Global Grid Forum 10, Berlin, March 9, 2004
Workflow in Grid Systems

Job workflow in the Virtual Laboratory

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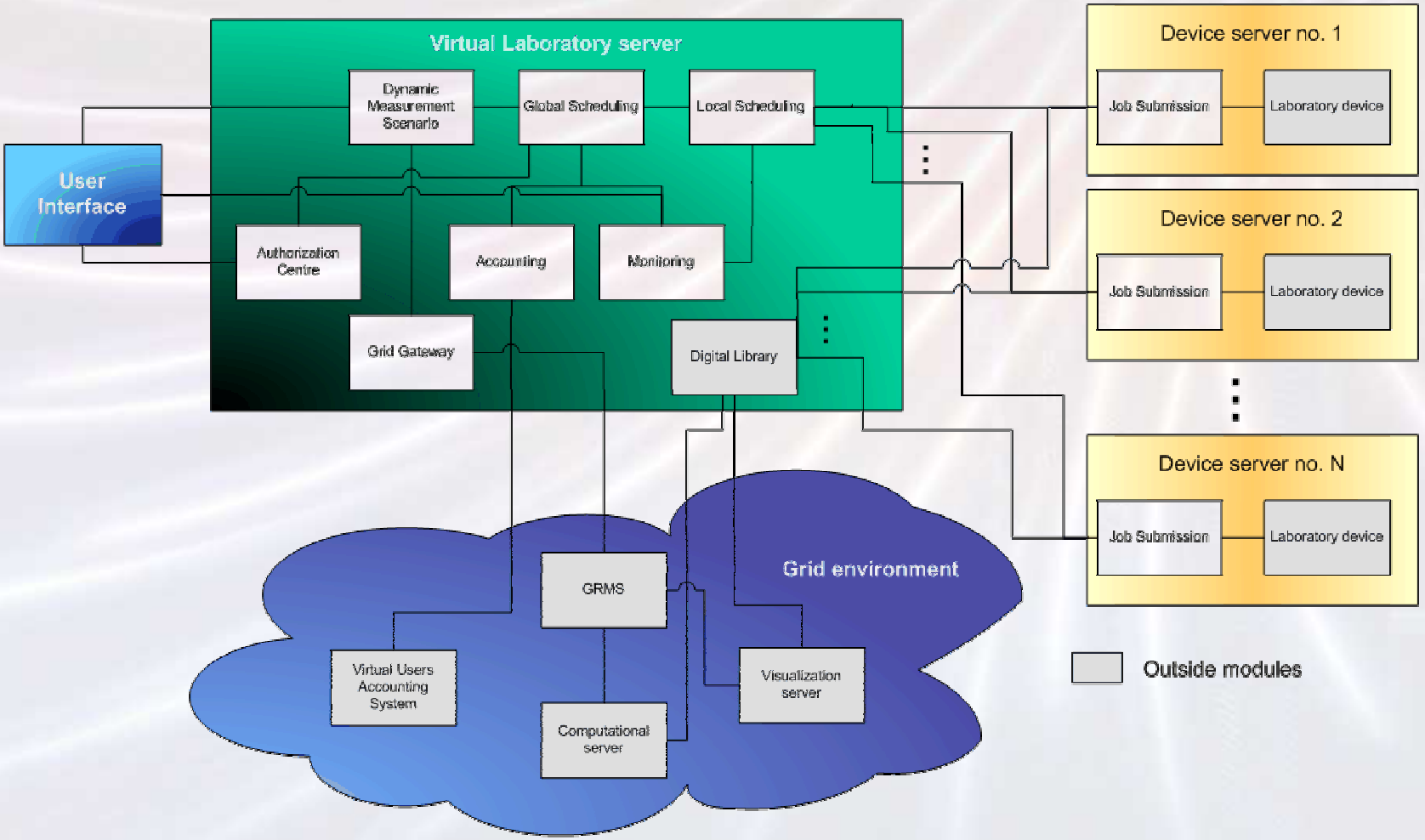
Virtual Laboratory overview

