



Remote Engineering Virtual Instrumentation 2004

Generalization aspects 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.

Where is the problem?

The Virtual Laboratory is a complex system, providing its users complex functionality.

Most known virtual laboratories are specialized for a given science laboratory.

Most virtual laboratories are developed from the beginning, so:

- many similar operations under development are repeated by developers,
- developers have to concentrate on the wide spectrum of problems, instead of given laboratory specific problems,
- different laboratories are incompatible,
- it takes much time and costs a lot.



What we can do?

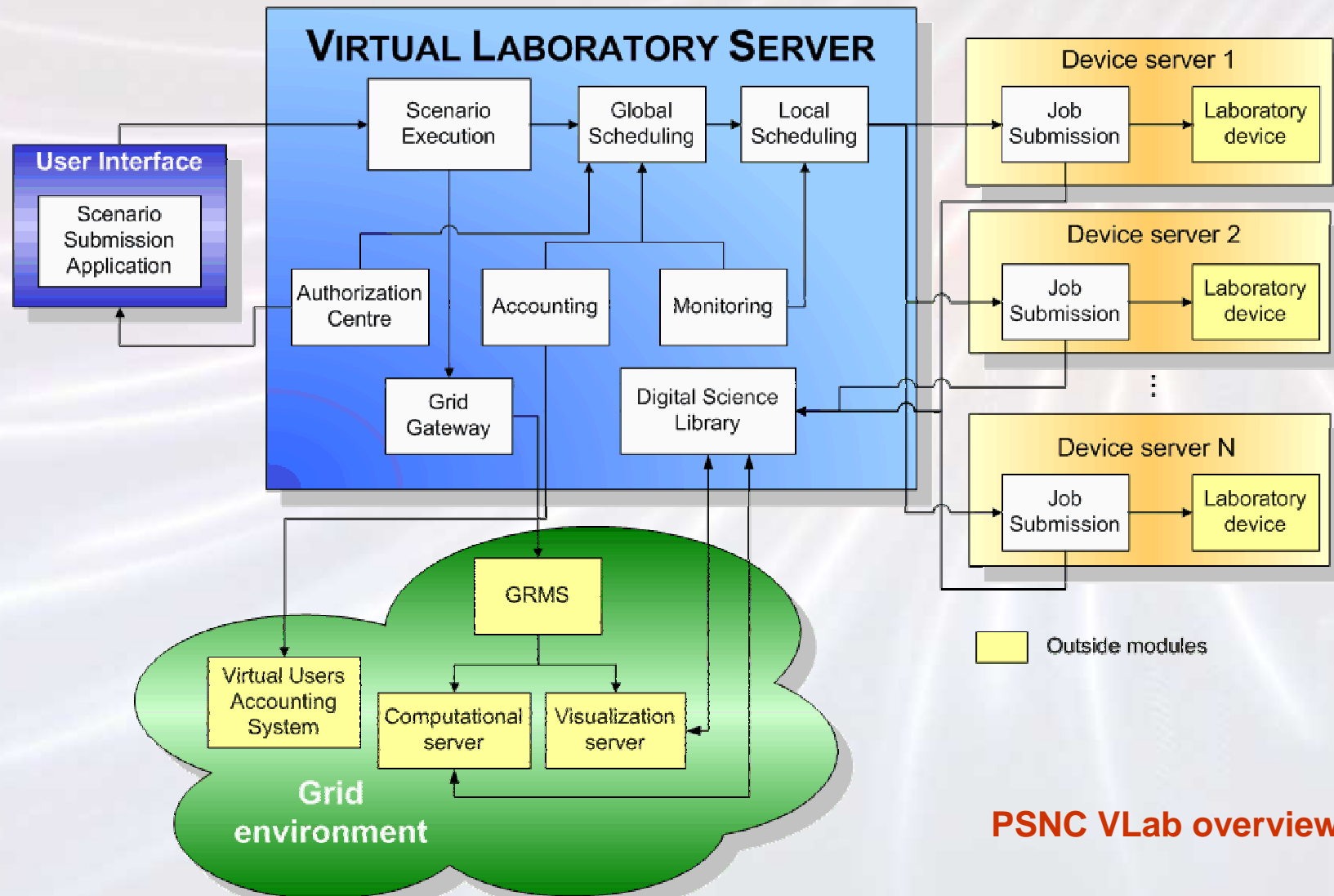
Creating general virtual laboratory is impossible, because of different nature of each laboratory.

