility of user-supplied images in the network of the infrastructure provider and (2) hiding network complexity, when two clusters separated on national networks can be connected by single virtual layer 2 network, providing the clusters with a logical local network.

In both scenarios, the cluster consists of user supplied images, potentially with images managed only by the user (i.e., insecure from infrastructure administration point of view). Such cluster is encapsulated into a private VLAN and it is enriched with an additional node which serves as a VPN access-point. The user can propagate the cluster under his/her own address space (thus taking responsibility for its network traffic). In the second scenario, nodes of private clusters serve as transparent extension of user's local network environment and potentially also as extension of private cluster, conforming local addressing and naming schemes.

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New Multi-Resource Fairness and Performance Metrics for MetaCentrum

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Abstract. This work is inspired by the current needs of the Czech National Grid Infrastructure MetaCentrum. MetaCentrum provides computational resources to various users and research groups. In such a system it is very important to guarantee that computational resources are shared in a fair fashion with respect to different users. while maintaining reasonably effective utilization of resources and low turnaround times for jobs. These requirements are typically solved using the services of the applied resource manager, in this case the TORQUE [3]. Based on the analysis of existing system and using the historic workload logs we conclude that one of the most important parts are the applied job priority scheme. In this work we propose new job priority scheme and a new system performance metric.

1 Introduction

The main contribution of this work is the proposal and analysis of a new, multi-resource fairshare metric. Based on the analysis of the existing workloads that come from different instances of production TORQUE servers running in parallel, we have identified several weaknesses in the existing fairshare metric. Fairshare is an integral part of the process of establishing job priorities [6, 2]. It is a mechanism that allows historical resource utilization information to be incorporated into job feasibility and priority decisions. Priorities are responsible for the proper job ordering within the queues in the system. The problem with current setup is that it uses fairshare metric that only considers consumed CPU time. Other resources such as RAM, GPUs, occupied HDD storage or software licenses are not considered. The problem here is that jobs requiring few CPUs but a lot of (all) memory on given machine or cluster are not adequately penalized. For the same reason a new system utilization criterion is proposed as it is also questionable whether the classical machine utilization metric that expresses the ratio of consumed and available CPU time is a proper metric to measure the effectiveness of heterogeneous systems.

The proposed fairshare metric has been frequently discussed with the MetaCentrum team. Of course, state of the art results [4, 8, 10, 6] were applied in the proposed solution. Job scheduling simulator [9] has been used frequently in order to evaluate new scheduling concepts prior their application in a production system.

In the following section we introduce the considered problem and the related work. Section 3 presents the newly proposed multi-resource fairshare metric and the system utilization function. Finally, the future work is presented in Section 4.

2 Related Work

All existing resource management systems allow to flexibly adjust system settings by means of queue settings and queue priorities mechanisms including fairshare [3, 1, 6]. However there is no "general recommendation" concerning proper system setup. Clearly, it is not possible to create some universal efficient setup that would be usable across different systems. In general, we can only say that the number of different queues should be as low as possible in order to remain understandable both for the system user and the administrator. Moreover, large number of queues usually leads to potential resource fragmentation and related drawbacks [6]. If possible, the final "tunning" should be performed using the combination of suitable scheduling strategy (e.g., suitable backfilling algorithm) and proper job/user prioritization strategy [6]. In this case, the proper fairshare mechanism is the integral part of the prioritization process and thus will be further analyzed.

There are several works that propose and describe suitable fairshare mechanisms. However, most of them such as max-min, Quincy or Hadoop Capacity Scheduler only deal with a single resource situation [5, 7]. It means that the fairshare is computed with respect to a single resource only, e.g., the CPU time. Based on the analysis of existing MetaCentrum's workloads we have quickly identified that such an approach is not efficient. The problem with a single-resource metric is more apparent when some nodes in the Grid are large shared memory machines. For example, CERIT-SC's zewura cluster available in MetaCentrum contains 20 machines, each having 80 CPUs and 512 GB RAM. In the historic workloads we can see several situations when some users utilize very few CPUs but require (nearly) all the memory. Such an examples can be seen for several jobs executed on zewura (see Figure 1 (left)).

The problem is that remaining free CPUs cannot be utilized by other users since there is no free RAM left. Second, classical metrics used to analyze the performance of the system such as CPU utilization are now misleading as they show dramatically low utilization but do not "explain" it via the high RAM consumption. Real-life example of such a situation is presented in Figure 1 (right).

Finally, classical — single-resource — fairshare mechanism computed according to the consumed CPU time is absolutely unacceptable as the users with high RAM requirements are not adequately penalized w.r.t. the users who only need (a lot of) CPUs[1].

Surprisingly, the so called multi-resource fairness seems to be a rather new area of researchers' interest as there are only few works that address this problem specifically [7, 4, 8]. Moreover, there is no common agreement about "what is

[1] Detailed discussion will be presented in Section 3.1.

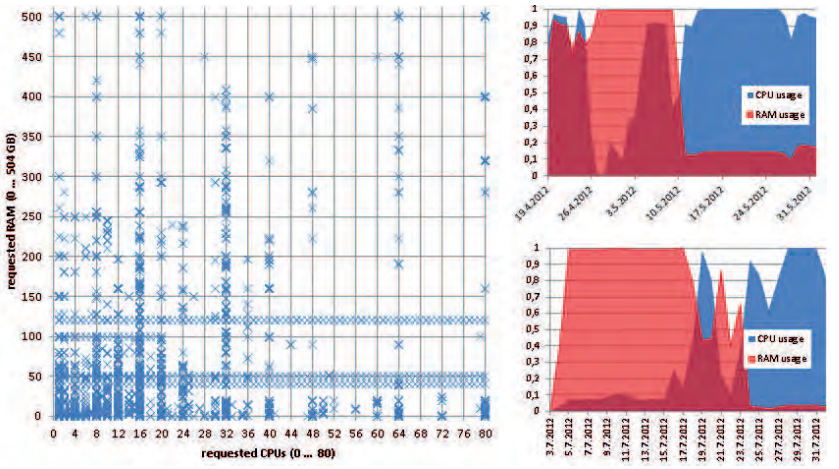

Fig. 1. Jobs' CPU and RAM requirements within the zewura cluster (left) and an example of CPU and RAM utilization for two selected nodes in zewura cluster (right).

fair" when consumption of multiple resources is considered [7]. Few existing multi-resource techniques represent several drawbacks. For example, the recent Dominant Resource Factor (DRF) [4] performs scheduling decisions according to so called dominant user's share, which is the maximum share that the user has been allocated of any resource. However, DRF does not consider previous scheduler's actions, i.e., it only allocates jobs according to current users' shares of resources ignoring previous, historic decisions.

Several resource managers such as Torque and corresponding schedulers like Moab or Maui allow the system administrator to somehow combine CPU and, e.g., the RAM consumption within the fairshare function [6, 2] using for example the processor equivalent (PE) mechanism [6]. The problem is that it is not very clear how these different mechanisms interact together.

For these reasons we have decided to propose and analyze new multi-resource fairshare formulas that are closely described in following Section 3.1 and the new system utilization metric (Section 3.2).

3 Proposed Solution

As we already discussed in Section 2, we seek for a solution of several problems. Especially, proper job and user prioritization is necessary [6]. Therefore, proper fairshare mechanism that is computed as a function handling multiple resources is to be found in the first place. It represents a multi-criteria decision making problem. Notably, we need to decide "what is fair" when multiple resources are considered and consumed together. Second, we also discuss suitable modification of the system utilization metric.

3.1 Fairshare Metrics

In general, the user's priority within the system is established using a function that is similar to Formula 1.

$$F_u = \sum_{j=1}^{n} (P_j * walltime_j) \tag{1}$$

Here, the F_u is the resulting priority of given user u that so far computed n jobs. The final value is the result of the sum that summarizes the products of job penalty P_j and the job's walltime ($walltime_j$). Such a formula is a general form of a function that can be used to establish ordering of users. It represents the simplest version, that do not use so called decay algorithm [6] which is usually used in order to reflect aging factor. For simplicity, we do not use aging in this report as its inclusion is straightforward [6]. The user with the smallest value of F_u gets the highest priority. The key problem here is how the job's penalty P_j is computed. We discuss several variants of P_j computation in the following text.

Single-resource Fairshare Metric The current solution applied in MetaCentrum uses a single-resource fairshare approach that prioritize users according to the amount of consumed CPU time. In this case, the penalty function P_j for given job j is described by Formula 2, where CPU_j is the number of CPUs allocated to given job j and $total\ CPUs$ is the total amount of CPUs available in the system.

$$P_j = \frac{CPU_j}{total\ CPUs} \tag{2}$$

Clearly, the penalty of given user's job j is proportional to the number of CPUs it requires as P_j expresses the ratio of consumed to available CPUs. The resulting distribution of such penalties can be illustrated by the graph shown in Figure 2 (left). This figure shows the penalty obtained according to the amount of requested CPUs.

Obviously, the penalty function has no relation to RAM consumption. Let us consider a simulated scenario that uses such a penalty function to prioritize various users in the system. In this scenario, each user has different requirements concerning CPU and RAM. We consider 8 different CPU requirements (1, 2, 4, 8, 16, 32, 64, 80) and 8 different requirements concerning the amount of available RAM (1, 5, 10, 20, 50, 100, 250, 500)[2], i.e., there are 64 different users with different combinations of CPU and RAM requests. With such a setup we ran an experiment where the amount of completed jobs in given time interval was measured for all 64 users.

The results are shown in Figure 2 (right). The two horizontal axes represent the CPU and RAM requirements while the vertical axis depicts the number

[2] The value depicts the requested amount of free RAM in GigaBytes.

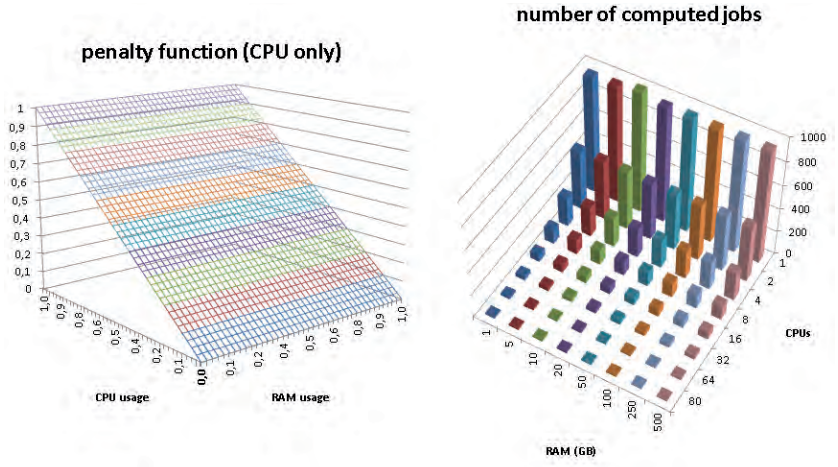

Fig. 2. Single-resource penalty function (left) and corresponding distribution of job completions among users of the system (right).

of completed jobs. Clearly, when such a single-resource penalty is applied the resulting amount of completed jobs (see the vertical axis in Figure 2 (right)) is clearly unfair as all users requesting the same amount of CPUs gets roughly the same number of completed jobs within considered time interval, disregarding their RAM requirements[3]. This simulated example demonstrates that the current single-resource penalty function is impractical and obviously unfair.

Multi-resource Fairshare Metric In order to resolve the inefficient single-resource fairshare metric we have proposed several different candidates that somehow incorporate also the RAM requirements [8]. In this report we present the two most suitable candidates. Again, we will only describe the penalty associated to given user's job as the extension to all user's jobs is straightforward. Two candidates as seen in Formulas 3–4 are considered in the following text.

The first candidate is based on a square root function and is shown in Formula 3 while the corresponding distribution of penalties is depicted in Figure 3.

$$P_j = 1 - \sqrt{\left(1 - \frac{CPU_j}{total\ CPUs}\right) * \left(1 - \frac{RAM_j}{total\ RAM}\right)} \tag{3}$$

As can be seen in the Figure 3 (left) the function assigns reasonably high penalties both for "symmetric" as well as for (highly) asymmetric jobs, i.e., for those jobs whose relative CPU and RAM requirements are unbalanced. Still,

[3] In this experiment, every job has the same duration, i.e., the number of completed jobs is a measure showing the level of priority of given user.

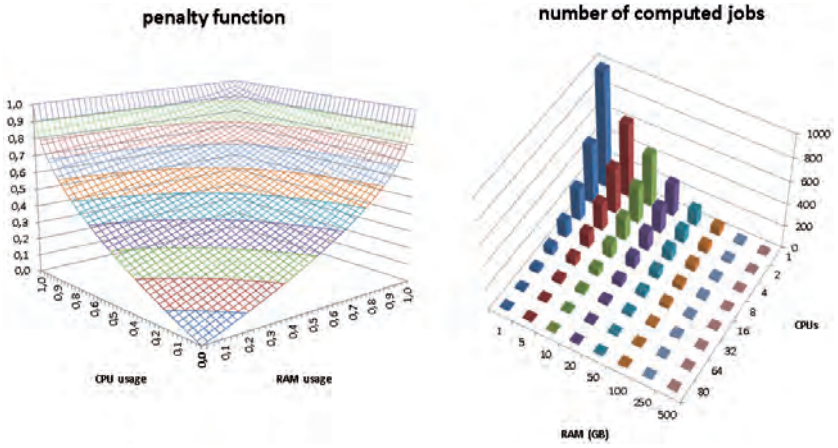

Fig. 3. Penalty function as computed by Formula 3 (left) and corresponding distribution of job completions among users of the system (right).

some problems remains. When focusing on the single resource the penalty is not linear. From some point of view this can be considered as desired behavior, however it is not desirable as it allows users to cheat in some situations. For example, instead of one large job the user can submit two smaller jobs. As a result, he or she will receive smaller penalty. Also, asymmetric jobs get smaller penalty than the symmetric ones. This feature can be useful as it may encourage the users to better estimate their CPU and RAM requests. In another words, those users who do not overestimate their requirements will obtain smaller penalty.

The second presented function is based on the findings presented in [4]. Instead of combining the CPU and RAM together, only the maximum request (so called "dominant share") is considered and penalized accordingly. The penalty is then computed using Formula 4 and the corresponding distribution of penalties is depicted in Figure 4.

$$P_j = MAX\left(\frac{CPU_j}{total\ CPUs}, \frac{RAM_j}{total\ RAM}\right) \tag{4}$$

This penalty represents several benefits. First of all, the penalty is not influenced by the less dominant resource. Therefore, it is very simple so both the users and the system administrators will find it easy to understand. Second, the penalty is linear, therefore it does not make much sense to cheat as it was possible in case of the square root-based Formula 3.

Further Problems So far, the Formula 4 seems to be a promising solution. Still, there are several things to be solved in the future. First of all, it is not very clear whether it makes some sense to incorporate different resources into

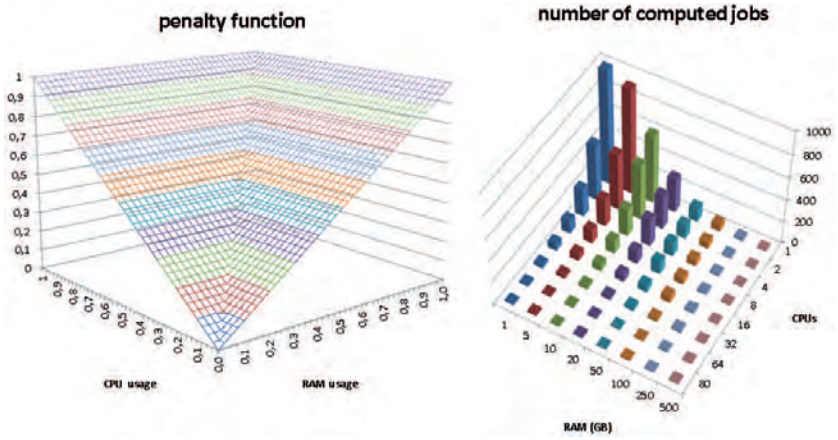

Fig. 4. Penalty function as computed by Formula 4 (left) and corresponding distribution of job completions among users of the system (right).

the MAX function. For example, it is questionable whether we can include the amount of consumed HDD storage into this formula and expect reasonable behavior. From this point of view, those functions that somehow combine several resources (see Formula 3) together seems to be more promising. Moreover, as the fairshare formula uses job's walltime it is necessary to first benchmark the whole infrastructure. Otherwise, those users that use slower machines will obtain lower priority (due to higher walltime) which is not fair.

3.2 System Utilization Metric

For the same reason why we need a a multi-resource fairshare function we also need a new multi-resource utilization metric. Currently, the utilization of MetaCentrum is measured using standard machine usage criterion that only covers the percentage of used CPU hours. However, as the existing workloads indicate (see Figure 1 (right)), such a metric does not really say whether the machines are used. The problem is that it indicate low "utilization" even when the system is (fully) utilized by means of consumed RAM.

For starters, we propose to use simple MAX function that for each time interval considers the maximal value of CPU and RAM utilization. Corresponding formula called System Utilization (at time t) SU_t is shown in Formula 5.

$$SU_t = MAX\left(\frac{used\ CPUs}{total\ CPUs}, \frac{used\ RAM}{total\ RAM}\right) \tag{5}$$

With such a SU_t function we will obtain more "self explaining" results concerning system utilization as is demonstrated for given zewura node in Figure 5.

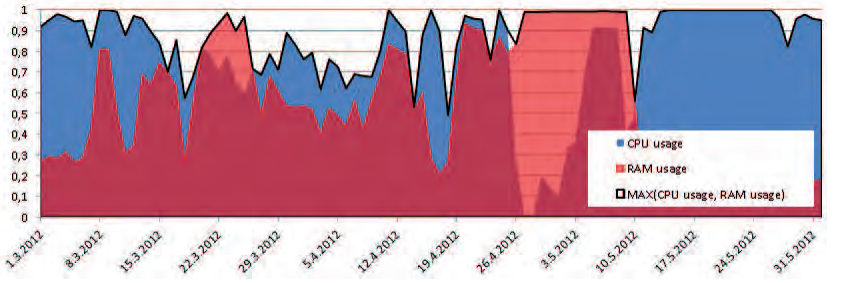

Fig. 5. An example of CPU and RAM utilization and the new system utilization metric.

4 Future Work

In the near future the proposed extensions of fairshare mechanisms will be further tested both through the simulation and in a real testbed. Next, the most promising solution will be applied in the production MetaCentrum schedulers. Then, fairshare metric will be further extended in order to incorporate other consumable resources such as HDD storage, software licenses or GPUs.

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Alea – Job Scheduling Simulator

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Abstract. Newly proposed scheduling algorithms must be heavily tested and evaluated before they are applied in the real systems. Due to many reasons, such as the cost of resources, the reliability, the varying background load or the dynamic behavior of components, experimental evaluation cannot be mostly performed in the real systems. To obtain reliable results, many simulations with various setups must be performed using the same and controllable conditions that simulate different real life scenarios. This is often unreachable in the real Grid or cluster system. For this purpose many simulators have been developed. If properly designed, such simulators are very useful since different setups and different data sets can be used to evaluate existing or proposed solutions. While for some purposes an ad-hoc simulator is sufficient, there are also general Grid and cluster simulators allowing to simulate various scenarios and problems. This works presents the Alea Simulator, an advanced job scheduling simulator which we have been developing since 2007.

1 Overview

The Alea [7, 5] job scheduling simulator is an extension to the widely used GridSim [15] simulation toolkit[1] written in Java. It represents "ready to use" centralized scheduling system allowing to apply and compare various scheduling algorithms and scheduling scenarios similar to those used in the production scheduling systems such as PBS Pro, TORQUE or LSF. It is therefore very useful when analyzing the influence of modifications in existing setups of production schedulers, e.g., in MetaCentrum.

The solution consists of the scheduler entity and other supporting classes which extend the original basic functionality of the GridSim. The main benefit of our solution is that the Alea allows immediate testing by inclusion of several popular and widely used scheduling algorithms such as FCFS, Earliest Deadline First, Shortest Job First, EASY Backfilling, Conservative Backfilling, Flexible Backfilling, etc. Beside the queue-based algorithms, it also enables the use of algorithms that construct the schedule (scheduling plan) [4]. Over the time, many core improvements have been done concerning the design, the scalability [9] and the functionality [7]. Also, several new scheduling algorithms and objective functions were included as well as the support of additional job and machine characteristics [8].

[1] Gridsim is available at: http://www.buyya.com/gridsim/.

The Alea now also provides complex visualization tool which supports an export of simulation results into several bitmap formats. The simulation speed and the simulator's scalability have been significantly improved through the newly developed or redesigned classes. This covers a new memory-efficient job loader and a redesigned job allocation policy, which speeds up the whole simulation. Moreover, the support of standardized workloads formats has been included as well as the simulation of machine failures using the real life failure traces [7].

The paper is organized as follows. In the next section we describe all features of the simulator including the overall design. We will also closely describe the crucial scheduler entity. Next, the correctness of the simulator is discussed. Finally, we present the applicability of the simulator on several problems. Also, the use of Alea for solving problems related to the job scheduling in MetaCentrum is discussed in this work.

2 Simulator Design

The Alea extends existing GridSim classes and also offers brand new classes to provide a "ready to use" job scheduling simulator. It has been designed with respect to our needs concerning simulation capability. This involves the ability to perform complex simulations that involves realistic features of real systems. To be more precise, Alea is able to simulate sequential and parallel jobs, computational clusters, specific job requirements as well as system dynamics such as machine failures or users' activity. It also supports various optimization criteria including utilization, slowdown, response time, wait time and fairness related criteria including the support of various fairshare methods [6]. Using these complex functionality we are able to simulate various scenarios that are of interest in MetaCentrum [8, 6].

Same as the GridSim, the Alea is an event-based modular simulator, composed of independent entities which implements the desired simulation functionality (see Figure 1).

It consists of new centralized scheduler, the Grid resource(s) with the local job allocation policy, the job loader, the machine and failure loader and additional classes responsible for the simulation setup, the visualization and the generation of simulation output. As in GridSim, simulator's behavior is driven by the event-based message passing protocol. The simulator is fully compatible with the latest GridSim 5 release since no changes were made in the GridSim package itself. All extensions were made by implementing child classes which extend the standard GridSim (parent) classes. Similarly, easy extension of current functionality is possible thanks to the object oriented paradigm used by the GridSim and the Alea. In the following text all important extensions on top of the GridSim package are mentioned and explained.

The simulation is initialized by the `ExperimentSetup` class which creates instances of the scheduler, the job and machine loader, the failure loader and other entities as required by the standard GridSim.

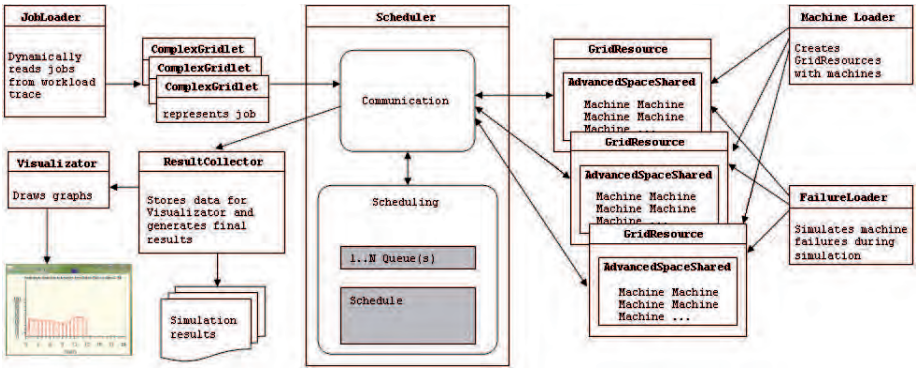

Fig. 1. Main parts of the Alea simulator.

The `MachineLoader` initializes the simulated computing environment. It reads the data describing the clusters and machines from a file and creates Grid resources accordingly. The `JobLoader` reads the file containing the job descriptions and creates jobs' instances dynamically over the time. The `JobLoader` supports several trace formats including the Grid Workloads Format (GWF) of the Grid Workloads Archive [2] and the Standard Workloads Format (SWF) of the Parallel Workloads Archive [3]. When the simulation time is equal to the job submission time the `JobLoader` sends the job to the scheduler.

The job itself is represented by the instance of the `ComplexGridlet` class. The GridSim provides only trivial implementation of a job in its `Gridlet` class. The `ComplexGridlet` extends this class, allowing to simulate more realistic scenarios where each job may require additional properties such as the deadline, the estimated runtime, the specific machine parameters, and other real life based parameters and constraints.

The `FailureLoader` reads the file containing descriptions of machine failures. Once the simulation time reaches the failure start time, the appropriate machine is set to be failed, killing all jobs being currently executed on that machine. When the failure period passes the machine is restarted. Machine failures can be used to simulate addition of a new machine or permanent machine removal [8, 7].

As in the GridSim, the resource is represented by the `GridResource` instance and is managed by the local scheduling policy. Unfortunately none of the currently provided policies support the execution of parallel jobs and the simulation of machine failures at the same time. Also the co-allocation of several machines for job execution is not available. Therefore, new allocation policy called `AdvancedSpaceShared` was developed for the Alea based on the GridSim's `SpaceShared` policy. It enables to simulate more realistic scenarios involving the parallel jobs as well as the simulations of machine failures.

The newly developed `Visualizator` class generates the simulation's graphical output. It displays information useful for tuning and debugging of scheduling algorithms. So far, several outputs covering different objectives are supported

and displayed. Those are the overall utilization of resources, the cluster utilization, the number of waiting and running jobs and the number of requested, utilized and available CPUs. Beside that, also the percentage of failed and running CPUs per cluster can be displayed. The `Visualizator` may work in two different fashions. In the first case, the visualization is generated continuously as the simulation proceeds (see Figure 2).

