Central European Grid Infrastructure for Generic Applications

Jan Kmuníček and Daniel Kouřil*

Abstract. *Grid computing as new paradigm of distributed computing is currently seen as major enabler of fulfilling up to date science research requirements demanding extreme computing power and/or large storage capacities. This has led to formation of the worldwide research infrastructure available for everyday scientific work providing access to massive computational/data resources. These resources are geographically dispersed, span multiple trust domains and are heterogenous. They can be dynamically contributed by different owner institutions, thus forming virtual pools accessible to users showing the appropriate credentials. This article describes VOCE - Virtual Organization for Central Europe - a grid production infrastructure available for researchers from the Central European region.*

1. Introduction

Grids can be seen as huge distributed systems composed of organizationally individual elements that can be individual computing and storage facilities, middleware services and information services mutually interconnected by a computer network. The potential of grid systems is immense and many large research projects benefit from their use. However, current grids are very complex systems with long and slow learning curve causing they are only used by large user communities with enough resources for training their researchers. Also deployment and mainly everyday operation of core services providing access to the Grid resources is a difficult task that requires skilled administrators who have to be well trained first. Therefore, the potential of current grids is not fully utilized yet and especially small research groups, which do not have resources to build and administrate such a sophisticated infrastructure and train users are not able to even test the grid environment and evaluate if it fits their needs.

Users in current grids are organized within *virtual organizations* (VO) that reflect real hierarchy of users coupled to solve joint problems. A VO usually spans multiple administrative domains and even countries providing an abstraction of the user community. Each VO provides basic user management and also provides all resources necessary to solve the research problems.

European Union (EU) project Enabling Grids for E-SciencE (EGEE)[1], currently in its second stage EGEE-II, brings together experts from more than hundred organizations and almost thirty countries from all around the world with the common aim of building and operating a production grid infrastructure, which is available to scientists 24 hours-a-day. The operation activities of the project are organized according to the geographical principle segmenting the participants into several *federations*

*CESNET z. s. p. o., Zikova 4, 160 00 Praha 6, Czech Republic, email: {kmunicek,kouril}@ics.muni.cz

[1] http://www.eu-egee.org/

that operate their local resources and provide support for users from their region.

The Central Europe (CE) federation consisting of institutions from Austria, Croatia, Czech Republic, Hungary, Poland, Slovakia, and Slovenia must deal with high level of heterogeneity in both partners and organizations. Despite this fact all the members of the federation are able to cooperate to provide a useful heterogeneous set of tools for the end users day-to-day work in established grid environment. In order to bring the grid facilities closely to the end users the CE federation established and operates a grid environment available to all users from the Central European region. This infrastructure is open for every user from the region and is meant as a general *catch-all* virtual organization serving users not covered by other application specific environment. The environment targets primarily at users without any experience with grid computing who look for possibilities to test the environment and try using their applications there.

2. VOCE Environment

Most VOs is designed for a particular group of users that are collaborating on common problems to provide them with a common platform that can be used as the basis for their work. For example a set of scientists working on the same research project could establish a VO that allows them to coordinate the work by sharing data and providing computing resources. Such VOs are usualy tied closely with the end community and are concerned only with problem of this specific environment and mechanisms implemented by the VO aim primarily at the main focus of the users.

The Virtual Organization for Central Europe environment[2] currently consists of computational resources and storage capacities provided by the Central European resource owners. Unlike majority of other virtual organizations, VOCE tends to be a generic virtual organization providing an application neutral environment. Such environment is especially suitable for grid newcomers allowing them to get quickly first experience with grid computing and to test and evaluate grid environment towards their specific application needs. Primary purpose of VOCE is to provide an easy access for users who already use computing techniques to solve their problems but are not familiar with utilization of grids. According to our experience, individual researchers and/or small research groups cannot often penetrate through the complex environment provided by the grids to start their using. Such groups also usually do not have access to any established grid infrastructure and are not willing and able to build a separate environment just to test it. Targeting at these user communities, VOCE tries to motivate new application communities to use the immense power provided by current grids. The VOCE application neutrality can be also seen as an important feature that allows provision of an environment where different application requirements meet and different expectations can be fulfilled.

