



6th CARNet Users Conference

Workflow with Dynamic Measurement Scenarios in the Virtual Laboratory

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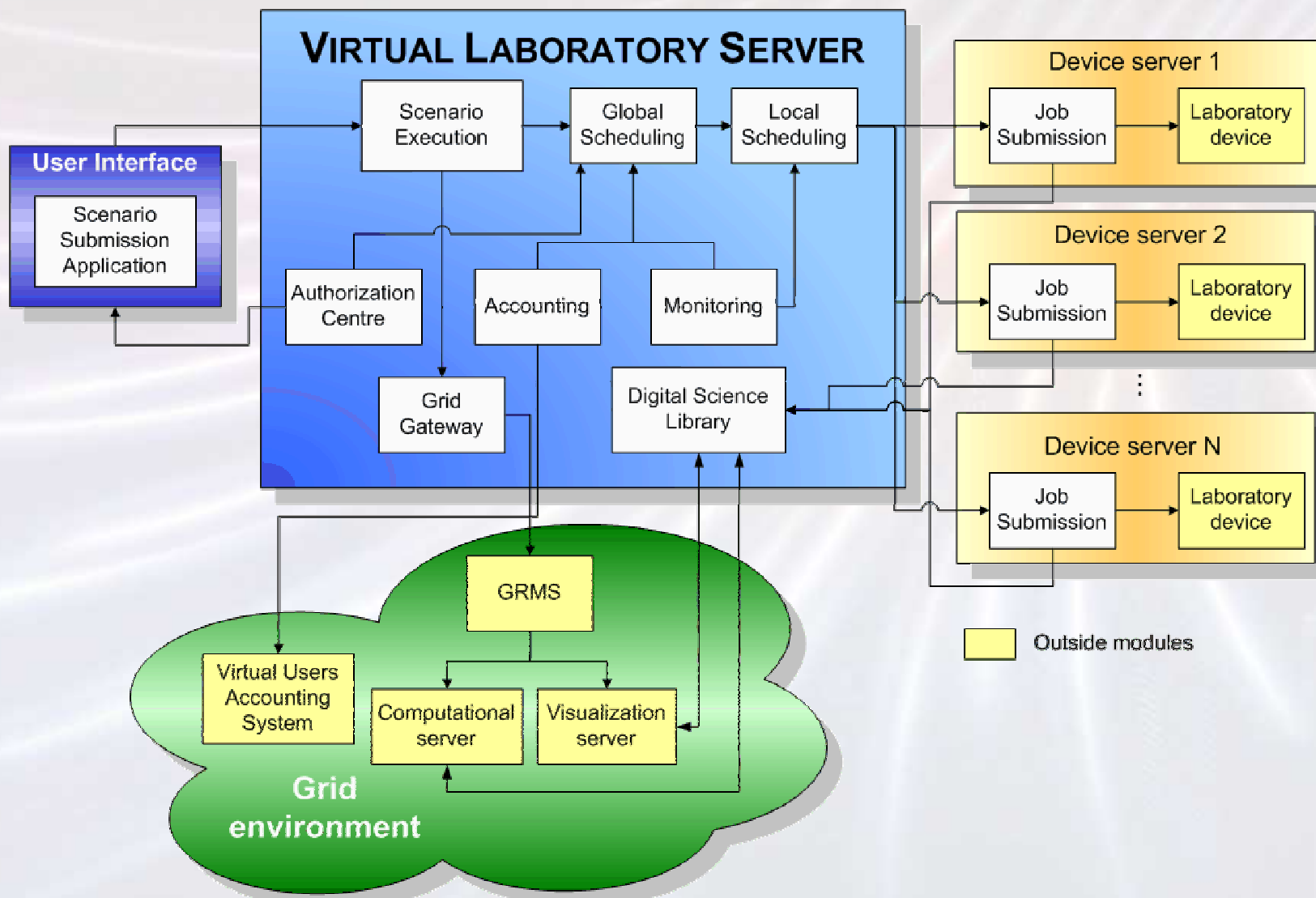


Virtual Laboratory overview

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

The Virtual Laboratory workflow



Motivation to create MDS

The most important advantages of MDS:

- connection of different types of jobs (experimental and computational),
- speed up of tasks sequence execution,
- simplifying scenario monitoring,
- possibility of multiple use of a given scenario,
- legible way of the workflow control,
- possibility of defining many measurement execution ways.