We can think about some aspects of the system which we can try to generalize.

Subjects on which we want to focus on:

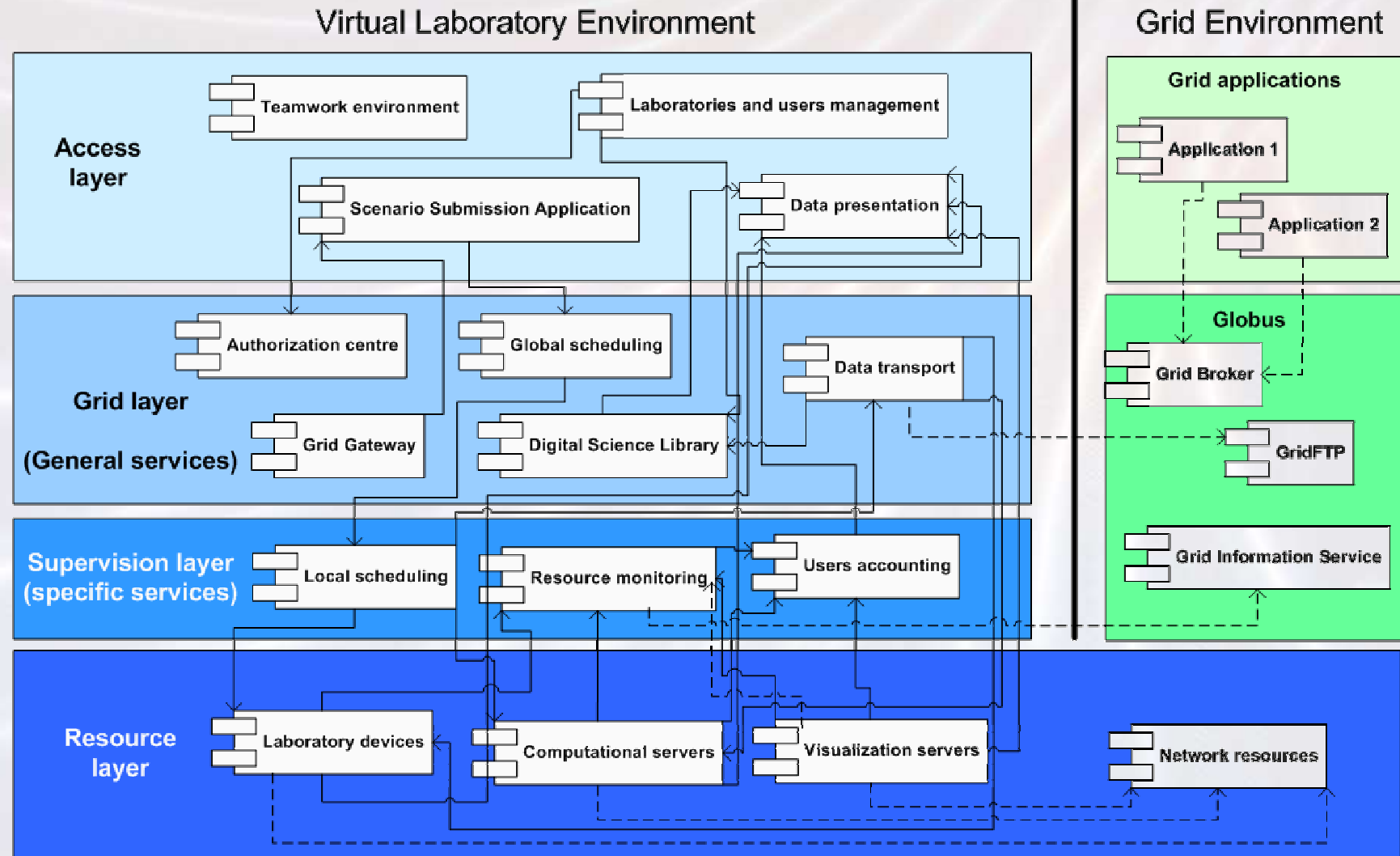
- virtual laboratory framework,
- communication and modules architecture,
- jobs submission.