2.1. VOCE Infrastructure

VOCE currently provides a complete grid infrastructure running all necessary grid services to serve scientific end users solving their research projects and problems. The core services (e.g. scheduler, file catalogs, *etc*.) are based on the Lightweight Middleware for Grid Computing (gLite) software stack[3], which is being developed by EGEE and Worldwide LHC Computing Grid (LCG)[4]. In some cases we provide multiple different versions of the services to extend features set supported by VOCE.

[2] http://egee.cesnet.cz/en/voce/
[3] http://glite.web.cern.ch/glite/
[4] http://lcg.web.cern.ch/LCG/

For instance, we run two installations of the scheduler, the LCG Resource Broker (RB) providing a tried and tested service and the latest gLite Workload Management System (WMS) providing new functionalities and features.

The core VOCE infrastructure is entirely independent of any services operated outside CE and thus can be configured very flexibly on demand if any special needs arise. End resources (i.e. computing and storage elements) are provided by the CE institutions that are distributed all over the region and are usually shared with other VOs supported by the sites.

In order to provide a flexible and efficient user support the VOCE also operates a well-known system Request Tracker (RT)[5], which allows coordination of actions among the administrators even if they are often geographically dispersed. It also provides additional features useful to assist in problem solving, such as detailed history of all tickets, different ways of communication, *etc*.

Users in VOCE are maintained by sophisticated tool Perun [1] that was developed specifically to cover the user management needs in distributed environments. Beside usual user management operations (accounts creation and removal, notification sent to the users, *etc*.) it is also able to propagate information into LDAP and VOMS [2] servers. These services are used extensively in current Grid environment as a basis for authorization of users. Moreover, VOCE supports some non-standard features, such as parallel execution of jobs using MPI.

2.2. Current VOCE Status

VOCE currently provides access to approximately 1260 CPUs and nearly 30 TB of disc space for its 178 registered users. Several hundreds user requests have been sent to dedicated VOCE support RT system containing both infrastructure as well as application problems. This evidently proofs that the provided email interface of VOCE RT is increasingly being used by new users and is seen as useful gateway for getting proper help with accessing VOCE environment. VOCE approach tried to tackle the slow learning curve problem bothering grid newcomers through provision of access to the open grid environment supporting generic application portfolio and hiding the complexity of generic grid environment.

Moreover, VOCE removes the necessity of building VO from scratch and allows outsourcing of all necessary VO-related services to dedicated administrators who perform routine VO management & administration. To maximally simplify research day-to-day work of the end users VOCE provides a set of high-level middleware tools as Charon Extension Layer toolkit[6], portals (P-GRADE, GENIUS) and VOCE-UIPnP[7] that represents a modified version of User Interface Plug anf Play (UIPnP) originally prepared by National Institute of Nuclear Physics (INFN)[8].

VOCE represents a model how so-called *catch-all* VO approach enables an easy way for accessing the grid environment. Furthermore, dynamic building of VO complicates the establishment and subsequent VO utilization due to necessity to set number of policies, find proper technical solutions and guaranty of day-to-day operation thus preventing users from direct immediate usage of the grid environment.

[5] http://www.bestpractical.com/
[6] http://egee.cesnet.cz/en/voce/Charon.html
[7] http://egee.cesnet.cz/en/voce/UIPnP.html
[8] http://www.infn.it/indexen.php

2.3. Users' Utilization of VOCE Resources

VOCE is open for all users from the region who are interested in the grid technologies. The only requirement for the users is a possession of a digital certificate issued by a certification authority approved by the IGTF. This requirement makes the VOCE different from other similar projects, which allow users to use arbitrarily certificates, often issued using very weak identity vetting procedures. Such users cannot be identified properly and it is hard (or even impossible) to trace them if they cause an incident. The VOCE users, on the other hand, can be easily contacted by the resource owners if they harmed the resource. Last but not least such a precaution helps educate users in proper credential management. The VOCE membership can be applied for using a simple web form, which generates a request to the administrators. Users accounts and all arrangements are then created within a few days. The applicants are not required to have any prior experience with grids, for such inexperienced users VOCE provides an ideal platform for getting experiences with grid as the environment provides real services and not limited facilities.

Moreover VOCE partners also organize training events where users can learn how to use the grid. After getting familiarized with the environment the users are ready to use VOCE for their own research. They gradually move from examples to real work and prepare their application for the grid environment. When the applications are tested and ready the users use the VOCE infrastructure for everyday routine production. VOCE resources provide efficient background for complex problems solving and VOCE experts are available to assist and help users. When the users gain enough knowledge with the grid their needs may grow. If the features provided by VOCE do not fulfill their requirements, such users can establish a new VO providing dedicated resources and/or services for their purpose. In this case the VOCE experts can provide necessary expertise in building and operating the VO.