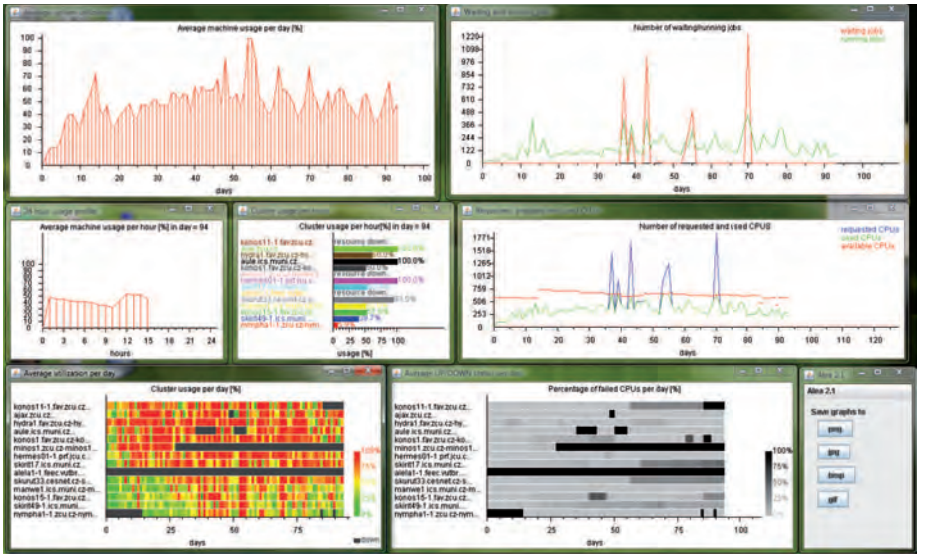

Fig. 2. Visualization interface of the Alea during the simulation.

Results are continuously collected by the `ResultCollector`. When the simulation completes, the `ResultCollector` stores them into csv files that can be easily used as an input for other tools (Calc, Excel, Spreadsheet, etc.) and it also saves generated graphs into a preferred bitmap file (png, jpg, bmp, gif).

The `Scheduler` is the main part of the Alea. Its behavior is driven by events and corresponding messages. Using the events, the Scheduler communicates with the `JobLoader` (job arrivals), with the `GridResources` (job submission/completion and failure detection) and with the `ResultCollector` (periodical result collection). Also the internal events are used to manage the scheduling process. The Scheduler (see Figure 1 middle) is responsible for performing scheduling decisions according to the selected scheduling policy. It was designed as a modular, extensible entity composed of three main parts which are discussed in the following text.

The first part stores dynamic information concerning the Grid resources (see Figure 1 right). For each `GridResource`, one `ResourceInfo` object is created that holds up-to-date information regarding the current resource status. It stores information about jobs currently in execution, about jobs that are planned for

execution (if the schedule is being constructed) and it implements various functions that help to compute or predict various values, e.g., the next free slot available for specific job, etc.

The second part is responsible for the communication with the remaining simulation entities (see Figure 1 middle). It accepts incoming messages (events) and reacts accordingly. Typically, the `Scheduler` receives newly incoming job from the `JobLoader`. It takes the incoming job and places it into the queue or schedule according to the applied scheduling algorithm. Next, new scheduling round is performed and an attempt to submit jobs present in the queue or schedule is performed. If some resource is available and a suitable job is selected, it is submitted to the resource where it will be executed. Moreover, appropriate scheduler's `ResourceInfo` object is updated according to the new situation. Once some job is completed, it is returned to the Scheduler and the `ResourceInfo` object is updated as a result of the new state. Similar update is performed when some machine fails or restarts. Next, a new scheduling round is started. The cycle finishes when no new job arrivals appear and all submitted jobs have been completed. Then the simulation ends and the results are stored into the output files.

The last part of the `Scheduler` contains plugins implementing several popular and widely used scheduling algorithms. Both the queue and the schedule-based (planning) techniques are supported. Concerning the queue-based techniques following algorithms are implemented in the `Scheduler` entity: First Come First Served (FCFS), Shortest Job First (SJF), Earliest Deadline First (EDF), EASY Backfilling (EASY), Conservative Backfilling (CONS), Flexible Backfilling (Flex-BF), and a PBS-like (PBS) multi-queue and priority-based scheduling algorithm [14, 10]. Schedule-based techniques use a schedule — instead of a queue(s) — to store the jobs. In this case, each job is placed into the schedule upon its arrival which defines its expected start time, expected completion time and the target machine(s). The use of the schedule allows to use advanced scheduling and optimization algorithms such as the local search-based methods. These techniques are represented by the Best Gap – Earlier Deadline First (BG-EDF) and Best Gap (BG) policies and local search-based optimization routines Random Search (RS), Gap Search (GS) and Tabu Search (TS) [10].

Several objective functions are supported which can be used for decision making or optimization. During the simulation, the `Scheduler` is capable of collecting various data such as the number of waiting and running jobs, current machine utilization, etc. Once the simulation is finished, output files containing these data are generated. Moreover, selected objectives can be used as an input for either the "on the fly" or the "post mortem" visualization provided by the `Visualizator` graphical tool.

3 Correctness of the Simulator

The correctness of the simulator was checked by analyzing the implementations of algorithms and simulation outputs. First, the implementations of scheduling algorithms were checked against their known pseudo-codes. Next, the simulation outputs of existing algorithms such as FCFS, EDF, EASY or Conservative Backfilling were compared with the known results from the literature. In case of PBS [13] and Flexible Backfilling [12], both the implementation details and the simulation outputs were directly checked by the authors of these algorithms. Proposed policies and optimization algorithms were checked through several experiments where the expected behavior (algorithm's specification) was compared with the simulation trace and simulation outputs. Also the graphical simulation output played an important role when analyzing the implementation. When some anomaly was identified, the code was traced and analyzed using classical debugging techniques and the implementation was fixed accordingly.

4 Applications of the Alea Simulator

The Alea has been used in our several works that covered wide area of problems related to Grid scheduling. In [1, 10, 12] it has been used to compare and evaluate several queue-based and schedule-based scheduling algorithms. In [8], it was used to demonstrate the importance of using truly complex workload traces when simulating job execution. Also, several problems related to the user-to-user fairness have been described and their possible solution evaluated using the Alea simulator [11, 6]. These particular issues related to maintaining fairness with respect to various consumed resources such as CPUs, RAM, GPUs, software licenses, etc., are very important and are highly important for MetaCentrum these days. Here, Alea plays an important role when simulating efficiency of newly proposed fairshare metrics [6] before these are applied in the production MetaCentrum environment. In [9], newly proposed time and memory efficient data structures designed to represent job schedules have been experimentally evaluated using our simulator. We have also received positive feedback from several researchers from around the world who found using it very helpful[2].

The Alea, including the sources and full documentation, can be freely downloaded from `http://www.fi.muni.cz/~xklusac/alea`. Further discussion about Alea's performance with respect to other available simulators and simulation toolkits is available in [7]. Also, exhaustive related work is presented there.

[2] Since 2007, we are aware of more than 30 foreign Alea users.

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e-Infrastructure Research and Development:

Identity Management, Operation and Tools Development

Beyond Contemporary Identity Federations

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Abstract. Identity federations enables users to use the authentication credentials they use at their home institutions to access services operated by other institutions. The concept is attractive for both the end-users as well as the resource providers because it simplifies the credential and identity management. We contribute to development of systems focusing on better utilization of the federated model. After several years of production utilization of the concept we also identified several weaknesses present in the model and designed solutions addressing them.

1 Identity Federations

MetaCentrum provides access to its resources to users originating from a lot different institutions and therefore it has always been important to focus on proper authentication and identity management in such an environment. We seek to provide users with access to the resources, which is simple yet secure enough. The model of federated identity that has evolved over past few years is a viable option for this effort.

An identity federation is an infrastructure connecting identity management systems from different institutions and services providers, which require user authentication. Identity federations enable to share information about the users through a standardized protocol that is accepted by every party in the federation. Every organization participating in the federation manages its users by a local user management system. An identity provider (IdP) service is built on top of such an existing user management system, providing an interface to access authentication information and other attributes about the user, like name, affiliation and unique identifier. Every service provider (SP) in the federation can obtain this information by calling the IdP service. SPs process the data returned by the user's home IdP and use it to make access control decisions. Before users are allowed to use a service, they have to present a set of attributes issued by their IdP. These attributes are provided to users or to a service working on their behalf upon proper authentication of the user with the IdP.

First integration of federated model with the user management system of MetaCentrum was done a few years ago. After that we witnessed a sudden grow of applications, since the users could apply for a membership purely in an electronic way.

For many years MetaCentrum has contributes to operation and development of atlas of medical images. We managed to establish a service that is integrated

with 18 identity federations. This number of supported federation makes the atlases service rather unique world-wide. Experiences and links established with Atlases allowed us to quickly integrate a group of users from Austria collaborating with Czech researches.

In addition to exploring current technologies we also perform additional research and development of areas that target on addressing shortcommings of contemporary identity federations.

2 Moonshot

Moonshot[1] is a set of technology for providing federated access to applications. At a technical level, federation decouples management of credentials within an organization from authentication proofs between organizations. Many existing technologies such as Security Assertion Markup Language (SAML), RADIUS, and Diameter support federation. However these existing technologies are focused on a single application domain. SAML provides federation for the web and web services. RADIUS and Diameter provide federation for network access. Moonshot uses the Generic Security Services Application Programming Interface (GSS-API) to integrate RADIUS federation into most application protocols. At the same time, SAML is fully supported and provides rich attributes to describe federated subjects. Unlike other federation middlewares (e.g., Shibboleth), Moonshot is not tied with the web environment and can be utilized by non-web applications. The Moonshot architecture is based on open standards and the Moonshot community actively contributes to the ABFAB working group of the IETF. The Moonshot architecture is developed in a project funded jointly by JANEK-UK and the Geant EU project.

Unlike the majority of other systems that provide federated model, Moonshot does not rely on the web environment. Therefore, using Moonshot it is possible to adapt non-web services to leverage from federated model. The focus of the project is to support common services, ranging from Jabber to distributed filesystems. MetaCentrum seesk to explore ways how the Moonshot technology could be used to mediate access to the grids systems, both on the national and international level.

As a MetaCentrum contribution to the project, we intergated the Mooshot with the MyProxy service, which provides a bridge between the world of X.509 digital certificates and identity federations [1]. Later on we focused on utilizatio of the technology in the fields of common distributed filesystems, like NFSv4 and CIFS. We finished integration with the NFSv4 protocol and piloted an NFSv4 storage exposing Moonshot-authenticated shared [2].

[1] `http://www.project-moonshot.org/`

3 Aditi

Despite they are a big step forward, current identity federations also have several drawbacks like complete user control over the user's data, the ability to verify trustworthiness of the attributes issued by the IdP, the ability to combine attributes from different IdPs into one set, resistance against phishing and man-in-the-middle attacks. Therefore, we have designed a new system called Aditi [3], which is based on a concept of user centric identity federations.

The Aditi system enhances the standard federated model with new IdP and SP components operated directly by the user (user IdP and user SP, respectively) to provide an interface between the user and the services in the federation. Utilizing the User IdP (uIdP) the user maintains the attributes issued to them by other IdPs. The attributes are managed separately and can be organized into the cards, therefore the user can use the cards as a representation of different users' digital identities. Digital cards are analogous to the physical cards like payment or national ID cards. A user can provide the created cards through the uIdP to the SPs. Compared to the reality, a user can select only the subset of attributes (information) from the card that will be exposed to the SP, or can combine the attributes from different IdPs. A component, that helps users manage digital cards and attributes is called card selector. The card selector is responsible for requesting attributes from the IdPs and for preparing the set of attributes, which will be sent by the uIdP to the SP. Card selector in the Aditi is from the user's point of view similar to the CardSpace card selector, but in the inside it works completely different. CardsSpace card selector has a cards as a representation of the identity at the IdP, but the Aditi uses cards as a container of the attributes acquired from the IdPs.

The design of the architecture has been discussed at several events [4]. Since it builds up on the existing infrastructures without requiring huge modifications we believe that it will provide a reasonable way to address issues of current identity federations.

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Security Monitoring

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Abstract. In order to recognize the security risks and to address potential vulnerabilities in a timely manner, every larger infrastructure needs to maintain an oversight of the infrastructure from the security standpoint. Information produced by security monitoring is also important during assessment of new risks and vulnerabilities since it enables to identify the scope and impact of a potential security incident. The security team MetaCentrum focuses on development of security tools that enables to collect security-related information from the infrastructure and evaluate it easily.
Our main focus during the last was on the management of security patches and development of the Pakiti service, and on gathering syslog messages from the whole infrastructure and their efficient processing.

1 Pakiti

It is common practice for current cyber-attackers to misuse known vulnerabilities in operating systems and applications. It is therefore important for system administrators to make sure that security fixes are applied properly and in timely manner. Hence, one key area of operational security is monitoring how security patches have been applied. Knowledge gathered by several years of incident response teaches us that security patches not being applied properly significantly increase potential damage caused by the attackers since they have simpler access to the infrastructure.

In order to implement sufficient monitoring of patch management, we have been involved for several years in development of service Pakiti[1] [1]. The development is co-funded by the EGI CSIRT, which is another example of the fruitful collaboration among security teams on the European level.

Pakiti is a client/server solution with the server collecting information about installed software packages that is reported by the clients running on particular nodes of the infrastructure. The server evaluates the information and make the results of the evaluation available for further check

Pakiti is primarily focused on the Linux environment. The Pakiti client is a simple script that uses common commands to collect a list of RPM and/or DEB packages installed on the system. The Pakiti client does not require root privilege to be executed. Apart from the list of installed software package, Pakiti

[1] http://pakiti.sourceforge.net/

client also collects some additional information such as the version of the running Linux kernel and name of the Linux distribution etc. The Pakiti server is a central services which collects information reported by the Pakiti clients.

The Pakiti instance in MetaCentrum is integrated with the Nagios-based monitoring of the infrastructure, which ensures its complete monitoring coverage.

2 Monitoring based on system logs

A good security practice, which ease the operations of infrastructures as well as handling security incidents is a centralized log management. In the course of deploying a centrall syslog server we encounter several drawbacks that were necessary to address. One issue concerned with the way how log records are gathered. This step is usually easy to be done in a single institution for which common tools available today are just sufficient. However, if logs are collected from multiple different institutions and/or the infrastructure gets more complex, issues appear that did not expose at the smaller scope or were even not deemed important. hile collecting logs from a local environment it is usually acceptable for the institution to rely on physical security of the local network, which also provides a reasonably stable environment, so log records sent over UDP get lost only rarely. On the other hand, log collectors receiving data from multiple institutions (or multiple branches of a single institution) that are interconnected via the Internal must ensure confidentiality of the data transferred as well as a high level of fault tolerance. In order to provide a secure way of collecting the data we utilized the syslog-ng tools. In the course of its deployment, however we found out that it does not provide the functionality and we have to implement a few changes and improvements to the implementation. Most of the changes have been accepted by the syslog-ng maintainers and they will appear in mainstream.

Another principal problem concerns with the way how data is processed once it is collected and stored on the central service. The traditional way is setting up series of filters that detect some known patterns in incoming data. This mechanism can only be employed for patterns that are known in advance and can only be applied to new data. Sometimes it is therefore necessary to analyze the data collected. There are several common tools that can be utilized for that, like grep and other standard Unix commands. However, processing a large amount of data with these tools is very intensive, which makes them unusable for interactive work.

Based on these limitations we decided to explore alternative ways how logged data can be processed and examined. We combined together several open source solutions and built up an infrastructure to fast index log record and manipulate them in an easy and quick way. The solution is based on an internal cloud that runs the indexing tools, which continually process received logs. Being provided in a cloud, the indexing service can shrink or enlarge on demand, based on current amount of the data and requirements of the operators. On the top of the pre-processed results we run visualization tools that are used to access the data and manipulate with it via web interfaces, see e.g. Fig. 1.

Fig. 1. Web GUI showing SSH attacks

We also produced a set of tools to perform routine checks above the data collected. Using them it is possible for the security staff to obtain a quick overview of the whole infrastructure. The screenshot in Fig.2 shows an example of such a query.

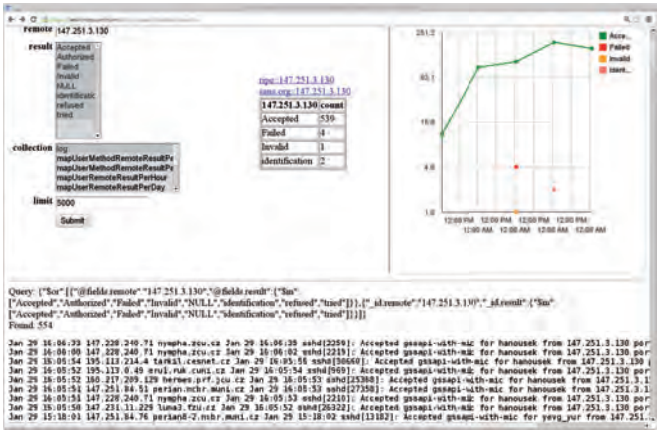

Fig. 2. SSH connections a cluster headnode to other nodes

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Perun

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Abstract. MetaCentrum became Czech National Grid Infrastructure (NGI) which means that apart from maintaining its own users and resources it also coordinates all national activities towards European Grid Initiative (EGI). That puts new requirements on all management systems used in MetaCentrum. Current user and resource management system used by MetaCentrum for more than 10 years has reached its technical and conceptual boundaries. It will be very hard to add new functionalities in order to accomplish new requirements. Therefore it has been decided to developed a new system called Perun as well as the old one. Apart from basic functionality which were adopted from the old Perun, new Perun additionally supports management of virtual organizations, users' registrations, acknowledgements via publications and many more. MetaCentrum NGI is able with new Perun easily support local as well as global virtual organizations and let them manage theirs users by theirs own.

1 Conceptual Schema

As Perun tries to cover management of the whole ecosystem around distributed services like distributed computing and storages, it must provide functionality to manage all the entities and theirs relationships. Core part of the Perun manages virtual organizations (VO), users, groups, facilities, resources and services. Other things like applications, notifications, configurations deployments, publications, data exports are managed by separated modules. As the concept of VO is well established in area of distributed computing like grids. VOs can be used also outside the grids environment for they ability to delegate responsibilities among its members, therefore Perun uses VOs as a core unit for user management. Facilities are managed separately from the VOs, so facility manager can provide his/her facility to the VO by defining rules under which VO users can use his/her facility.

2 Perun

As was mentioned, Perun consists of core and additional components which enhances the core. Perun core can be split into two parts. The first takes care of organizing users into the VOs and groups within the VOs. The second is targeting management of the facilities and resources. Currently Perun has components which manage users' publications, service configuration propagations, VO's applications, LDAP exporter, notifications, auditer and RPC. Next sections will highlight some interesting features of core and component.

Virtual Organizations Concept of virtual organization (VO) is well established in grid environment and MetaCentrum also runs one called MetaVO. VO can be briefly defined as a group of people which have similar interest. Membership in VO is defined by set of rules. Each VO has at least one person who represents the VO, he/she is responsible for making an agreements with resource providers. Perun has capabilities to support such VOs. Administrators, members and groups within the VO can be easily managed as well.

Group, User and Identity Management Most of the users have several different digital identities, such as an email account, institutional login, login to some social network, digital certificate, therefore we cannot force users to get another one in order to get access to the Perun. Perun was not designed as a primary source of the users' identities, all identities which can be managed by Perun must be from external sources. Perun only provides an evidence of such identities.

Identity consolidation is crucial in a world of federated identitites where services do not know user's identity in advance, therefore it is nearly impossible to make any authorization rules prior user access. User can register all his/her federated identities in Perun and than Perun can distribute that identities together with additional information like group memberships to the end servivces.

Users can be organized into the groups within VO, because in most cases only membership in the VO is not sufficient. Not only single group management is possible in the Perun, but also managing administrators of the groups. The right to the management of the group can be delegated to any member of the VO. Groups can be assigned on the resources which means allowing access to the group members on the resource.

Registrations Each VO manager can define set of prerequisites which have to be satisfied by the user in order to become member of the VO. Prerequisites are usually transformed into the registration form aka application. Registrar component provides necessary functionality to create such application. Applications can contain various input fields, each with its own value checking mechanism. Also extending user's membership in the VO can be managed by Registrar component. VO manager is able to set manual or automatic approval on the applications.

Publications Perun primarily targets on academic sphere, where users "pays" for the used resources by the acknowledgement in articles or publications. Every user can enter a citation of his/her publication into the Perun and select to which resource provider he/she wants to thanks. After that the resource provider can reward the user. In order to ease reporting of publications, Perun has a connector to the existing systems for publication management at the institutions, so that users can import citations directly from theirs home institution information system. Currently Peurn supports connectors to the information system of Masaryk University and University of West Bohemia.

2.1 Facilitites Management

Usually VO doesn't possess any resources, they are lend by academic or national institutions or commercial providers. Every resource has to be properly configured for every VO, therefore Perun provides tools for resources providers. Perun uses slightly different naming for the resources, it distinguishes resources and facilities. Facility is an entity which provides some services and needs to be configured. It can be cluster, software, data storage, web server and so on. Resource is basically virtual binding between a facility and a VO which specifies how exactly the VO can utilize the resource. Perun provides tools for creating facilities and setting up resources for VOs based on a mutual agreement between resource provider and VO. Such agreement is called service level definition (SLD) and specify conditions by which VO users can use the resource.

Services and Propagations To provide fine grained control over facilities and resources for individual VO users, Perun presents mechanism called *Perun services*. There are used to set up real services like access to host via SSH or creates unix accounts in some other system. Perun service ensures that target service will receive all necessary configuration information. Some of the information required by the service can be automatically generated by Perun, therefore an administrator of the facility and VO is requested to provide only basic information.

Component called *Engine* maintains configuration propagation on target services. It monitors all actions made in Perun and if some of the event represents change in any configuration file it fires processes which ends with updated configuration on all affected facilities. Engine plans propagations, so they are not flooded after every change occurred in Perun. Moreover, it monitors each propagation and tries to deliver configuration files repeatedly in there was an error.

2.2 Application Interfaces

There are several ways how to communicate with Perun. Users can access web based GUI or use CLI. Application developers can use Perl library, PHP binding or Java library in order to integrate Perun with theirs own applications. Online services can communicate using REST interface over secured HTTP.

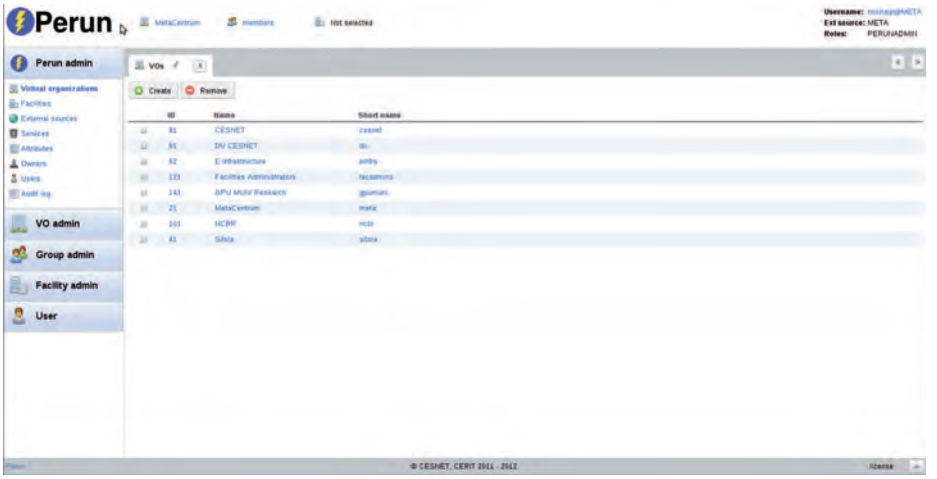

Fig. 1. Perun graphical user interface

2.3 Current Status

Perun currently manages over 1800 users organized in 18 virtual organizations, which have international as well as national scope. Over 27 services are managed and configured on more than 1500 machines.

2.4 Conclusion

As the old version of Perun didn't meet all requirements of the national grid infrastructure and lack support for managing virtual organization, development new Perun based on the latestes technologies was the only way. New Perun is designed not to support only national grid infrastructure, but also research communities outside the Czech Republic and also local partners of eInfrastructure initiative.

RT and RT/GGUS Interface

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Abstract. The RT: Request Tracker[1] [1] is the leading enterprise-grade open source issue tracking system. Metacentrum has been maintaining the RT instance already for more than 8 years. During the last two years the RT system used by Metacentrum was quite heavily modified to fit everyday needs of its users. The usage of the system shows a steady growth. Metacentrum provides another instance of the RT system for the EGI community, maintains the interface between the RT system and GGUS trouble ticket system and disseminates the know-how obtained through all these efforts. This article gives a brief overview about current RT development for Metacentrum needs.

1 RT4 Development and Deployment Status

A new major stable version of the RT system 4.0 was released last year, hence the RT instance maintained by the Metacentrum will inevitably become obsolete in the near future. Also direct upgrading of the current Metacentrum RT instance to any up-to-date RT version is very hard if not impossible at all mainly due to the number of modifications and customizations of the RT code made over the course of last couple of years. Moreover, CESNET maintains another small RT 3.7 instance for internal purposes which is rather ineffective. Under these circumstances we have decided to merge both Metacentrum and CESNET RT instances and deploy a new RT instance based on up-to-date stable upstream RT version 4.0.7. We have made some major decisions while modifying the RT4 to fit our needs:

- We have developed new authentication mechanism for the RT4 instance based on federated infrastructure allowing to accommodate users from different institutions and also allowing the users to use various authentication mechanisms based on what is provided by their identity providers.
- Users and groups management is done completely through the Perun user management solution[2] developed by MetaCentrum. RT then pulls the users and groups data from the Perun LDAP interface.
- We stick with the upstream RT version as much as possible to allow for easier future maintenance and updates.