DMS designing

The designing of the DMS consists of the following stages:

- application analyzing,
- connection diagram preparing,
- describing additional dependencies in the connection diagram,
- applications and links description generating,
- measurement scenario description generating.

Application analyzing

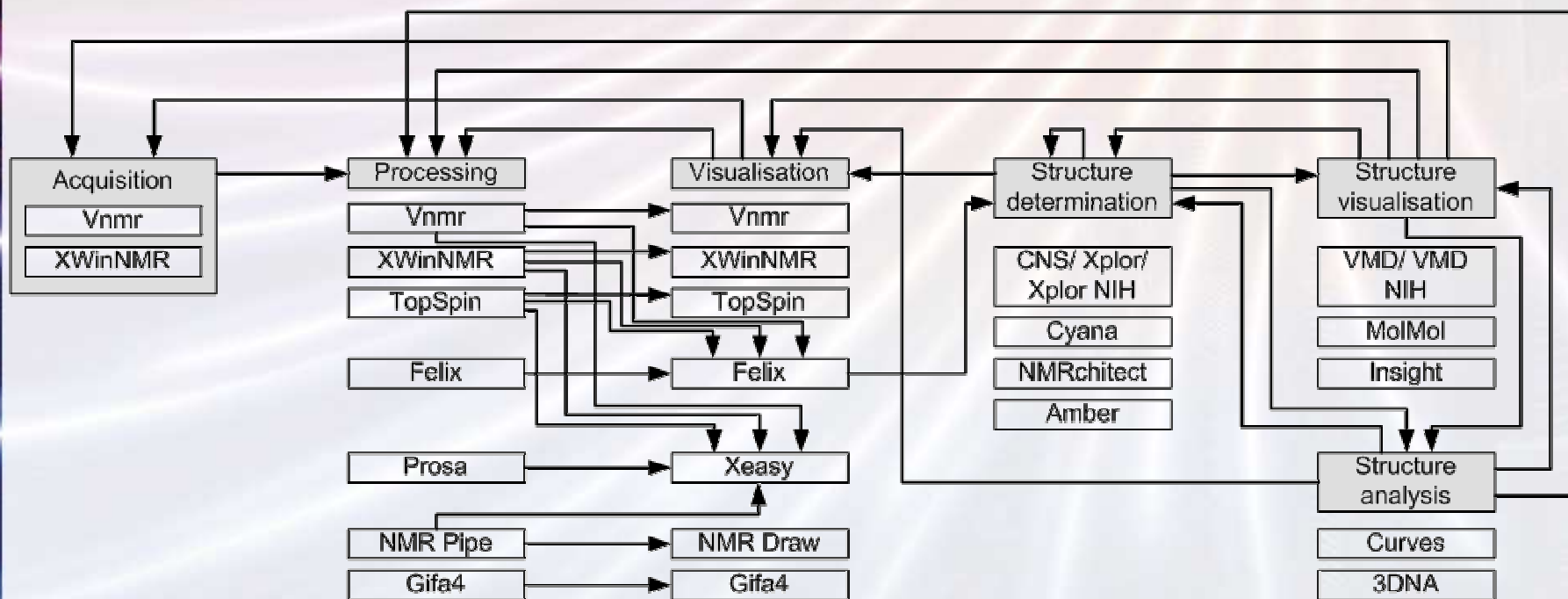
The most important issues to analyse:

- hardware requirements (scalar or vector processors, amount of RAM),
- software requirements (additional software, libraries),
- input and output parameters,
- input and output format files (binary, text),
- filename format (if exists): filename mask, filename extension,
- file structure analysing (in case of a text file),
- taking into consideration the security aspect.

Connection diagram

Which applications can be connected and how?

What are the main stages of scenario execution?



Exemplary stages for the laboratory of NMR spectroscopy

Additional dependencies in the connection diagram

Now we focus our attention to:

- connection conditions - they are verified after the end of each application and in this way the following execution path is determined,
- conversion issues - performed when two connected applications have a different input-output file format, administrator should determine the type of conversion
- files types related to links - determine which type of file can be used as an input file to the target application

Applications and links description

Description is generated using the Scenario Submission Application (SSA)

DMS is encoded in the Dynamic Measurement Scenario Language (DMSL).