Research goals

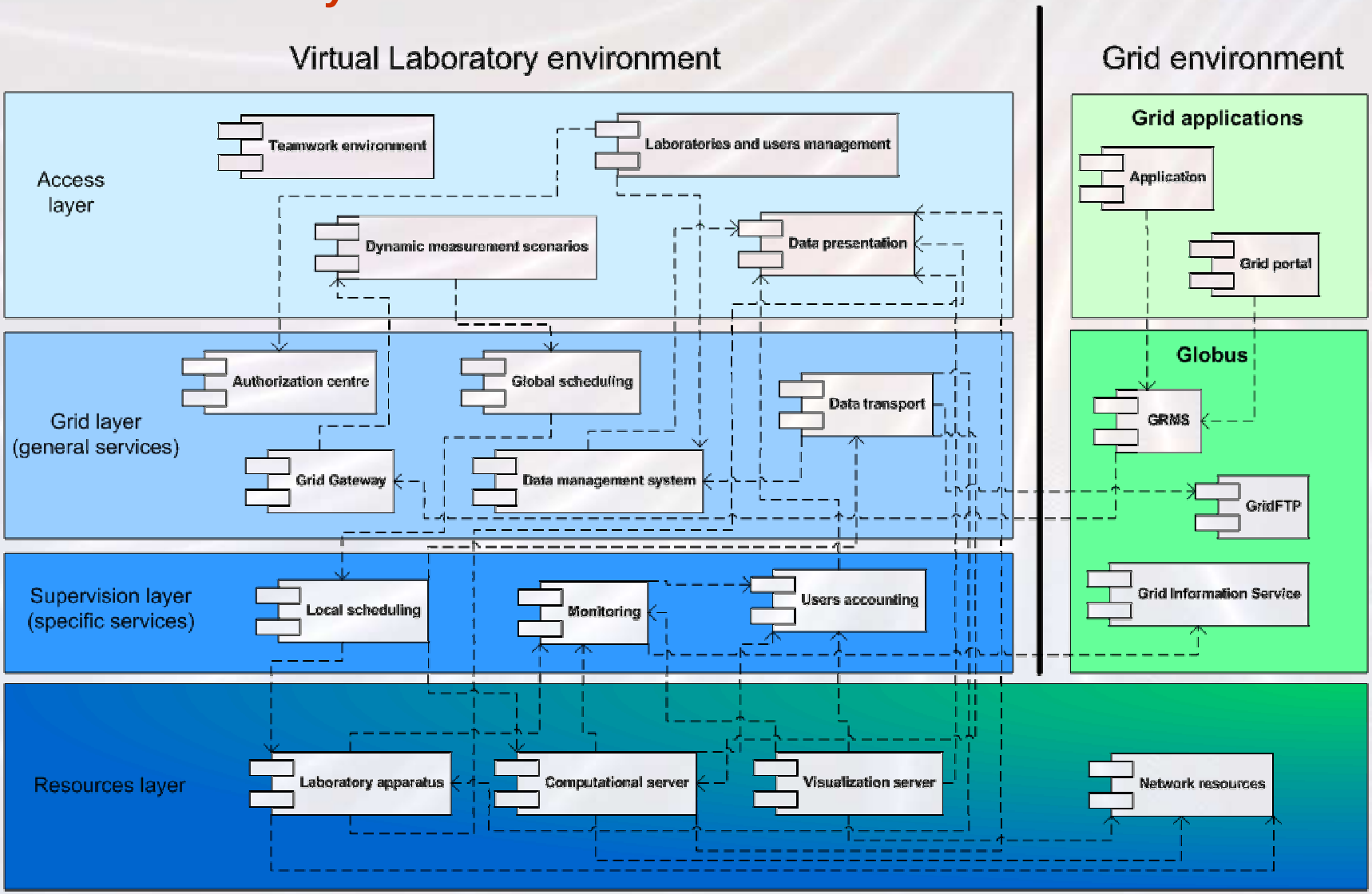
- Defining general VLab architecture
- Defining dynamic measurement scenario
- Device allocation in distributed environment
- Load balancing
- Taking into consideration the human factor