Workflow of the virtual laboratory



PSNC VLab overview

The Virtual Laboratory architecture



Communication - VL datagram

1/2

VL datagram should:

- be appropriate to many laboratory types,
- supports both: experimental and computational jobs.

We divide datagram into two parts - general and specific:

- **General** – for any type of laboratory, consists of data which can be implemented and used for any task (device),

datagramId – ID of datagram
validTaskId – ID of task
userId – ID of user
groupId – ID of group
inetAddress – destination IP address
operationId – operation ID
operationStatusId – operation status
contentId – ID of specific part
contentSize – size of specific part
datagramNumber – no. of datagram
datagramCount – total no. of datagr.
VL specific part

Structure of general part of VL datagram

Communication - VL datagram 2/2

- **Specific** – datagram consists of data only for given task (experiment or computational job).

scenarioid - id of the scenario	taskExecMode - execution mode
taskStatusId - initial task status	taskMaxCost - maximum cost allowed
deviceId - id of the device	sampleId - id of the sample
taskTypeId - type of the task	probId - id of the NMR probe
taskArchive - bool - archive or delete the data	impseqId - id of the impulse sequence
taskDesc - short description	filterId - id of the NMR filter
startTime - timestamp - task start time	solventId - id of the NMR solvent
deadline - timestamp - task deadline	expNucleusIdsArray - array of nucleuses
reservedFrom - timestamp - time reserved	expTemp - experiment temperature
reservedTo - timestamp - time reserved	experimentType - type of the experiment (description)
taskInput - initial input for the NMR task	usrPresence - required user presence (in minutes)
taskExecProfile - execution profile	oprPresence - required operator presence (in minutes)

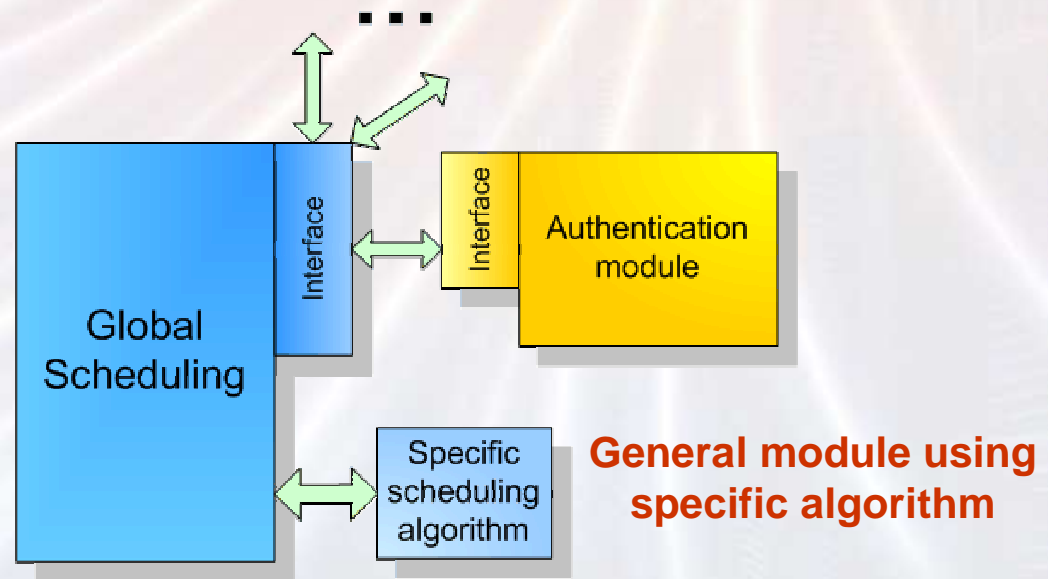
Specific part of VL datagram for NMR laboratory