[1] http://bestpractical.com/rt/
[2] http://www.metacentrum.cz/en/devel/perun/

- Nevertheless, we have ported parts of the functionality from our old RT3 instance. This applies especially to the RT/GGUS interface and processing of emails coming from international grid infrastructure (usually from various dashboards or other ticketing systems). The modifications to incoming email handling, email notifications handling and some minor changes related to the RT authentication procedure related to the adoption of Shibboleth[3] are the only modifications to the code of the vanilla RT system so far.
- As many modifications as possible are based on official RT extensions by Bestpractical or on extensions provided by the community through Perl CPAN. The rationale behind this is that much of the functionality we have developed for our current RT3 instance is now in some way available through supported extensions. On one hand this decision means that some functions will behave slightly differently (such as the accounting which we have completely developed in the past and now replaced by similar extension), on the other hand this decision considerably simplifies the RT maintenance and namely future updates. We currently use namely the following extensions on top of the default RT installation:
  - *LDAP Import* to allow for importing the users and user groups from external LDAP directory,
  - *Merge Users* to solve the issues of having affiliated with multiple institutions and thus having multiple identities. It is quite common that a user is affiliated with Cesnet and with his home university at the same time. Such users are coming with different identities when using different institutions identity providers. However, we sill want these users to have their tickets and user rights available in the RT system no matter which identity they used for authentication.
  - *Activity Reports* to provide a tool to gather accounting and statistical data based on the tickets in the RT database.
- We have developed tools allowing partial merge of both RT instances databases. This means especially merging existing tickets from both RT instances and the import of existing users including their user rights and merging them with user identities obtained from Perun.

The new RT instance based on RT 4.0.7 is due to be deployed in Q1 2013. The deployment will most probably happen early during the January 2013 in close cooperation with other groups within CESNET. We also suppose that the decisions we made through the course of RT4 development should allow to use this tool not only for Metacentrum and CESNET purposes but for the whole national e-Infrastructure and its users.

[3] `http://shibboleth.net/`

2 RT/GGUS Interface

The RT/GGUS interface saw a first major rewrite after the legacy GGUS web service interface was abandoned and replaced by a new one in the year 2012. The new GGUS web service interface was considerably simplified by dropping unused methods and method parameters[4].

We have been also further working on the RT/GGUS interface dissemination to other NGIs and groups interested in building their own ticketing system and connecting it to the GGUS. We have provided especially consultations and parts of the source code of our RT/GGUS interface to provide implementation guides for other ticketing systems than RT. In this way we have disseminated the interface to the following NGIs and groups in the year 2012:

- Spanish NREN RedIRIS for their RT ticketing system instance,
- National institute of nuclear and particle physics (IN2P3) of the CNRS for their OTRS ticketing system.

We were also shortly in contact with the team deploying a RT system for the PRACE association and offered our expertise for their RT/GGUS interface deployment.

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e-Infrastructure Research and Development:

Middleware Development

Middleware Development

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Abstract. Besides operating its own national grid environment—the MetaCentrum—CESNET has been a traditional participant in international projects to develop, operate and evolve large-scale high-throughput grids, and to promote their use within as well as outside Europe.

CESNET has been a partner in EU-driven grid deployment efforts since the European Data Grid project was first conceived in 2001. Since then, we have participated in a series of EU-funded Grid Computing projects to develop a comprehensive suite of grid middleware products. They were: the original *European DataGrid* project (EDG, 2001 – 2004), the *Enabling Grids for E-sciencE I–III* series of projects (EGEE, 2004 – 2010) and most recently the *European Middleware Initiative* (EMI, 2010 – 2013).

Currently, within the EMI project, CESNET maintains and develops several distinguished products providing grid security and monitoring solutions. Some of the products have started life as a part of the gLite middleware stack originally developed in the EDG/EGEE series of projects. Others were taken over or started afresh within EMI, where providers of different European grid platforms (gLite, dCache, ARC and Unicore) came together to consolidate, harmonize, evolve and extend their original products.

The middleware is used by the Worldwide LHC Computing Grid (WLCG), which is essential to the operation of the Large Hadron Collider (LHC) at CERN. Indeed, when CERN held a press conference in early Summer 2012 to announce the discovery of a new particle—presumed to be the theoretically predicted Higgs boson—grid computing was mentioned as a key element of that achievement. Through its participation in EMI, CESNET is also an important technology provider for the European Grid Infrastructure (EGI), a major European effort to provide access to high-throughput grid computing resources across Europe not only to particle physicists but also to scientists in other fields.

Grid Security Products

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Abstract. Having participated in a series of European grid middleware projects, CESNET has—over the years—assumed responsibility for several security products, which it now maintains and develops for use in the European Grid Infrastructure, the World LHC Computing Grid, and other distributed computing infrastructures. This article gives an overview of those products, explaining their purpose, history and current status.

Grid Security requires complex solutions to allow various grid components as well as end users access or delegate access not only to inputs and results but also to jobs at runtime, to their status, monitoring or accounting information, etc. Middleware solutions grouped in EMI implement GSI—the Grid Security Infrastructure specification—based on public key encryption, X.509 certificates, and the Secure Sockets Layer (SSL) communication protocol, with extensions for single sign-on and delegation.

CESNET participates in EMI's Security Area activities and assumes responsibility for several different products.

1 gLite ProxyRenewal

The grid security infrastructure uses short-lived security tokens in the form of proxy certificates to store and pass user credentials. The short-term credentials are used by grid components during the lifetime of a job to access various services such as storage or computing elements.

ProxyRenewal is a simple service intended for keeping proxy certificates valid throughout the lifetime of their respective compute jobs. Since a proxy certificate is typically issued for a few hours, which can be easily spent by the compute job waiting in queues, ProxyRenewal—in conjunction with the NCSA MyProxy service—maintains a repository where proxy certificates can be requested by the workload manager any time they are required.

ProxyRenewal was conceived in the EGEE project as a part of the gLite stack and is used in gLite WMS (Workload Management System) installations.

2 caNl—EMI's Common Authentication Library

As an original development in EMI, a set of libraries has been introduced to provide common authentication functions uniformly across different programming languages and different grid middlewares. Besides essential functions to open and maintain authenticated connections using X.501 certificates, there is also an interface for managing certificates and proxy certificates, performing functions such as proxy creation or signing. Development of the library still continues, and the newest additions include support of additional standards such as PKCS #11 (cryptographic tokens API) or OCSP (Online Certificate Status Protocol).

There are three language versions of the library following the same specification and maintaining compatibility on protocol level. CESNET is responsible for the C part of the library, while the Java and C++ versions are being developed by the University of Warsaw and the University of Oslo, respectively. CESNET has also been leading the overall caNl development effort within EMI.

3 GridSite

GridSite started life as a web application at the GridPP (UK Particle Physics Community) and gradually grew into a set of extensions to the Apache web server and a toolkit for Grid credentials, GACL access control lists and HTTP(s) protocol operations. The primary role of GridSite consists in controlling resource access (both read and write) based on X.509 user certificates loaded in standard Web browsers such as Mozilla Firefox. Access control is achieved through the mod_gridsite module for Apache.

During the EGEE series of project, GridSite was developed and maintained at the University of Manchester. CESNET took over at the start of the EMI project in April 2010 and since then was maintaining the product. As a new major development, GridSite was significantly refactored using caNl and a new major release (2.0) is scheduled for release with EMI-3 Monte Bianco in early 2013.

e-Infrastructure Research and Development:

Complex Monitoring and Accounting Development

Logging and Bookkeeping—Grid Process Monitoring

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Abstract. Logging and Bookkeeping (L&B) is a widely available job-centric grid monitoring service conceived by the European DataGrid project and subseqently evolved in successor grid middleware projects – the Enabling Grids for E-sciencE series and the European Middleware Initiative. With its generic design it now proves useful in monitoring all kinds of processes relevant to distributed computing. This article is going to introduce the motivation and essential principles of the L&B service.

Although originally envisioned as a part of gLite's Workload Management System, Logging and Bookkeeping (L&B) has evolved into a stand-alone service in its own right, used in monitoring all kinds of processes relevant to grid computing.

During their lifetime, grid jobs pass through multiple grid components and the execution path is not necessarily a straightforward one. It may branch off, for instance, when jobs get resubmitted for lack of response by the originally selected computing element. This makes the task of discerning the current status of a job or reconstructing its history rather complicated since no component has the complete picture and, what is worse, it is impossible to know which component has seen the job most recently in the first place. That is why the gLite middleware designers introduced L&B—a service to collect event messages from various grid components, keep their history and interpret them to make out their current state. In essence, L&B performs the following tasks:

- Unique identification of any single process, achieved through a hierarchical identifier (JobID).
- Reliable asynchronous (non-blocking) delivery of event messages. This is achieved by a two-stage delivery model where the local logging daemon accepts the message, authenticating the caller but performing no authorization, and stores the contents of the message locally. In the second step, the local copy is delivered by an interlogger daemon to its final destination—the L&B server. In this way, the synchronous part of the operation does not comprise any remote calls.
- Interpretation of the event messages. L&B supports different types of processes and implements state diagrams for all of them. The present solution has been designed to overcome irregularities in the incoming messages, such as events delivered out of order or not at all. This was made possible by the

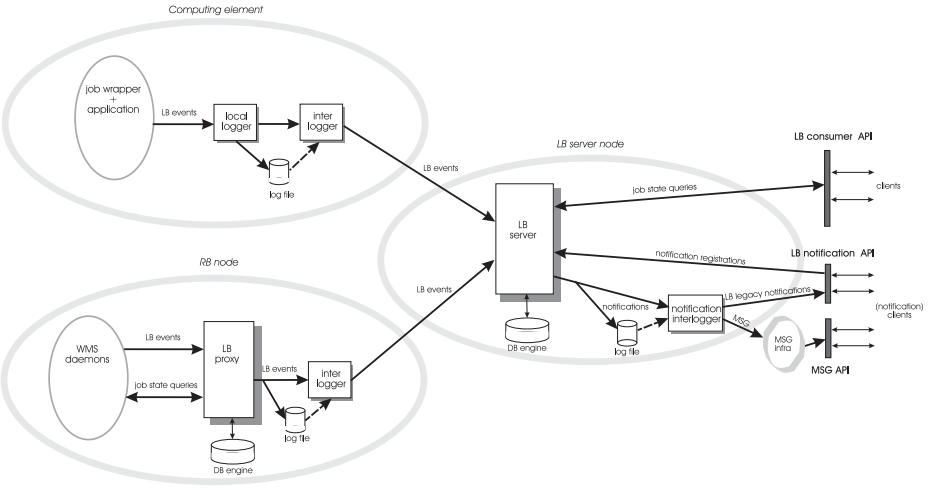

Fig. 1. Interactions of individual components in the delivery chain and the L&B server itself

introduction of event sequence codes—hierarchical counters wherein different components are incremented by different sources.

The overall architecture of the solution is illustrated by Fig. 1, which shows individual components of the L&B service deployed not only 0n the L&B server node but also in computing elements (CE nodes) and workload management systems (RB – Resource Broker nodes).

Information collected by L&B is made available over different channels following either the query/response model (L&B queries, HTTPs interface, Web-Services) or the subscribe/publish model (L&B notifications, messaging, RSS) – see Fig. 1.

Although originally intended primarily for gLite jobs and logical groupings thereof (collections, acyclic graphs), L&B also supports other types of grid-related processes such as native CREAM CE jobs or input/output sandbox transfers. A solution to monitor native PBS/Torque jobs has been prototyped in MetaCentrum and a demonstration was given at the EGI Technical Forum 2012 in Prague [2].

In a very recent development, we have acknowledged the obvious similarities between grid jobs and virtual machines, especially those provided by cloud or node-on-demand services [1]. The ability to monitor virtual machines together with their payload, i.e., grid jobs running on the virtual resources, and keep track of the mutual connection, has also been prototyped in MetaCentrum. Both virtualization solutions used in MetaCentrum—the widespread OpenNebula toolkit and the Magrathea manager for virtual clusters—have been tested with the new functionality.

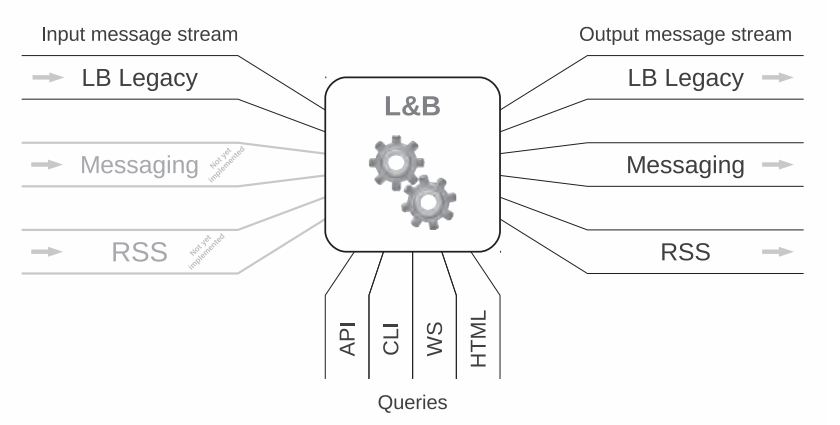

Fig. 2. LB as a message processor making processed information available over different channels

L&B has been present in all gLite and EMI releases and with over 120 L&B Server instances, it is a widespread and commonly available service across the European Grid Infrastructure. A new major version of the service will be released with the EMI-3 release in early 2013.

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PBSmon and Accounting

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Abstract. The MetaCentrum infrastructure is rather complex. It consist of clusters of physical machines hosting virtual machines which can be started or throttled back on demand. It employs two job planning systems with queues with various priorities. It is used by hundreds of users, who have different priorities based on their membership in groups owning physical machines and on their number of publications with acknowledgements to MetaCentrum.
And all of this can and does evolve over time. Physical machines get upgrades in their number of CPUs, or are moved from one cluster to another cluster. Both physical and virtual machines can also be reserved for certain purposes or can be in maintenance.
To make this complex infrastructure more comprehensible, MetaCentrum has a web application named **PBSmon**, which displayes the **current state** of the infrastructure. It displays the state of physical and virtual machines, jobs, job queues, and users, in the real time.
MetaCentrum also has another system, named **accounting**, which keeps **historical records** of the state of all the entities mentioned above. It is used to compute statistics over time periods.
This section describes how the PBSmon and Accounting systems work.

1 The Current State Visualisation - PBSmon

The PBSmon system is a web application featuring web pages representing the basic entities – jobs, users, machines, etc. – linked together by hyperlinks.

PBSmon reads its data from various sources. The most important sources are the PBS servers (Portable Batch System, Torque is a clone of PBS). The PBS servers provide information about *computing nodes*, which map to virtual or physical machines, *node properties, jobs* and *job queues*. Users' lognames are extracted from data about jobs.

Another source of information is a supportive system called **pbs cache**, which stores various information that the PBS server uses for job planning. It includes information about the mapping of virtual machines to physical machines, information about states of virtual machines, information about fairshare user rank, and information about sizes of local disks for scratch directories.

Other source of information is the Perun system, which generates lists of physical machines and their physical properties like the number of CPUs, and lists of users with more detailed information than is available from the PBS servers.

Information from all these sources – PBS servers, pbs cache, Perun – is integrated and made available in the form of web pages to MetaCentrum users.

The PBSmon system also features a so called *Personal View* page. The personal view is different for each user, and it displays the queues and machines that are accesible to the particular user. Not all users have access everywhere. There are dedicated job queues with assigned dedicated machines, available only for selected users. The selected users are usually described as members of a group. So PBSmon reads information about user membership in groups from system files on the machines hosting the PBS servers, reads the ACL (Access Control Lists) of job queues and machines from PBS servers, combines them together, and so it can tell to each user which job queues and machine the user can use.

The Personal View page also features *Command qsub refining* form, where a user can select parameters like number of CPU, size of memory, or node properties, for the **qsub** command that is used for submitting jobs, and the page then displays the machines that would fit the used parameters. Thus a user can see how many machines fit a given set of parameters, and estimate how long a job with such parameters would wait in a queue before start.

2 The MetaCentrum Historical Records - Accounting

While the PBSmon system displays the current state of MetaCentrum resources, the Accounting system keeps historical records.

The Accounting system consists of a relational database keeping the records, a set of sensors collecting data from computing nodes and the PBS servers, a cron script computing statistics on daily basis, and web interfaces for displaying the collected data and statistics about resources usage.

The database structure is rather complex, because it is modeled after the complex MetaCentrum infrastructure. The database must be able to answer queries like *Which physical machines with how many CPUs were in a give cluster on a given day?* or *What portion of available CPU-time of the physical machines was utilized by jobs running on the virtual machines that were running on the physical machines on a given day ?*

The database keeps information about entities and their relations in time, for example in which time interval a physical machine had a certain number of CPUs, in which time interval it belonged into a given cluster, etc.

The sensors collect data about jobs from the PBS servers by reading their logs, and also collect data about processes of jobs from kernel accounting of operating systems on computing nodes.

The data collected by sensors are on daily basis processed to statistics. The processing is complex. Basically it computes the number of CPU-seconds that were available on a given cluster on a given day by multiplying the number of CPU in the cluster on that day with the number of seconds in that day, taking into account machines in maintenance and the special days with change in daylight savings time. That resulting number of CPU-seconds is considered as

100 %. Then the number of CPU-seconds utilised by jobs and special reservations is computed, taking into account mapping of jobs to computing nodes and mapping of computing nodes to physical machines. The ratio of utilized CPU-seconds to available CPU-seconds is considered as the cluster utilization on that day and saved to the database.

Web interface then enables generating graphs of this computed utilisation of clusters for selected time periods.

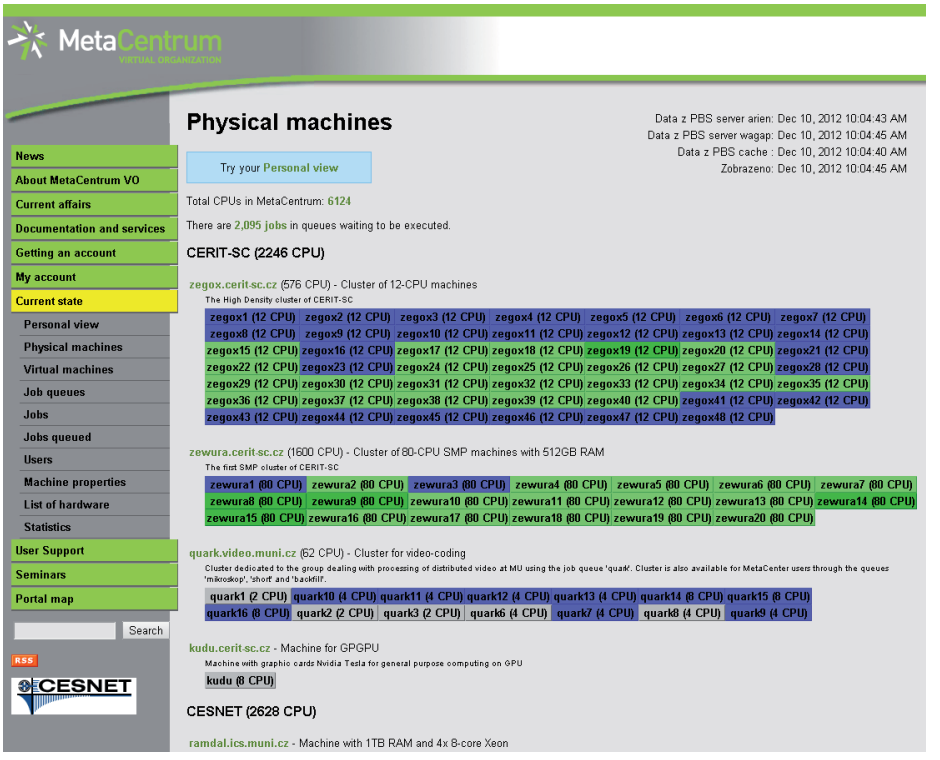

Fig. 1. Screen shot of the web page with overview of state of physical machines in PBSmon.

Part III

Research Collaboration/Support

Foreword

Apart from providing a computing and storage resources as well as coordinating the national grid infrastructure, MetaCentrum supports research collaborations with its end users and research teams. These close collaborations aim to apply cutting-edge ICT technologies on the research problems the users cope with, trying to help them to get over specific IT-related issues that require non-trivial e-infrastructure support (e.g., paralelisation, new computation methods, computer modeling and simulation, huge data manipulation, new algorithms, etc.). The goal of these collaborations is to help the users to overcome their current research problems/limitations, so that new research problems/areas may arise. These collaborations are primarily coordinated by the Center CERIT-SC (CERIT Scientific Cloud)—the national center providing significant computing an storage resources integrated to the MetaCentrum national grid infrastructure, thus being an important partner of the national e-Infrastructure. In this part of the Yearbook, a few such collaborations are described.

Research Collaboration/Support:

Research Collaborations

Three-dimensional Tree Reconstructions from Terrestrial LiDAR Scans

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Abstract. In 2012, the CERIT-SC centre has started a new research project with the *Global Change Research centre AS CR, v.v.i (CzechGlobe)* (directed by Proff. Michal V. Marek), specifically with its *Remote Sensing department* (led by assoc. prof. František Zemek).
The goal of this project was to find a method for automated creation of tree mock-ups (especially spruce trees, which the group mainly focuses on) like 3D objects from their laser scan measurements (performed by LiDAR scans)—actually, such a method would significantly reduce the manpower necessary for proper parameterization of the subsequently used DART model (which is able to import 3D tree mock-ups and perform its automated parametrization), and mainly improve the details of such a parametrization.
Even though several methods for tree reconstructions based on their LiDAR scans exist, no one is applicable on the data the CzechGlobe centre is working with—the reasons are that the required precise and high-resolution LiDAR scans are very hard to obtain for mature spruce trees (because of large "gaps" in the point cloud induced by the tree foliage), or the proposed methods do not focus on precise reconstruction of branches (which, however, would result in an inaccuracy in the subsequent use). Because of these reasons, we have proposed and implemented a novel, fully-automated method for tree reconstructions, which is able to cope with occlusion-induced artefacts.

1 Introduction

The Remote Sensing department of the *Global Change Research centre AS CR, v.v.i (CzechGlobe)* focuses on physical-based retrievals of biophysical and biochemical parameters of vegetation from remotely-sensed airborne/satellite spectrometric image data, and on laboratory/field spectroscopy of plants in general. One of the approaches developed by CzechGlobe is based on coupling the leaf radiative transfer model [4] with the discrete anisotropic radiative transfer [3] model in order to retrieve total chlorophyll content of a complex Norway spruce

canopy from airborne hyperspectral data acquired at very high spatial resolution [5,7].

The DART model provides rather realistic representation of forest canopies, which requires a number of input structural parameters describing the optical and structural properties of canopy elements. Structural parameterization (tree dimensions and spatial distribution of leaf and woody elements within a crown) at very high spatial resolution is a difficult task, especially in the case of mature forests, because direct (destructive) measurements are hardly feasible. Therefore, structural parameterization of mature Norway spruce canopies is usually based on the in situ measurements and laser scanning.

The basic input model parameters, characterizing experimental spruce canopy, could be also obtained from the LiDAR point datasets—the datasets, that had been acquired by the *LiDAR (terrestrial Light Detection And Ranging)* systems that record the 3D position of objects (trees in this case) within the scanner field of view by measuring the time delay between the transmission of a laser pulse and the detection of the return pulse reflected from the target. Such datasets need to be manually processed in order to get the parameters characterizing the experimental spruce canopy.

Since recent developments of the DART model allow importing a tree mock-up into the model like a 3D object [1], a direct and automated creation of the tree mock-ups from the laser scan measurements could significantly improve the accuracy and details of the models, and even reduce the manpower necessary for proper model parameterization. To obtain the tree mock-ups from their laser scan measurements, there have been several methods [2,6] already proposed.

However, employing the existing methods on reconstructions the spruce trees, which the CzechGlobe centre focuses their study on, becomes impossible since these methods either require a precise and high-resolution LiDAR scans (densely and uniformly sampled data, which are—especially for the mature spruce trees—very hard to obtain because of large "gaps" in the point cloud induced by the tree foliage), or do not focus on precise reconstruction of branches (however, such an inaccuracy could significantly influence their subsequent use within the DART model).

To overcome these issues, we have started a collaboration with the CzechGlobe centre, which resulted in proposing a novel methodology for reconstructing 3D tree architectures from terrestrial LiDAR scans. Our methodology is fully automated, does not require high-resolution LiDAR scans, and is further fairly insensitive to occlusion-induced artefacts in the 3D point clouds.

1.1 Input Data

The laser scans we are working with were obtained by the CzechGlobe centre at selected locations around village *Kvilda* in *Šumava* mountains in the Czech Republic using the *OPTECH Ilris*–3_6D terrestrial laser scanner (Figure 1) in October, 2009.

A total of 15 spruce trees were scanned from 7 different standpoints in order to obtain 4 different scans of each intended tree: from its "front"/"back" side, both of which recording first/last reflection of the laser beam – thus getting a cloud of 3D points along with a beam reflection intensity of each of them.

The raw data files were processed using the *PolyWorks IMSurvey* software, where the scans were split into individual trees, and each tree points were manually divided into the *foliage* and *wooden* part via thresholding by the intensity value (the wooden parts do usually have a higher reflectivity than the leaves).

Fig. 1. OPTECH Ilris–3_6D

2 Proposed Algorithm

As mentioned before, we have developed a novel method for reconstructing the tree branch structure from a given 3D point cloud data that tries to overcome mentioned limitations of existing algorithms in order to be applicable on reconstructing the mature spruce trees, and thus be applicable on the data the CzechGlobe centre is working with.

Our method has been inspired by the algorithm described in [2]; however, we have adapted its steps in order to cope with "gaps" in the point cloud, and proposed several additional steps supporting the full reconstruction of the tree branch structure. The general idea behind our algorithm is to identify individual parts of the reconstructed tree (i.e., to find branch-like structure in every such part) and to interconnect all the components in order to form the final tree branch structure.

Currently, the capabilities of our algorithm are being checked by comparing its fully-automated reconstructions with reconstructions performed on manual/semi-manual basis. Once finished, we plan to present the details behind the method—besides going to present it in [9,10], we would like to present it in a conference/journal focusing on remote sensing of environment as well.

3 Conclusions

As stated before, the goal of this efforts arised from the impossibility of employing the existing approaches to tree reconstructions on spruce trees, being studied by our research partner—the Global Change Research centre AS CR, v.v.i (CzechGlobe)—who focuses on physical-based retrievals of biophysical and biochemical parameters of vegetation (including, but not limited to spruce trees) from remotely-sensed airborne/satellite spectrometric image data.