Virtual Laboratory general connection diagram



Simplified version of connection diagram in VLab

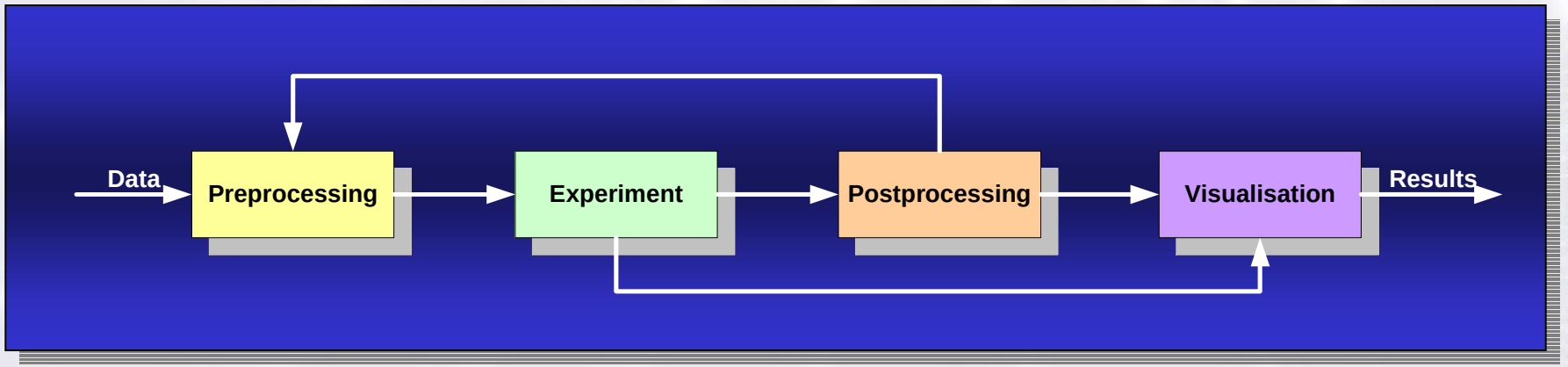
Virtual Laboratory architecture



Dynamic Measurement Scenario

Assumptions

- connection of experimental and computational jobs
- speeding up of execution tasks sequence
- simplification of tasks sequence control



Example of simple measurement scenario

How does the DMS is created?

