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Workflow with Dynamic Measurement Scenarios in the Virtual Laboratory

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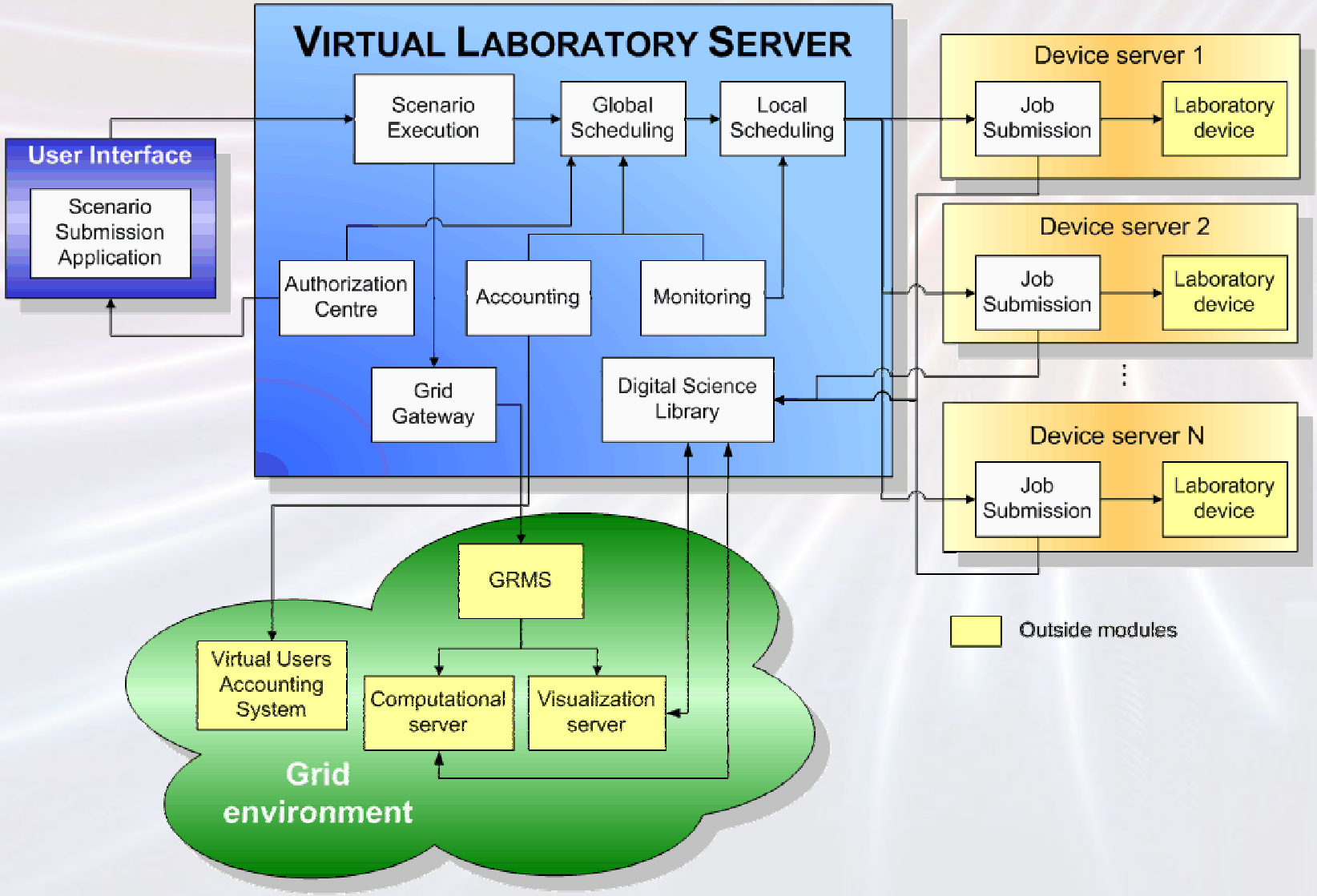
Virtual Laboratory overview

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 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.