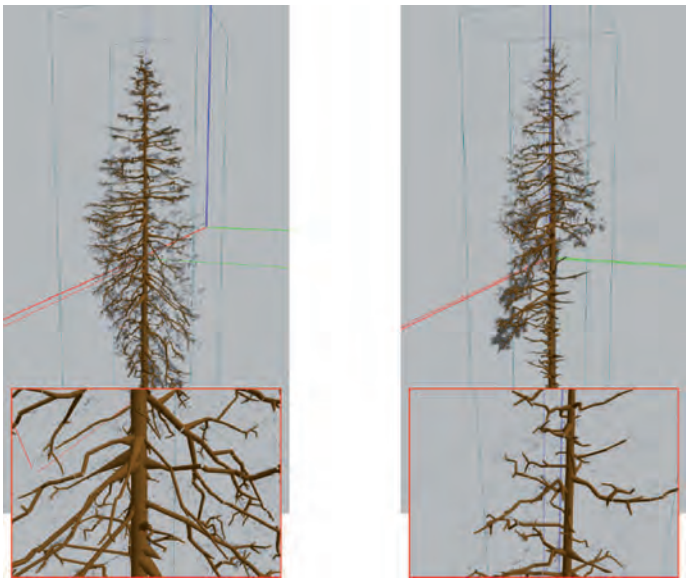

Fig. 2. An example of two fully-reconstructed spruce trees.

Since the existing approaches fail on reconstructing the trees being represented by a sparse and non-uniform 3D LiDAR point clouds, we have proposed a novel algorithm for as precise as possible reconstructions of the 3D spruce tree architectures—the proposed (and already implemented) algorithm is fully automated, does not require high-resolution LiDAR scans, and is further fairly insensitive to occlusion-induced artefacts in the 3D point clouds. Thus, the reconstructed mock-ups could be used for further processing within the DART model by the CzechGlobe centre.

Regarding the future work, besides its publication, we would like to implement the foliage reconstruction, most probably using an open L-System growth grammar [8], where each small branch/point will be attracted by the real-foliage points that were scanned. Furthermore, since most of the steps of the proposed algorithm are independent on the type of the reconstructed tree (the only step assuming the spruce trees is trunk construction, where a straight, non-dividing trunk is supposed), we would like to adapt and test it on trees of different type (which could be easier to reconstruct, since the deciduous trees are usually scanned during the non-vegetative period, which introduces better laser scans and smaller gaps in the dataset).

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Computational neurosciences

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Abstract. The field of neuroscience is currently enjoying vivid development due to recent improvements in relevant imaging technologies and available processing power necessary for the evaluation of acquired data. Moving towards more complex statistical methods and methods based on mathematical models of the brain function is contingent on availability of adequate computational resources.

Several groups in Brno collaborate on the study of human brain and mind. The neurology clinic of the St. Anne's University Hospital is responsible for the clinical part of the research, while the Institute of Scientific Instruments of the ASCR and the Department of Biomedical Engineering of FEEC BTU provide experience and theoretical background in the image and signal processing. All activities are coordinated by Prof. MUDr. Milan Brázdil, Ph.D. under the CEITEC Brain and Mind Research programme.

Neuroscience makes use of numerous imaging modalities to study the structure and function of the brain. The CEITEC group uses functional magnetic resonance (fMRI), scalp electroencephalography (EEG), simultaneous EEG and fMRI, and stereoelectroencephalography (SEEG). As the acquisition technology is evolving, processing of the measurement data and developing new methodologies requires nontrivial computational resources, both in terms of memory and processing power.

Refining the methods for the preprocessing and statistical evaluation of the time-volumetric fMRI data is done among others by Monte-Carlo simulations. These simulations are repeated for many values from given parameter space and are therefore well suited for processing on the computational grid in batch manner.

Main field of cooperation is currently the analysis of the intracranial SEEG recordings. In recent generations of the acquisition system the sampling frequency grew up to 5 kHz and the number of simultaneously recorder channels to 200. Processing of data of such size is behind the possibilities of sequential tools and requires parallelization of the algorithms and more complex tools to harness the power of contemporary high performance workstations. Moreover data of this size and the results of the analysis cannot be visualized by naive methods and more effective approaches need to be devised.

1 fMRI: functional and effective connectivity

It is agreed, that the brain is build according the principles of functional segregation and integration. The current challenge lies in formulating mathematical models capturing the basic principles of brain function on several levels of detail and validate them on measured data.

fMRI produces time-volumetric images of brain activity based on blood-oxygenation level dependent contrast. Several effects can attribute to distortion of these images: movement of the head, scanner field non-uniformities, physiological changes, etc. The methods involved in removing these artifacts contain numerous parameters, and the success of the preprocessing step depends on their careful setting.

In the next step, the data are analyzed in terms of both functional and effective connectivity [1]. The functional dependencies capture the statistical relationships in the brain activity patterns (correlations, coherence, transfer entropy, ...). The effective connectivity describes the causal relationship or coupling between the active areas. The methodology for reconstruction of this coupling from measured data is still under development and can easily run out of computational resources if too complex models are applied on large brain areas.

Dynamic causal modeling (DCM) [3] is one such a method, which has received a lot of attention recently. It models the brain as neural populations (consisting of excitatory and inhibitory subpopulations) coupled with possibly bidirectional connections. This model is described by differential equations describing the hidden (directly unobservable) states of the model and their influence on the observables (measured signal). Inversion of this model enables the researchers to make inferences on the neural interactions underlying specific responses of the brain on given event or task.

2 SEEG analysis

The measurements of brain activity are in the case of SEEG more direct compared to the fMRI. Deep electrodes implanted directly to the brains of patients with pharmacoresistant epilepsy can measure the electrophysiological activity of the surrounding brain matter. Resulting measurements have high temporal and low spatial resolution and the analysis requires therefore different set of methods. Processing these signals involves visual inspection, segmenting, frequency band filtering and statistical evaluation (cross-correlation of time-signal, coherence, power envelope, ...) [5]. With the high sampling frequency and a need for interactive analysis of the signals on various levels of detail, visualization becomes challenging task. Moreover the requirement of reasonable interactivity poses additional constraints on the tools and the used computational architecture.

Furthermore, to move beyond the analysis of functional dependencies it is necessary to tailor the methods for effective connectivity to the SEEG specific characteristics (limited spatial resolution, limited validity of the far field approximation, etc.) [4, 2]. Refinement and validation of suitable methods will require experience with implementation of demanding numerical computations and appropriate infrastructure.

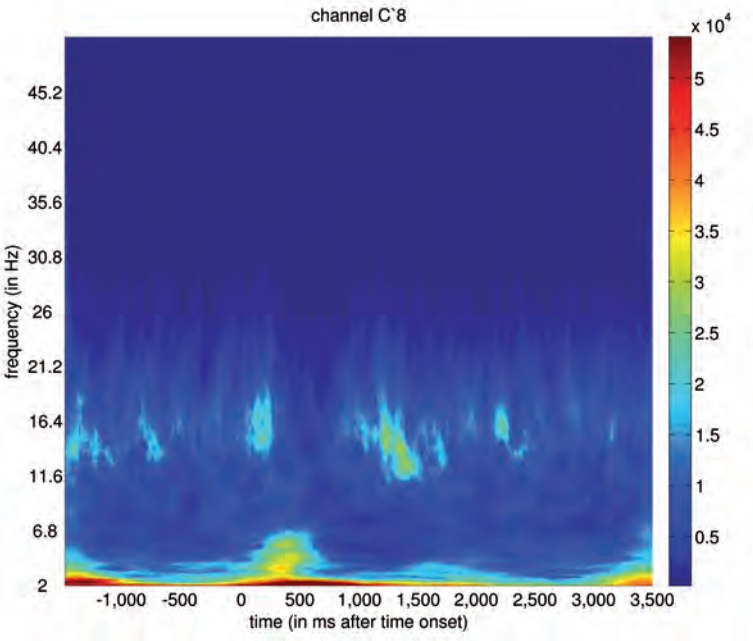

Fig. 1. Event-related SEEG time-frequency analysis: average response to target stimulus on one electrode placed in middle temporal gyrus. Currently in this resolution, the computation for 2 stimuli and 5 electrodes takes 7 hours and requires 49 GB of RAM.

3 Current state of collaboration

At present, we are helping the members of affiliated groups with moving the suitable parts of computations on the MetaCentrum resources. We are also working on modifying the SEEG analysis and visualization to cope with higher sampling frequency and number of channels with the help of modern hardware architectures. Furthermore, we are working on the application of the DCM on the SEEG data, previously studied with classical techniques. This should provide more detailed insight on the structure of the dynamical system underlying the generation of the observed data.

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Web-based Virtual Microscopy Using JPEG2000

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Abstract. Keeping high quality digital slides for purposes of virtual microscopy requires high capacity high performance storage system. Image compression algorithm used to compress and store digital slides can influence storage space utilisation, number of files stored, and overall latency of virtual microscope which affects user experience. In this paper, we show that using JPEG2000 storage format (1) size of stored files is reduced by 57% while image quality is preserved, (2) number of stored files is reduced, and (3) slides loading latency is reduced by up to 9×.

1 Introduction

Virtual microscopy [5] has been utilized for teaching or research purposes and is emerging technology in domain of diagnostic practice [4]. The idea of virtual microscopy being used for hypertext atlases for diagnostic purposes started at about 1996; in 1997 we had the first version of the Atlas of Dermatopathology. Later other atlases (Pathology of the Newborn, Pathology of the Bone Marrow, Fetopathology and Atlas of Pathology) were added.

In addition to elementary functionality (zooming and focussing), the digital technology behind the virtual microscope brings several benefits. First, the pathologist easily obtains photos of the examined tissue as they already exist in digital domain. Second, the virtual microscope can extend control possibilities. Virtual microscope can zoom selected areas, seamlessly change zoom levels, trace actions providing back and forward navigation through history of actions, show preview together with zoomed tissue and so on. Digital scans of the tissues can be stored online and thereafter they are instantly available for the virtual microscope compared to traditional archives of tissues for the real microscope. Virtual microscopy thus also enables instant remote consultation and telepathology [1].

From the beginning, the Atlases are supported by CESNET—the Metacenter computing facilities are used to prepare and store the images, and to design and optimize the web-based virtual microscope in terms of performance and usability as a whole. Over time, the Atlases gained high importance in the community—there is a long list of participating pathologists, dermatopathologists, dermatologists and clinicians (prof. Günter Burg from Zürich university, prof. Jeffrey Cao from Loma Linda Medical Center, California, Spasoje Radovanovic, prof. Hana Jedlikov and many others, as well as authors of individual atlases, Marta

Jeov, Mojmr Moulis, Vra Feitov). Recently, we have also obtained the grant support for creation of teaching atlas of human pathology with clinical correlations: PATH-atlas: using hypertext documents for teaching pathology (OPVK, CZ.1.07/2.2.00/28.0045). This hypertext teaching material should contain texts and images of different modalities (histology, clinical pictures, images from CT, MRI etc.).

In this paper, the optimization of the processing required to process the images, which are provided by the virtual microscope application, is discussed.

2 Virtual Microscope

We designed the virtual microscope as a client-server application. Digital images of scanned tissues are stored on the server and are downloaded to a displaying device (client) when required.

Scanned images are, however, extremely large. Their size is above 100,000 × 100,000 pixels taking several gigabytes of disk space. Therefore it is not feasible to read and send the whole scanned image to the display device—the transfer of several gigabytes is not instant and displaying such a huge image is computationally very intensive. Instead, we send the image piecewise and on demand, i.e., only actually visible parts of the image are sent. But common image compression standards do not support extremely large images together with fast extraction of required pieces. Therefore, we split the image into the small pieces (tiles) which are adequately compressed and stored on disk. Each such tile is then directly accessible and can be sent to the display device on demand. In this way we process each focus level of every tissue. The described procedure is satisfactory for manual focusing and panning. For zooming, further processing is needed. We scale down the scanned images to get smaller zoom levels. We scale them to half of the original size then scale the result to half size and so on, until we get small enough image that can fit into virtual microscope. In each step of scaling procedure, we split the scaled image into tiles which are stored on disk. We call this design *traditional storage organisation*.

2.1 Limitations of our Traditional Storage Organisation

Huge number of files. The image tiles must be small enough (commonly used sizes are 256 × 256 pixels or 512 × 512 pixels) so that bandwidth between the server and the client is not wasted and the tiles are displayed almost instantly. Small tiles results in enormous explosion in number of files stored. E.g., single tissues scan, having 100,000 × 100,000 pixels in dimension, presents about 530,000 tiles including 7 focus levels.

Zoom levels. For every additional zoom level a scaled clone of the original image has to be stored. This introduces further storage capacity consumption and also further explosion in number of files stored. For 8 zoom levels the disk usage and number of files grows about 33%.

3 JPEG2000

JPEG2000 [3] is recent image compression standard providing not only compression performance superior to the current JPEG standard but the intent was also to provide advanced features which include lossless image compression for immutable image archiving. Effective file organization enables fast access to particular locations of large images therefore there is no need to split original image into many smaller tiles and store them as separate files. Without any volume growth, JPEG2000 compressed file can contain several resolution representations of original image and also several quality layers.

3.1 Multiple Resolution Representation

Once compressed, JPEG2000 file can be decompressed directly into different resolution representations without a need for explicit resizing. A smaller resolution representation can be then used for preview or image overview purposes. This can be also of advantage in case when zoom-like behaviour is to be implemented by an application as in case of virtual microscope where zooming is the essential functionality.

Another advantage over other image formats is the fact that all resolution levels are contained within a single file, so there is no explosion in number of stored files. Moreover, due to the DWT decomposition property, the growing number of zoom levels does not have undesirable impact on size of resulting JPEG2000 file—i.e. the size of compressed file remain approximately the same regardless the number of zoom (DWT decomposition) levels. In fact, the DWT levels have positive impact on compression performance.

4 Web-based Virtual Microscope Interface

Further we describe our prototype implementation of the virtual microscope. It comprises two parts: (1) Image preparation and (2) Image presentation. Image preparation process begins at digital camera equipped microscope that creates digital image if the tissue (image acquisition). This digital image is further processed as described in the following subsection. Image presentation describes required processing to present the stored tissue to the users.

4.1 Image Preparation

Image acquisition process stores gigapixel images into PNG graphic container. This PNG file is further converted into JPEG2000 format using lossy compression to save disk space, the PNG file is offloaded to tapes. JPEG2000 format is not ready as archiving container because of its limited support in existing applications such as image viewers or editors.

There are several encoder tools for JPEG2000 such as OpenJPEG[3], Jasper[4], or Kakadu [5]. The former two are free encoders, the latter is commercial encoder. Unfortunately, neither of them supports PNG format in usable form. Kakadu and Jasper do not support PNG at all, OpenJPEG supports PNG format but it decompresses whole image into memory buffer which is not possible with 10 gigapixels images (such image consumes about 40 GB of memory). Therefore, the PNG image has to be converted into PPM format before conversion can be done. We use Kakadu encoder as this is the fastest encoder from mentioned set.

JPEG2000 Compression Process The converted image has to be virtually split into tiles so that whole image does not have to be loaded into memory. We use 16384×16384 pixels and their size influences the speed of extraction of small zoom levels from JPEG2000 container (the bigger tile, the faster extraction, however, the bigger tile, the more memory during compression is used).

4.2 Image Presentation

We utilise JPEG2000 features which allow us to quickly extract a desired tile of particular zoom level from the file. This extracted tile can be either in JPEG2000 format or in uncompressed RGB format. While the web browsers are unable to display JPEG2000 format directly, we use uncompressed RGB output and convert it into JPEG. This re-compression is provided by image server[6] (IIP Image server). The image server runs on web servers that have direct access to JPEG2000 files. Benefits from JPEG2000 formats are moderated by required CPU processing power (for JPEG2000 $\rightarrow$ raw RGB $\rightarrow$ JPEG conversion).

IIP Image server supports several clients (i.e., prefabricated web based applications) such as Zoomify[7], IIPZoom, IIPMooViewer, Jiip[8], and 3rd party clients. According to our experience, Flash and Java clients are not supported in all browsers without problems (Flash blocking add-ons are popular, some platforms do not support Flash at all, Java is commonly disabled rather than enabled). This experience makes Zoomify (Flash based) and Jiip (Java based) clients unsuitable. IIPMooViewer has only limited features for virtual microscope usage. Prefabricated clients usually supports only zoom and pan on a single image. Virtual microscope needs to switch images as users switch focus layers on the fly. Our microscope also supports annotations which are graphic marks on the image that show interesting spots to the user. This is feature which prefabricated clients do not possess. Therefore, we developed our own client purely in Javascript language.

[3] `http://www.openjpeg.org/`
[4] `http://www.ece.uvic.ca/~mdadams/jasper/`
[5] `http://www.kakadusoftware.com/`
[6] `http://iipimage.sourceforge.net/`
[7] `http://www.zoomify.com/`
[8] `http://iipimage.sourceforge.net`

5 Prototype Evaluation

The prototype implementation had to find answer whether transition from traditional storage organization in many JPEG files to JPEG2000 is worth of. We considered and evaluated several criteria. With transition to JPEG2000, we expected that 1) disk space usage and number of stored files will be reduced, 2) server load will be high.

5.1 Disk Space Reduction

Traditional storage organization in many JPEG files took significant amount of disk space. Up to day, we store about 3,000 scanned tissues taking about 3.4 TB of disk space and also taking 150 millions of files. Largest scans ($180,000 \times 150,000$ px) take 70 GB (including all five focus planes) and have 2.7 millions of files.

Conversion to JPEG2000 can save 33% of disk space using same compression ratio as stored JPEG tiles as we do not have to store individual zoom levels. Disk space saving is derived from the following equation:

$$\sum_{i=1}^{zoom\_levels} image\_size * \frac{1}{4^i} \doteq 0.33$$

The same equation holds for the number of files, without zoom levels, the number of stored files is cut by 33%. However, as we do not store individual tiles in JPEG2000 but the whole tissue in a single file, we reduce the number of stored files to one single file.

Our JPEG tiles were stored using quality level 95 which corresponds according to PSNR metrics [2] to 6 bits per pixel in JPEG2000 for small files below 2000 pixels width and to 2.4 bits per pixel (1:10) for large files above 16384 pixels width. Using compression 1:10 and storing only a single file, we can save additional 26% of disk space.

Using JPEG2000, we can significantly reduce number of stored files from millions to few for a single tissue and disk space can be halved.

5.2 Server Load

Traditional storage organization in many JPEG files did not impose high server load. The server performance was limited by disk subsystem power—i.e.,how fast can be a tile looked up in a directory and how fast can be read from the disk–rather than CPU power.

Using JPEG2000 for image storage demands CPU power in two tasks: 1) JPEG2000 decompression, 2) JPEG compression. In the former task, part of JPEG2000 has to be read from disk and decompressed (CPU intensive task). In the latter task, the decompressed image has to be compressed into standard JPEG format so that browser is able to display it.

We compared both traditional JPEG tiles with JPEG2000 tile extraction. We used our production server hosting `http://atlases.muni.cz` so that tests are from real environment. The server is equipped with 24GB RAM, 12 physical CPU cores at 2.93GHz. The server is equipped with 1Gbps NIC. The server used directly attached RAID 5 disk array consisting of 16 disks. The client is equipped with 4GB RAM, 2 physical CPU cores at 2.4GHz and 1Gbps NIC. We use standard Debian distribution except two libraries: 1) We use Kakadu library for fast JPEG2000 decompression/extraction, 2) We use MMX enabled libjpeg[9] for fast JPEG compression. For our tests, we used gigapixel image having $176,000 \times 148,000$ px.

We measured duration of HTTP GET request for 300 of tiles. We compared latency for individual zoom levels of traditional JPEG storage organisation with new JPEG2000 storage schema including recompression to JPEG. Results can be found in Fig. 1.

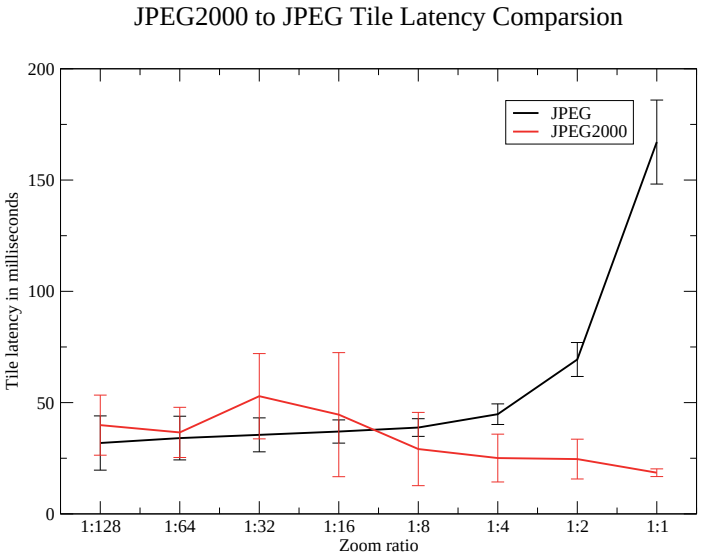

Fig. 1. Latency of request-response action of getting tile from JPEG an JPEG2000

Traditional JPEG tiles were served at rates 6 to 32 tiles/sec. JPEG2000 tiles (extracted and recompressed) were served at rates 19 to 54 tiles/sec. These numbers correspond to 0.2 to 1 full HD (1920×1080) frames per second for JPEG tiles and to 0.6 to 1.7 full HD frames per second for JPEG2000 tiles.

[9] `http://sourceforge.net/projects/libjpeg-turbo/`

Traditional JPEG tiles suffer from large number of tiles for zoom ratio close to 1:1. In such a case, our testing image had 500,000 tiles. Looking up individual tile takes some time. For this reason, latency increases with decreasing zoom ratio. JPEG2000 does not have this problem, tile latency for individual zoom ratios is dependent on internal JPEG2000 structures.

6 Conclusions

Our web-based virtual microscopy application[10] contains over 3,000 of scanned pathological images. These images are stored as hundreds of millions JPEG files which a) becomes running of of available disk space, b) poses a problem with archiving and maintaining.

Using JPEG2000, we were able to reduce consumed disk space by 57% while image quality is preserved, able to reduce number of files from hundreds of millions to tens of thousands. We demonstrated that these benefits further improve slides loading latency in some cases by up to 9×.

Our approach of adoption of JPEG2000 for tissue storage enables us to use the same web-based virtual microscope application that we were using with standard JPEG files. Such approach eases gradual transition from JPEG to JPEG2000.

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[10] `http://atlases.muni.cz`

De novo sequencing of *Trifolium pratense* genome, assembly software and read error correction evaluation

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Abstract. New generation sequencing (NGS) technologies enable us to generate large amount of sequence data with sufficiently low costs but it is compensated by our increased reliability on computer processing of these data. Red clover (*Trifolium pratense*) is very important plant from leguminous family from which already three species have been sequenced. Nevertheless, its medium sized genome seems to be challenging for the recent possibilities of hardware and software as well. Therefore, we firstly used a testing datasets with different error rates created from chromosome 2 of *Medicago truncatula* for assessment of several quite often used and a few just recently developed de novo assembling programs in terms of contiguity and accuracy of the assembly. Afterwards, we used the best one in the *de novo* assembly of the real datasets of *T. pratense* (original, two 3'-end trimmed and quality trimmed dataset).

1 Introduction

DNA sequencing is the process of determining the precise order of nucleotides within studied DNA molecule. Due to our technological inability to sequence whole length of one DNA molecule, this molecule is fragmented into smaller parts which are sequenced and the original sequence is being reconstructed based on the overlaps. Sequencing project often aims at very long DNA strands, such as chromosomes or whole genomes. Until recently, Sanger sequencing was the most common method used for sequencing [1]; however, it was expensive and laborious. This sequencing approach includes cutting of large DNA pieces into shorter DNA fragments, which are then cloned (amplified) and individually sequenced. Due to long read lengths, the assembly back to sequence matching the original one, is relatively easy task. However to sequence the human genome (3.2 Gbp), the costs were $2.7 billion and project lasted for 13 years[2].

Recently, new generation sequencing (NGS) technologies are revolutionizing molecular biology[3], as they have lowered the costs per sequenced nucleotide and increased throughput by orders of magnitude. New sequencing approaches allow to generate gigabases of nucleotide per week (1Gbp for $41; generating up to 600

Gbp per 11 days long run in Illumina HighSeq 2000[4]). However, compared to Sanger sequencing, NGS high-throughput techniques produce reads of shorter length which increases both hardware and software demands on reconstruction of the original sequence.

Initially, the NGS were successfully used in resequencing projects[5] aiming to describe the variability within previously sequenced model organisms. With the progress of read lenght from 36 bp to 100 bp also *de novo* sequencing project appeared (*de novo* translates from Latin as 'from the beginning', and it means determination of sequence in species with no previously known pattern of the sequence = reference). Since then, many projects have aimed at *de novo* sequencing or re-sequencing of various organisms ([6],[7], [8], [9]) and many more projects are currently in progress.

Nowadays, the most prevalent sequencing technologies are based on generating paired-end reads. In this approach, DNA fragment is sequenced from both ends[10]. Reads arrising from one fragment sustain their pair information and in addition their distance is equal to the length of the original DNA fragment. This enables us to determine the distance between the sequences even if the sequence in between is not covered by other reads (see Fig. 1).