2.4. VOCE Application Portfolio

One of the VOCE major features differentiating VOCE from other VOs is its application neutrality. VOCE is not bound to any particular application or application domain and therefore it is designed to allow users from arbitrary application area to test/evaluate the environment towards their particular applications needs and subsequently use the environment without any additional requirements (learning new tools, switch to different middleware, accessing different resources, *etc*.).

Currently there are already active users from various application communities (e.g. computational chemistry, physics, astrophysics) but apparently there is place for other potential VOCE customers from other scientific research domains (e.g. bioinformatics, material simulation, *etc*.)

2.5. Access to VOCE Resources

VOCE provides different ways for accessing available resources. On one hand, VOCE resources are accessible through well-known graphical user interfaces (GUIs) - P-GRADE portal and GENIUS portal - forming nowadays *de facto* standard of grid computing GUI approaches each with different focus on provided services.

- Portal P-GRADE [3] offers mechanisms for solving complex problems. P-GRADE portal is a workflow-oriented grid portal enabling the creation, execution and monitoring workflows in grid environments through high-level, graphical web interfaces. Overall, it supports powerful workflow management (components of the workflows can be sequential and MPI jobs), comfortable execution of parallel applications and provides support for legacy applications together with access to multiple grids.

- Portal GENIUS [4] was originally developed in order to support training and demonstration grid activities and to make the use of available EGEE II grid environment easier and more intuitive for non-expert users. It is often used as a standard tool during training events, induction courses, and grid schools that aim to teach grids utilization and to allow smooth transition in production grid usage.

On the other hand, an unique, modular system - Charon Extension Layer (CEL) - offering command-line interface (CLI) approach with standard gLite and LCG users' commands being used as the default has been jointly developed by computational chemistry community members of National Centre for Biomolecular Research (NCBR)[9] and Czech Education and Scientific Network (CESNET)[10] operator for utilization within VOCE environment.

3. Charon Extension Layer System

Charon Extension Layer toolkit [5] is a universal framework[11] creating a layer upon the basic grid middleware environment and making an access to the complex grid infrastructure much easier compared to native middleware. CEL provides a command-line oriented interface and is supposed for users that require a full control over their running computational jobs. CEL system provides uniform and modular approach for complex computational jobs submission and management and forms a generic system for the use of application programs in the Grid environment independently of Grid middleware present at specific fabric infrastructure. CEL can be easily used for powerful application management enabling single/parallel execution of computational jobs without the job script modification. Simultaneously, standard job management involving easy job submission, monitoring, and result retrieval can be performed without any additional hassle or requirements on users.

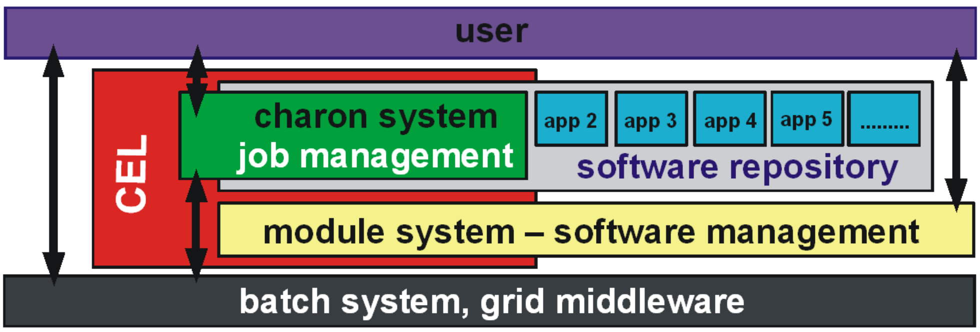


Figure 1. A basic scheme of CEL architecture composed from two main parts - Module system and Charon system forming together a layer between a grid end user and a grid middleware.

The complete Charon Extension Layer is combined from two distinct subsystems Module System and Charon System (see Fig. 1). Module System is used for the management of available application

[9]http://ncbr.chemi.muni.cz/
[10]http://www.cesnet.cz/
[11]http://troll.chemi.muni.cz/whitezone/development/charon/wiki/index.php/Introduction

portfolio. It solves problems connected with execution of applications on machines with different hardware and/or operation systems and it is also capable to simplify the execution of applications in parallel environments. Charon System is a specific application managed by Module System that introduces complete solution for jobs submissions and their subsequent management.