Module types

We divide modules into:

- **General** – can be implemented in most types of virtual laboratory instances e.g. authorization and authentication modules,

- **General with specific functionality** - e.g. General Scheduling,

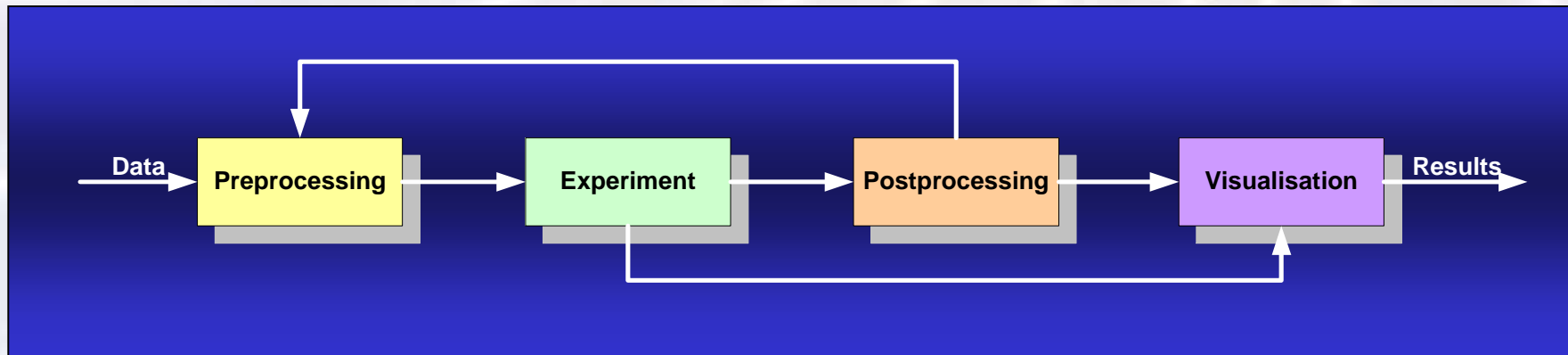


- **Specific** – has to know the context of activity, only these modules have to be exchanged entirely in new laboratory e.g. Local scheduling, Job submission.

Jobs submission

In the virtual laboratory user can submit measurement scenario which consists of many connected jobs.

To define and execute measurement scenario we use Dynamic Measurement Scenario (DMS).



Example of a simple measurement scenario

Motivation to create DMS

The most important advantages of DMS:

- 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,
- **laboratory independent language** – can be implemented in many lab. types

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 (DMSL).