DMSL base on the XML and XSD standard.

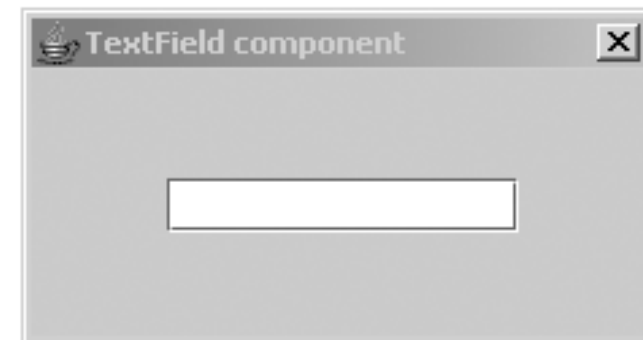
The general DMS consists of a description of all possible applications with all parameters available for users.

Components description

Defined list of components:

- used for describing the resource element type
- used for the visualization of the resource properties
- the current? component list: check box, date and time dialog, list, combo box.

```
<component id="2"  
  name="JTextField"  
  class="TextFieldElement"  
  document="TextDocument"  
  modelDataAttached="false">  
  ...  
</component>
```

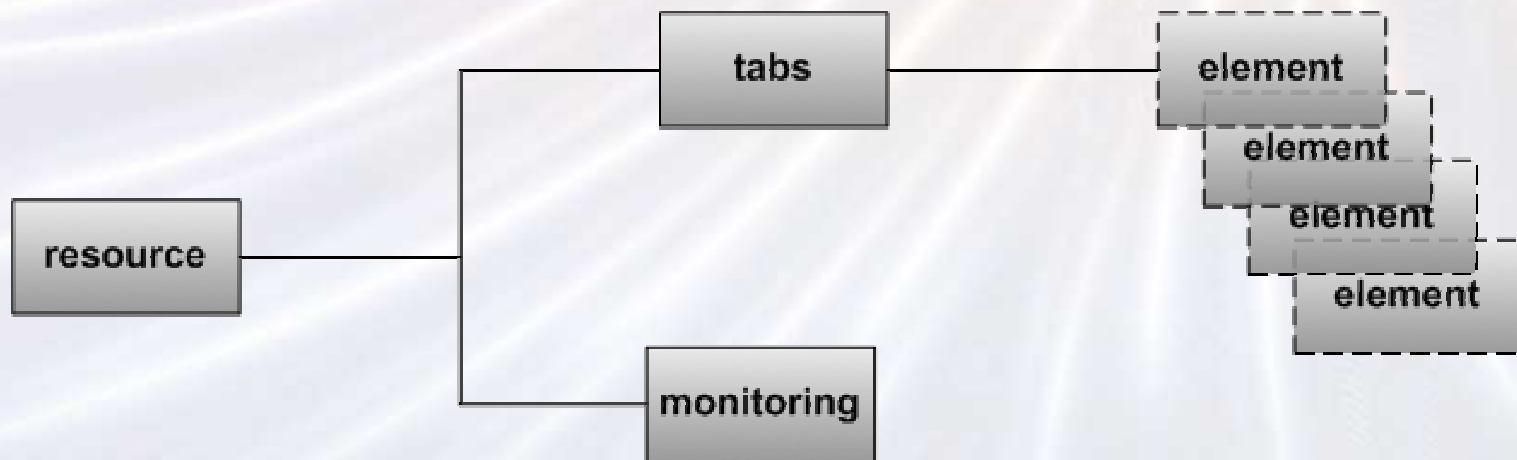


Example of TextField component

Resource type description

Every resource element contains the following sections:

- tabs - the tabs node is used to group the resource properties represented by the element node; there can be many tabs defined containing a different number of elements,
- monitoring - this optional section contains information about the state of the resource in the VLab system.



