

POZNAŃ

PIONIER



VLAB

VIRTUAL LABORATORY

NEW DIMENSION OF THE SCIENTIFIC WORK

<http://vlab.psnc.pl/>

e-science e-science



Virtual Laboratory – closer the eScience

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Grid Computing for Complex Problems
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Why VLabs?

VERY limited access

Main reason - **COSTS**

Main **GOAL** - to make commonly accessible

Added Value

virtual, remote, ...**Grid-enabled**



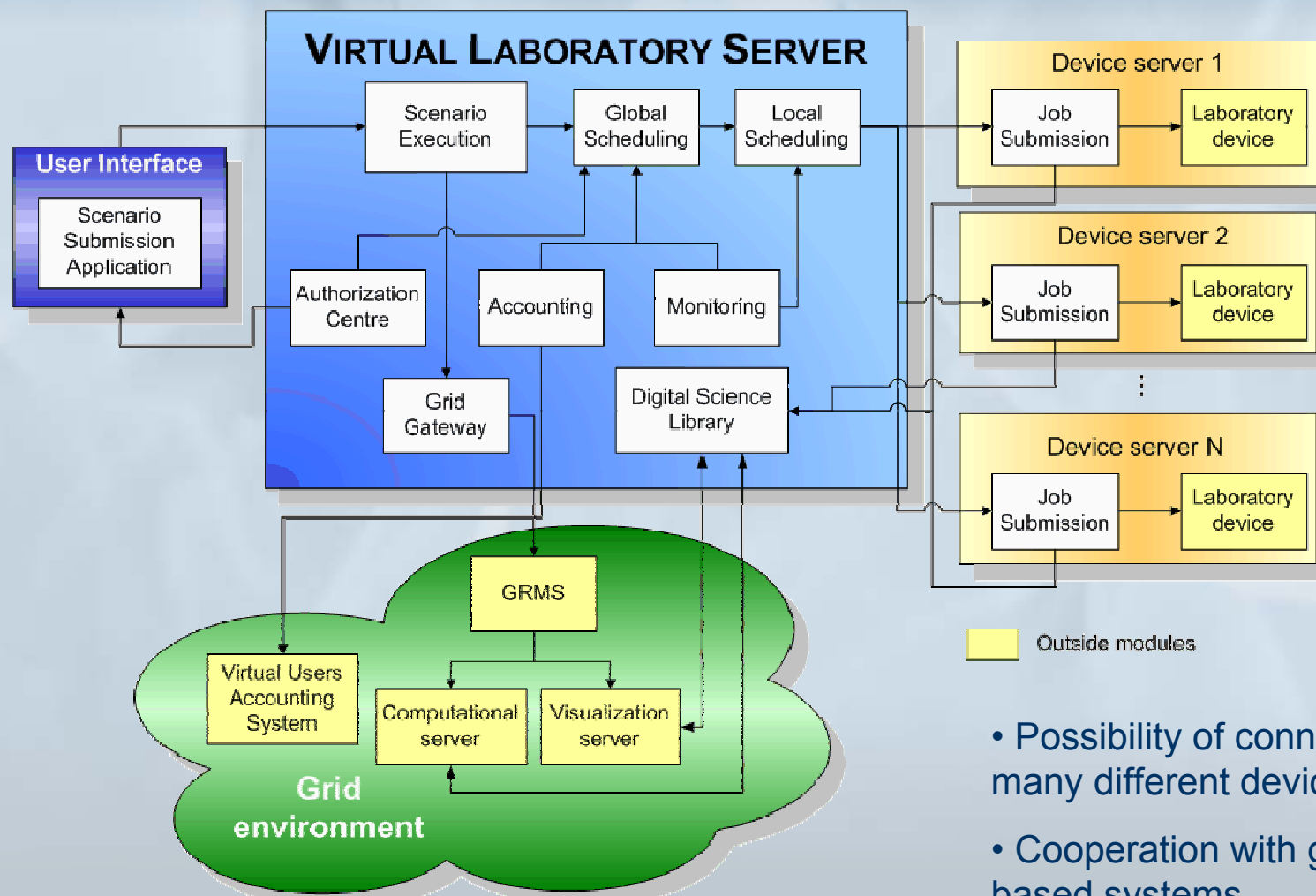


Virtual Laboratory overview

The Virtual Laboratory is a distributed environment, providing its users with the following functionality:

- **Remote access** to complex and expensive laboratory research equipment,
- **User-customized Dynamic Measurement Scenarios**,
- Digital Science Library,
- Data storage and management,
- Educational potential,
- Workgroup collaboration tools.