Application analyzing

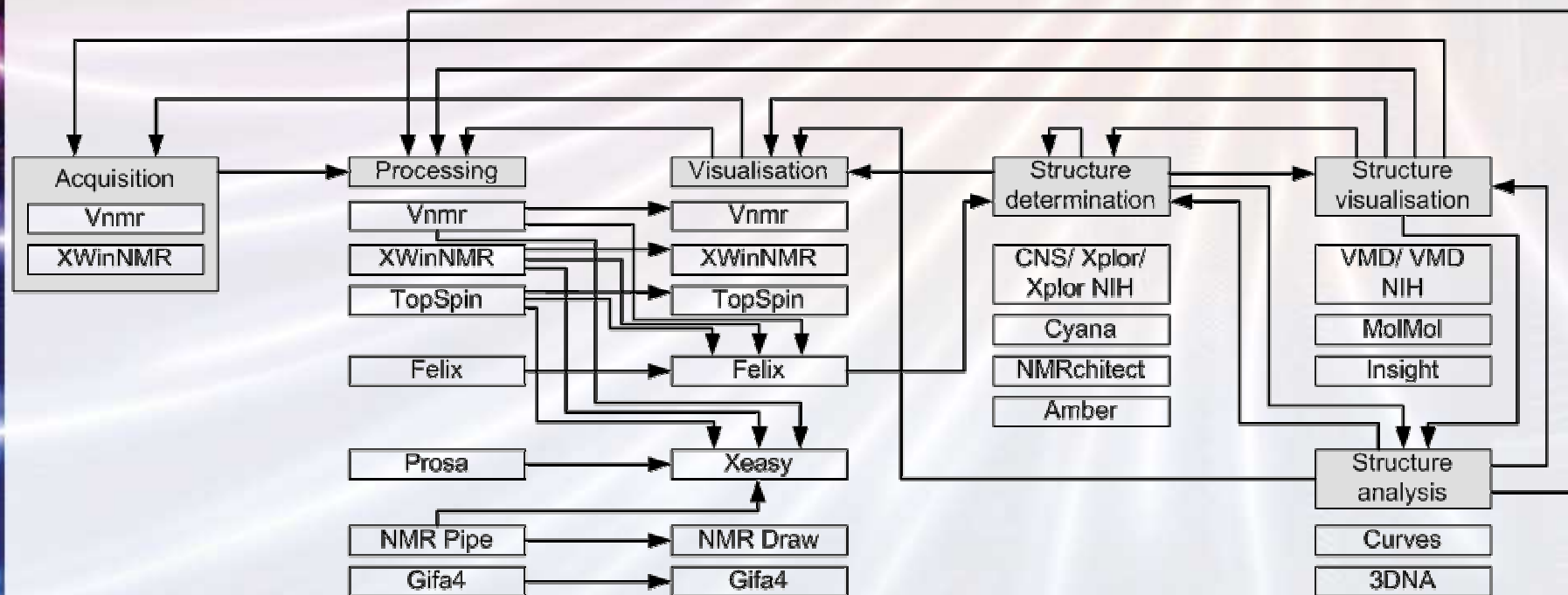
The most important issues to analyse:

- hardware requirements (scalar or vector processors, amount of RAM),
- software requirements (additional used 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 a case of text file),
- take into consideration the security aspect.

Connection diagram

What are the main stages of scenario execution?

Which applications can be connected and how?



An exemplary stages for the laboratory of NMR spectroscopy

Additional dependencies in the connection diagram

Now we focus our attention on:

- 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 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

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

DMSL basis on the XML and XSD standard.

Description is generated using Scenario Submission Application (SSA)

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 actual component list: check box, date and time dialog, list, combo box, text field.