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

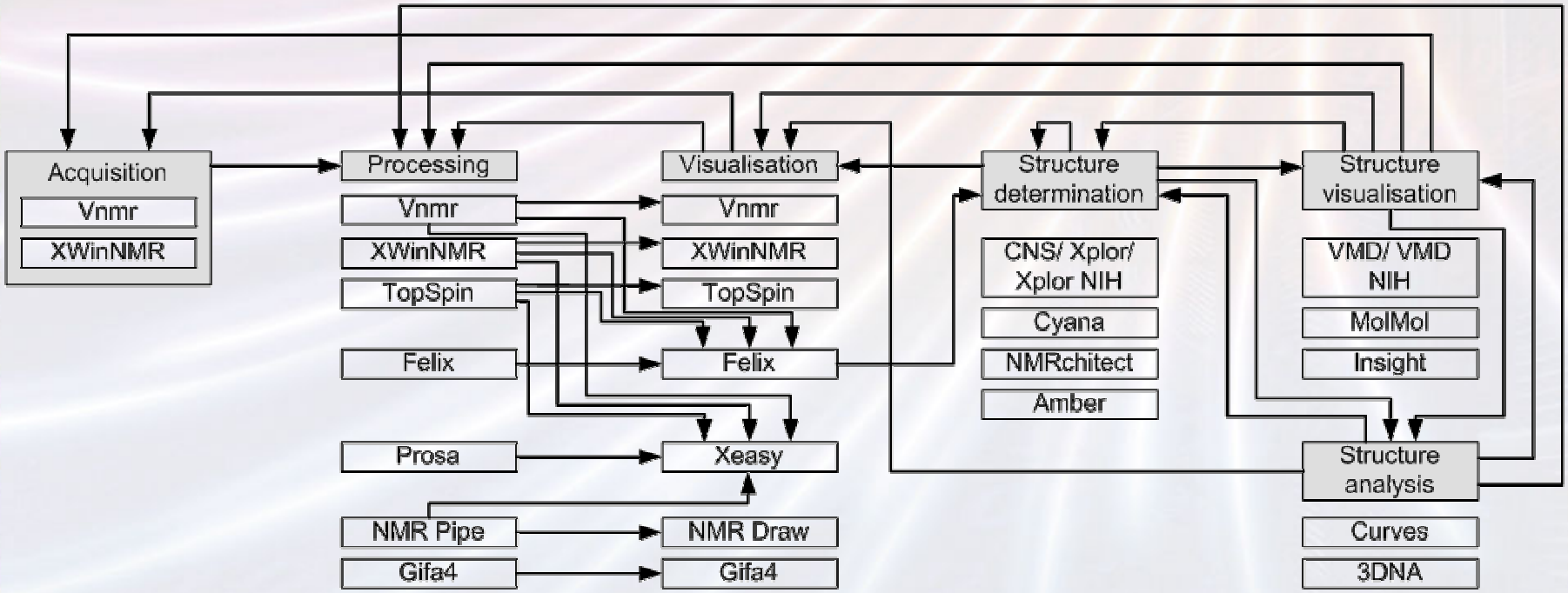
The most important issues to analyse:

- 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 a case of text file),
- take into consideration the security aspect.

Connection diagram

Which applications can be connected and how?

What are the main stages of scenario execution?



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
- file 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 Scenario Submission Application (SSA)

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

DMSL base on the XML and XSD standard.

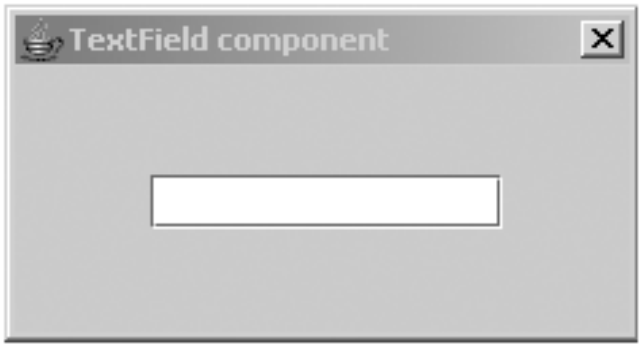
The general DMS consists of a description of all possible applications with all parameters available for users.