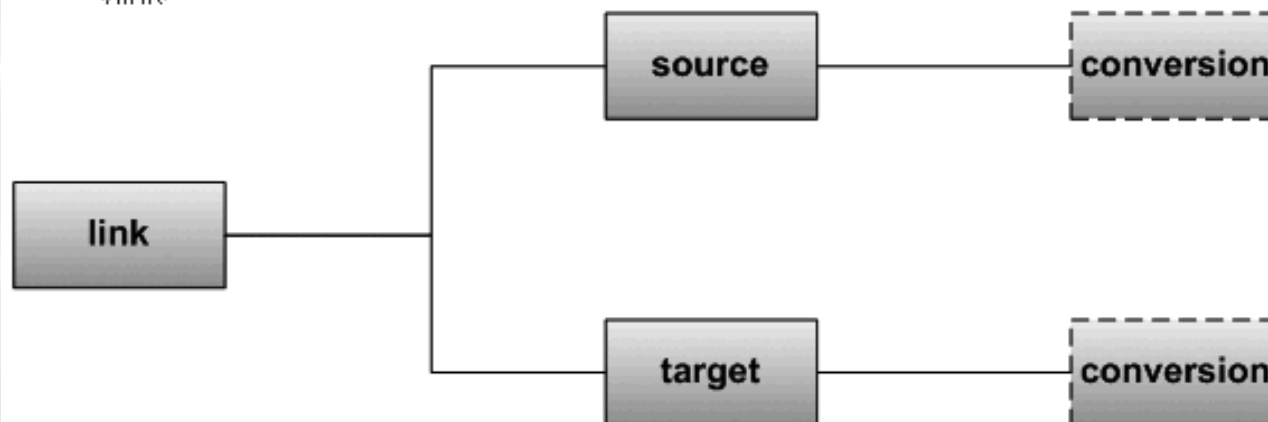
Resource description structure

Link description

The Link Description schema (LDS) describes:

- the available connections between resources,
- specifies the conditions which have to be taken into consideration while connecting resources.

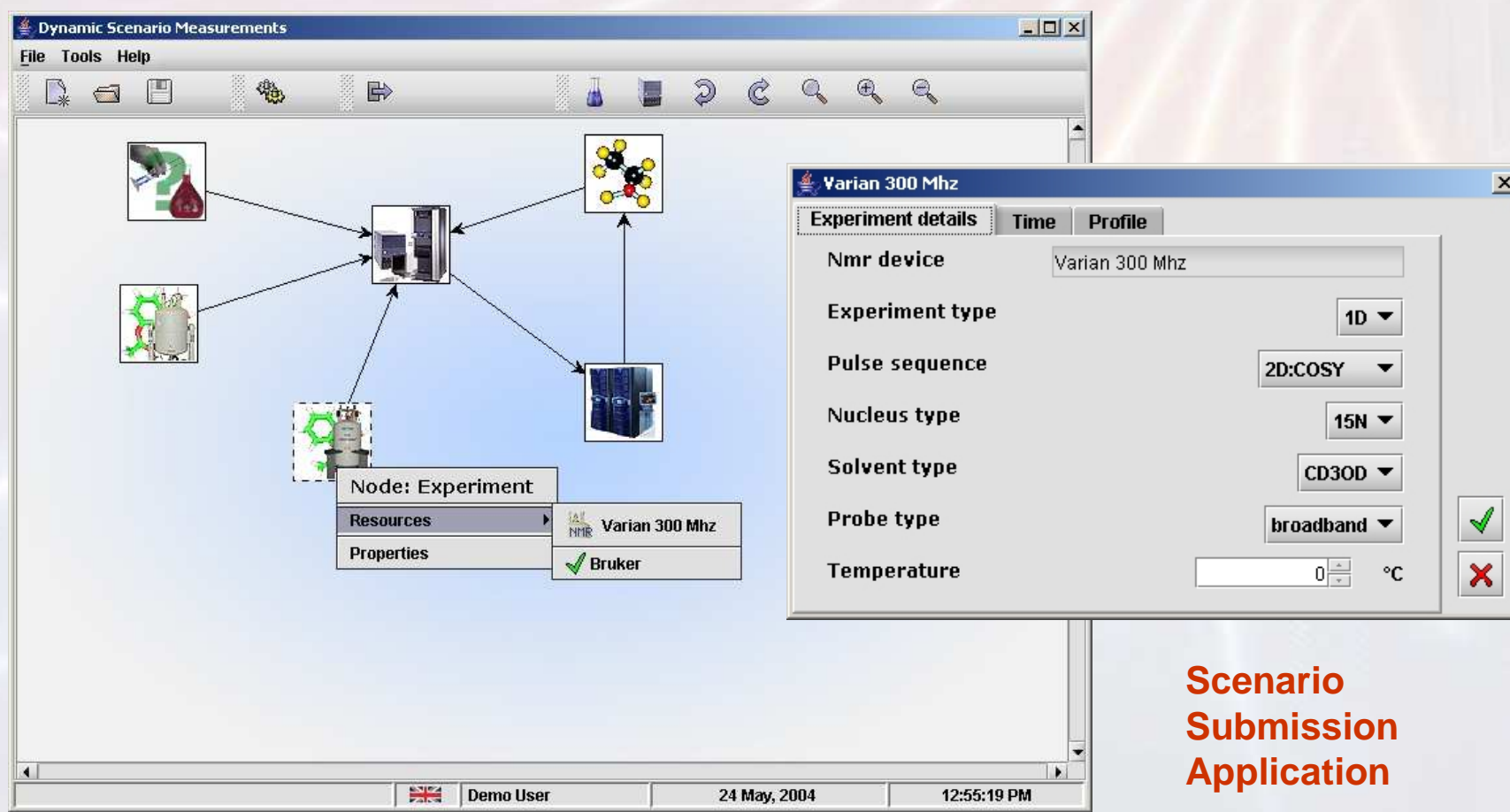
```
<link id="3" externalConversion="false">
  <source resourceId="2" conversionDefined="false" isExternal="false">
  </source>
  <target resourceId="4" isExternal="false" conversionDefined="true">
    <conversion id="1" appName="imageConverter">
      <params index="0" name="fileFormat">jpg</params>
    </conversion>
  </target>
</link>
```



