



Enabling Grids for E-scienceE

CESNET NA3 Activities

Jan Kmuníček

NA3/NA4 CESNET activity manager

www.eu-egee.org



Information Society



- **Approaching users**
- **Performed activities**
- **Achievements**

- **NA3 CESNET activities aims**
 - to inform end user about EGEE worldwide infrastructure and its services
 - to educate end users how to advantageously use the available environment and tools
 - to evangelize end users about grid computing and related domains

- **Local dissemination events organized**

- organized user education events

- § First Auger hands-on session (09. 01. 2007, Praha)
- § EGEE II project seminar (12. 12. 2006, Šlapanice)
- § Seminar for users of EGEE Grid (13. 12. 2005, Praha)
- § Advanced EGEE course (16. 12. 2004, Praha)
- § Induction EGEE course (26. 10. 2004, Praha)

- organized internal EGEE meetings

- § JRA1 All Hands Meeting (10. 07. 2006, Plzeň)
- § JRA1 All Hands Meeting (20. 06. 2005, Brno)

- **External dissemination**

- events with **our active contribution**

- § EGEE Industry Day (19. 09. 2007, Bratislava)
- § AUGER Offline Meeting (14. 09. 2007, Karlsruhe)
- § CE Joint Regional Summer School (25. 06. 2007, Budapest)
- § GCCP 2006 Conference (27. 11. 2006, Bratislava)
- § CE Joint Regional Summer School (03. 08. 2006, Budapest)

- **regular active participation** at worldwide grid meetings

- § Cracow Grid Workshop, EGEE Conference, EGEE User Forum, ...

- **CESNET dissemination / training**

— overview available at

<http://egee.cesnet.cz/en/info/results.html>

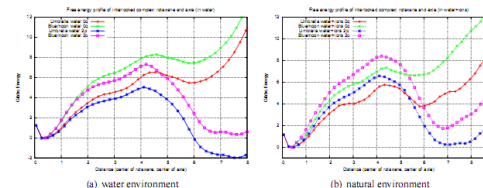


Figure 4. Free energy profiles of unprotonated/protonated rotaxane complex in water and natural (water and ions) environments.

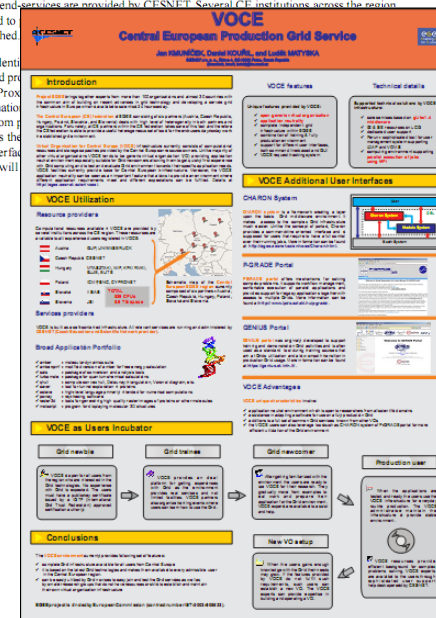
for unprotonated state. This behavior can be related to insufficient lengths of simulations needed for sampling the phase space.

5. VOCEI - 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 (Infrastructure) available for the grid end users. Generally speaking, a Infrastructure requires a stable, secure environment (preferably close to production) that could be available on-demand exible user management.

A VOCE training (VOCEI) infrastructure is being set up. The basic VOCEI features are as OCEI is VOCE sub-VO that is technically independent, VOCEI core services are shared and the end-services are provided by CESNET. Several CE institutions across the region promised to establish

users identification and provided on MyProxy International by random, which limits the web interface only and will



A Generic Grid Environment for Central Europe A Study of Pseudorotaxanes Behavior

Jan Kmuňeček, Daniel Kouřil, Petr Kulaňáček, and Martin Petříček

CESNET z.s.p.o., Žitkova 4, 160 00 Praha 6, Czech Republic
{kmuňeček,kouřil}@ics.muni.cz, {kulhaneč,petreček}@chemi.muni.cz

Abstract. Grid computing is currently becoming one of the best methods for fulfilling a research infrastructure by computing optimization for researchers utilization for access investigation of

Introduction can be seen as an independent element of the network. The process benefits from being slow and gradually implemented in everyday life. This is especially true for administrative support of the grid in the Europe region. In this paper we demonstrate

O for Central in current Grid hierarchy of