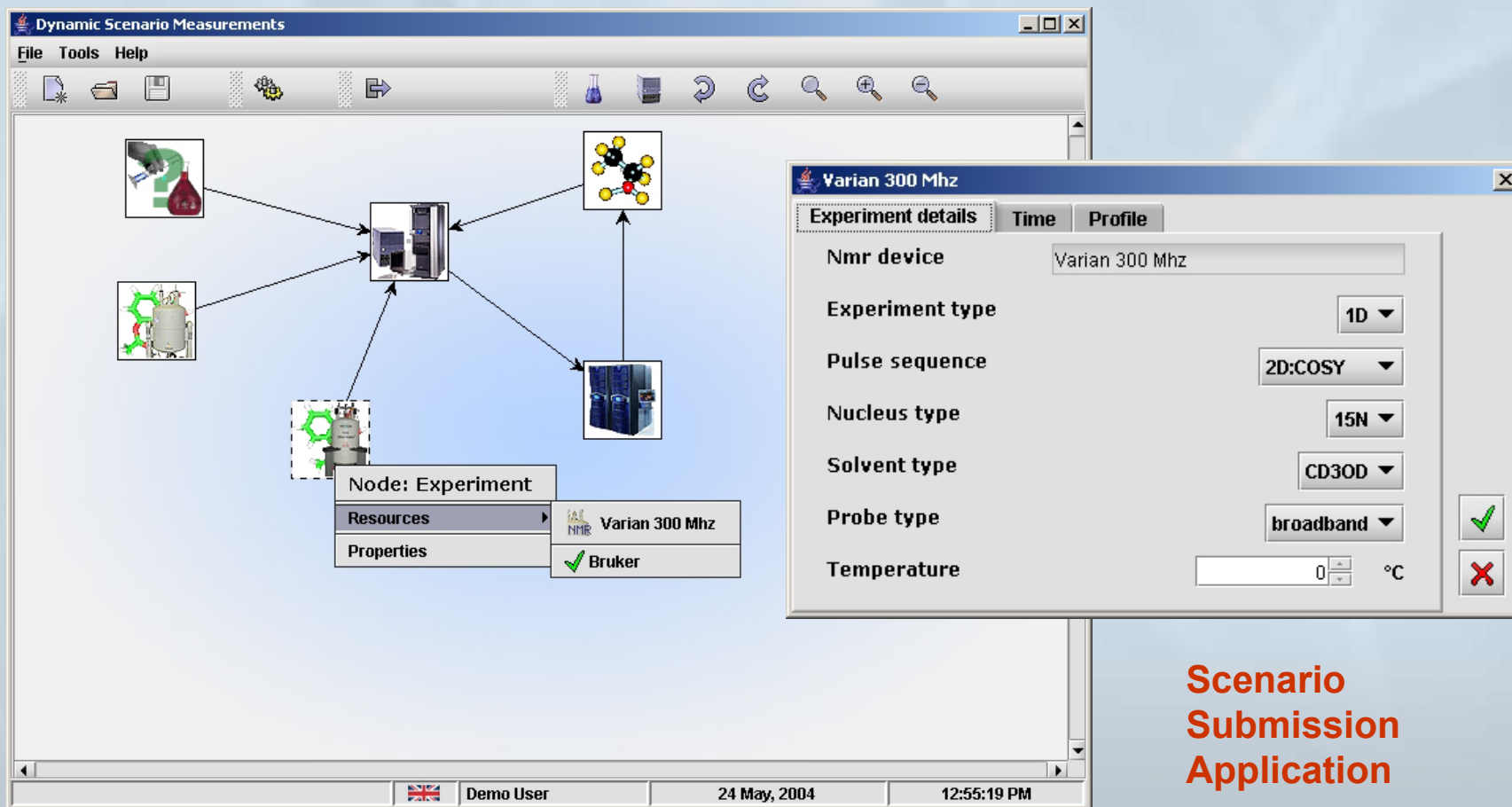
Jobflow in the Virtual Laboratory



- Possibility of connection to many different devices
- Cooperation with grid-based systems

Scenario Submission Application


The user is welcome to create the measurement diagram using the Scenario Submission Application (SSA).