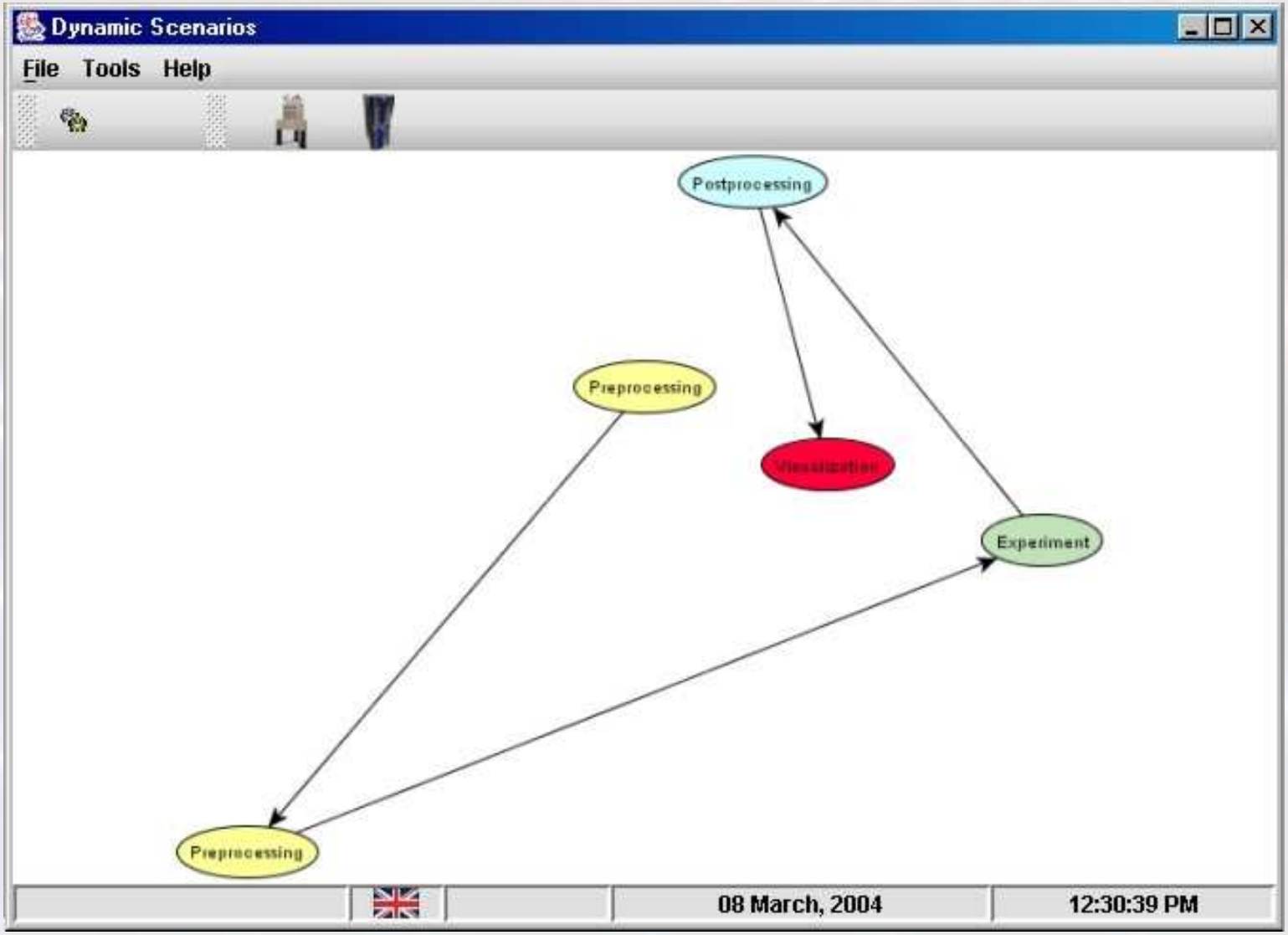
Virtual Laboratory

Creation process is devided into three stages:

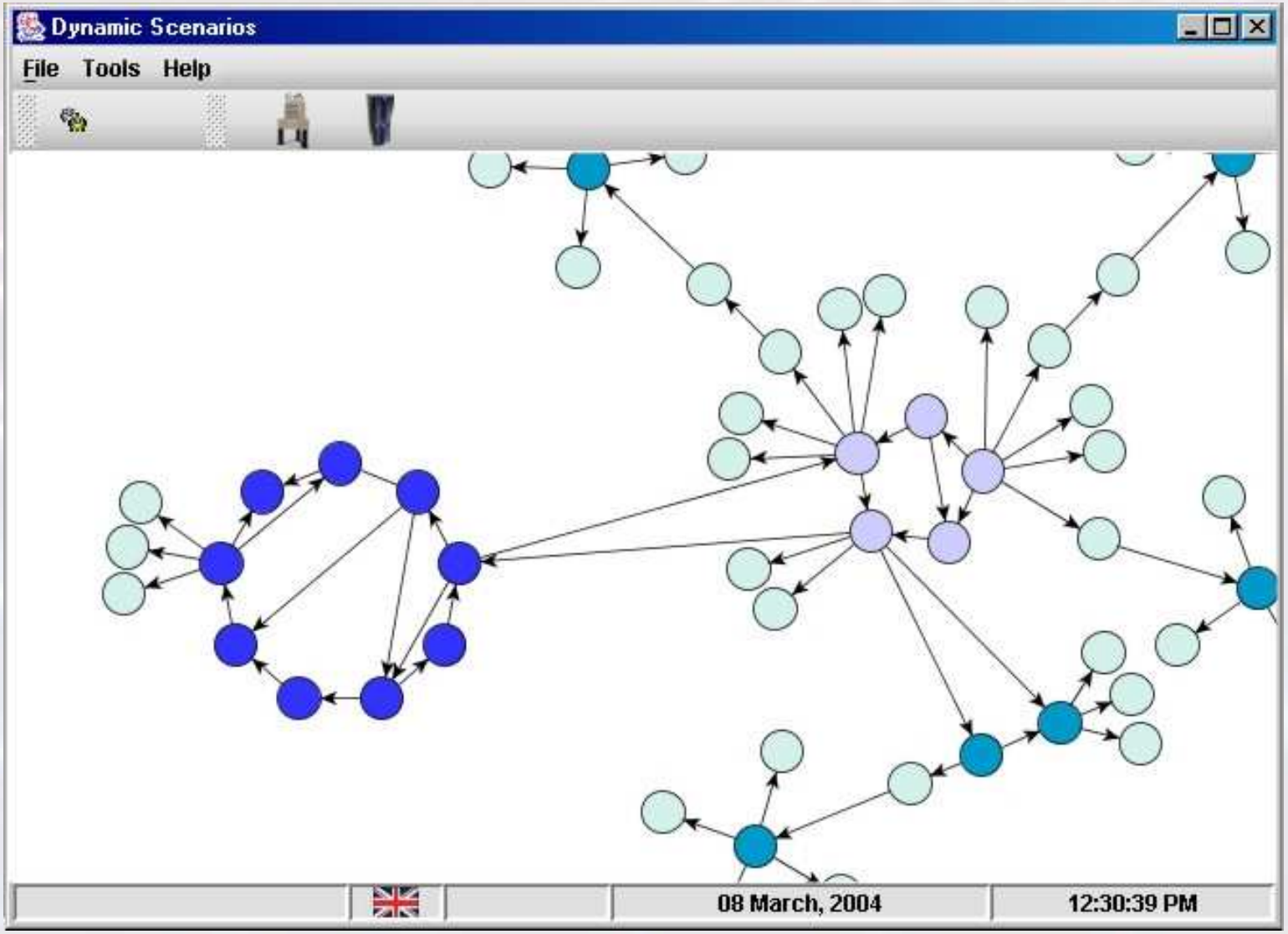
- preparation of connection diagram
- writing down diagram dependencies
- creation of the user DMS coded in Dynamic Measurement Scenario Language (written progressively during creation of workflow diagram by user)