Link description

Measurement scenario description

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 central server icon with arrows pointing to various experimental components: a pipette, a chemical structure, a gas cylinder, and a server rack. A context menu is open over the central server icon, showing 'Node: Experiment', 'Resources' (with a dropdown arrow), and 'Properties'. The 'Resources' dropdown is expanded, showing 'Varian 300 Mhz' and 'Bruker' with a checkmark.

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

| Parameter | Value |
|-----------------|----------------|
| Nmr device | Varian 300 Mhz |
| Experiment type | 1D |
| Pulse sequence | 2D: COSY |
| Nucleus type | 15N |
| Solvent type | CD3OD |
| Probe type | broadband |
| Temperature | 0 °C |

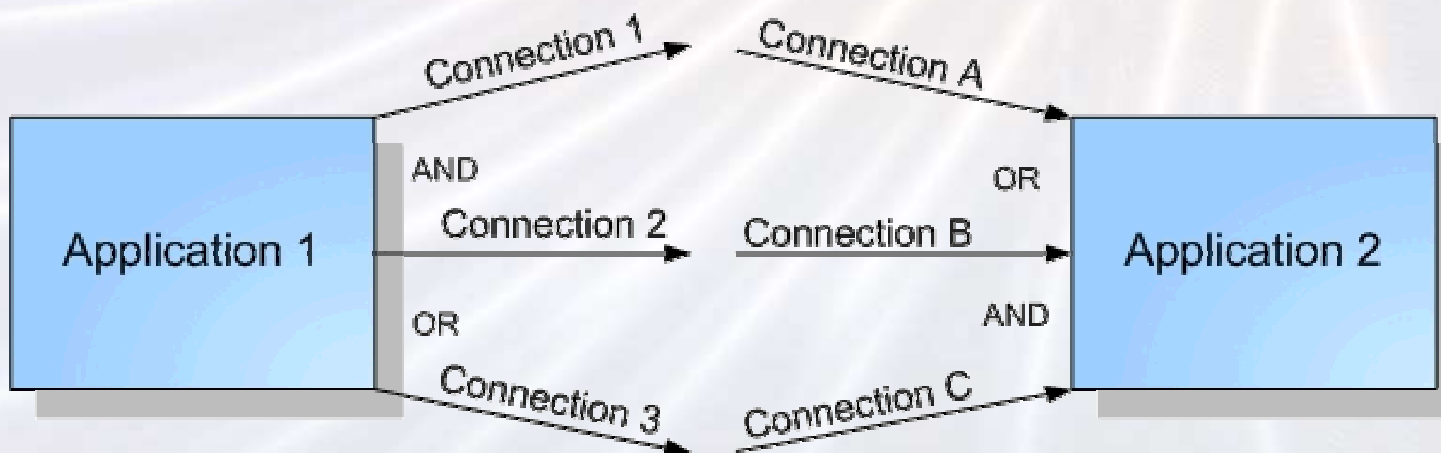
The status bar at the bottom of the application window shows: Demo User, 24 May, 2004, 12:55:19 PM.