The screenshot displays the 'Dynamic Scenario Measurements' application window. The main workspace shows a measurement diagram with a central NMR spectrometer icon connected to various input and output components. A context menu is open over the spectrometer, showing 'Node: Experiment', 'Resources' (with a dropdown arrow), and 'Properties' (with a checkmark and 'Bruker').

A 'Varian 300 Mhz' configuration window is open, showing the following settings:

Experiment details	Time	Profile
Nmr device	Varian 300 Mhz	
Experiment type	1D	
Pulse sequence	2D: COSY	
Nucleus type	15N	
Solvent type	CD3OD	
Probe type	broadband	
Temperature	0 °C	

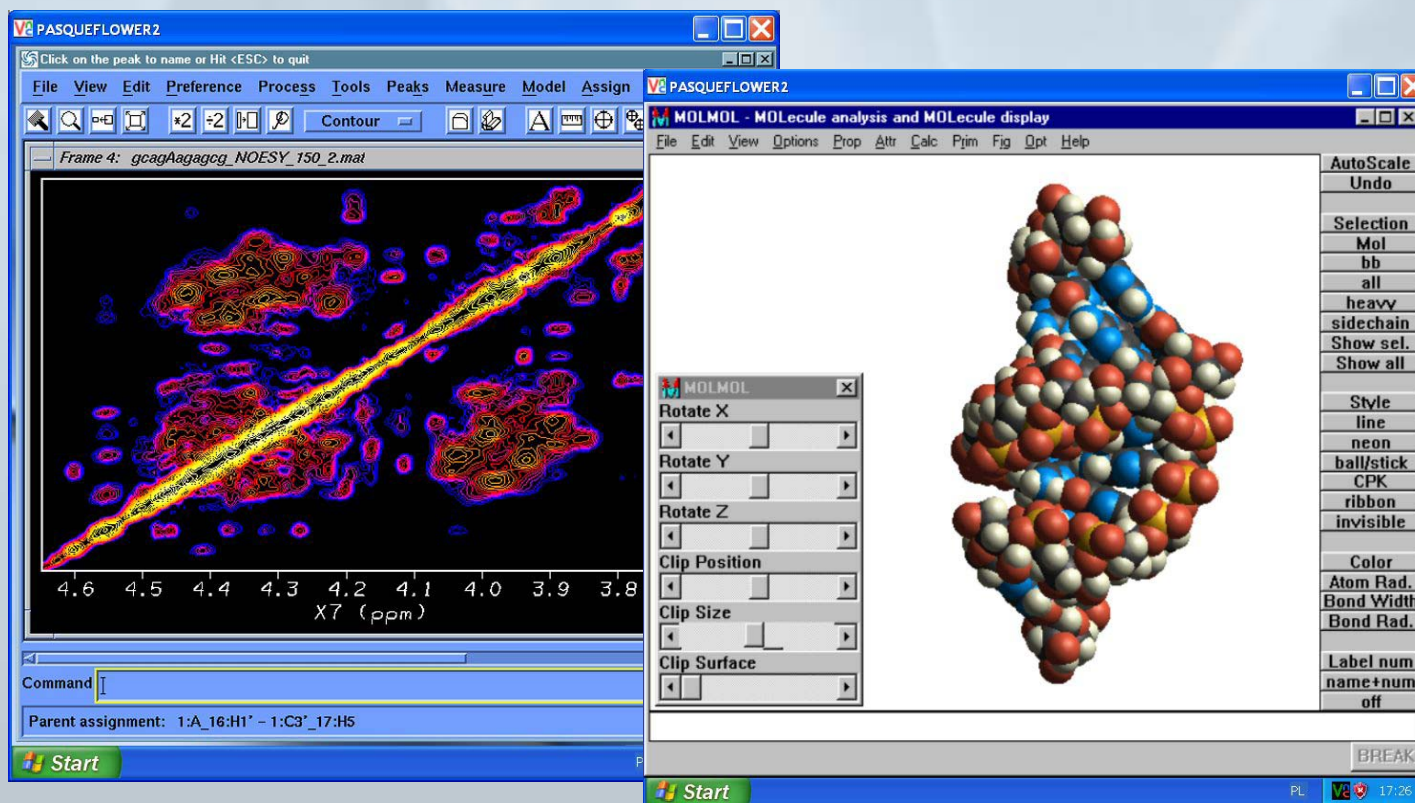
The status bar at the bottom of the application window shows:  Demo User | 24 May, 2004 | 12:55:19 PM