First prototype demonstration on Supercomputing Conference 2003

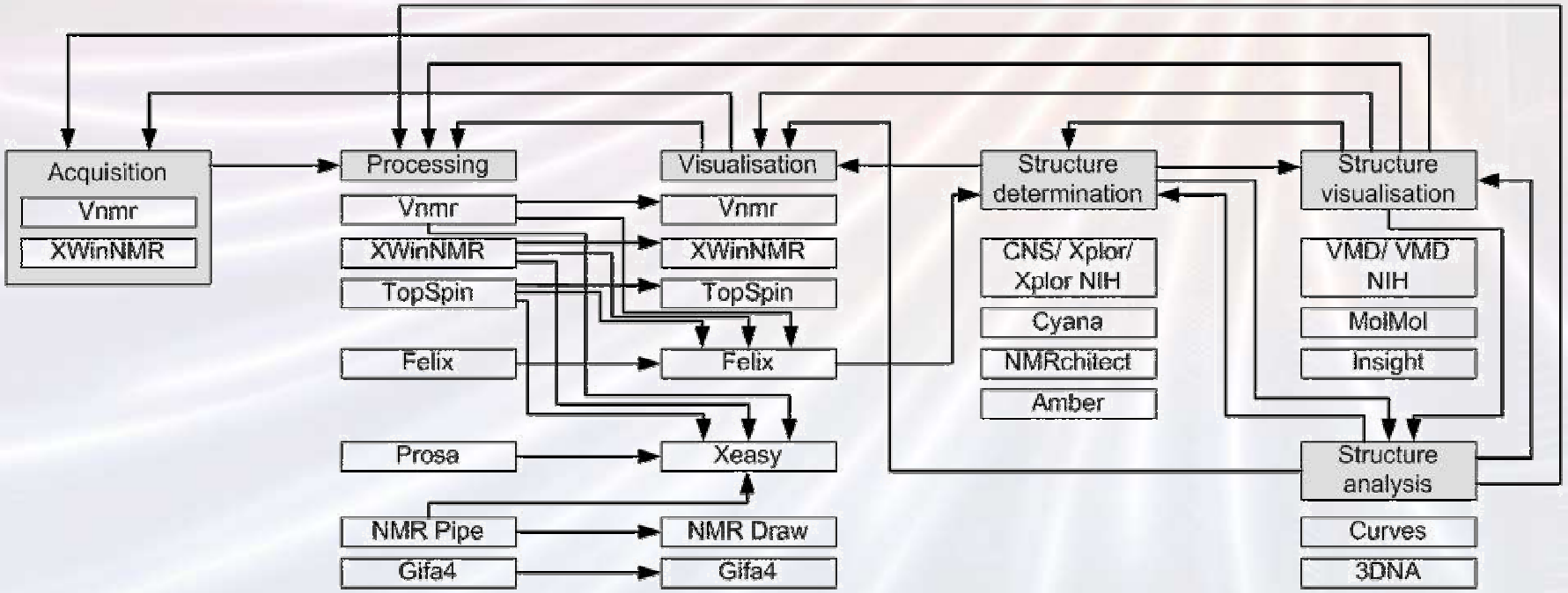
Example of DMS diagram



Example of DMS diagram



Stage 1: Preparation of connection diagram



Example of diagram for NMR scenario

Stage 2: Writing down connection rules

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<application ID="001">
  <devicename>Varian</devicename>
  <devicedesc>Varian 300MHz</devicedesc>
  <experimdesc>
    <expertype>1D,2D</expertype>
    <pulseseq>2D:COSY</pulseseq>
    <nucleustype>15N,20N</nucleustype>
    <solventtype>CD3OD</solventtype>
    <probetype>broadband</probetype>
    <temperature>10,20,25,30,40</temperature>
  </experimdesc>
  <cost>100</cost>
  <parameters>"-x -p -c"</parameters>
  <files>
    <inputfile1>input1.txt</inputfile1>
    <inputfile2>input2.txt</inputfile2>
    <outputfile1>output1.txt</outputfile1>
    <outputfile2>output2.txt</outputfile2>
  </files>
  <availableconnections>
    <connectedapp>
      <appID>"002"</appID>
      <conversion>"NO"</conversion>
    </connectedapp>
  </availableconnections>
  <timespec>
    <deadline>   </deadline>
    <reservation>
      <from>YYYY:MM:DD:HH:NN</from>
      <to>YYYY:MM:DD:HH:NN</to>
    </reservation>
    <userpresence> </userpresence>
    <adminpresence> </adminpresence>
  </timespec>
</application>
```

Simplified example

Stage 3: Creation of the user DMS

Virtual Laboratory

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<section secID="0">
  <diagapp ID="1">
    <applicationID ID="12">/
    <connectedapp>
      <connapp ID="3">/
      <connapp ID="4">/
    </connectedapp>
  </diagapp>
  <diagapp ID="2">
    <applicationID ID="5">/
    <connectedapp>
    </connectedapp>
  </diagapp>
</section>

<section secID="1">
  <diagapp ID="3">
    <applicationID ID="2">/
    <condition>
</condition>
    <inputfile1>

    </inputfile1>
    <connectedapp>
      <connapp ID="5">
    </connectedapp>
  </diagapp>
  <diagapp ID="4">
    <applicationID ID="5">/
    <condition>

    </condition>
    <inputfile1>

    </inputfile1>
    <connectedapp>
      <connapp ID="6">
    </connectedapp>
  </diagapp>
</section>
```

Simplified example

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