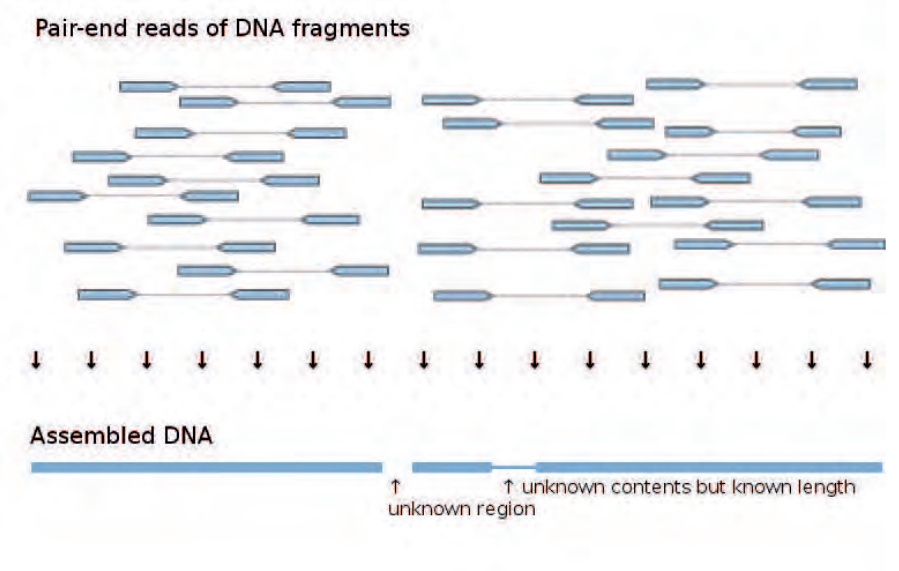

Fig. 1. Genome sequencing

Assembling *de novo* sequencing data is quite a difficult task in spite of ever improving technology. To handle such amounts of data, we are using the resources and support from Metacentrum[11] and CERIT-SC[12]. The assembly process

performed on computers is roughly as follows: Firstly, in the pre-assembly phase, read errors are attempted to be identified and fixed based on either knowing which base sequences are unlikely to occur or by statistical methods. Then the assembler compares the millions of fragments against each other, finding all common segments between two fragments that are sufficiently long. Since these overlaps could not have occurred by chance, they become the foundation of the assembly. However, since many non-informative parts of DNA sequences are repetitive (these parts are simply called 'repeats'), some of the overlaps that were found are not true, they are 'repeat-induced'. The assembler identifies and excludes the repeat-induced overlaps by looking at the 'depth' of the total number of fragments in them: repeat-induced overlaps would generally arise from more fragments than true overlaps. Once the true overlaps are identified, so-called contigs (contiguous parts of the original DNA) are formed from fragments constituting them. Eventually, in a phase called scaffolding, these contigs are ordered and oriented based on the mate-pair information (knowing the mutual distance and orientation of the two reads in each pair)[13].

2 Red clover (*Trifolium pratense*) sequencing

Red clover (*Trifolium pratense* L.) is very important forage plant in many countries around the world. It is used as inter-crop plant and coverage of temporarily unused soil. Red clover belongs to leguminous plants and due to symbiosis with bacteria of *Rhizobium leguminosarum* bv. *trifolii*, it is capable of air nitrogen fixation. Leguminous order belongs among the most examined one in the plant kingdom. Already three plants from this group have been sequenced; however, red clover is neither case. Its medium sized genome, estimated to 418 Mbp (1C = 0.43 pg)[14], is suitable for assessment and also challenging for many of contemporary *de novo* assembly software as they were until recently focused mainly on bacterial genome assembly[15].

In our study, we focus on comparison of number of available assemblers which adopted different assembly approaches. The assemblers are firstly tested on shorter datasets from closely related plant of *M. truncatula*. Assembly results on these datasets are used to provide insight into algorithm specifics influencing the posssible outcomes of red clover assembly. On these datasets, we compare also several read error correction software and their impact on assembly statistics (contiguity and accuracy) and the gain of read error correction for subsequent studies thanks to the known reference (*M. truncatula*). Our study should offer not only the comparison of the assemblers, as their algorithms are very likely to change very soon. It should provide also a counsel for the scientist interested in *de novo* sequencing and *de novo* assembly from NGS data as it is (also from our work) obvious that the number of the available software need to be tested before relying on their results.

3 Computing resources

With the development of sequencing technology, new algorithms followed in wake to handle the problem of large amount of short reads, as the previously used overlap and string graphs[16] used for Sanger sequencing[1] showed predominantly incapable of solving this problem. Several assembly programs have been developed, adopting different algorithmic approaches. Some assemblers like Edena[17] improved overlap layout extension approach, some like CABOG[18] were fitted to handle NGS data, but the assemblers based on de Bruijn graph were mostly released. As the projects grew in scale they had to deal with fitting larger datasets into memory, e.g. Velvet[19], ABySS[20], SOAPdenovo[21], Pasha[22]. However, these programs require great volumes of available operating memory – typically hundreds of gigabytes[7,23], if they are even able to manage such amount of raw data. On that account, these types of projects cannot be run on desktop computers, which rise up the need of using computer clusters[20,24]. Therefore large computing resources available to the scientific community (like Metacentrum[11] and CERIT-SC[12] we used) or paid service like Amazon EC2[25] are needed. Also new advanced algorithms are being developed that are capable of handling billions of reads without the need of significant investments into computer hardware. For example, Conway and Bromage[26] described method of encoding a de Bruijn graph using sparse bitmap, which was recently implemented in Gossamer[27], or the SGA assembler which take advantage of prolonging of the read length and uses the string graph and compressed index of the sequence reads[28].

To make use of high-quality data from NGS technology, the error correction should be implemented among the steps of data processing[29]. Correcting the wrong base calling of sequencing technologies, which are unique among different NGS platforms (the Roche/454 sequencing platform produces mostly InDel errors due to homopolymers, whereas the SOLiD and Illumina platforms are susceptible to substitution errors with error rate rising towards 3'-end of the read), helps both assembly and variant calling[30]. Highly redundant coverage of genome in NGS data fortunately enables correction of these errors. Several algorithms have been developed, mainly those based on the k-mer frequency: e.g. Quake[30], ECHO[31], Reptile[32]; multiple alignment: e.g. Coral[29]; and generalized suffix trie: SHREC[33]. Since the majority of these programs need a fine-tuned parameters to run properly (frequently unknown *a priori* the correction), it is quite tricky to choose the right one.

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Research Collaboration/Support:

Research Support

Environmental Chemistry & Modelling Computations in MetaCentrum

Research Centre for Toxic Compounds in the Environment (Recetox), Faculty of Science Masaryk University, Brno, Czech Republic

1 Group Introduction

Research Centre for Toxic Compounds in the Environment (Recetox) is an independent department at the Faculty of Science, Masaryk University, with its own research and development, educational programmes, and expert activities within the field of environmental contamination. The centre focuses on persistent organic pollutants (POPs), polar organic compounds, toxic metals and their species, and natural toxins—cyanotoxins.

One of its working group—*Atmospheric processes and modelling*, led by prof. Gerhard Lammel (Max Planck Institute for Chemistry, Recetox)—is focused on modelling of processes, which influence concentration of persistent organic pollutants in atmosphere and other parts of an environment.

The group aims to understand the processes, important for geographical distribution of POPs in an environment, and time trends of their concentrations. The output of their research could be further used for impact assessment. An attention is focused on polychlorinated biphenyls (PCBs)—toxic substances, whose production and usage is controlled by European legislation. Current evidence suggests that the major source of PCB release to an environment is an environmental cycling process of PCBs previously introduced to the environment.

2 The Benefit of Running Computations in MetaCentrum

The collaboration with MetaCentrum started in late 2011. Since the complex numerical models, such as those studied by Recetox, are computationally very intensive, it has been decided to make use of the powerful MetaCentrum clusters in order to perform these modelling computations efficiently. This performance benefit would further allow the group to study more complex situations of environmental contamination.

The Atmospheric processes and modelling working group deals with diagnostically simulations of the meteorological conditions and air quality of Europe during 2009-2010 (hourly temporal resolution, space resolution 12 x 12 km, 28 vertical layers). They use a chemical transport model—CMAQ (Community Multiscale Air Quality Model), developed by USEPA and a network of academic collaborators worldwide—to model the fate of PCBs in an environment. So, the software has been prepared within the MetaCentrum infrastructure; besides

other, the CMAQ has been prepared to allow distributed computations, and thus allowing to perform the computations in an efficient way.

Another software—WRF (Weather Research and Forecasting Model)—produces meteorological input fields for the CMAQ model, which then performs modelling of advection, diffusion and chemistry of gas phase, aerosol and clouds. The WRF has also been prepared within the MetaCentrum infrastructure. Even though the first version supported just parallel computations, currently we are testing a new version, which supports distributed computations as well.

Last, but not least, the MetaCentrum is starting a closer collaboration with Recetox—currently, there is a collaboration topic being discussed, which would help the Recetox with their simulations.

Running BOINC and Windows-based applications in MetaCentrum

Laboratory of Security and Applied Cryptography (LABAK), Faculty of Informatics, Masaryk University, Brno, Czech Republic

1 Sensor Security Simulator

The Laboratory of Security and Applied Cryptography (LABAK), Faculty of Informatics, Masaryk University, Brno uses its simulation platform to run a wide set of computations generated by its current research focus – genetic programming of security protocols and optimization of intrusion detection systems for wireless sensor networks (WSN)[3]. Its demands exceed the capacity of the available 16 computers (32-CPUs total) in local computer lab. The research group has a strong potential to achieve more results if short-term peaks in demand of computing power are satisfied. The application is an in-house Windows-based development of the research group with port to the MetaCentrum (Debian Linux, batch manager) possible, but costly. To satisfy such needs MetaCentrum have advanced but less known service called virtual cluster. We started the experiment to use this service to boosts LABAK research.

The virtual cluster service[2] is based on the idea that providing a virtual machine is just another form of a computing job. Our scheduler controls resource assignment regardless of job type (job/virtual machine) and we want to demonstrate that even Windows-based infrastructure controlled by BOINC workload manager can be seamlessly provided by our resources.

The experiment was successful, MetaCentrum resources seamlessly integrated the original BOINC infrastructure run on local PC lab. The provided additional computational capabilities allowed to find new secrecy amplification protocol that outperforms existing, human designed protocols, in terms of provided level of security as well as the message complexity. The vast search space was explored to obtain robust information about protocol behavior [3]. Availability of high peak computation resources shortened parallel search for partial hash collisions with complexity of 2^{47} SHA-2 operations used for novel key predistribution protocol from several days down to the tens of hours, allowing us to quickly abandon nonviable initial settings and focus on the viable ones. The experiment helped to achieve results in the form of two improvements of random key predistribution for WNS[1].

2 Architecture of integration into MetaCentrum

The architecture of used solution is shown on Fig. 1. The Sensor Security Simulator runs on virtual cluster service provided by MetaCentrum which allows to run the same environment like local resources (PC lab in our case). This is achieved by virtualization where we start new worker nodes running the same image of machine as the original local infrastructure. The workload manager stays untouched – in our case the current BOINC server stays working as usual while the new resources provided by MetaCentrum appears as new worker nodes asking for its tasks. Moreover the BOINC workload manager proved itself suitable for such usage – coping well with dynamic environment (discovery, recovery/resubmits, robustness).

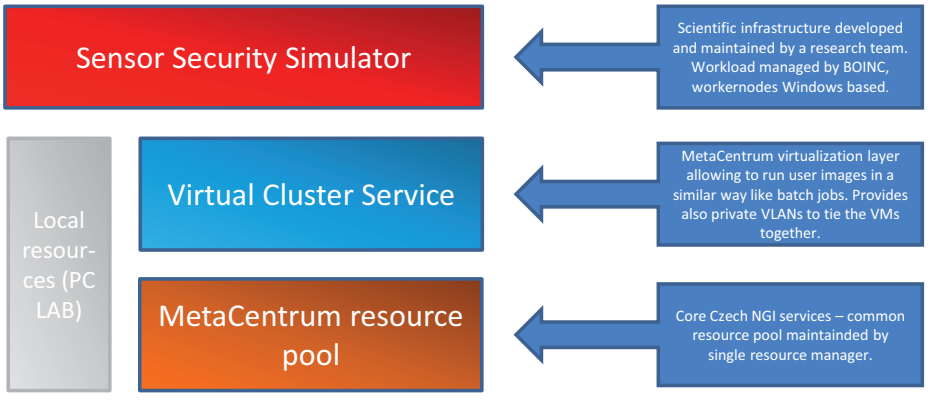

Fig. 1. Architecture overview.

The virtual cluster service networking part provides dedicated virtual network (VLAN) for each set of virtual machines so the created infrastructure can be encapsulated if needed. In our case we connected the VLAN with the existing infrastructure to form one virtual networking segment, accessible only by the BOINC server. As shown on the figure, the virtual cluster service sits on top of the existing MetaCentrum resource pool managed by a central resource broker, so the resources are managed in the same way as batch jobs. So the users can dynamically ask for new resources getting it in the form of new worker nodes of their existing infrastructure.

3 Virtual cluster service summary

This experiment is a demonstration of Czech NGI's strategy to be flexible and easy to use for established or emerging research groups who have specific requirements or already operate their own infrastructure. We show the possibility

to expand established infrastructures using MetaCentrum resources without any changes in software or computational model. With the virtual cluster service the end users do not need any new training, only a local administrator interacts with MetaCentrum. The users can stay focused on the scientific essence of their problem. This is valuable because the need of extra computing power usually arises in the stage of scientific project when there is no room to change computing model or tools. Moreover the resources can be provided fully respecting local security and network policies and conventions and configuration (authentication, storage namespace and protocols, software versions).

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Photometric Archive of Astronomical Images

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The MetaCentrum NGI via the integrated CERIT-SC center cooperates with Miloslav Zejda and Marek Chrastina of the Department of Theoretical Physics and Astrophysics of the Faculty of Science at Masaryk University (the department is lead by prof. Rikard von Unge) on creation of a Photometric[1] Archive which will collect CCD images from astronomical telescopes.

The archive will collect images from both professional and amateur astronomers, which are not, so far, collected in any systematic manner (they are kept only by their respective authors, not accesible to other astronomers for research). The goal of our support/collaboration is to create an archive, which will automatically identify all astronomical objects on all images, measure the instensity of all such objects, and allow searches in the resulting database.

The current usual practise is that images are taken as rectangular parts of the sky around the main observed object, which is solely identified in the image metadata. The other objects that happen to be in the vicinity of the main object and end up in the image are not identified. Thus identifing all such objects on all images will hugely increase the number of known recorded observations of each object.

In the first phase covered, we will create the archive database and its web interface—this phase is nearly done and it is expected to be fully finished in the first months of the year 2013. During the second phase, an identification of all objects on all images will be implemented. In the third phase, a standardised interface to so-called Virtual Observatory will be proposed and implemented.

A considerable challenge of the first phase is to unify metadata of the images. The astronomical images are stored in FITS format, which allows arbitrary text attributes to be stored in each image file. However, the images are produced by various CCD cameras and software processing tools, and the set of attached attributes is not fully standardised. Various attribute names are used for the same image property, or various units (meters, millimeters etc.) are used in values of the same attribute. Thus a set of required attribute names and their allowed values was defined by the scientists of the Department of Theoretical Physics and Astrophysics, and the archive performs a transformation of FITS attributes of each image to this defined set.

Another considerable challenge we faced is the mechanism for uploading images, because images are usually taken in series of hundreds or thousands, with average size around 1 MB per image, so a series of images from a single observation can be in the order of hundreds of megabytes. The amateur astronomers

[1] Photometry is a technique of astronomy concerned with measuring the intensity of an astronomical object's electromagnetic radiation. Photometry is used for example for finding variable stars or exoplanets.

may have slow internet connections, so progress of an upload should be observable over long time periods. Also the astronomers' computers may have various operating systems, so the upload mechanism should cover as many of them as possible. Various solutions were considered, and the chosen solution is to use modern web browsers with HTML5 support on the client side. HTML5 browsers allow users to choose many files or even whole directories for upload, and then upload the many files one by one using `XMLHttpRequest`, which allows displaying of upload progress for each file separately.

Experimental Simulation of Deploying a Large Smartmeters Network

[1] Mycroft Mind, Jundrovska 618/31, Brno, Czech Republic,
[2] CEZ Group, Duhová 2, Prague, Czech Republic

Currently the operator of the Czech national electric power distribution network runs a pilot project of testing deployment of approx. 35,000 smartmeters – devices which measure various quantities related to power consumption at the end-user side. The measured data are gathered along the distribution to concentrator devices (each serving several hundreds of smartmeters typically) which push it further to a cluster of central servers for complex analysis. This pilot will be followed by deployment of approx. 100x more such devices; however, such deployment is unprecedented with the software in use. Therefore a simulation experiment is required to discover and mitigate potential scaling issues.

The simulation is run in the cloud infrastructure of CERIT-SC (managed by the OpenNebula stack). The central servers are deployed on hardware of similar scale and in the same software configuration as intended for the production. The data sources – smartmeters are simulated at the level of concentrators. The implementation allows to simulate varying patterns of measurements (different quantities, properties of time series etc.) Unchanged communication protocols between the concentrator and the central server are used then. Because the target setup assumes up to 50,000 concentrators, up to thousands of concentrators must be handled by a single simulator instance.

The target environment uses data links of varying qualities, starting even at GPRS links. Therefore the simulator also includes modules which emulate packet loss, delay, and jitter in the network communication in a controlled way. This setup allows testing sensitivity of the entire system on network properties.

The communication also operates in two modes – push (data are sent from concentrators actively) and pull (data are requested by the central servers). The push model may yield saturation of the central servers because of lack of communication planning. Experiments to test sensitivity to this problems are planned. On the other hand, the pull model is challenging to simulate (technically, thousands of network addresses must be handed by single machine).

The cloud is an essential flexible infrastructure to run such an experiment. With the exception of the RDBMS server running on a large SMP machine all the servers (both the central cluster and the data source simulators) are run in virtual machines in the cloud. This allows multiplatform setup (Windows and two Linux flavours are used) and, in particular, servers can be added to various groups (simulators, front-ends, application logic, etc.) easily. On the other hand, resources which are not required in a certain stage of the experiment, can be easily released to other use, which makes even such a large experiment affordable.

The whole usecase also serves as a good example of collaboration between academia and industry in development and experimental use of novel technology.

Grid Virtual Organisation for the Pierre Auger Observatory

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1 Pierre Auger Observatory

In 2012 we celebrated the 100-year anniversary of discovery of cosmic rays. Even after such a long time the origin and nature of the cosmic rays with the highest energies is not known. These particles are measured indirectly via the observation of extensive air showers developing in the Earth's atmosphere. Currently the largest and most advanced experiment designed to investigate the highest energy cosmic rays is the Pierre Auger Observatory.

The Pierre Auger Observatory (PAO) is located in the vicinity of the small town Malargue in Argentina. It covers an area of about 3000 km^2 at a mean altitude of 1400 m close to the Andes mountain range. The goal of the PAO is to improve our knowledge of the highest energetic particles and answer questions about their origin and composition. The PAO started to collect data in January 2004 with a subset of detectors, the construction of the base design was finished in 2008. Two different techniques are used for measurement: surface detector (SD) and fluorescence detector (FD). SD is made up of 1660 stations containing about $10m^3$ of purified water each. Three photomultipliers in each tank can record Cherenkov photons emitted by muons passing through a tank. Signals from different tanks are combined and used for reconstruction of cosmic ray showers. Base FD consist of 24 telescopes located at 4 stations overviewing the atmosphere above the field covered by SD. Telescopes record fluorescence light emitted by particles propagating through the air. FD can trace the development of the shower and reconstruct the energy of the originating particle with smaller model dependence, but has only about 15% duty cycle, because it can take data only during nights not close to the full moon. SD can measure showers without interruptions and use FD reconstruction for energy calibration.

Recently new detectors were added to a smaller area to decrease the lower energy threashold of observable showers to about 10^{17} eV. The HEAT telescope extends the field of view of the FD in order to detect showers that develop higher in the atmosphere. The so called Infill array of SD stations has distance between detectors reduced to 750m. The Auger observatory will continue to record and analyze data for several years.

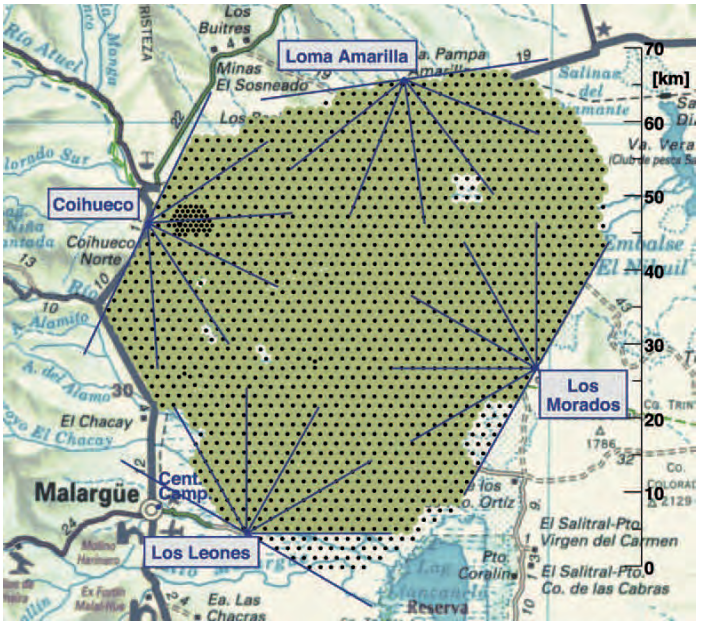

Fig. 1. Schematic positions of PAO detectors.

2 Monte Carlo Simulations

The reconstructed showers are compared to various models using Monte Carlo simulations. Detailed simulations require a lot of computing and storage capacity. We mostly use CORSIKA [1] program, which allows user to choose from different models for the most important hadronic part of interactions. A particle with energy of 10^{20} eV produces shower with too many particles and it is impossible to track all of them using ordinary computers. In fact, in 2012 one shower with a primary energy 10^{20} eV was simulated in full details using a customised version of CORSIKA and a cluster of computers with 1200 cores. The ouptut was stored in several files with a total volume of 7 TB. This attempt shows why we had to adopt another solution for simulations of many thousands of showers. This solution is called thinning. Bellow defined threashold energy we track only a smaller number of secondary particles with an increased statistical weight. Good choise of thinnig parameters produces usable simulations running maximum tens of hours on one core.

The simulations were originally run on a few computing sites by our collaborators with a local access. Results were difficult to share because either a local user account was needed or a copy to another site was done. Also local producers could use different settings in programs and it was difficult to compare simulations from different sites. The PAO collaboration consists of more than 500 physicist from 94 institutions in 19 countries. We decided to unify access

to computing facilities by using grid tools. We used our experience from high energy physics and in 2006 we founded Virtual Organization auger. This is a basic group of grid users sharing data and resources. The support of the VO *auger* gradually increased from 6 sites in 2007 to 23 in 2012. We prepared tools for semiautomatic job submission and output retrieval. Using grid we could use all supporting sites in the same way with exactly same settings of simulations. CESNET servers provide central services for the VO *auger* - registration portal, database of users (VOMS) and file cataloque (LFC). Other servers are replicated on several sites.

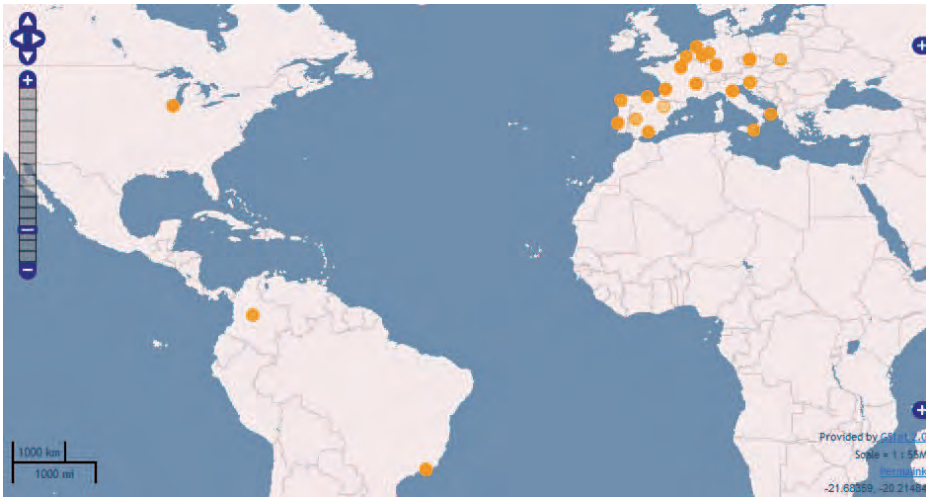

Fig. 2. Sites supporting VO *auger* are located in Europe and America

3 Grid Production

We group simulations into collections called libraries. Each library is characterised by a type of a primary particle, its energy and interaction models. The actual production is now managed by a team at the University of Granada using a Job Management Module described in [2]. This set of tools is based on an earlier version developed by the Prague group [3] with added MySQL database, which stores job states. Thousands of jobs are submitted every day in collections via WMS servers. These servers do not scale well, we use several instaces on different sites. The LHC VOs ceased to use WMS server and further support of this component is not clear, we investigate other options for job distribution.

The production system automatically reacts on different states of jobs. Aborted and cancelled jobs are resubmitted. Jobs running or waiting in a queue above

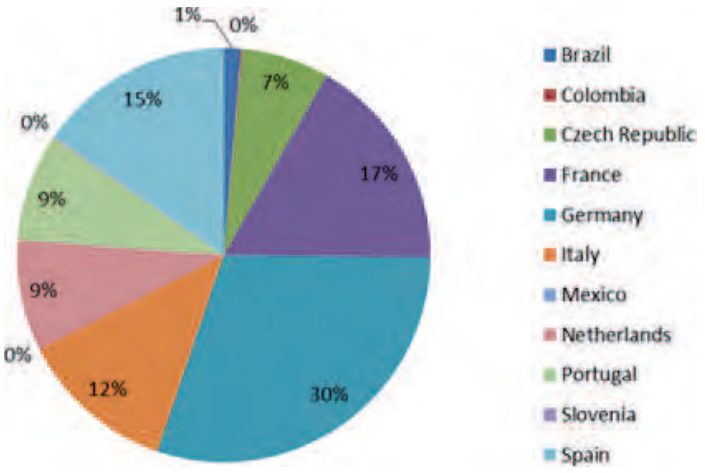

Fig. 3. The ratio of total elapsed time used by the VO *auger* per country. The total time consumed from January to November 2012 is 2860 years.

configurable limit are cancelled and also submitted again. Each job in the beginning checks if the output file is already registered and signals inconsistencies from failed jobs. Simulations with lower primary energy take considerable shorter time, such showers can be grouped and produced in one grid job. Also we started to run in the same job the reconstruction part done by Auger Offline package. It saves time for download of the simulated shower and increases effieciency.