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

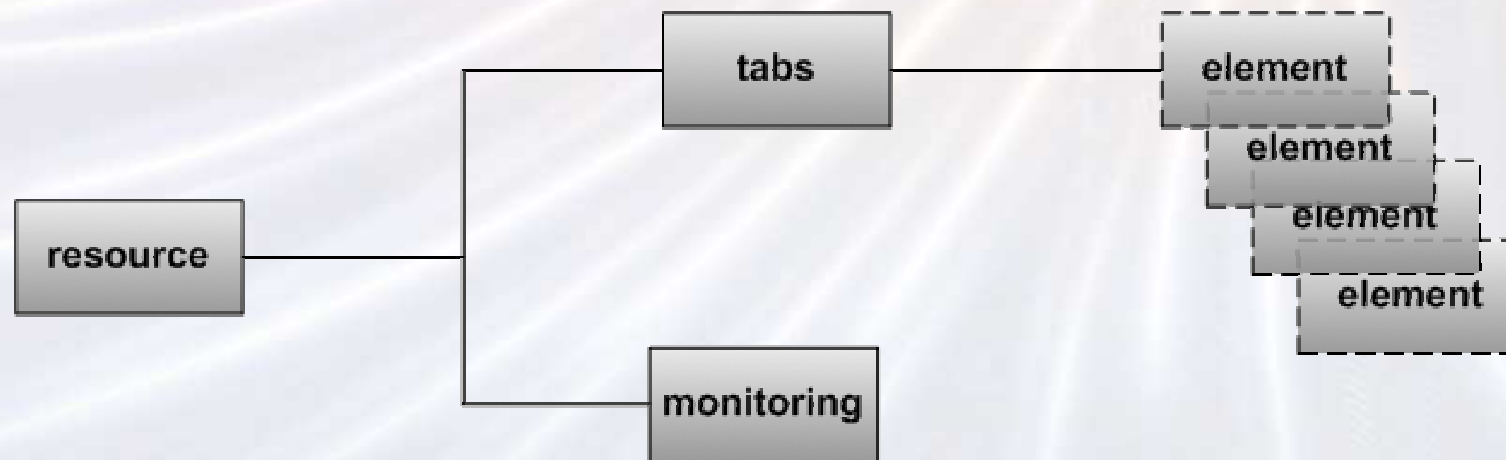


Example of TextField component

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 different number of elements,
- monitoring - this optional section contains **information about the state** of the resource in the VL system.



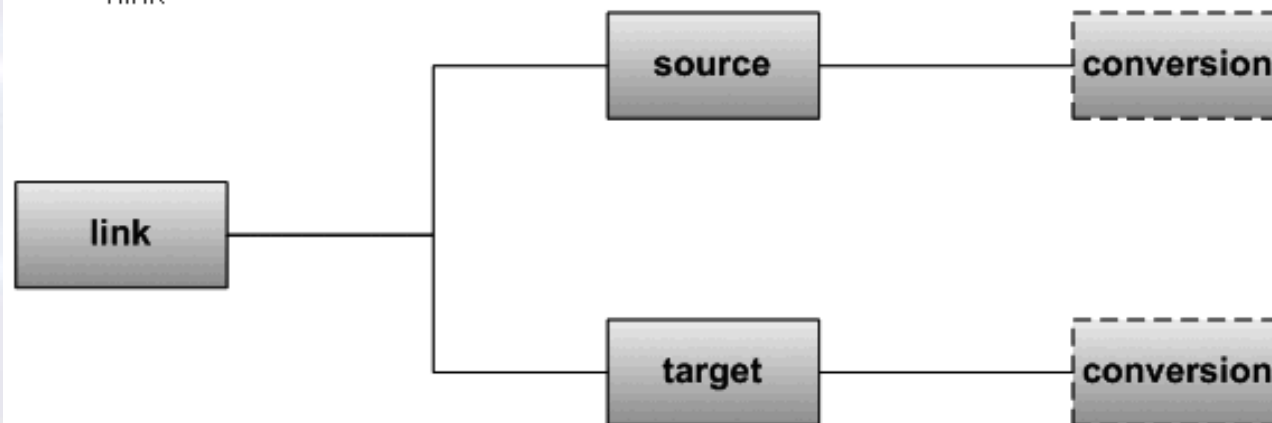
Resource description structure

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.