These two parts of CEL form together a unique and consistent solution not only for job submission and administration but also for easy job preparation. Moreover, CEL does not limit original batch systems in any way. It just extends their functionality and simplifies their usage as much as possible for everyday submissions and monitoring of tens up to hundreds of complex computational jobs.

Currently Charon Extension Layer provides following set of unique features:

- easy access and utilization of heterogeneous grids in an easy and smoothly integrated way
- transparent access to distinct grids
- powerful software management and administration
- comfortable enlargement/modification of available application portfolio
- easy job submission, monitoring, and results retrieval
- interactive software repository

3.1. Module System

The very generic requirements on a system that could be used for easy yet powerful administration of application programs within a grid environment should involve following set of features: easy application initialization, application versions conflict handling, inter-application conflicts and/or dependencies handling, very same utilization for single/parallel jobs execution, support for different levels of parallelizations. All these basic demands are currently supported by Module System that is one of the essential CEL parts serving for management of applications available in a specific grid environment.

3.2. Interactive Software Repository

Recently, the Module System was extended with interactive browser of the module database containing real-time list[12] of available software realizations (see Fig. 2). This service can show the list of available applications with or without the accessible application versions. Moreover, this information is integrated with the detailed description of applications, i.e. with documentation of particular compilation and installation in the MediaWiki format.

3.3. Charon System

The administration of a computational job through its complete lifetime within a grid environment would definitely demands easy job submission, easy parallel executions of applications. The system should naturally allow user to focus only on desired task not to all things related to submissions; often

[12] http://troll.chemi.muni.cz/whitezone/development/charon/isoftrepo/

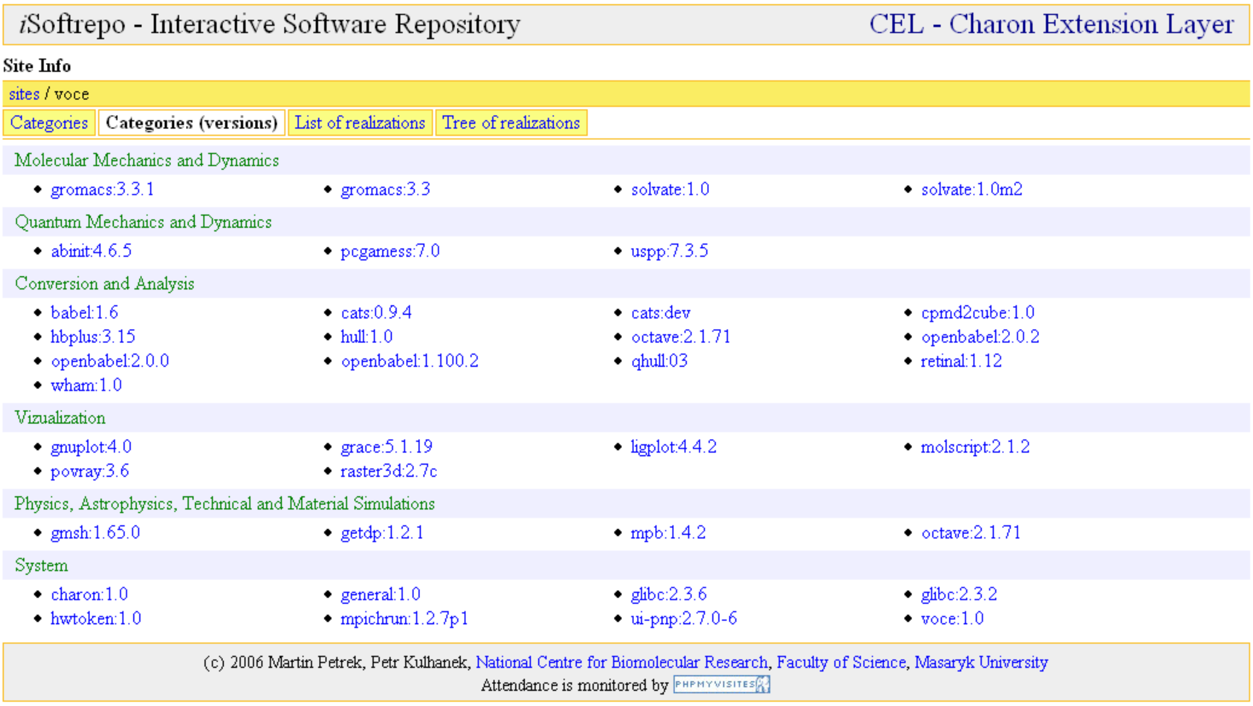


Figure 2. Software repository of programs currently ported and available within VOCE environment through Charon Extension Layer