**Scenario
Submission
Application**

More about connection aspects

The user is also welcome to define logical conditions between links. There are two types of conditions: OR (default) and AND. Their meaning depends on their localization:

- Beginning – AND – the next applications are executed when all link conditions are met, OR – applications are executed independently;
- Ending – AND – the given application is executed when all previous applications are finished, OR – the given application is executed regardless of the state of other previous applications

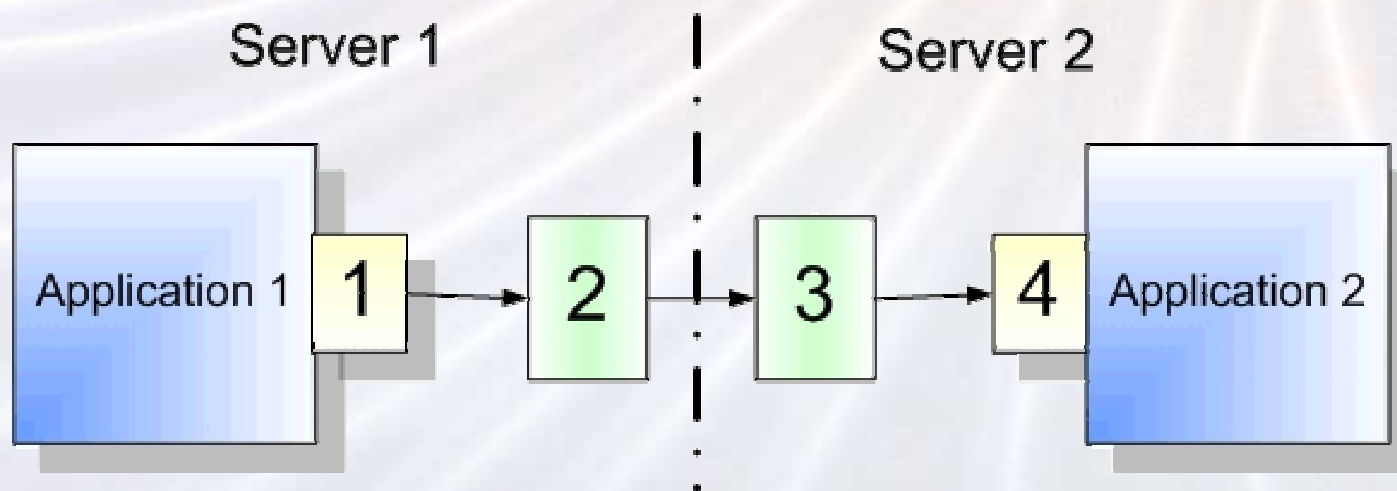


Defining the beginning and ending connection conditions

More about conversion aspects

Conversion may be done in four different ways:

- setting up the switch in the source application to export data in an appropriate format (1),
- using a program on the source server to convert the output file (mini postprocessing) (2),
- using a program on the source server to convert the output file (mini preprocessing) (3),
- setting up the switch in the target application to import data in an appropriate format (4).