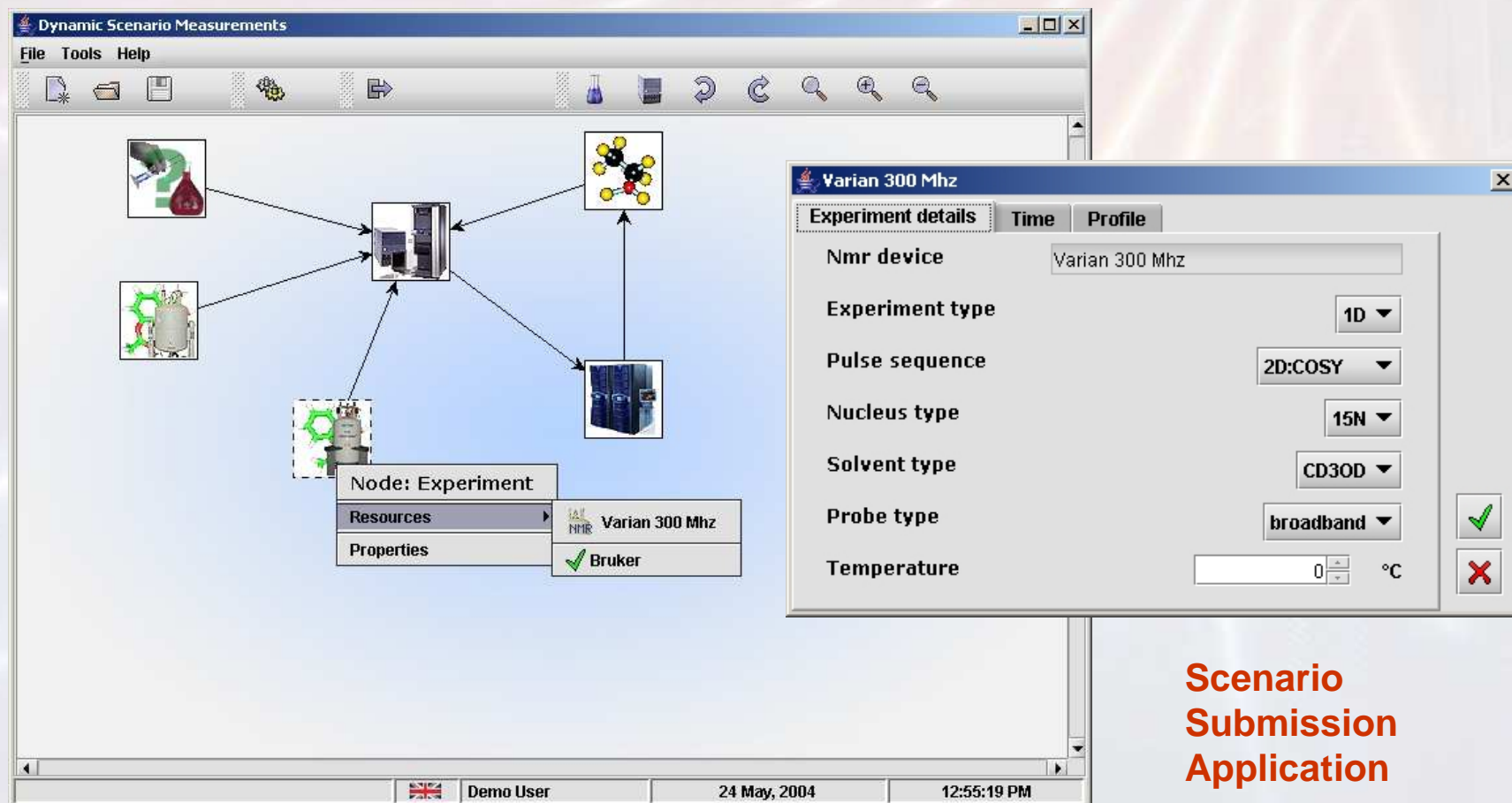
```
<link id="3" externalConversion="false">
  <source resourceId="2" conversionDefined="false" isExternal="false">
  </source>
  <target resourceId="4" isExternal="false" conversionDefined="true">
    <conversion id="1" appName="imageConverter">
      <params index="0" name="fileFormat">jpg</params>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



Link description

Scenario Submission Application

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



Node: Experiment

- Resources
 - Varian 300 Mhz
- Properties
 - Bruker

Varian 300 Mhz

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	

Demo User 24 May, 2004 12:55:19 PM

**Scenario
Submission
Application**

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



VLAB

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