Remote access to NMR spectrometer using the Virtual Laboratory

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Outline

- Introduction
- Characteristic
- Research goals
- Security
- Accounting
- Team Work
- Putting into practice
- Prototype
Introduction (1/2)

- Project „Big scale computation and visualisation for virtual laboratory using SGI cluster” – co-founded by State Committee for Scientific Research (project no. 6 T11 0052 2002 C/05836) and SGI company. Duration time: December 2002 – October 2004

- Partners:
  - Academic Computer Centre CYFRONET
  - Institute of Bioorganic Chemistry PAS - Poznań Supercomputing and Networking Center
  - Computer Centre of the Technical University of Lódź
Introduction (2/2)

- Research grant „Building general architecture for virtual laboratory” founded by State Committee for Scientific Research. Duration time: May 2003 – April 2005.

- Partners:
  - Institute of Bioorganic Chemistry PAS - Poznań
  - Supercomputing and Networking Center
  - Radioastronomy Department of Mikołaj Kopernik University in Toruń
Characteristic

- Remote access
- Load balancing
- Users accounting
- Result digitalisation
- Team work
- Communication with the laboratory staff
- Time slot reservation for experiment executing
Research goals

- Defining general VLab architecture
- Device allocation in distributed environment
- Load balancing
- Taking into consideration the human factor
- A method of delivering and presenting information
- Support for collaborative work
- e-Learning
Security

- Access to the VLab environment only with certificate
- Multistage authorization for users’ processes
- Encryption of communication channels
- Single point of entry
- Firewalls
Accounting

- Users accounting – monitoring of resources usage
- Limits for using resources
- Reporting system
- Integration with the Grid accounting system
- Virtual Users System (PSNC)
Team work

- Many types of communication:
  - sending messages
  - chat
  - audio
  - video

- Collaborative work support for scientists from geographically distant places
Putting into practice

- Virtual Laboratory of Nuclear Magnetic Resonance Spectroscopy – cooperation with Institute of Bioorganic Chemistry PAS

- Virtual Laboratory of Radiotelescopy – cooperation with Radioastronomy Department of Mikołaj Kopernik University

- Implementing based on PIONIER network
User interface

Jobs management
- Submit new scenario
- Monitoring
- Accounting

Digital library
- NMR database
- Radio-astronomy database
- Publications database

Communication tools
- Chat
- Audio
- Video

Educational area
- Depends on laboratory profile

User profile
- User information
- Customizing tools
Measurement scenarios
Experiment submission (1/2)

- NMR Device: JCHB Varian 300MHz
- Experiment type: 2D
- Pulse sequence: 2D: COSY
- Nucleus type: 15N
- Solvent type: methanol CD3OD
- Probe type: Broadband
- Temperature: 25°C
Postprocessing submission (1/2)
Visualisation (1/2)

Program: VNMR

Visualization data file: Browse...

Use previous processing task output data

Parameters: None

Graphic mode: 1024x768

Output file format: JPG

Execution profile: Quickest
Visualisation (2/2)
Experiment executing
Educational area

- For a given science discipline area (e.g. NMR, Radioastronomy)
  - Beginner user
  - Advanced user
  - Comprehensive tests
- User guide
- VLab management course
- VLab devices description
Thank you for your attention

http://vlab.man.poznan.pl/
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