Development of Problem-Oriented Services for Distributed Computing Environments Based on the UNICORE System

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Outline

• South Ural State University
• Supercomputer Simulation Laboratory
• Problem-Oriented Environment
• Distributed Virtual Test Bed Concept
• Practical Engineering Problems Solution
South Ural State University
South Ural State University

South Ural State University: National Research University
South Ural State University

- **History**
  - Founded in 1943
  - 32 faculties
  - 2,700 professors and assistant professors
  - 55,000 students
  - 400 international students
  - 300 programs of higher professional education
  - 200 programs of further education
Centers and institutes

- Center of metallurgy and material study
- Center of mechanical engineering
- “Nanotechnology” Research and Education Center
- Research-manufacturing institute “Educational engineering and technologies”
- Supercomputer Simulation Laboratory
Supercomputer Simulation Laboratory
Supercomputer Simulation Laboratory

- **Supercomputer Center**
  - supercomputers administration and software license management
  - scientific research in the field of parallel and distributed computing and software development for grid computing and supercomputer systems

- **Distributed Computing and Embedded Systems Department**
  - development of software for distributed calculations, embedded systems, mobile platforms, electronic resources

- **Support and Training Department**
  - consultation for the users of the applied and system software on solving problems on the SSL supercomputers
  - training courses based on the SSL resources

- **Data Mining and Virtualization Department**
  - research in the field of data mining and virtualization technologies, solutions of practical problems based on these technologies, implementation and maintenance of appropriate software
Supercomputer Resources Evolution in SUSU

Physics
Computer cluster
Peak performance
1 Gflops
2000 г.

Infinity
Computer cluster
Peak performance
333 Gflops
2004 г.

SKIF URAL
Supercomputer
Peak performance
24 Teraflops
2010 г.

Intel Pentium 3
0,8 GHz
Intel Xeon64 DP
3,2 GHz
Intel Xeon E5472
3 GHz

SKIF-Aurora
SUSU
Supercomputer
Peak performance
117 Teraflops
2011 г.

Intel Xeon x5570
2,93 GHz
Intel Xeon x5680
3,33 GHz
SKIF-Aurora SUSU Supercomputer Specifications

- Ranking TOP50 CIS list: 3rd
- Ranking TOP500: 87 (June 2011)
- 117 Teraflops
- 8832 computing cores
- RAM: 9 TByte
- Disk space: Intel SSD 108 TByte

Communication networks:
- System network: 3D torus, 60 Gbit/s
- InfiniBand QDR, 40 Gbit/s
- Gigabit Ethernet
SUSU Supercomputers Workload Characteristics

Distribution of tasks among priority areas of science

- Strategic information technologies (52.2%)
- Energy efficiency and conservation (33.7%)
- Space technology (9.4%)
- Medical technology (3.5%)
- Nuclear technology (1.2%)

Distribution of tasks among branches of knowledge

- Natural science (65%)
- Engineering (33%)
- Socio-economic (2%)

Tasks
Distributed Problem-Oriented Environments
Distributed Problem-Oriented Environments

Goal:

- The principal objective is to develop a technology allowing to take into account the specifics of the problem-oriented subject areas while providing the recourses of distributed computing environments.
- This technology aimed to create “intelligent” middleware providing users with easy, transparent and secure access to distributed computing resources and allowing them to solve specific classes of applied problems.
Example of Distributed Problem-Oriented Environment

- **CFD (Computational Fluid Dynamics)-Environment** is a distributed problem-oriented environment for computer-aided engineering in the Computational Fluid Dynamics problem domain on the basis of ANSYS CFX package
“Simulating Flow in a Static Mixer”

CFD problem example

- A static mixer consists of two inlet pipes delivering water into a mixing vessel
- **Inlet in1**: $V_1 \text{ m/s}$, a temperature of $T_1 \text{ K}$
- **Inlet in2**: $V_2 \text{ m/s}$, a temperature of $T_2 \text{ K}$
- Radius of the mixer: $R \text{ m}$
The Basic Definitions: Job

- **Job** is a set of *Tasks* organized as a workflow aimed at achieving of a useful result.

- Job determines the order of tasks execution, the conditions under which this or that task will be started, mutual synchronization of tasks and information flows between tasks.
The Basic Definitions: Tasks

- **Task** describes the process of transformation of input parameters into output parameters.