repeated things should be process automatically and it would be useful to keep information about job during its execution and/or after its execution. All of mentioned requirements are fulfilled in the Charon System – the second major part of CEL framework.

4. VOCE Data Challenge

One of crucial factors showing the real usability of the VOCE environment is its ability to enhance solving of research tasks that require extreme computational resources. An example of such large-scale application utilization can be demonstrated by accomplishments achieved by the computational chemistry community utilizing the VOCE grid environment through Charon Extension Layer toolkit.

4.1. Research Study Purpose

One of the currently intensively studied areas of modern material design and drug discovery is chemistry of interlocked supramolecules and their mutual interactions. A rotaxane – a supramolecular complex – and its behavior were thoroughly investigated during a VOCE data challenge. Rotaxanes [6] are interlocked molecules in which macrocycle (the 'wheel') is threaded by a long 'axle' component. Our system consists of a molecule cucurbit[7]uril (CB7) and a 4,4'-bipyridinium derivate (see Fig. 3). Experiments [7] show switch-like movements along the axle in this supramolecular complex. To give a detailed insight to the switch-mechanism we calculated the free energy profile along reaction coordinate related to this movement.

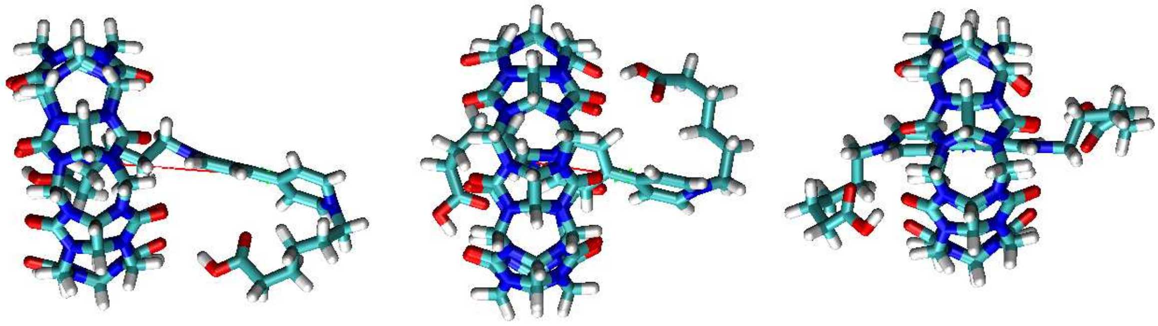


Figure 3. Supramolecular complex of cucurbit[7]uril (CB7) and a 4,4'-bipyridinium derivate

4.2. Computational Methods Used

We focused on two methods for the free energy estimations that are used currently — umbrella and bluemoon.

The main idea of the umbrella method is to add an artificial restraint to the system. This restraint keeps a value of a reaction coordinate in a small interval (so-called window) about a prescribed value. The whole interval is then covered by these windows. Windows should overlap partially. A molecular dynamic simulation is then performed in each window holding the reaction coordinate in the window. A histogram of reaction coordinate values for the window range is obtained from the each simulation. These histograms are consequently combined into a single one by the weighted histogram analysis method (WHAM) [8]. Then, relative frequencies are estimated from it and used to calculate free energy in whole range.

In the bluemoon method, the whole interval is covered by a satisfactory amount of points, not necessarily equidistantly distributed. A constraint molecular dynamic simulation is calculated for each point with the reaction coordinate being fixed at the point value. So-called mean force is followed during the simulation. Mean force denotes the force that has to be applied on the system in each time-step to hold the constraint fixed. The mean-value of this force quadrate with a derivation of the free energy with respect to the value of the reaction coordinate. The mean-values of forces are merged together from all windows to get the dependence of the derivative in the whole range. A numerical integration is then used and a resulting free energy profile is obtained. The key point of the method is constraint keeping and mean force estimating. This is solved by an iterative algorithm that adjusts system coordinates to reach the state where the difference between the real and desired values of reaction coordinate vanishes. The Lagrange multiplier that is used to get mean force estimate is retrieved from that algorithm as well as new atoms coordinates with fulfilled constraint.