Some sites contributing to the production are associated with a group participating in the PAO and pledge minimum amount of cores and disk space for the VO *auger*. However there are also sites which offers for free only they spare resources otherwised unused. The resource sharing effectively increases VO *auger* computing capacity for free. This works well with CPU time; usage of unpledged storage is more problematic because we faced rapid needs to move a large amount of data in short time. We protect against data lost by creating a copy of final results in one central place - IN2P3 Computing Centre in Lyon. Data management is still quite complicated. We cannot use solutions adopted by biger LHC VOs, they are too specific and require a lot pf dedicated effort. On the other hand the grid middleware offers only basic tools not suitable for management of millions of files occupying hundreds of TB on many places. We plan to test new solutions using DIRAC [4] for job and data management in 2013.

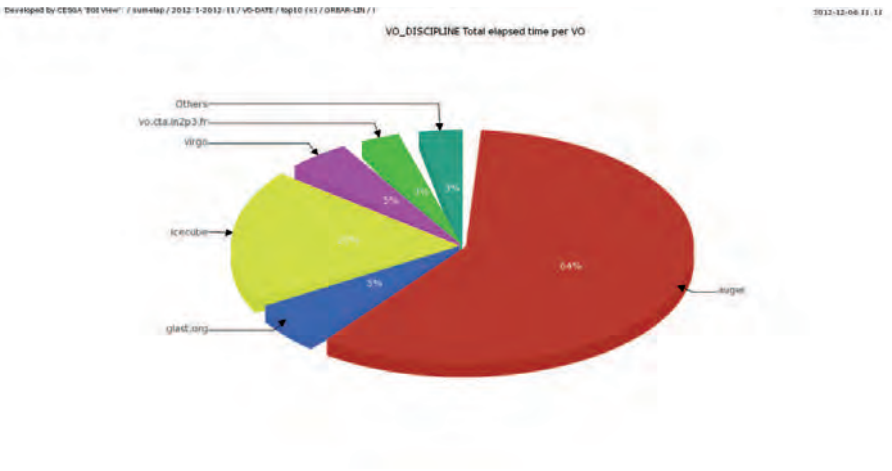

Fig. 4. The ratio of total elapsed time used by different astroparticle physics projects. The VO *auger* dominates with 64% share.

4 Conclusions

Monte Carlo simulations are needed to produce scientific results described in papers signed by the whole Pierra Auger collaboration. The impact of these papers on the astroparticle community can be ilustrated by the fact that one quarter of the 25 most downloaded articles from Astroparticle Physics journal [5] comes from Pierre Auger collaboration with number 1 and 2 in the list. The EGI grid provides necessary computing resources and is heavily used by the collaboration.

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Parallelization of Regression Algorithm for Identification of Biomarker Areas in SELDI-TOF Mass Spectra

Department of Medical Biophysics, Faculty of Medicine in Hradec Kralove,
Charles University in Prague

The researcher Jiří Knížek from the Department of Medical Biophysics of Faculty of Medicine in Hradec Králové of Charles University in Prague contacted the MetaCentrum user support with a problem how to process large amounts of data which could not be processed on his personal computer in time.

The data he works with were several sets of 431 files containing tabular data. Each file required about two days of computation on a personal computer in order to be processed by a program written by Jiří Knížek in MATLAB. Clearly, processing of the whole sets would take several years on his PC, so some high performance computing resources were needed.

Fortunately, such a processing could be highly parallelized, because each file could be processed independently. The MATLAB program spent most of its time in matrix multiplication, which itself could also be parallelized to many processors within a single machine.

When the unmodified MATLAB program was run on MetaCentrum resources, each file got processed in somewhere between 20 and 60 minutes of wall clock time thanks to high counts of CPU cores in MetaCentrum machines.

Each data file could be submitted as an independent computing job, thus many machines were used in parallel. In effect, a set of 431 files took just several hours of wall clock time to be processed. Of course, during the several hours of wall clock time, many thousands of hours of CPU time were used because of the high parallelization.

Except from the necessary hardware, the MetaCentrum also provided this highly parallel computation with the MATLAB software and the hundreds of its licenses needed to run it. Since the pool of available MATLAB and its toolbox licenses is shared not only by all the MetaCentrum users, but also with teachers and students of large Czech universities, the main challenge in performing such a large parallel computation is to use a system for allocation of the MATLAB licences, so that these are available once the computation is scheduled for processing. Even though the basic support of detecting the available licenses is provided directly by the MetaCentrum job scheduler, there had to be a second stage established, waiting in a loop for licences of needed toolboxes. Once all the necessary toolbox licenses became available, the computation has been started.

Experimental Biology Agenda Database

Department of Experimental Biology, Faculty of Science, Masaryk University

The CERIT-SC center cooperated with the Department of Experimental Biology, Faculty of Science, Masaryk University, on creation of a web-based system for integration of key production information of gene-specific chemicals used in the department and all available information about functionality of molecular-cell reagents – antibodies, siRNA, plasmids, cell lines, primers.

The system was developed as a diploma thesis of a student of Faculty of Informatics, Masaryk University.

The system allows storing information about primary entities – genes, primers, siRNA etc. – and their mutual relations, which can be accompanied by arbitrary documents, usually PDF or MS-Word documents or images.

Before the system was created, the information was not integrated, it was dispersed usually in Excel files and separated documents on disks of personal computers of various individuals, which led very often to losing information when students who performed some studies left the department. With this integration system in place, the information is all kept in one place, and is stored with back-up copies in professional way on resources provided by the CERIT-SC center.

Part IV

Selected Users' Reports and Publications in 2010-2012

Foreword

National grid infrastructure users are obliged to acknowledge the usage of provided computing and storage resources they took advantage of for creating their research publications. These acknowledgements should be regularly reported to MetaCentrum, since these positively influence the users' fairshare, and thus may help them to easily (i.e., faster) access the infrastructure resources in cases of their saturation.

During 2010–2012, we've received 274 acknowledgements, which are listed in the Appendix B of this Yearbook. In this part of the Yearbook, we proudly present research reports of the user groups, which regularly use the infrastructure resources, and which have provided us with at least 5 acknowledgements during the particular period.

Central European Institute of Technology & National Centre for Biomolecular Research

Faculty of Science, Masaryk University, Brno, Czech Republic

Structural Biology Programme is one of seven main research programmes of *Central European Institute of Technology (CEITEC)*, lead by prof. Jaroslav Koča. The Programme integrates information concerning the structure of biologically important macromolecules – proteins, nucleic acids and their complexes. The aim is to obtain the knowledge necessary to understand the basic functions and life processes at the molecular and cellular levels. Progressive high-resolution methods of structural analysis such as X-ray diffraction, nuclear magnetic resonance, cryo-electron microscopy and tomography is used in combination with modern methods of molecular modelling, theoretical chemistry, and bioinformatics. There is a tight synergy between CEITEC and *National Centre for Biomolecular Research (NCBR)*. NCBR is an independent institute of the Faculty of Science, Masaryk University, Brno. The main activities of the Centre involve research in specific areas of chemistry and biology as well as teaching, especially at advanced and Ph.D. levels. This report summarizes utilization of MetaCentrum and CERIT-SC computational and data storage resources by Laboratory of Computational Chemistry and independent computational divisions of NMR Laboratories, GlycoBiochemistry Laboratory and Laboratory of RNA/Protein Interactions, which are members of both NCBR and CEITEC.

Selected Research Topics

Structure Determination by NMR Techniques

Nuclear magnetic resonance (NMR) spectroscopy has been developed into very important tool in the repertoire of methods suitable for study of biomolecules. We use NMR to determine 3D structures of RNA recognizing protein domains. Unlike in the X-ray crystallography, investigated samples are usually in liquid phase, which allow studying them close to the physiological environment. Molecular dynamics simulations are then used to find models that fulfill majority of experimentally determined distances via NMR measurements (Figure 1).

Protein Dynamics by Molecular Dynamics

BsoBI is a homodimeric DNA binding restriction endonuclease. The crystal structure shows that DNA is completely encircled by the enzyme. Moreover, experiments revealed that enzyme does not break up to monomers without the DNA, which indicates that the enzyme must undergo large conformational changes during the DNA binding (Figure 2). Using molecular dynamics biased by metadynamics the various pathways how the DNA can enter to the active site are studied.

Fig. 1. Distance information (in yellow) used to create a structure model of protein (purple)

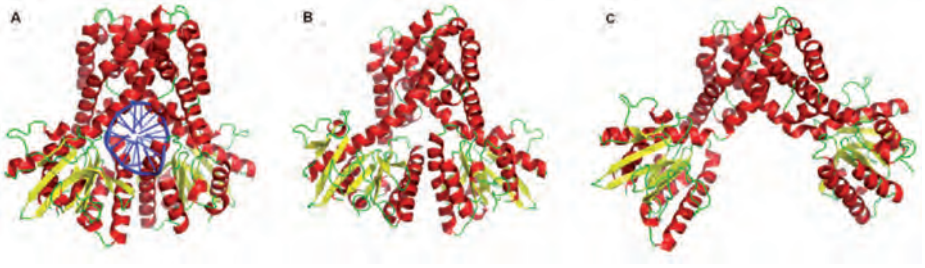

Fig. 2. Studied BsoBI enzyme. (A) native crystal structure of BsoBI with DNA (in blue); (B) without DNA – closed state; (C) without DNA – opened state

Calculations of NMR Parameters

Solid-state NMR spectroscopy is a powerful technique routinely used for the study of powdered and pollycrystalline samples of biomolecules, polymers and pharmaceutical compounds at an atomic resolution. However, the relationship between the structural parameters of interest and NMR observables is seldom straightforward. We examined the influence of the crystal packing for three purine derivatives (hypoxanthine, theobromine, and 6-(2-methoxy)benzylaminopurine) on the principal components of the NMR chemical shift tensors (CSTs). We employed density functional calculations to obtain various molecular properties (the ground-state electron density, the magnitudes and orientations of the components of NMR chemical shift tensor, and the spatial distribution of the isotropic magnetic shielding) for the isolated molecules and for the molecules embedded in supramolecular clusters modeling the crystal environment, and evaluated their differences. The concept has enabled us to rationalize the effect of the crystal packing on the NMR CSTs in terms of the redistribution of the ground-state electron density (EDD) induced by intermolecular interactions in the solid state (see Figure 3).

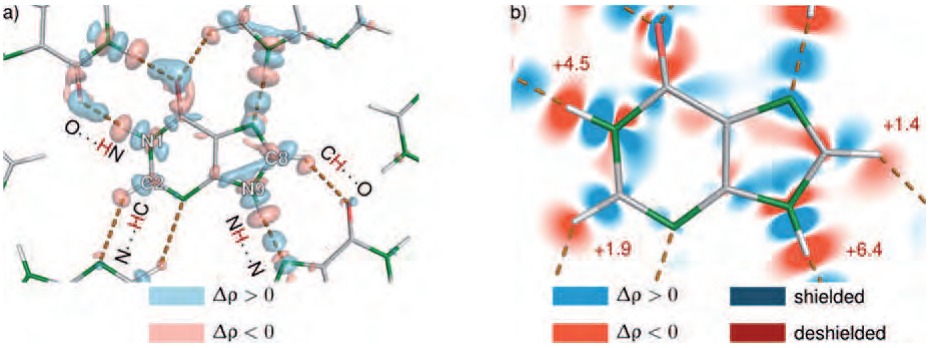

Fig. 3. Visualization of (a) the EDD for a hydrogen-bonded cluster of hypoxanthine and (b) in-plane slice of the EDD with calculated changes in the ^{1}H NMR chemical shifts for the individual hydrogen atoms trapped in standard and weak hydrogen bonds

Mechanisms of Enzymatic Reactions

Enzymatic reactions are essential in many biochemical and biological processes. Using various computational techniques, we study reaction mechanisms of DNA cleaving enzymes and several glycosyltransferases. Many glycosyltransferases are used in posttranslational modification of proteins. In higher eukaryotes, their misregulation can be linked to a wide variety of diseases, such as diabetes, cancer, and neurodegenerative diseases, including Alzheimer disease. The knowledge of their function is thus a key step in the better understanding of such diseases. Reactions are studied by quantum mechanics/molecular mechanics (QM/MM) hybrid approaches. The reaction pathways are probed by potential energy scans and/or by advanced free energy calculation methods such as string method (see Figure 4).

Quantum chemical study of CH-π interactions

Molecular recognition plays a crucial role in many biological processes, such as bacteria-host identification. Some of these recognition processes are performed by proteins called lectins, which are able to bind saccharides in very specific way. Various studies on lectin-carbohydrate interaction have shown that the interaction is predominantly driven by hydrogen bonds and dispersion interaction. The CH-π interaction is one of such dispersion interactions. Its nature requires employing high quality quantum chemical methods for its correct description. Furthermore, the additive properties of CH-π interaction with respect to number of aromatic rings interacting with carbohydrate moiety were studied too (Figure 5).

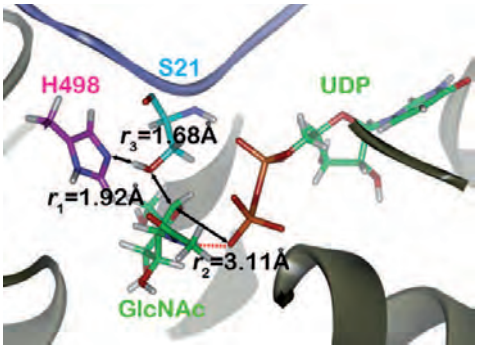

Fig. 4. The QM/MM optimized transition state structure of studied glycosyltransferase. The donor, acceptor and the catalytic base are represented in stick representation.

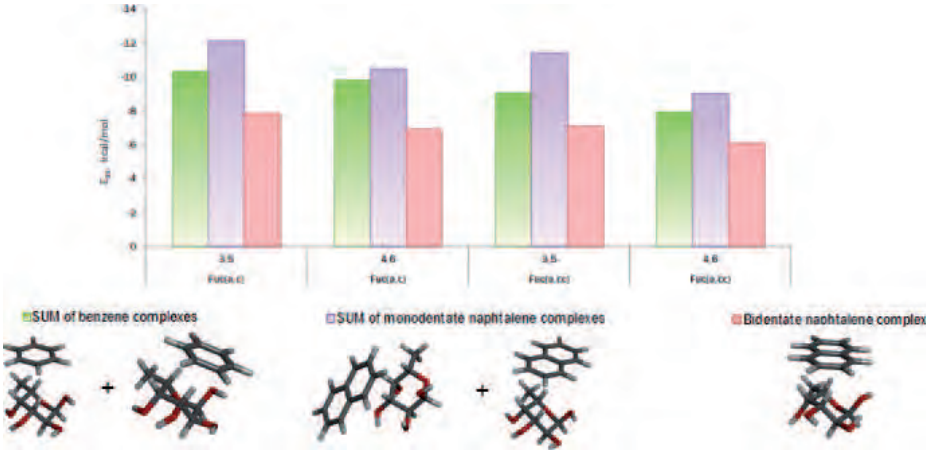

Fig. 5. Comparison of interaction energies of benzene and naphthalene with L-fucose moiety

The role of MetaCentrum resources & services

Computational resources provided by MetaCentrum and CERIT-SC are used in broad range of directions spanning many methods of computational chemistry, chemoinformatics and bioinformatics.

Quantum chemical (QM) calculations are used to uncover details of specific interactions occurring in biomolecular systems. They are also used to study reaction mechanisms of enzymatic reactions. Moreover, they are important in prediction of spectroscopic properties such as NMR chemical shifts and spin-spin coupling constants. Calculations are performed employing Gaussian, Turbomole, MolPro, ADF, Schrödinger, and CPMD packages. Common bottleneck of QM calculations is that they are very memory demanding and in a few cases also disk space demanding, especially in cases where high-quality quantum chemical methods are used. MetaCentrum and CERIT-SC have several computational nodes that are equipped with both large memory and disks thus we are able to perform such calculations.

Other calculations employ molecular dynamics or Monte Carlo simulations on both atomistic and coarse-grained levels. In majority of simulations, the free energy, which is connected with chemical equilibrium and kinetics, is the point of our interest. Its calculation requires very long simulations. In many cases, they might be run independently on many computational nodes, which allow us to obtain converged free energies faster. From this perspective the architecture of MetaCentrum as large aggregation of small SMP computational nodes is very beneficial. Simulations employing molecular dynamics and Mote Carlo simulations are used to study conformational changes of large biomolecules, interaction energies in biomolecular complexes and interaction of various particles with biomembranes. Simulations are performed in Amber, Gromacs and own packages for coarse grained simulations.

Composition of complexes containing large biomolecule and small ligands is studied by molecular docking. Most prominent packages used in docking studies are AutoDock, AutoDock Vina, and Dock. Moreover, they are also used in virtual screening studies, which aim to find specific high affinity binders to selected biomolecules and thus having possible pharmacologic impact. Trajectories obtained by molecular and *ab initio* dynamics simulations represent the largest portion of all data produced. Possibility to store them on data storages is highly acknowledged.

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Loschmidt Laboratories

Department of Experimental Biology, Faculty of Science, Masaryk University, Brno, Czech Republic

Loschmidt Laboratories (LL), lead by prof. Jiří Damborský, conduct research aimed at dissecting fundamental principles of structure-function relationships of dehalogenating enzymes haloalkane dehalogenases (HLDs). HLDs convert halogenated aliphatic hydrocarbons to alcohols and find their use in biodegradation of toxic chemicals, decontamination of warfare substances, detection of hazardous chemicals in the environment and synthesis of optically active compounds. Activity of natural HLDs for such environmental, chemical and biomedical applications is often rather low and must be improved. HLDs have been found in various bacteria colonizing diverse ecosystems (water, soil, plants and animals) rising the intriguing question of biological role of these enzymes.

The specialty of LL is high integration of experimental and theoretical approaches in the study of enzyme function. The former comprises techniques for construction and biochemical characterization of mutant proteins, while the later molecular modeling techniques used for analysis of structure-function relationships and rational design of mutations. The experimental data provide essential feedback to get more understanding of structure-function relationships and to guide next round of rational design.

Contributed hardware
LL contributed to the MetaCentrum infrastructure with 264 CPU cores divided into two clusters: loslab (14 nodes, 2x six-core Intel Xeons) and losgar (2 nodes, 4x 12-core AMD Opteron). These resources are available to other users via the queues short, normal, backfill, and preemptible.

Developed software
CAVER 3.0 is a software tool widely used for the identification and characterization of transport pathways in macromolecular structures. The latest version of CAVER enables automatic analysis of tunnels and channels in large ensembles of protein conformations. CAVER 3.0 implements new algorithms for the calculation and clustering of pathways. A trajectory from a molecular dynamics simulation serves as the typical input, while detailed characteristics and summary statistics of the time evolution of individual pathways are provided in the outputs. CAVER 3.0 paves the way for the study of important biochemical phenomena in the area of molecular transport, molecular recognition and enzymatic catalysis. The software is freely available as a multiplatform command-line application at `http://www.caver.cz`.

Projects solved with the use of resources provided by MetaCentrum

- **Prediction the effect of amino acid substitutions on protein function.** Single nucleotide polymorphisms are the substitutions of one nucleotide in the DNA sequence that may have phenotypic consequences. Since approximately half of the known disease-causing mutations are the result of amino acid substitutions, it is very important to distinguish non-neutral substitutions that affect protein function from those that are functionally neutral. In this study, the performance of nine tools designed to predict the effect of substitutions were compared according to their confidence scores and reliability coefficients acquired from validation on the dataset consisting of about 30000 substitutions.
- **Assessment of reactivity of potential substrates of haloalkane dehalogenase DmmA by QM/MM simulation.** Previous projects utilized docking based virtual screening methods for almost 45000 potential substrates of HLDs. This enzyme possesses a larger entrance tunnel and wider active-site cavity than other dehalogenases which poises this enzyme for development of a new biotechnology tool. In this project, a coupled QM/MM simulation was applied to the top 10 screened molecules to assess their potential reactivity. In total, 4 molecules revealed barriers of the reaction matching values reported for the common substrates of haloalkane dehalogenases representing new classes of substrates.
- **MD simulations of 1-bromohexane stabilization in DatA enzyme.** Catalytic residues of haloalkane dehalogenase DatA and other members of the family significantly differ by one amino acid. Instead of W109 acting as the second halide stabilizing residue, DatA enzyme employs a tyrosine in the equivalent position. The single point mutation Y109W in DatA, mimicking the traditional composition, results in dramatic changes in substrate specificity of DatA enzyme. This project employed molecular dynamics of DatA wild-type and Y109W mutant complexed with docked 1-bromohexane to verify improved stabilization of the substrate in the mutated enzyme.
- **Evaluation of Stability Effects of Mutations in Tunnel Residues.** Tunnels mediate transport of small molecules, ions and water solvent in a large variety of proteins. The aim of this project was to assess the previously proposed concept of protein stabilization by tunnel engineering. We evaluated the stability effects of mutations in the tunnel residues and compared them with the effects of mutations in other protein regions. For this purpose, twenty six different proteins from all six enzyme classes were analyzed. The tunnels were calculated using CAVER 3.0 software. The effect of 227924 mutations, out of which 43681 were localized in the access tunnels, was predicted computationally using FoldX. The obtained results showed that saturation mutagenesis targeting the tunnel residues has almost two times better chance to produce protein variants with significantly improved stability than mutagenesis targeting other protein regions (see Figure 1).

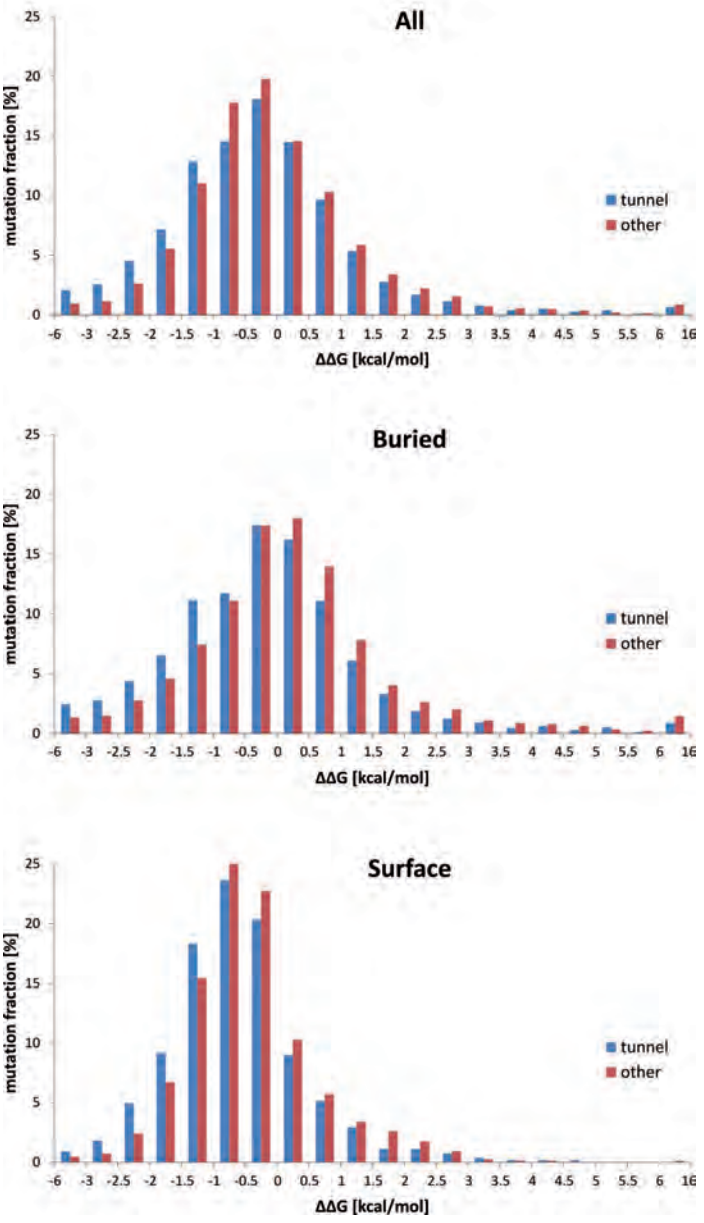

Fig. 1. Distribution of the stability effects of mutations located in the access tunnels and in other protein regions for the whole dataset (All), dataset of buried residues (Buried) and dataset of surface residues (Surface). For each protein from the test set, the $\Delta\Delta G$ values of all possible single point mutations were calculated by FoldX. The mutation with the lowest $\Delta\Delta G$ was selected for each amino acid position. The selected mutations were divided into 20 bins according to their $\Delta\Delta G$ values.

The role of MetaCentrum in the research projects
The computational resources of MetaCentrum enables us to run computationally demanding projects for prediction of various enzyme properties involving long molecular dynamics simulations as well as highly parallel virtual screening campaigns to identify novel inhibitors. We also use the MetaCloud component of MetaCentrum to access fully controlled environment needed for execution of numerous computational tools needed to evaluate effects of mutations on large datasets. Our laboratories also benefits from continuous monitoring of performance of our submitted jobs by administrators of MetaCentrum, which resulted into several proposals leading to their increased efficiency or even collaboration in the development of more suitable platform for the job execution. Last but not least, the professional administration of our private cluster is provided by MetaCentrum.

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Thermal Plasma Department

Institute of Plasma Physics, Academy of Sciences, Czech Republic

The research interests of the *Thermal Plasma Department (Institute of Plasma Physics AS CR)*, lead by assoc. prof. Milan Hrabovský, focuse on generation of thermal plasmas, properties of thermal plasma jets and fundamentals of plasma processing technologies. This area includes generation of thermal plasma in arc discharges at atmospheric and reduced pressures, theoretical and experimental investigation of electric arcs with liquid stabilization or with combined gas-liquid stabilization, as well as examination of properties of the thermal plasma, dynamics of thermal plasma jets, interaction of plasma jets with ambient atmosphere and with substances of different state of matter, primarily with solid state particles, liquid substances, and gaseous jets. Moreover, methods for diagnostics of thermal plasma jets with extreme values of temperature, enthalpy, and flow velocity are being developed, and physical processes decisive for technological applications of thermal plasmas are being studied by the department.

Research interests of Ing. Jiří Jeništa, MSc., CSc., include physics and numerical modeling of thermal plasmas including electric arcs operating in different configurations, namely, swirl and hybrid-stabilized arcs. His close co-workers are experts in calculation of the transport, thermodynamic and radiative properties of thermal plasmas (Dr. Petr Křenek – IPP AS CR, Assoc. Prof. Milada Bartlová and Prof. Vladimír Aubrecht – both from Brno University of Technology). Since 2005 he has a collaboration with Japanese colleagues (Assoc. Prof. Hidemasa Takana and Prof. Hideya Nishiyama) at Institute of Fluid Science (IFS), Tohoku University, Sendai, Japan.