- **Task** represents a solution for some part of a job.

```
Converter

Problem parameters
Template
Converter

Input parameters
Transformation
Output parameters

JScript

Geometry

DesignModeler Service
```
“Simulating Flow in a Static Mixer” Job and Tasks example

- Design Modeler
- CFX-Mesh
- CFX-Pre
- CFX-Solver
- CFX-Post

- Creation or correction of a geometric model
- Creation or correction of a mesh
- Creation or correction of problem definition
- Problem Simulation in CFX-Solver
- Visualization in CFX-Post

Values of the optimization criteria are not satisfactory
The accuracy of the calculation is not satisfactory
The Basic Definitions: Services

- **Service** is a specification of resources to solve a specific class of Tasks. Service defines format of the input and output data.

```json
{
  ApplicationName: "DesignModeler",
  ApplicationVersion: 1.0,
  Environment: ["SOURCE=input.js"],
  Imports: [
    {File: "input.js", To: "input.js"},
  ],
  Exports: [
    {File: "output.agdb", To: "output.agdb"},
  ]
}
```
The Basic Definitions: Resources

- **Resource** is a hardware and software required to perform a *Task*
The Basic Definitions: Activity

- **Activity** is allocation of necessary resources and launch of a specific service on a specific resources to execute a specific *Task*

- Activity = Task + Values of input parameters + Service + Recourses
Technological Process (T-Process) is a workflow of activities aimed to implementation of a specific Job.
Distributed Virtual Test Bed Concept
Test Bed

Real

Virtual
Virtual Test Bed - As-a-Service
Distributed Virtual Test Bed (DiVTB) includes:

- an **interface** for a CAE-problem statement;
- a **driver** (a set of software tools enabling the use of grid resources for virtual experiment);
- a set of **grid services** (a set of supercomputers in a distributed computing environment, with the installed software components)
Distributed Virtual Test Bed

Features:

• A web-access to a remote simulation of engineering tasks on a supercomputer

• Providing a safe and transparent access to the resources of a distributed computing environment (UNICORE)

• The use of idle resources of supercomputer centers
DiVTB levels

- **A conceptual CAEBean** defines problem-oriented interface for DiVTB in terms of its CAE-parameters.

- **A workflow CAEBean** implementing a CAE-workflow for a certain CAE-problem.

- **Physical CAEBeans** convert a problem-oriented description of a CAE-problem into the set of files which are needed to launch a single **CAE-action** (mesh generation, simulation, post processing, optimization etc.)

- **System CAEBean** - a computing resource in a distributed computing environment.
Conceptual CAEBean

Input parameters

Output parameters

Workflow CAEBean

Physical CAEBeans

Complete descriptor

d_1=3 d_2=2 l_1=10 ...

Action generation

Action results

CAE System

UNICORE
CAEBeans System

Engineer

Application programmer

CAEBeans Portal

CAEBeans Server

CAEBeans Broker

Grid
CAEBeans Constructor
CAEBeans System

- **CAEBeans Server, CAEBeans Broker** – WSRF services
- **CAE-Resources** – UNICORE Target Systems
DiVTB for practical engineering problems solution
DiVTB for common CAE-systems

- We developed DiVTB to solve problems by using common CAE systems
  - ANSYS CFX,
  - ANSYS Mechanical,
  - ABAQUS,
  - DEFORM,
  - LS-DYNA.
Pressure distribution in flow tube of vortex flow meter
Customer: JSC Chelyabinsk Tube-Rolling Plant

Purpose of study: simulation of tube deformation during hardening during production on tube rolling plants

Result:
- rejection rate reduced by 10%

Temperature distribution during water sprayer pipe cooling
Optimization of Pneumatic Transmitter Cap DiVTB

Customer: EMERSON

Purpose of study: Optimization and design of pneumatic transmitter cap with the following properties:

- strength - as the original version of the design;
- technological effectiveness - as in "alternative" option (forging instead of casting);

Result:
- 15% less material requirements maintaining the required strength

Equivalent stresses at 56 MPa pressure (color scale – stress in MPa)
Simulation of Deformation of Flat Knitted Products Structure

Customer: Kyshtym knitwear Ltd.

Purpose of study: development of new methods of clothes design that take into account properties of the tissue

Result:
- automation of design process
- time to design new models reduced
- product range growth
- volume of output increased by 20%

Equivalent Mises stress (Pa)

The mechanism of “dressing” jerseys on the dummy
Increase of Turbulence Coefficient of Airflow which is Fed into the Cylinder Combustion Chamber of the Diesel Engine

Customer:
UAB “CTZ-Uraltrack”

Purpose of study:
Develop a rotary-vane turbulence promoter and implement it into swirl inlet port of the cylinder head

Result:
Coefficient of turbulence is increased by 20%
Deformation and Destruction of Fabric Bulletproof Vest by a Bullet Strike

Customer: UAB “FORT Technology”

Purpose of study: development of new body armor design

Result:
- profit margins increased from 10% to 30% due to reduction of field experiments and use of virtual prototyping
- bulletproof vests are on arms of special units of the Russian Federation and foreign countries (Germany, France, Israel, Poland, Czech Republic, etc.)
Interactive example

http://skif-ural.susu.ac.ru:82
What’s next?

- Development of billing services for DiVTB
- Development of CAEBeans Constructor Web-application
- Development of scheduling algorithms for CAEBeans Broker
- Development of remote 3D-visualization services
- Integration of authorization and authentication with UNICORE services
- Integration with UNICORE workflow system
- Integration with multi-criteria optimization systems
Questions?

http://supercomputer.susu.ac.ru/en/