The evaluation of the free energy is a computationally demanding task requiring extensive computational resources due to necessity to properly sample large phase-space. Both the umbrella and bluemoon methods as well as other that are used nowadays (such as the adaptive biassing force method) require a calculation of a huge amount of middle-length molecular dynamic simulations that can run independently in parallel. Therefore, these types of computational tasks are very well suited to exploit large grid environments like VOCE. The complete solving of the described research problem comprises approximately hundreds thousands of CPU hours at 1.6 GHz CPU with 1 GB RAM.

4.3. Simulation Details

There have been performed several simulations of rotaxane complex in various environment. As experiments indicate a dependence of the molecular switch on the environment acidity simulations for both protonated and unprotonated system have been launched. The 'axle' molecule within the protonated system was enriched at the both ends by two hydrogen atoms (total charge 2+). These hydrogens are missing in the unprotonated system and the 'axle' molecule is neutral (total charge 0). Two types of explicit solvent - pure water (tip3p) and natural conditions environment (water and Na+, Cl- ions) were selected as an external environment. Moreover, a separate simulation within vacuum has been carried out.

Charges and the input structure was obtained for both systems (protonated and unprotonated) from *ab initio* calculations using program Gaussian 03 [9] (basis 6-31G*). Subsequent parametrization for the molecular dynamics was carried out by program 'antechamber' from the AMBER 8 program package using the GAFF (General AMBER Force Field) parametric model. Program Solvate 1.0m2[13] was used for solvation of the model. Program AMBER 8 [10] was used for simulations themselves together with an additional library for calculations of free energy using methods Umbrella and Bluemoon. The reaction coordinate ξ was set as the distance of centers of individual parts of the complex ('wheel' and 'axle'). The same calculation of so-called main ridge of reaction coordinate was accomplished for both the explored methods. Such a calculation gradually increases the reaction coordinate from zero (interlocked state) up to 8 Å.

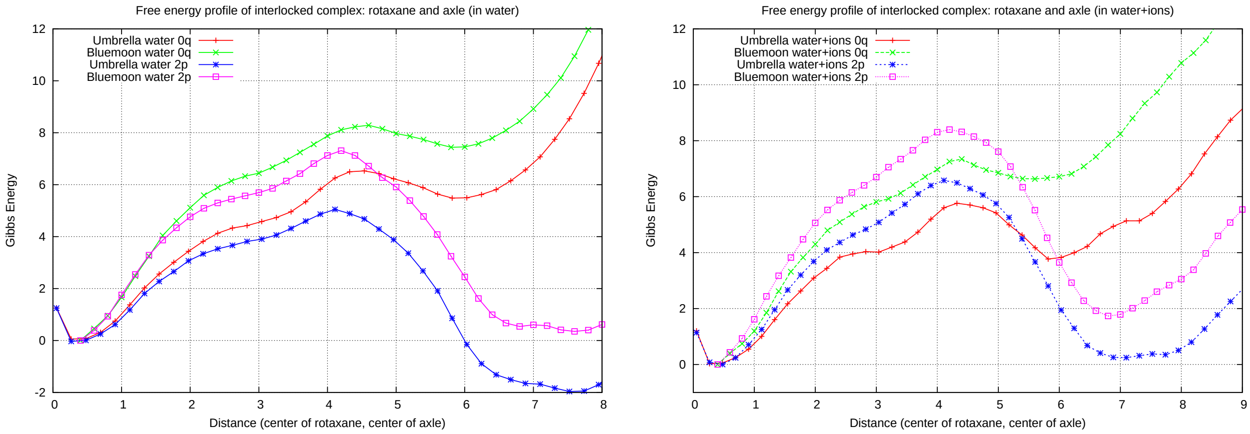
Individual subjobs suitable to be solved in the grid environment have been generated in consecutive steps of the main computational job. Each subjob simulated 250 ps of constrained or restrained molecular dynamics, respectively. The integration step was chosen as 2 fs with the SHAKE algorithm option switched on. Concerning the size of the system (17 000 atoms) the length of the particular subjobs was around 4 up to 5 days.