Assoc. Prof. H. Takana is involved in the numerical simulation of thermal and non-equilibrium plasma flow, as well as in their application of material and environmental processing and energy conversion devices. Prof. H. Nishiyama is the head of the Electromagnetic Intelligent Fluids Laboratory. His research fields include fluidics (fluid mechanics), plasma science (plasma science and technology) and thermal spraying (heat engineering). He is currently involved in numerical simulation of plasma flow systems, electromagnetic control of plasma flow and its intelligent systematization, synthesis of magneto-rheological suspensions and functional evaluation.

Dr. J. Jeništa has been participating in the so called "Collaborative Research Project" at IFS since 2009. The aim of the Collaborative Research Project is a cooperation between the researchers of other institutes and those of IFS. Dr. Jeništa was the leader of the project "Investigation of supersonic hybrid-stabilized argon-water arc for biomass gasification" in 2009-2011, currently he is the leader of the project "Investigation of subsonic-supersonic hybrid-stabilized argon-water electric arc with inhomogeneous mixing of plasma species".

In 2011-2012 we focused in our research on the influence of turbulence and radiative tranfer method on parameters in the discharge and near-outlet regions

of the hybrid-stabilized arc. The results between laminar and turbulent flows have been discussed and compared with available experiments.

The so-called hybrid stabilized electric arc, developed a decade ago at IPP AS CR in Prague, utilizes a combination of gas and vortex stabilization. In the hybrid argon–water plasma torch, a thermal plasma generator, the arc chamber is divided into the short cathode part, where the arc is stabilized by tangential argon flow, and the longer part, which is stabilized by water vortex. The arc is attached to the external water-cooled rotating disk anode at a few millimeters downstream of the torch orifice. At present, this arc has been used for plasma spraying using metallic or ceramic powders injected into the plasma jet, as well as for the pyrolysis of waste (biomass) and production of syngas, which seems to be a promising environmentally friendly application of thermal plasma jets.

Radiation losses from the argon-water arc are calculated in our numerical model in two ways: by the net emission coefficient for the required arc radius of $3.3mm$ and by the partial characteristics method for different molar fractions of argon and water plasma species as a function of temperature and pressure. Continuous radiation, discrete radiation consisting of thousands of spectral lines, molecular bands of O_2, H_2, OH and H_2O have been included in the calculation of partial characteristics. Broadening mechanisms of atomic and ionic spectral lines due to Doppler, resonance and Stark effects have been considered.

Turbulence is modelled by Large eddy simulation with the Smagorinsky subgrid-scale model, the Van Driest damping function near the walls, and standard values of the Prandtl number $Pr = 0.9$ and the Smagorinsky coefficient $C_S = 0.1$.

The set of conservative governing equations for density, velocity and energy (continuity, momentum and energy equations) is solved numerically by the LU-SGS method, which is coupled with Newtonian iterative method. To resolve compressible phenomena, convective term is calculated by using a third-order MUSCL-type TVD scheme. For the electric potential, the TDMA algorithm enforced with the block correction method is applied. The task has been solved on an oblique structured grid with nonequidistant spacing for the total number of 38553 grid points.

The principal results for currents 300-600 A and for argon mass flow rates 22.5-40 standard liters per minute can be summarized as follows:

1. The partial characteristics method gives somewhat lower temperatures at the arc axis near the outlet nozzle, but in most cases higher outlet velocities and the Mach numbers (compared to the net emission coefficients).
2. The results for fluid, thermal and electrical characteristics, calculated by the two radiation methods, exhibit the relative difference below 15 %.
3. Reabsorption of radiation in colder part of the discharge (the partial characteristics method) ranges between 31-45 %; it decreases with current and slightly decreases with argon mass flow rate.
4. Turbulence is not significant phenomenon in the discharge and near-outlet regions of the hybrid-stabilized argon-water electric arc:

   - The maximum relative difference of each of the monitored physical quantities calculated at the arc axis, along the radius and within the volume of the discharge and of the near-outlet region reaches less than 10 %.
   - The difference generally increases with current; the maximum value of the difference occurs for the Reynolds number.
5. Turbulent effects are stronger in small regions near sharp edges of the outlet nozzle and in the transition region between hot plasma and surrounding atmosphere in the near-outlet region with high radial temperature and velocity gradients.
6. Comparison with available experimental data demonstrates very good agreement for temperature. Agreement between the calculated radial velocity profiles and the profiles derived from experiments is worse.

Our numerical code developed in co-operation with Japanese colleagues is written in Fortran. The code is not parallelized, all jobs are running one a single processor. The compiler `intelcdk-12` is our choice number one. The average time for completing one task is about four days, depending on the grid size. In Metacentrum we appreciate the great advantage of a possibility to submit and execute many jobs at one time (30), it helps us to obtain a lot of results quickly. The web-based interface for job submission is very nicely done in Metacentrum.

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Department of Cybernetics

Faculty of Applied Sciences, University of West Bohemia in Pilsen, Czech Republic

The *Department of Cybernetics (KKY)*, lead by prof. Josef Psutka, is one of the five departments of the Faculty of Applied Sciences at the University of West Bohemia in Pilsen. The aim of KKY's research activity is the building and development of systems theory and its application in the area of objectively and subjectively uncertain systems as well as in the planning of information and control systems. The basic activity of artificial intelligence is the research into sophisticated computer algorithms and methods of intelligent machine decision-making and classification. The research is mostly focused on the area of man-machine voice communication in natural language.

Research activities are chiefly aimed at:

- Building and further development of a general systems theory with emphasis on creating a correct axiomatic theory (continuous systems, systems with distributed parameters, etc.)
- Solving tasks of optimal control and optimal estimation using the latest knowledge of structural characteristics of stochastic systems
- Solving tasks of adaptive control and estimation
- Developing systems of intelligent decision-making and communication with application mainly in the area of voice dialog systems (speech recognition and synthesis, dialog control) and technical and medical diagnostics (integration of knowledge- and feature-based approaches)
- Methodology of planning of information and control systems using methods of object-oriented analysis.

1 Continous Speech Recognition group

An automatic speech recognition comprises a conversion of human continuous speech to the text. We focus on real-time applications in different acoustic environments including speech understanding and related applications. Our speech recognition system is developed and deployed in many research projects funded by Czech government and industry as well.

Since computer algorithms used in the state-of-the-art automatic speech recognition system have massive computing demands, we appreciate accessibility of many high-performance computers managed by MetaCentrum. We use common computing tools such as Matlab for development of methods employed in robust acoustic modeling. Many applications of neural networks in this field require fast training algorithms using parallel computing power of GPUs. On the other side, openFST tools are applied during a task of speech understanding. To search for optimal parameters of the whole recognition system, we use our tools developed for multi-core CPUs available at MetaCentrum.

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2 Computer Speech Synthesis group

The aim of speech synthesis is to generate speech, in such form and quality that synthetic speech follows as closely as possible the characteristics of human speech (often even the voice of a concrete person); not just the voice itself and its quality, but also the style of speaking, etc. To produce speech automatically by a machine, text-to-speech (TTS) technology is used. Its task is to convert any text to the corresponding speech. Our group deals with all sub-tasks within the TTS process – text processing, conversion of text to its pronunciation form, prosody generation, and speech production itself. Our speech synthesis system is developed and deployed in many research projects funded by Czech government and industry as well.

Since the current speech synthesis algorithms use very large speech corpora and have massive computing demands, we appreciate accessibility of many high-performance computers managed by MetaCentrum. More specifically, we use the computing resources to develop fast, efficient, and highly optimized algorithms of unit selection in large speech corpora, statistical modeling of speech units and their phonetic segmentation, statistical parametric speech synthesis, etc.

Publications with MetaCentrum/CERIT-SC acknowledgement

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Computational Chemistry and Materials Science

Faculty of Natural Science at Masaryk University in Brno, Czech Republic

Project CEITEC is a supra-regional centre of scientific excellence, whose results will be comparable to those of top centres and will thus contribute to strengthening the position of Brno as a recognized European scientific centre. CEITEC strives to be completely on par with the world's leading institutions of this kind, taking advantage of the unique opportunities arising from synergies between life and traditional sciences. One of the main goals is innovative research in the field of Quality of Life and Human Health.

The group *Computational Chemistry and Materials Science* (principal investigator prof. M. Šob) constitutes a part of the Laboratory for Synthesis and Analysis of Nanostructures headed by prof. J. Pinkas. Its research concentrates on theoretical modelling of intermetallics and nanoalloys. Aminy others, the group investigates properties of phases of potential industrial importance. The results obtained are used in prediction of phase equilibria and calculations of phase diagrams. This research is realised via the ab initio (VASP, WIEN2k) and semiempirical CALPHAD (THERMOCALC, MT DATA) codes. Sophisticated techniques on gaining thermodynamic and phase equilibrium data for technically important systems with intermetallic phases (ordered structures, Laves phases etc.) and prospective lead-free systems are applied. In combination with theoretical calculations, they focus on preparation of metallic nanoparticles with functionalized surfaces suitable for further applications and on directed research on metallic nanoparticles applicable both in the material and life sciences. Theoretical investigations of mechanical and magnetic properties of interfaces in selected advanced materials and of stability of nanoparticles are performed. Recent discovery of magnetically dead layers at grain boundaries and surfaces may provide a solid basis for construction of new materials for spintronics.

In MetaCenter, the group performs large-scale calculations of electronic structure, total energies and other properties of selected advanced materials. One of the main goals is to gain a deeper understanding between the structure and properties of materials and to be able to predict new materials with desired technologically important properties. These calculations are very demanding and MetaCentrum provides an excellent opportunity to perform them. In a way, the group conducts measurements in a computer, predicting properties of various solids and proposing those with desired properties.

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Optoelectronic Phenomena and Materials

Institute of Macromolecular Chemistry of the Academy of Sciences, Czech Republic

The department *Optoelectronic Phenomena and Materials* of the Institute of Macromolecular Chemistry AS CR focuses on studies of photo- and electroactive polymers and their low-molecular-weight analogues. Physical phenomena, such as electrical conductivity, photoconductivity, photochromism, photorefractivity, electroluminescence, as well as the injection, generation, recombination, and transport of charge carriers are investigated with respect to their dependence on the chemical structure of the materials. Both π- and σ-conjugated polymers are studied. Understanding the processes associated with photon absorption and emission, like photoexcitation, excited state dynamics, photoinduced electron transfer, changes in molecular conformations, dissociation and recombination of ion-pairs enables us to determine the basic principles of designing organic solar cells. The transport of free charge carriers and polarons are studied on polymer photoconductors and structures of organic FET transistors.

Theoretical activities of the group are focused on quantum mechanical and semi-classical modeling of the processes connected with the charge carrier transport, photogeneration, and recombination in organic materials. Special attention is paid to the materials and structures perspective for the construction of the sensing and switching devices. An important part of this research is determination of the molecular parameters of the proposed models by means of the quantum chemical methods (e.g. density functional theory methods). These calculations are partly done in Metacentrum using the Gaussian 09 program package. The calculated properties include geometry optimizations, study of the conformational properties, IR vibrational spectra, weak intermolecular interactions, complexation, solvation effects, electron densities (population analysis), absorption spectra, properties of polarons and excitons. Computational resources of Metacentrum are also used for the Monte Carlo calculations of the charge carrier mobility in organic materials, which is performed using own programs compiled by high performance Fortran compilers (Portland, Intel).

Publications with MetaCentrum/CERIT-SC acknowledgement

[1] S. Ehala, E. Makrlík, P. Toman, V. Kašička: *ACE applied to the quantitative characterization of benzo-18-crown-6-ether binding with alkali metal ions in a methanol-water solvent system.* Electrophoresis 2010, Vol. 31, No. 4, pp. 702–708.

[2] J. Kříž, P. Toman, E. Makrlík, J. Budka, R. Shukla, and R. Rathore: *Cooperative Interaction of Hydronium Ion with an Ethereally Fenced Hexaarylbenzene-Based Receptor: An NMR and Theoretical Study.* J. Phys. Chem. A 2010, Vol. 114, No. 16, pp. 5327-5334.

[3] E. Makrlík, P. Toman, P. Vaňura, and R. Rathore: *Cooperative interaction of protonated hexamethylenetetramine with a hexaarylbenzene-based receptor:*

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[6] P. Toman, E. Makrlík, and P. Vaňura: *A combined experimental and theoretical study on the complexation of the ammonium ion with benzo-18-crown-6.* Monatsh Chem 2010, Vol. 141, No. 3, pp. 301-304.

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Department of Physical and Macromolecular Chemistry

Faculty of Science, Charles University in Prague, Czech Republic

Department of Physical and Macromolecular Chemistry was founded in 1921 by Prof. J. Heyrovský (Nobel prize winner in 1959). Aside electrochemistry, that was the main research topic of the department in 60s, many other (both theoretical and experimental) fields including spectroscopy, theoretical, biophysical and macromolecular chemistry are intensively studied.

In the group of Prof. K. Procházka, a wide variety of polymer systems is studied both experimentally and theoretically. The later include conformational behavior of linear, block and branched polymers (stars, combs, dendrimers) both uncharged and polyelectrolytes (weak or strong), their association, complexes with surfactants, persistance length of semiflexible polymers and polymer dynamics in the context of dynamic light scatttering and fluorescence correlation spectroscopy studies.

Besides polymers, systems composed by smaller molecules are studied by Dr. F. Uhlík, including fullerenes (both pristine and endohedral, their electronic structure and thermodynamic properties), organometallic compounds (electronic structure and electrochemical behavior), water (from small water clusters to description of ice) and others

The extensive computations by the members of the department would not be possible without generous resources provided and maintained by the Metacentre together with cooperative user support.

Publications with MetaCentrum/CERIT-SC acknowledgement

[1] P. Bačová, P. Košovan, F. Uhlík, J. Kuldová, Z. Limpouchová, and K. Procházka: *Double-exponential decay of orientational correlations in semiflexible polyelectrolyt.* European Physical Journal E 35 (2012) 53.

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MUFIN

Faculty of Informatics, Masaryk University, Brno, Czech Republic

The goal of the project *Multi-Feature Indexing Network (MUFIN)*, lead by prof. Pavel Zezula, is to develop a general purpose technology solution to the problem of searching in various and very large databases. The project represents a joint research effort towards a scalable and extensible similarity search system for many applications. Its extensibility is achieved by accepting the metric space model of similarity, so the technology works for any metric distance measure and finds applications as diverse as biology, geography, multimedia, data cleaning and integration, etc. In order to scale into billions of object searched on-line for hundreds of queries processed real-time, structured peer-to-peer similarity search networks are applied. In order to tune performance, MUFIN keeps a clear separation between the logical P2P structure and the hardware physical infrastructure.

During the years 2011 and 2012, the research of the MUFIN project has focused on algorithms for distributed similarity processing, extraction of image-content descriptors and techniques for multi-modal data processing.

The research of the MUFIN distributed technologies requires large infrastructure of networked computers with diverse computing power. For comparions of various techniques, the MetaCentrum resources offer easy and quick access to large hardware platforms that would be otherwise too costly to utilize. Since the MUFIN system works with rather huge data collections that require extraction of content descriptors, the MetaCentrum classical GRID jobs allow to speed-up the processing that would otherwise take weeks to complete.

Publications with MetaCentrum/CERIT-SC acknowledgement

[1] Michal Batko, Fabrizio Falchi, Claudio Lucchese, David Novák, Raffaele Perego, Fausto Rabitti, Jan Sedmidubský, and Pavel Zezula: *Building a Web-scale Image Similarity Search System.* Multimedia Tools and Applications, Springer Netherlands, 47, 3, od s. 599-629, 31 s. ISSN 1380-7501. 2010.

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[8] Jan Sedmidubský, Vlastislav Dohnal, and Pavel Zezula: *On Investigating Scalability and Robustness in a Self-organizing Retrieval System.* In Proceedings of CIKM 2011 and the co-located Workshops. New York, NY 10087-0777: ACM Digital Library, 2011. od s. 33-38, 6 s. ISBN 978-1-4503-0717-8.

Department of Chemical Physics and Optics

Faculty of Mathematics and Physics, Charles Univesity in Prague, Czech Republic

Experimental and theoretical research of the *Department of Chemical Physics and Optics at Charles University in Prague* is carrying out in related fields like the primary processes of photosynthesis, femtosecond laser spectroscopy of molecules, investigation of protein complexes, fast relaxation processes in semiconductor nano structures, quantum theory of molecular processes, quantum chemistry of biologically important molecules, simulation of complex molecular structures, classical and quantum nonlinear phenomena and applied research in collaboration with beer industry.

Quantum chemical sub-group of the Department (DCPO/KCHFO), lead by prof. J. V. Burda, concentrates mainly on ab initio, DFT and QM/MM calculations of organometallic complexes with biomolecules like nucleobases, models of oligonucleotides in ds-DNA, peptides or short protein sequences. (cf. papers 2-5 in the list of publications below). Further, calculations of structures concerning various photosyntetic problems were performed recently (cf. paper 1). Some additional interests deals with polymeric (polyaniline) models, their interaction in nanocomposites and further characterizations of such materials.

All these interests reflected in our calculations are performed in the frame of Metacentrum projects. Without utilizing computational power (using programs like Gaussian, Amber and our own interfacing tool QMS for combined QM/MM calculations) of the Metacentrum we would not be able to successfully finished most of the above mentioned studies.

Publications with MetaCentrum/CERIT-SC acknowledgement

[1] J. Alster, M. Kabeláč, R. Tuma, J. Pšenčík, and J. V. Burda: *Computational study of short-range interactions in bacteriochlorophyll aggregates.* Computational and Theoretical Chemistry 998 (2012), p. 87–97.

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[3] Z. Chval, Z. Futera, and J. V. Burda: *Comparison of hydration reactions for "piano-stool" RAPTA-B and [Ru(?arene)(en)Cl]+ complexes; DFT computational study.* Journal of Chemical Physics 2011, 134, 2, 024520. 2011.

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Part V

Appendices

Appendices:

Appendix A: Detailed Resource Usage Statistics

Appendix A

1 MetaCentrum Operational Statistics in 2011-2012

This report summarizes the use of MetaCentrum VO computing resources in 2011-2012. The overall results were as follows. Data from 2011 are in parentheses.

- Number of completed jobs: 1080 thousands (609 thousands)
- Number of used CPU years: 2.5 thousands CPU years (742 CPU years)
- Number of users with active account: 613 (491)
- Number of extended accounts: 301 (314)
- Number of new accounts: 312 (177)
- Number of active users (with min. 1 job running): 322 (240)
- The amount of data in the storage: 350 TB (85 TB)

By the end of 2012, MetaCentrum registers 613 active users. Out of this number 301 accounts were extended and we gained 312 new users in 2012. At least one job was run by 322 users. Some of our members use their membership in MetaCentrum only for access to storage capacities and other services, some of them were never active.

In 2012, the users and their jobs utilized 22 millions CPU hours in over in over one million jobs via Torque. Comparing to 2011, the number of CPU cores and the total CPU time increase by approximately the same factor of three (see Fig. 1). This is a strong confirmation that the massive investments to the infrastructure are appropriate because there is a matching user demand. At the same time, the MetaCentrum services and organization were clearly able to handle this growth.

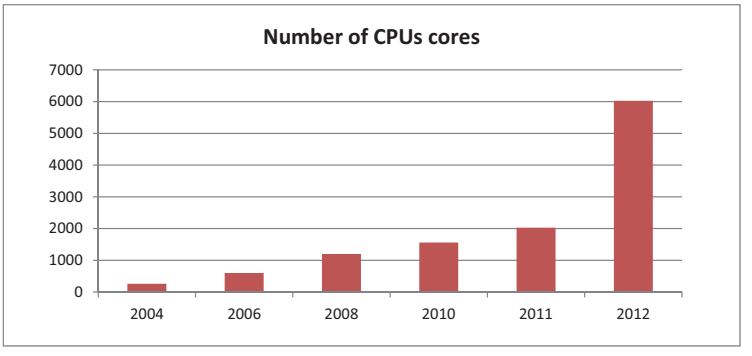

Fig. 1. Increase of the number of CPUs.

The rapid grow in number of the available CPU was realized in 2011–2012 thanks to the significant investments into the national e-Infrastructure supported by the ICT projects defined in the National Roadmap of Large Infrastructures for Research and Development, CESNET and CERIT-SC.

Major HW resources owners are CERIT-SC (2200 CPU) and CESNET (2600), having 80 % of all CPU cores available, the remaining resources are owned by other academic or research institutions, however, management of the clusters is done by MetaCentrum: *NCBR/CEITEC*, MU Brno (580 CPUs), *Loschmidt Laboratories*, MU Brno (260 CPUs), *West Bohemian University*, Pilsen (140 CPUs), FEKT VUT, Brno (100 CPUs), *Bohemian University*, Ceske Budejovice (100 CPUs), *FZU*, Academy of Sciences in Prague (70 CPUs), or *Faculty of Informatics*, MU Brno (60 CPUs). Up-to-date number of machines, CPUs and their utilisation are displayed on the MetaCentrum portal[1].

1.1 Utilization

Figure 2 shows hardware utilization of all clusters (with the exception of those included in the experimental cloud environment, i.e. Dukan and some nodes of Zegox) in 2012. The base (100%) is the total number of available CPU-core-seconds minus the CPU-core-seconds of machines under maintenance. The values are CPU-core-seconds of running jobs and reservations. Utilization above 60 % is considered as optimal; on the other hand utilization higher as 90 % means that cluster is fully saturated and users have to wait long time before their jobs are executed. The main part of clusters are in the range 60 % to 90 %, thus they are in the optimal range.

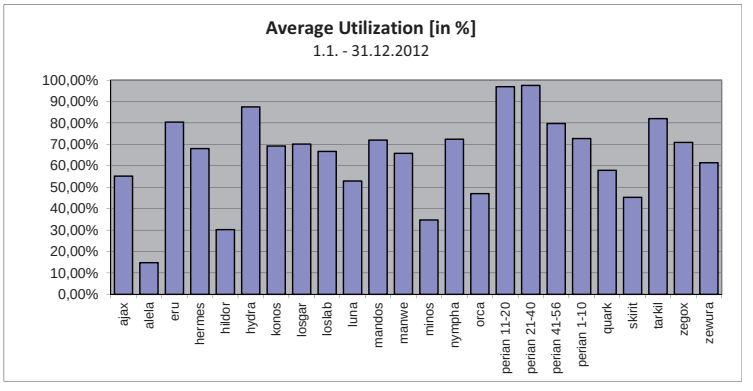

Fig. 2. Average utilization of MetaCentrum clusters

The most demanded clusters are the most powerful multiprocessors ones with sufficient memory. In general, the demand on newer (hence faster) CPUs is

[1] `http://metavo.metacentrum.cz/`

higher, yielding higher utilization as well. On the other hand, scheduling many-cores or huge-memory computations is more difficult (machines must be drained off smaller computations first), therefore utilization of SMP clusters is slightly lower.

New SMP Clusters Zewura and Mandos *Zewura* is the largest cluster with 1600 (20x80) CPUs and with the largest memory of 512 GB per each node. The first part of the cluster was made operational in December 2011, the second part half year later. *Mandos* is the second largest cluster in MetaCentrum. It contains 896 (14x64) CPUs and 256 GB RAM per each node. Zewura and Mandos represents SMP-clusters (Symmetric MultiProcessing) with single shared main memory. They are suitable for applications with enormous memory requirements and/or parallelized, composed from number of processes communicating through the shared memory.

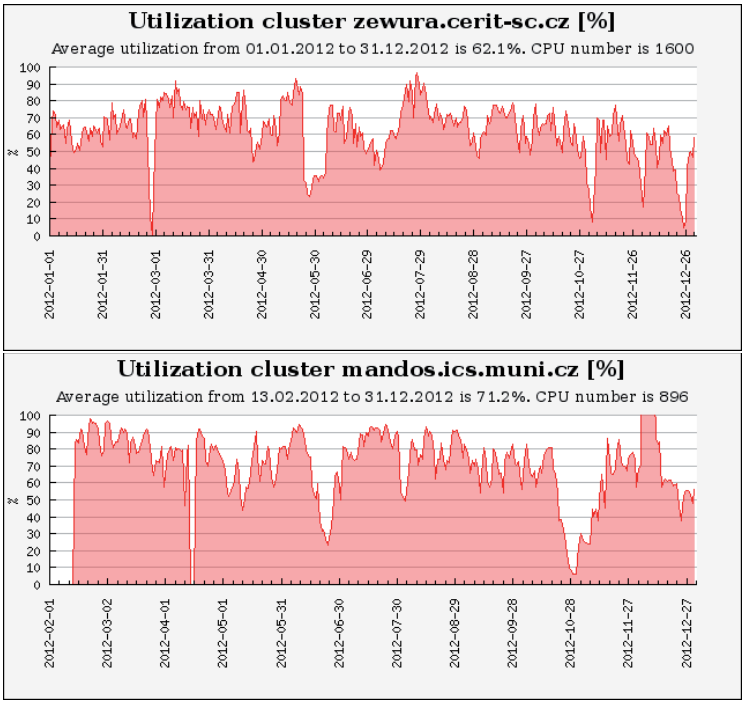

Fig. 3. Utilization of Zewura and Mandos (SMP)

Both the clusters are very popular for large memory demanding jobs running on small number of CPUs. Therefore, the situation when one user utilize just few CPUs, but concurrently whole machine memory often appears; consequently no more users can use the node, but processors in node stay idle and the node

seems to be free in the accounting. The utilization of the Mandos is above 70 %. From the beginning and in both deliveries, Zewura has faced HW problems, some nodes were available for supplier's testing purposes. Therefore its utilization is slightly below 65 %.

Figure 4 of total computed time per cluster shows that Zewura and Mandos became very popular clusters with the highest computed time in 2012.

