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Enabling Grids for E-sciencE

NA4 Activities
within Central Europe region

Jan Kmuníček

NA4 activity regional coordinator

Information Society

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- **NA4 VOs services**

- **Related support tasks**

- **Recent issues**

- **Plans concerning EGEE-III**

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- **VOs within Central Europe region**

  - VOs run and managed by CESNET & CYFRONET

  - CESNET provides all EGEE services WMS, LB, BDII, Myproxy, LFC, UI, ...) for **VOCE and Auger VOs**

  - CYFRONET manages **GAUSSIAN VO** and and newly created **TURBOMOLE VO**

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- **VOCE – Virtual Organization for Central Europe**

  resources from

  CESNET (Czech Republic)
  PSNC, CYFRONET, ICM (Poland)
  II-SAS (Slovakia)
  SRCE, IRB, FESB (Croatia)
  BME, KFKI, ELTE, NIIF (Hungary)
  GUP, HEPHY (Austria)

  more than   **324 registered users**

  from 14 institutes and 6 countries

  in total   **1387 CPUs**
  51 TB disc space

  currently   **19 sites supporting VOCE**

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- **Virtual Organization for astrophysics**

  – **Pierre Auger Cosmic Ray Observatory**

    http://www.auger.org

  – studies the universe's highest energy particles which shower down on Earth in the form of cosmic rays

  – Auger Observatory is a hybrid detector employing two different independent detection methods

  – one of them tracks the development of air showers by observing ultraviolet light emitted high in the Earth's atmosphere, to this AUGER community task will employ

  Grid environment with VO AUGER

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- **AUGER – Virtual Organization for astrophysics**

Pierre AUGER Collaboration

more than **300 scientists, 17 participating countries**

Argentina, Australia, Bolivia, Brazil, Czech Republic, France, Germany, Italy, Mexico, Netherlands, Poland, Portugal, Slovenia, Spain, United Kingdom, United States, and Vietnam

in total   **530 CPUs**
                        cca 10 TB disc space

currently   **3 sites supporting AUGER VO**

 more than   **19 registered users**
                        from 8 countries
                        (CZ, IT, FR, UK, US, SL, PL, MX)

The work mainly focuses on:

- **Computational chemistry management**

- **Commercial Software porting**

  – **Gaussian**
  – **Turbomole**

- **Management of VOs allowing access to above software packages**

- **Parallel execution of chemical packages**

Gaussian VO:

- Over 25 users since start in September 2006
- Open for every EGEE user
- VO manager -- Mariusz Sterzel (`m.sterzel@cyfronet.pl`)
- Registration at:

  `https://voms.cyf-kr.edu.pl:8443/vo/gaussian/vomrs`

Turbomole VO:

- Newly opened
- Enabled for every EGEE user as well
- Parallel execution allowed (over MPI)
- Registration at:

  `https://voms.cyf-kr.edu.pl:8443/vo/turbomole/vomrs`

More details at:

`http://egee.gridcyfronet.pl`

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- **Regular user support tasks (apart from VOs support)**

  – regular participation in **TPM** (Ticket Processing Managers)

    § one of CE TPM shifters teams together with Polish colleagues

  – regular participation in **ESC** (Executive Support Committee)

    § contribution to production utilization of GGUS/local helpdesk system
    § involvement in many related tasks
      - *ROC CE-GGUS documentation*

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- **Recent tasks being solved**

  - **VOCE/AUGER-specific SAM tests**

    § preparation of specific SAM tests to be published into central database to be used for sites exclusion using FCR

  - detailed analysis of **computing activity within VOCE**

    § access to LBs of individual WMS/LB installations

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- **EGEE-III NA4 CE plans**

  – activity NA4: **User Community Support and Expansion**

    § support for virtual organizaions

      - *virtual organization support*
      - *application porting support*
      - *direct user support*

    § strategic disciplines clusters
    § community building

- **EGEE-III NA4 CE plans**

  - **strategic disciplines clusters** composition

    - § high energy physics
    - § life sciences
    - § earth science
    - § grid observatory
    - § computational chemistry
    - § astronomy & astrophysics
    - § fusion

- **EGEE-III NA4 CE plans**

    – mapping of **working areas to CE institutes**

CESNET	computational chemistry, regional coordination
CYFRONET	computational chemistry
II-SAS	earth science, astronomy & astrophysics
JSI	regional coordination
MTA SZTAKI	application porting support
UIBK	computational chemistry, astronomy & astrophysics

- Computational chemistry management

- Software porting with particular focus on:

    - Commercial software packages
    - Parallel execution
    - Development of procedures concerning:
        § job check-pointing,
        § access to intermediate data generated by software packages
        § job restarting

- Development of Grid license models

- Web portal for chemical community