Conversion aspects

DMS performing

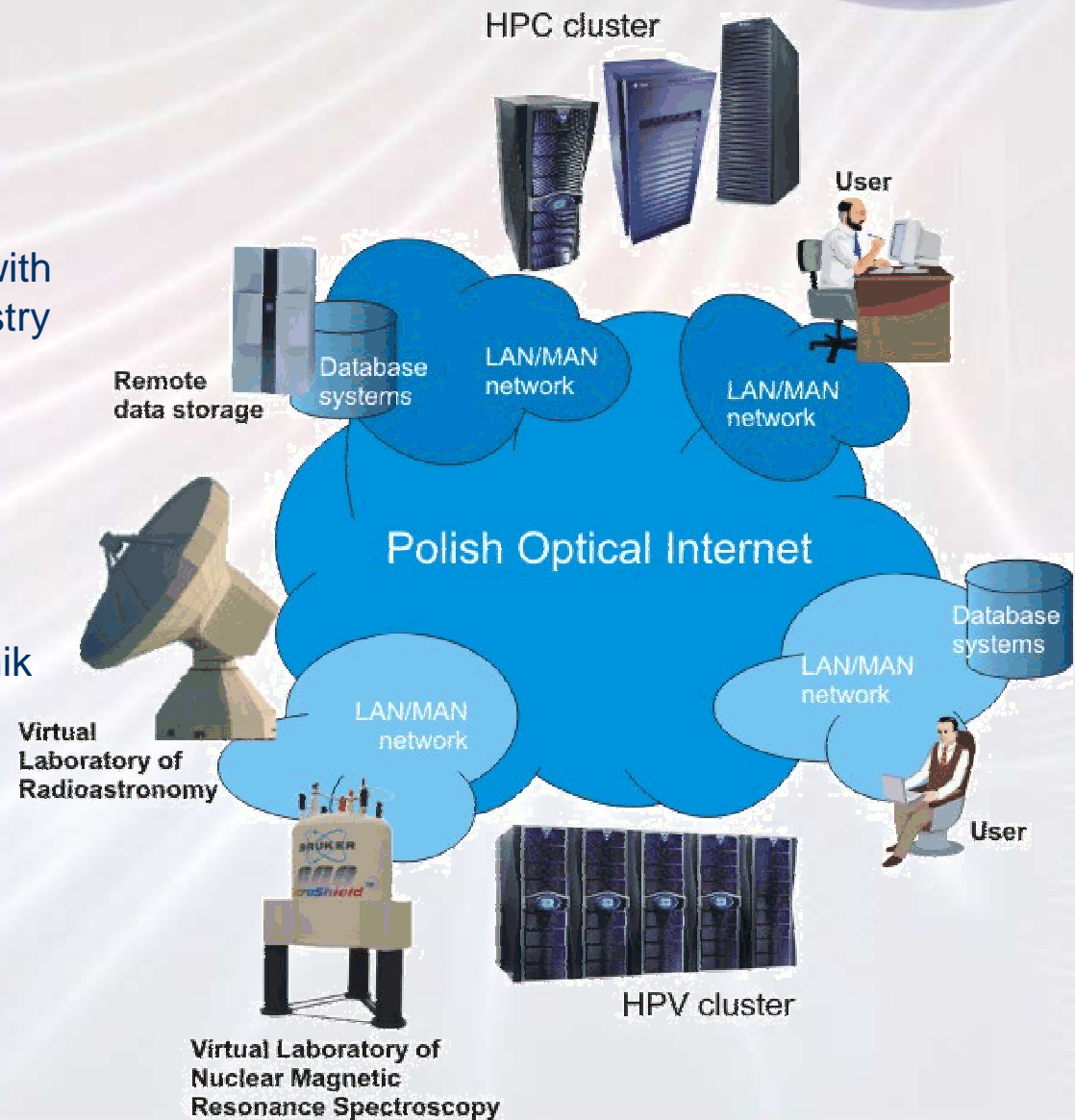
DMS prepared by SSA is performed by **Scenario Execution (SE)** module. The most significant SE steps follows:

1. Start by receiving client scenario data (XML structure describing graph connections and node details).
2. Create a directed graph and detect initial node(s).
3. Call the Monitoring module in a synchronous mode to create a new scenario - wait to receive new scenario identifier.
4. Create the first task description for a new scenario and call the Monitoring module to create an identifier for it.
5. Create a datagram with a task description and send it to the Global Scheduler module.
6. Check if other initial tasks exist. If so, go to step 4.
7. Wait for the response from Monitoring (as a separate thread) saying that the task has finished. Check if other tasks exist in the current scenario. If not, finish the algorithm, otherwise go to step 8.
8. Analyze graph connections.
9. Create new datagram(s) for new task(s) and send it(them) to the Global Scheduler module.
10. Go to step 7.

Putting into practice

Implementations of VLab:

- Virtual Laboratory of Nuclear Magnetic Resonance Spectroscopy – cooperation with Institute of Bioorganic Chemistry PAS
- Virtual Laboratory of Radiotelescope – cooperation with Radioastronomy Department of Mikołaj Kopernik University



V **LAB**

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