**Scenario
Submission
Application**

Visualization

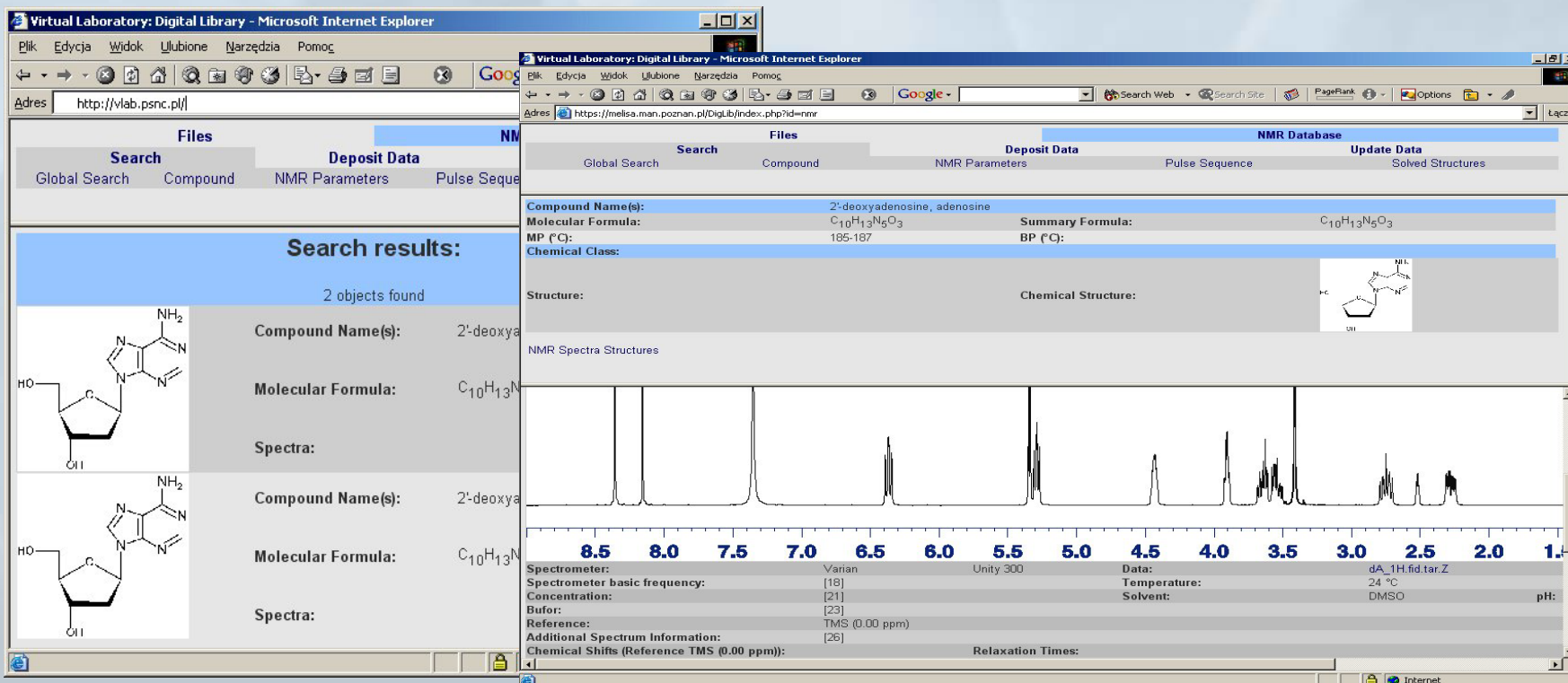
Support for interactive applications:

- taking into consideration user preference (e.g. presence, working hours)
- access to visualization applications from the VLab portal



Digital Science Library

- Storing, in organized way, experiment parameters and results
- Sharing data among scientists
- Browsing, searching and exploring of stored data
- References for external resources