4.4. Challenge Achievements

The simulations confirm the fundamental impact of the environment acidity on the free energy profile of studied system and therefore the possible molecular motion during pH change, too. There is an evident energy minimum for interlocked state ($\xi = 0$) at the unprotonated system (0q) in the pure water. On the other hand, the protonated system (2p) in the same environment allows also energetically identical (or even better) favorable state in which the 'axle' molecule is undocked ($\xi = 7.5$).

The situation within the natural environment differs as can be seen from Fig. 4(a) and Fig. 4(b). The global minimum for unprotonated state is confirmed again by both the used methods and the system tends to prefer a interlocked state ($\xi = 0$). While the situation is different for the protonated state (2p) where a minimum appears that is not energetically favorable compared with a interlocked state. When comparing both the methods it can be seen that for pure water i.e. homogeneous environment the lengths of the simulations are sufficient enough to properly sample the phase space and the graphs of both methods converge to a smooth curves that differ in a constant (cca 2 kcal). This is in agreement with continuity of the defined problem. There is no such convergence within the natural environment where freely moving ions play a crucial role and this results in the different shapes of curves especially

[13] http://www.mpibpc.mpg.de/groups/grubmueller/start/projects/solvate/solvate.html



(a) water environment (b) natural environment

Figure 4. Free energy profiles of unprotonated/protonated rotaxane complex in water and natural (water and ions) environments.

for unprotonated state. This behavior can be related to insufficient lengths of simulations needed for sampling the phase space.

5. VOCEt - VOCE Training Infrastructure

The need for effective training to deliver grid newbies basic utilization habits can be fulfilled through organization of training courses and proper mapping of potential users domains. To succeed in this critical mission there must be suitable environment available at which grid functionalities can be demonstrated properly. This clearly results in the necessity to have a training infrastructure (t-Infrastructure) available for the grid end users. Generally speaking, a t-Infrastucture requires a stable, reasonably secure environment (preferably close to production) that could be available on-demand allowing flexible user management.

Therefore a VOCE training (VOCEt) infrastructure is being set up. The basic VOCEt features are as follows: VOCEt is VOCE sub-VO that is technically independent, VOCEt core services are shared with VOCE and the end-services are provided by CESNET. Several CE institutions across the region has already promised to provide resources for VOCEt or join VOCEt later when the complete service will be fully established.

The VOCEt users identity management is performed using system Perun - already used for VOCE user management and proven in production utlization. PKI credentials will be issued by an on-line CA that is based on MyProxy service. The formal policy for the on-line CA are currently in preparation (following the International Grid Trust Federation (IGTF)[14] recommendations); the VOCEt users will be provided by random passwords, their email address will be used as the corresponding login name. Such approach limits the possibility of a login/password combination being lost/stolen and misused. Moreover, a web interface to MyProxy and Perun is under construction. It will be available for event organizers only and will be used for maintaining the trainees accounts.

Compared to currently default t-Infrastructure available in EGEE II grid - the GILDA service - VOCEt will provide higher level of security as it allows no anonymous users (this is especially important for

[14]http://www.gridpma.org/

the resource owners), all users will have their own personal certificate based on accredited CA's approved by the IGTF body. VOCEt CA is expected to issue short-term certificates (days) dedicated for training purpose and the users will be able to access only limited group of available resources. Furthermore, all resources available in VOCEt infrastructure are allocated, fully guaranteed resources (dedicated resources owned by CE partners) compared to best-effort approach provided by GILDA.

In summary, VOCEt makes it possible to organize accounts for an training event in minutes; it retains basic level of security through uniqueness of certificates that can be traced to the event or even particular trainee. On one hand, the sharing of the infrastructure with the production services guarantees high level of availability while on the other hand the users cannot influence much the production environment.

6. Conclusion

The VOCE environment provides a complete grid infrastructure, which is available for all users from Central Europe. Compared to standard virtual organization VOCE stands for an application generic grid environment serving production as well as training function, enabling utilization of its computational/data resources through a set of advanced distinct ways. The primary purpose of the infrastructure is to act as a user incubator, which allows novice users to get first outlook on grids and successively receive additional experiences with this new computing area until they are experienced enough to either form their own VO or join another specialized group. In addition to a full set of common grid services known from other VOs, the VOCE users can also leverage less usual tools such as the Charon Extension Layer framework or GUI portals for more efficient use of the grid environment.

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