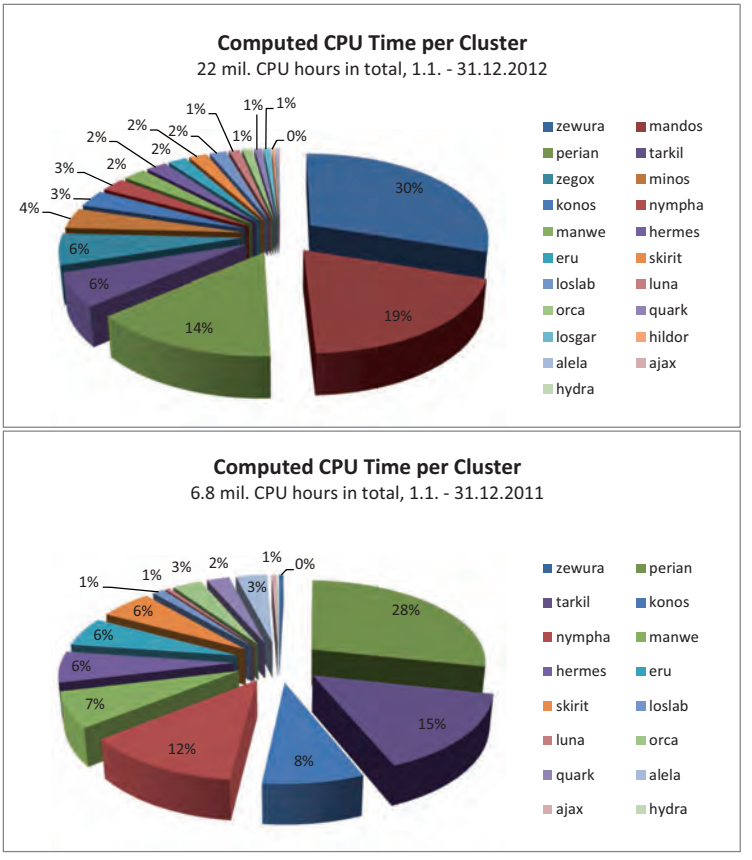

Fig. 4. Computed CPU Time per Cluster in 2011 and 2012

New HD Clusters Zegox and Minos High density cluster *Zegox* has 576 (48x12) CPUs and 90 GB RAM per each node, its utilization is nearly 80%. All nodes of the cluster are included in the OpenNebula cloud, thus being available to run user images of operating system when required. Complementarily, the nodes of the cluster which are not utilized by the cloud users run "CERIT-SC

standard" OS image which is a worker node of the Torque batch system. Hence the nodes become available in the batch system transparently.

Cluster *Minos* is the third largest cluster having 600 (50x12) CPUs together and 24 GB RAM per each node. Cluster is partially dedicated to virtualization experiments, therefore utilization by grid users noted in Fig. 5 is bellow MetaCentrum average. The jobs from experiments are not counted.

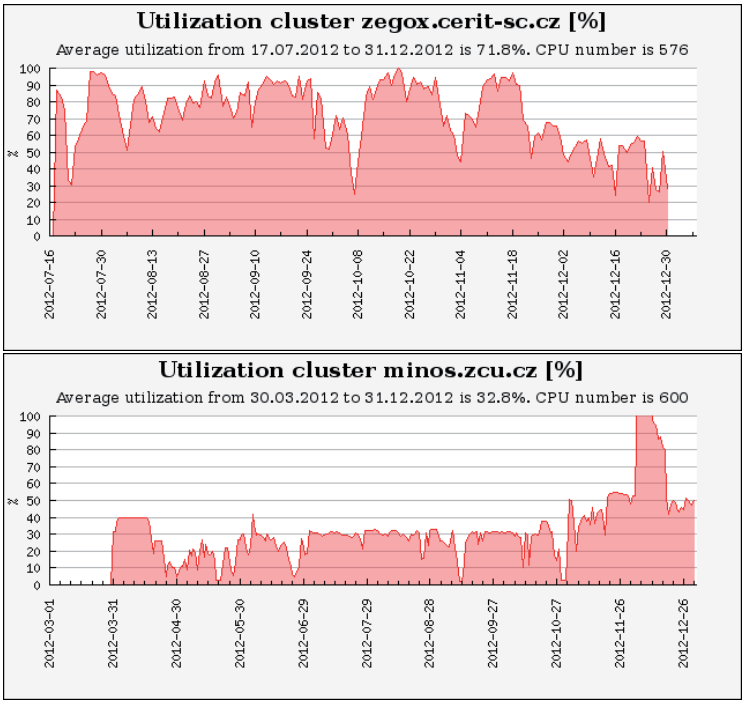

Fig. 5. Utilization of Zegox and Minos

Clusters owned by research groups Clusters with lower utilization (e.g. Loslab, Quark, and Orca) run in a restricted mode with significant capacity dedicated to their owners, therefore the total utilization is lower. On the contrary, Perian is owned by the group (NCBR) which generates the largest fraction of the whole MetaCentrum load, therefore it is well utilized too (See Fig. 6). Moreover, the jobs run there are specifically crafted to match number of CPU cores per node and available memory, hence using the resources optimally.

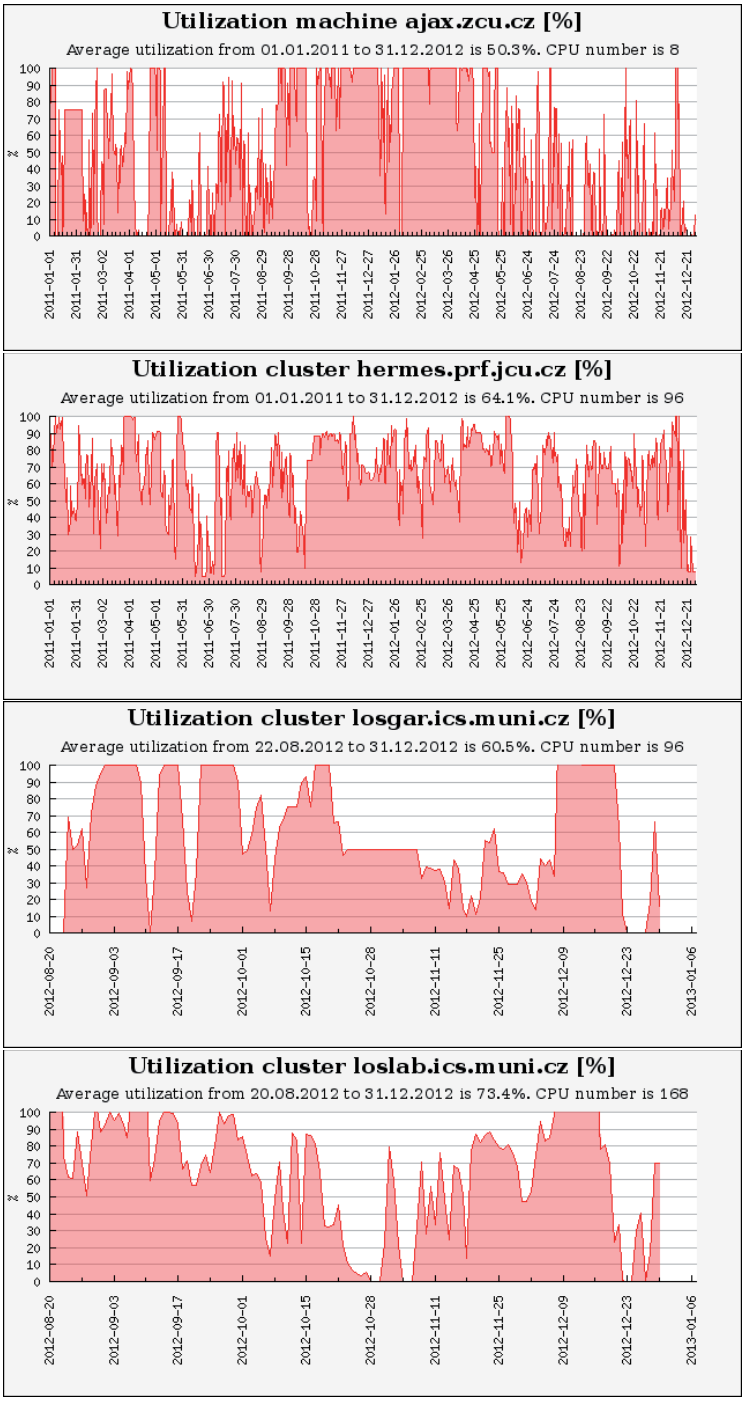

Fig. 6. Utilization of the clusters owned by research groups

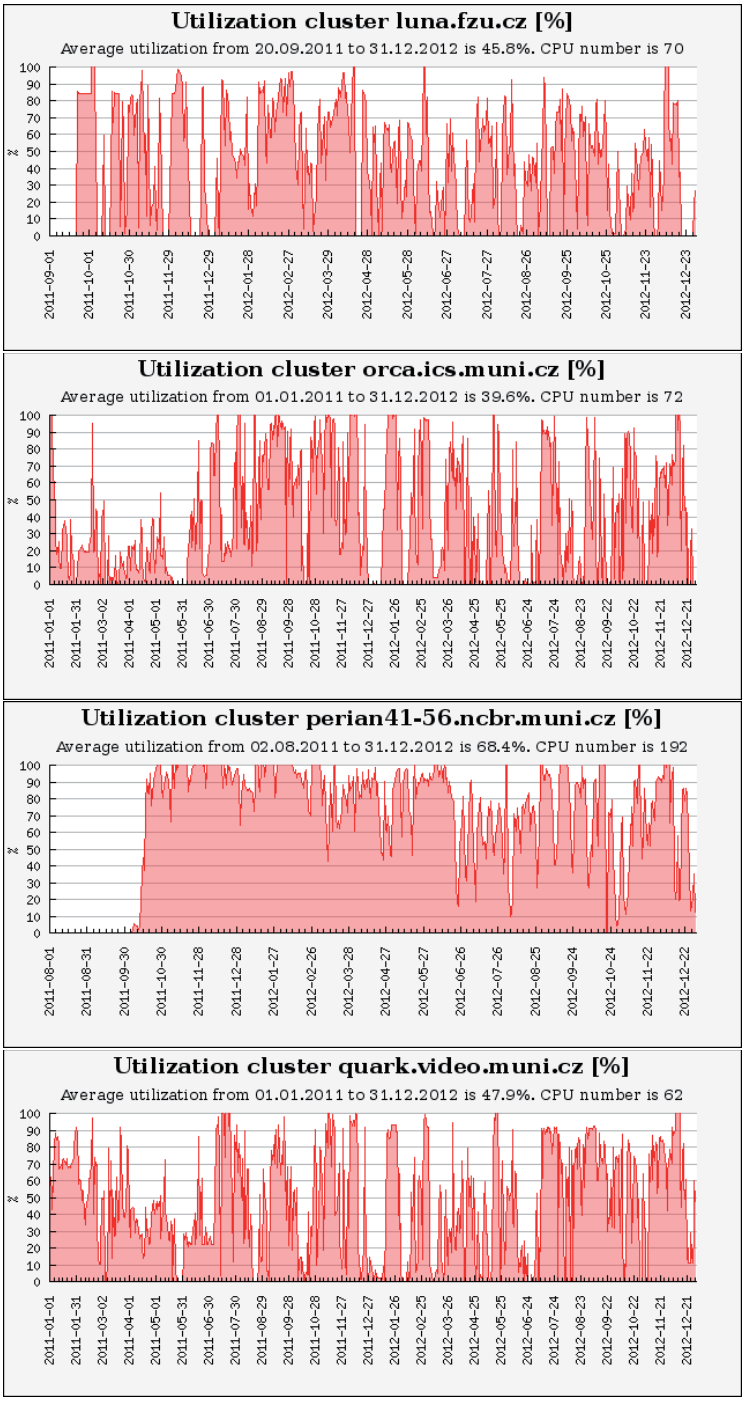

Fig. 7. Utilization of the clusters owned by research groups

1.2 Jobs in MetaCentrum

In 2012, the users and their jobs utilized 22 millions CPU hours in over one million jobs. Comparing to 2011, the number of the total CPU time increased three times, it corresponds with the increase of the number of CPUs (see Fig. 1). The number of executed jobs increased only with ratio 1.7 (see Fig. 8).

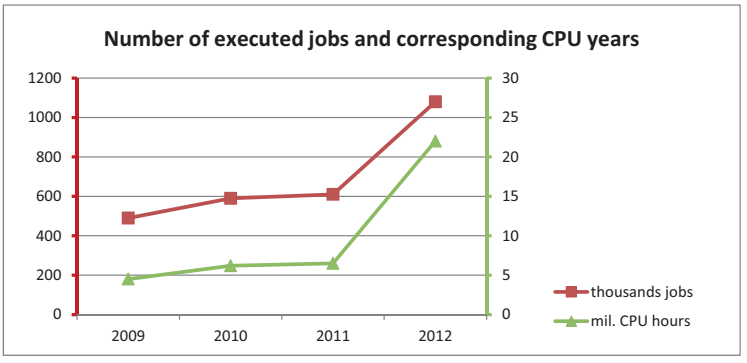

Fig. 8. Number of executed jobs and corresponding CPU time in past years.

This inproportion between the increase of the CPU time and number of executed jobs can be explained by the significant increase of the number of parallel jobs in 2012. For example, jobs requiring more than 16 CPUs were rather unusual in the past year while during this year they represent significant proportion of all jobs (see Fig. 9). This indicates that the users started to utilize new large SMP clusters and available from 2012. The largest jobs requested over 500 CPUs.

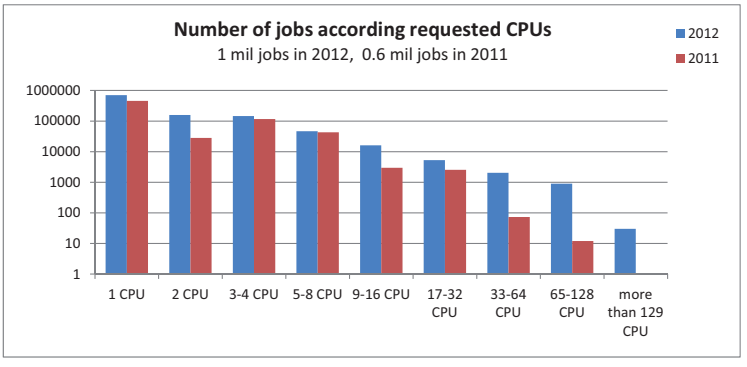

Fig. 9. Jobs utilizing given number of CPUs according to number of executed jobs

The most of jobs (over 65 % of all jobs) in 2011 and 2012 started immediately within 60 seconds. Almost 80 % of all jobs started within 24 hours. We noticed increase of the number of waiting jobs 1 hour and more in 2012, comparing to previous year (for details see Fig. 10).

Longer waiting time is very often for new, fast machines that are popular among the MetaCentrum users and also for parallel jobs with many CPUs or for memory demanding jobs. Other reasons of job waiting can also be very rare combination of machine properties, requested combination of properties that is not in MetaCentrum available, exceeding queue limits by the user, MPI jobs waiting until all required nodes are free etc.

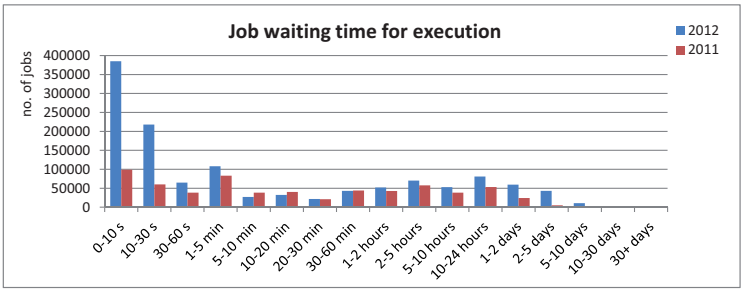

Fig. 10. Number of waiting jobs in 2011 and 2012.

Figure 11 shows increase of jobs execution duration in 2012 comparing to 2011.

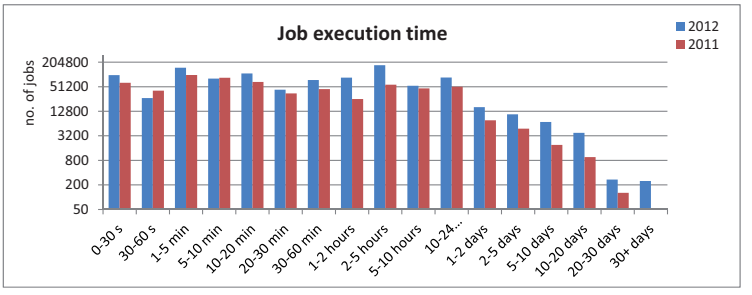

Fig. 11. Number of jobs according to execution time in 2011 and 2012.

Accoding to computed time, the most utilized were queues long@arien and default@wagap (See Fig. 12). The long queue is suitable for jobs with expected duration from 24 hours to 30 days. As compared to the MetaCentrum infrastructure, where the jobs' maximum run-time (influencing their scheduling) is implicitly specified by placing the jobs into a set of pre-defined, time-limited

queues (short, normal, long, etc.), all the jobs under the CERIT-SC computing infrastructure are placed into a single default queue.

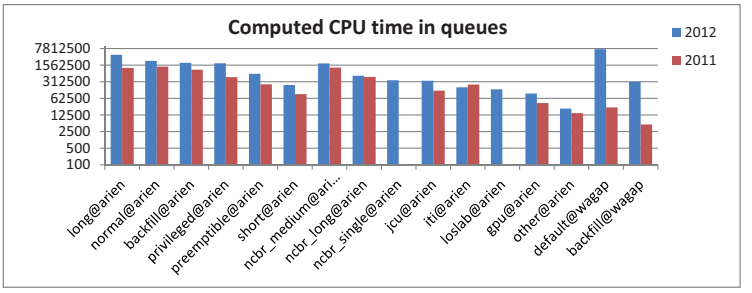

Fig. 12. Computed CPU time in queues

According to executed jobs (See Fig. 13), the most frequent was the queue backfill@arien, the low priority queue dedicated to many single CPU jobs (limit 1000 submitted job per user and 24 hours), that fills the nodes when there are free. Backfill is a low-priority queue; jobs from this queue "fill" free gaps in the schedule (e.g., when waiting for a completion of a job, which holds resources requested by a starving job). The queue accepts just single-node jobs with the specified maximum run-time in the length up to 24 hours. When necessary (e.g., reserving resources for a long-term job), the backfill jobs may be suspended or even terminated by us at any time.

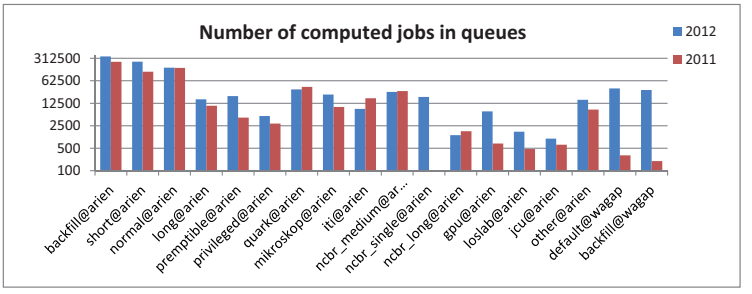

Fig. 13. Number of computed jobs in queues

1.3 Institutions, groups and users

There are 322 users that have executed at least one job during this time period. The number has increased from 240 in the year 2011. Metacentrum is utilized by several research groups from several academic or scientific institutions that covers computational groups. More detailed preview of computed time using by institutions is shown at Fig. 14.

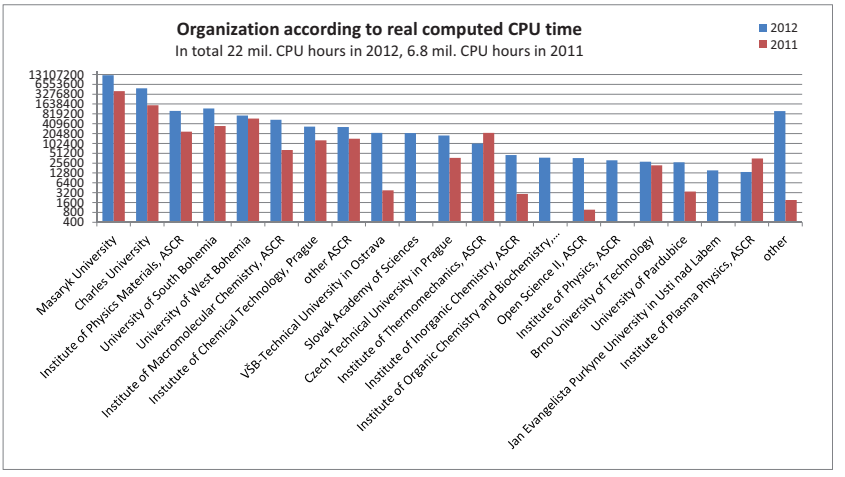

Fig. 14. Organizations and computed time

The most active users (according to consumed CPU time) are from the Masaryk univerzity, its members computed over 12 milion CPU hours (more than 50 % of total computed CPU time). There are more than 90 users from Masaryk university that have executed at least one job during this time period, the most of these users comes from NCBR (part of CEITEC) or Loschmidt laboratories groups. Both groups own clusters dedicated for their research, connected to MetaCentrum, and available also for other users. The second place according to real computing CPU time belongs to Charles univerzity with 32 users and 5 mil. CPU hours, the third position to Institute of Physisc Materials ASCR with 15 users and 1 mil. CPU hours, the fourth place to University of South Bohemia with 15 users and 1 mil. CPU hours, and the fifth position to University of West Bohemia with 38 users and 730 thousands CPU hours.

The same trend can be observed in the groups (see Fig. 15). Major part of user are not separated into research groups, the largest and most active is once again NCBR (41 members in MetaCentrum, part of CEITEC).

First ten users have computed more than 10 mil. CPU hours (see Fig. 16) that is almost 50 % of the whole computed time. According to the number of jobs they have computed over 800 thousands jobs, that makes nearly 70% of all jobs executed in MetaCentrum. Between the most active users belong users from

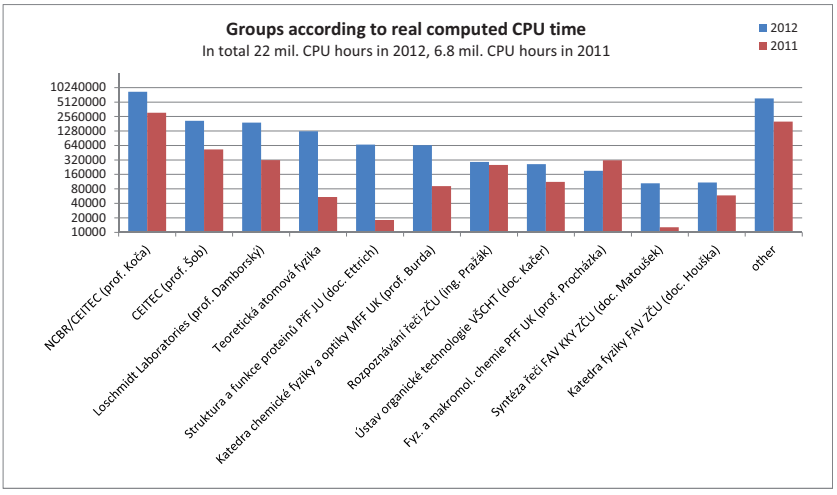

Fig. 15. Groups and computed time

NCBR and Loschmidt Laboratories groups (both from the Masaryk univerzity) and users from Charles university.

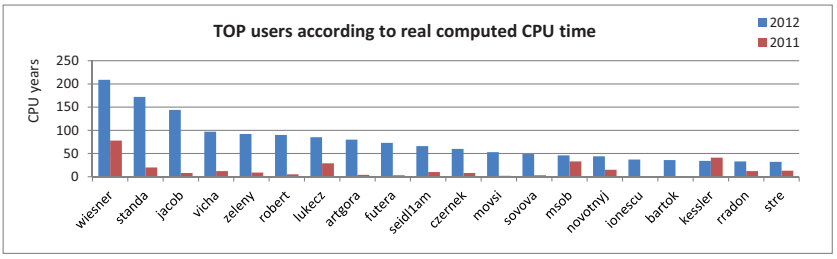

Fig. 16. MetaCentrum users with the highest computed time

Majority of recognized applications (see Fig. 17) that are utilized in MetaCentrum are from chemical domain. The unrecognized applications are often programs created by users.

- Amber package that contains cca 50 applications that covers methodes utilized in computational chemistry
- Gaussian package based on quantum mechanics to study molecules and chemical reactions
- VASP package for performing ab-initio quantum-mechanical molecular dynamics
- Gromacs package to compute molecular mechanics and dynamics – minimalization of energy of system and dynamic behaviour of molecular systems

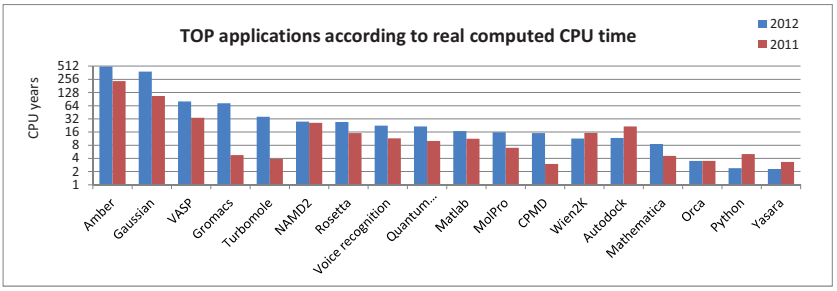

Fig. 17. Applications

1.4 Storage Usage

The NFSv4 volume, which is the main high-capacity online storage facility for MetaCentrum, has total capacity of 600 TB (124 TB in 2011). It consists of five disk arrays in three geographic locations (3 in Brno, 1 in Pilsen, 1 in Ceske Budejovice), One of the Brno's disk arrays is owned by the CERIT-SC Center (260 TB), all the other belongs to CESNET. End of 2012, user data occupied approximately 380 TB (60 % of total capacity) in 233 millions of files (last year it was only 155 millions of files). All disk arrays are available on all computing nodes as a */storage* volume.

Appendices:

Appendix B: Complete list of users' publications with MetaCentrum/CERIT-SC acknowledgements (2010-2012)

Appendix B: Complete list of users' publications with MetaCentrum/CERIT-SC acknowledgements (2010-2012)

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