The screenshot displays two browser windows. The left window shows the search results for '2'-deoxyadenosine' (Compound Name(s)), 'C₁₀H₁₃N₅O₃' (Molecular Formula), and '185-187' (MP (°C)). It includes chemical structures and NMR spectra. The right window shows the detailed NMR data for the same compound, including the chemical structure, NMR Spectra Structures, and a list of parameters:

Parameter	Value	Parameter	Value
Spectrometer:	Varian	Data:	dA_1H.fid.tar.Z
Spectrometer basic frequency:	[18]	Temperature:	24 °C
Concentration:	[21]	Solvent:	DMSO
Bufor:	[23]	pH:	
Reference:	TMS (0.00 ppm)		
Additional Spectrum Information:	[26]		
Chemical Shifts (Reference TMS (0.00 ppm)):		Relaxation Times:	

Security

- Important especially in the VLab: valuable lab equipment and scientific data
- User equipped with certificate
- Jobs proxy certificate
- Modules authentication
- Encrypted connection



Putting into practice

Implementations of VLab:

- Virtual Laboratory of Nuclear Magnetic Resonance Spectroscopy – cooperation with Institute of Bioorganic Chemistry PAS
- Virtual Laboratory of Radio Astronomy – cooperation with Radio Astronomy Department of Nicolaus Copernicus University



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VLAB VIRTUAL LABORATORY



VLAB

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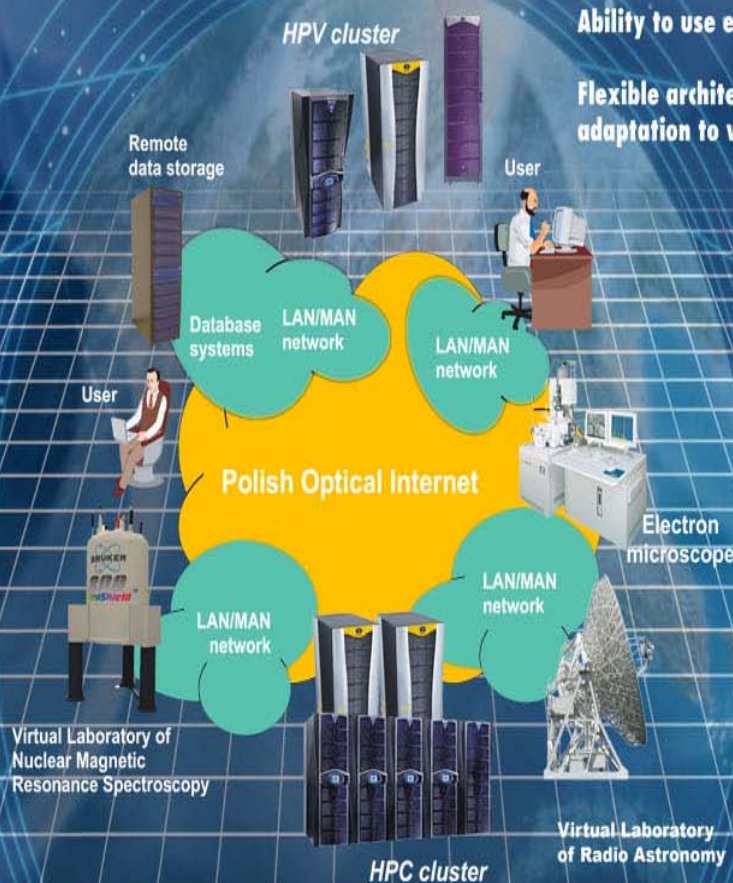
VIRTUAL LABORATORY

VLab overview

- Access via Internet
- Advanced job scheduling
- Resource accounting
- Single Sign-On
- Confidentiality of stored data
- Instrument access control
- Platform independence

Dynamic Measurement Scenario

- Flexible definition of various measurements
- Speed up of project realisation
- On-line progress experiments monitoring
- Taking into consideration the influence of a human factor
- Educational area



Ability to use expensive instruments remotely

Flexible architecture enabling adaptation to various types of instruments

Digital Science Library



Sharing the experiment results and bibliography

Communication with other scientists and cooperation within the confines of one project

NEW DIMENSION OF THE SCIENTIFIC WORK

CONTACT INFORMATION:

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