Components description

Defined list of components:

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

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

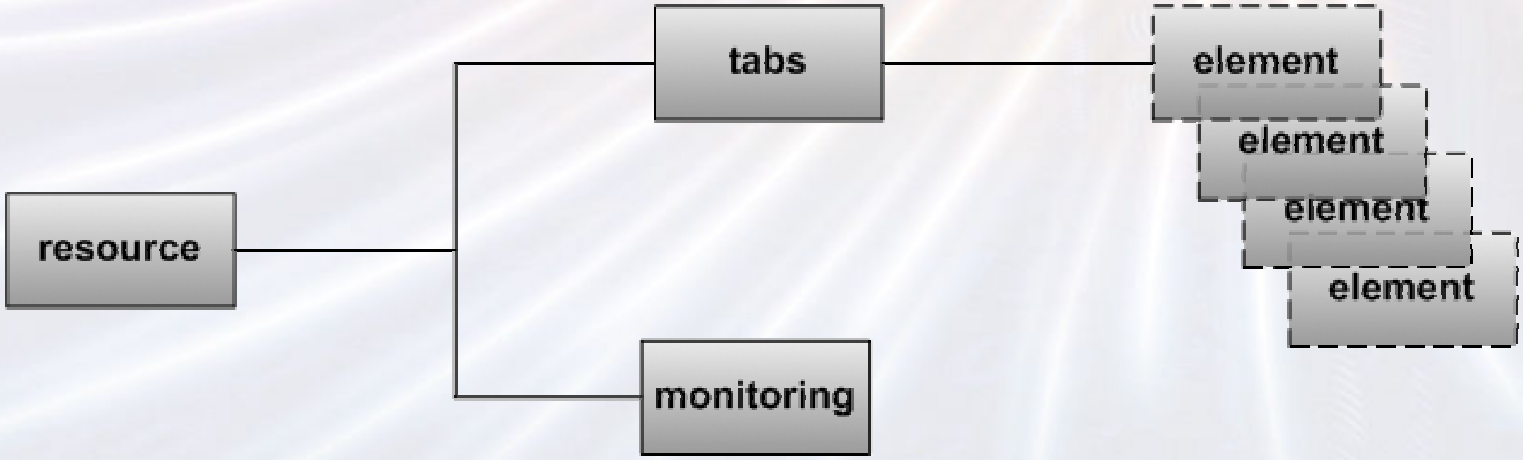


Example of TextField component

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



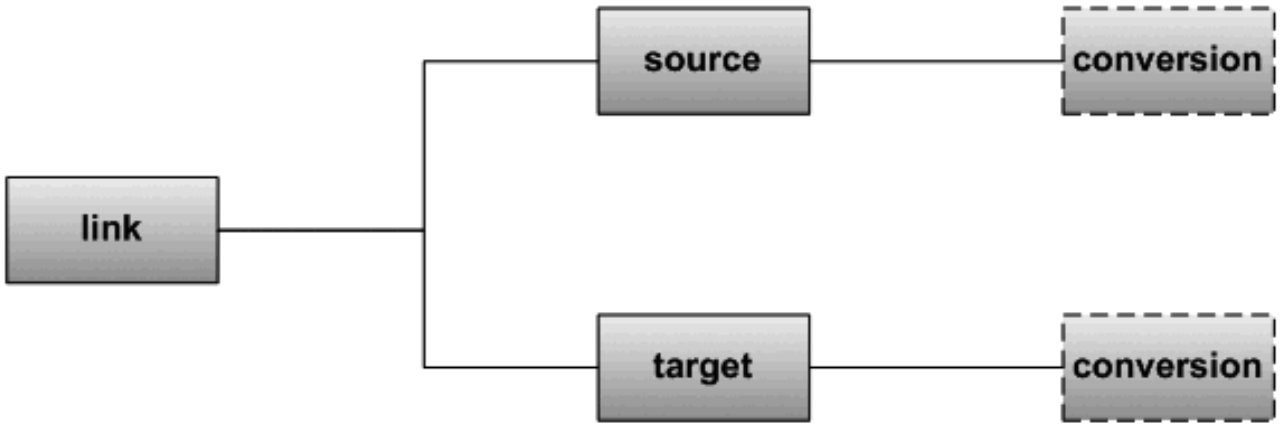
Resource description structure

Link description

The Link Description schema (LDS) describes:

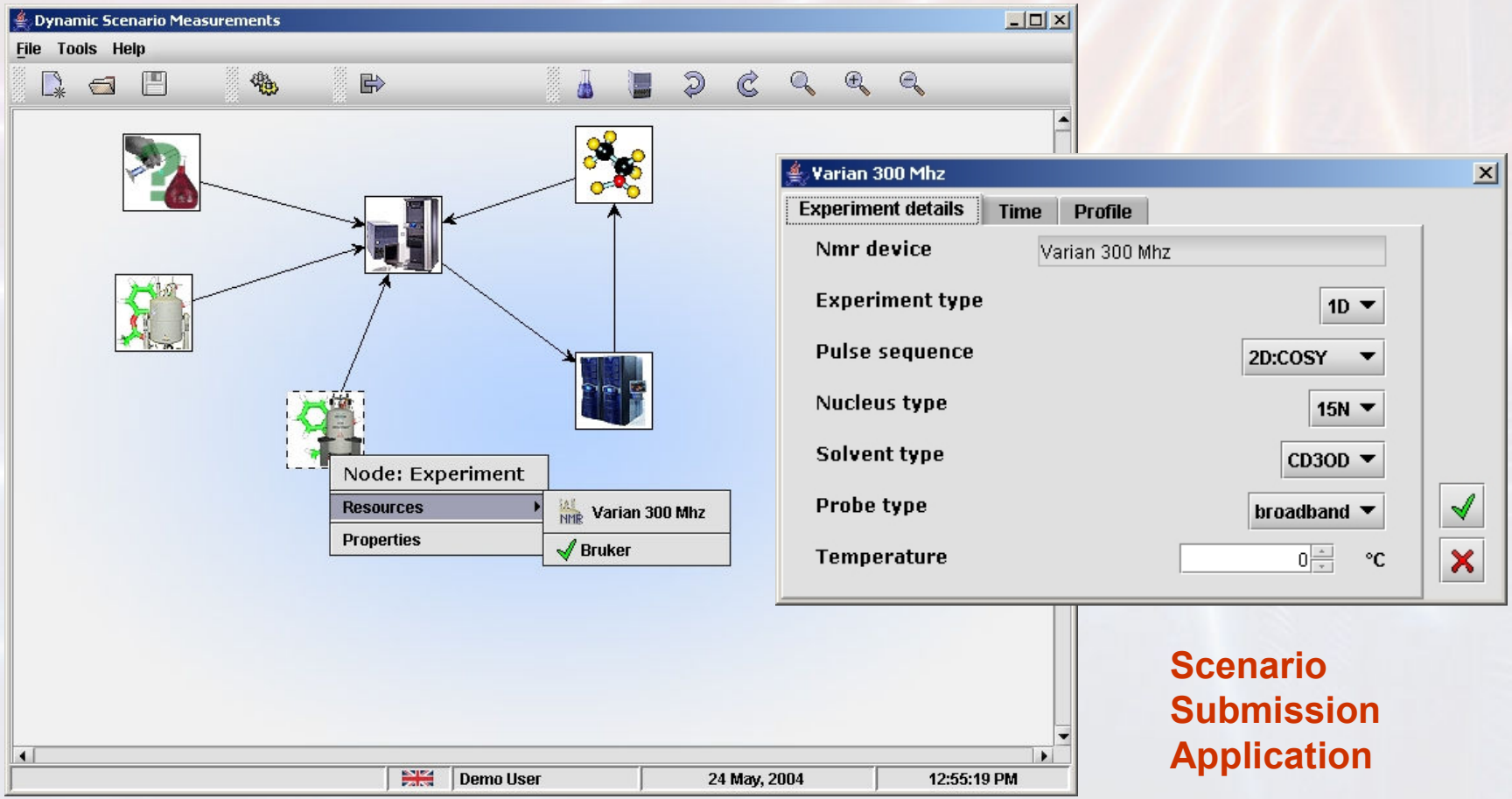
- the available connections between resources,
- specifies the conditions, which have to be taken into consideration while connecting resources.

```
<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>
```



