The DiVTB Platform: Some Experience Gained in the Application of UNICORE as Middleware in the "Mobility of Young Scientists" Project in Russia

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Outline

1. DiVTB system
   - Purpose
   - Architecture

2. Integration of external applications in the DiVTB system

3. Examples of applications
Purpose of the DiVTB system

• DiVTB (Distributed Virtual Test Bed) is a software system that provides the design and operation of distributed virtual test beds

• DiVTB provides a problem-oriented approach to specific classes of tasks in engineering design through resources provided by grid computing environments
Architecture of the DiVTB system
Integration of external applications in the DiVTB system
"Mobility of Young Scientists" Project

- The Federal Target Programme, entitled as "Scientific and Scientific-Pedagogical Personnel of the Innovative Russia" for the years 2009-2013

- "Technology of Creating Task-Oriented Services in Distributed Computing Environments“ as part of the above Programme
Materials for the participants

• A quick guide for the DiVTB system
• A virtual machine
• A guide for the virtual machine
• Examples of the project integration
• A visualisator for test beds
Virtual Machine of the DiVTB system

- Oracle VM Virtual Box
- OpenSUSE
- UNICORE-SERVERS
- UCC
Integration methodology of external applications

1. Describing an application in simpleidb

2. Creating a problem-oriented shell for the DiVTB Portal component to remotely trigger an external application as a grid service
Step 1. Describing an application in simpleidb

```
<idb:IDBApplcation>
  <idb:ApplicationName>Pow</idb:ApplicationName>
  <idb:ApplicationVersion>1.0</idb:ApplicationVersion>
    <jsdl:Executable>/bin/pow</jsdl:Executable>
    <jsdl:Argument>$FIRST_PARAMETER</jsdl:Argument>
    <jsdl:Argument>$SECOND_PARAMETER</jsdl:Argument>
  </jsdl:POSIXApplication>
</idb:IDBApplcation>
```
Step 2. Creating a problem-oriented shell

```xml
<?xml version="1.0" encoding="utf-8"?>
<problemCaebbean xmlns="http://caeserver.caebbeans.org" name="Concept_IH" author="Mr.Smith" version="1.0" caebbeanId="{pow-test}"

<categories>
  <category name="first_pair" data="first_pair_data">
    <parameter name="first_parameter" type="Float" visible="true">
      <text data="first_parameter_T" />
      <units data="first_parameter_U" />
      <comment data="first_parameter_C" />
      <enums />
      <default>2</default>
      <value></value>
    </parameter>
    <parameter name="second_parameter" type="Float" visible="true">...
  </category>
</categories>

<resources>
  <language xml:lang="ru">
    <data name="first_pair_data">First pair</data>
    <data name="first_parameter_T">X</data>
    <data name="first_parameter_U" />
    <data name="first_parameter_C">The X number</data>
    <data name="second_parameter_T">Y</data>
    <data name="second_parameter_U" />
    <data name="second_parameter_C">The Y number</data>
  </language>
</resources>
</problemCaebbean>
```
Visualisation of a test bed with the DiVTB Portal Test Bed Viewer

pow-test.xml

html-code

testbed.xsl
Final integration

1. Engineer transfers ProblemCaebean.xml VirtualMachine.vhd
2. DiVTB builds Project.xml for an engineer’s test bed
3. UNICORE integrates an engineer’s UNICORE/X component
4. DiVTB integrates a project of an engineer’s test bed

DiVTB
Engineer’s project

UNICORE
UNICORE/X
UNICORE/X
Examples of applications
Simulation of a chemical reaction of a metal complex catalysis

- Chemical reaction of a metal complex catalysis: a hydroalumination of olefins
- Calculation of a direct problem and checking the law of conservation
- Simulation of an induction period of the reaction for predicting the period’s behaviour under different input data

K.F. Koledina, Bashkir State University
Simulation of magnetic properties of nanomaterials

• Modelling of magnetic nanofilms
• Calculation of magnetic properties
• Solving of systems of nonlinear transcendental equations with many unknowns
• Writing of the application in the PYTHON programming language

Y. Kiriyenko, Far Eastern Federal University
Simulation of continuous media mechanics

- A model of two-dimensional acoustics
  - a parametrizable constant density
  - a parametrizable constant speed of sound
  - an initial exciting constant source of pressure

- Homogeneous boundary conditions of the first order

- Godunov’s method

I.M. Kulikov, an employee of the Institute of Computational Mathematics and Mathematical Geophysics, the Siberian Branch of the Russian Academy of Sciences
Remote visualisation service for problem solving

• SharpEye as a scientific visualisation system
• REST-server for SharpEye
• Two types of interfaces: graphic programmatic

P.A. Vasev, an employee of the Institute of Mathematics and Mechanics, the Ural Branch of the Russian Academy of Sciences
Results Yielded by the "Mobility of Young Scientists" Project

- Development of a technology for creating problem-oriented services in a distributed computing environment

- Creating of a methodology for the integration of problem-oriented applications

- Elaboration of a set of distributed virtual test beds for the solution of problems in various fields of knowledge