Measurement scenario description

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

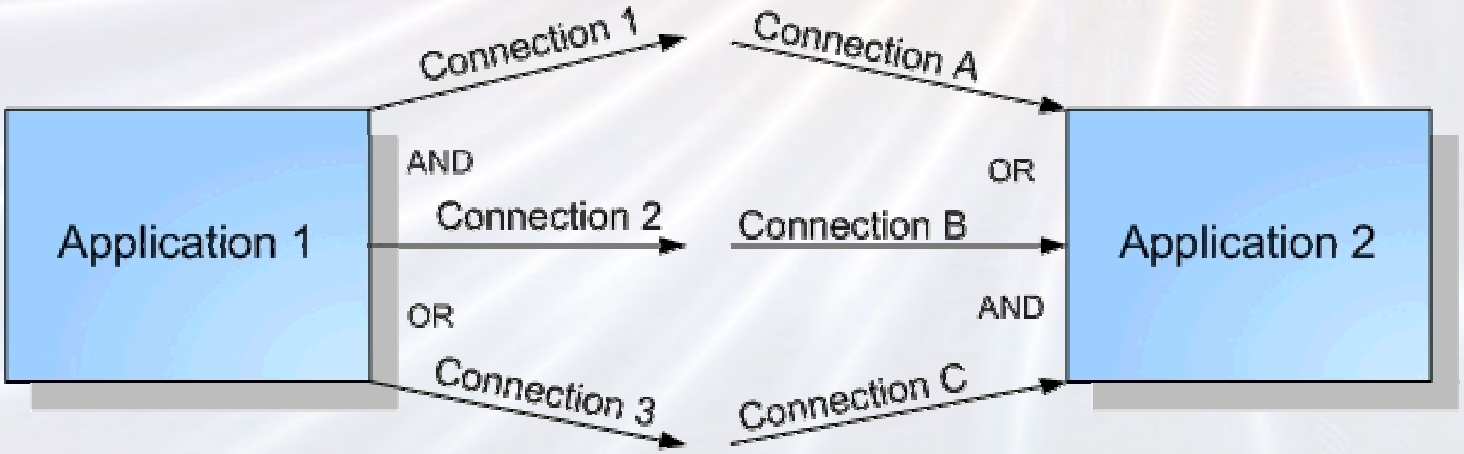


Scenario Submission Application

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:

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

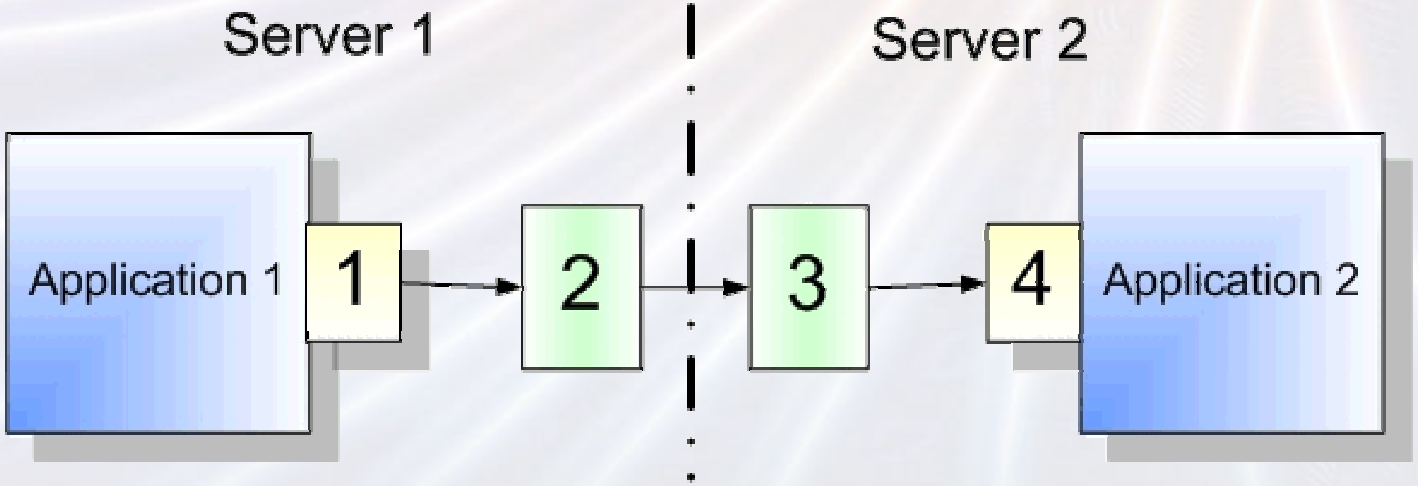


Defining beging and ending connection conditions

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 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 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 Radiotelescopy – cooperation with Radioastronomy Department of Mikołaj Kopernik University

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