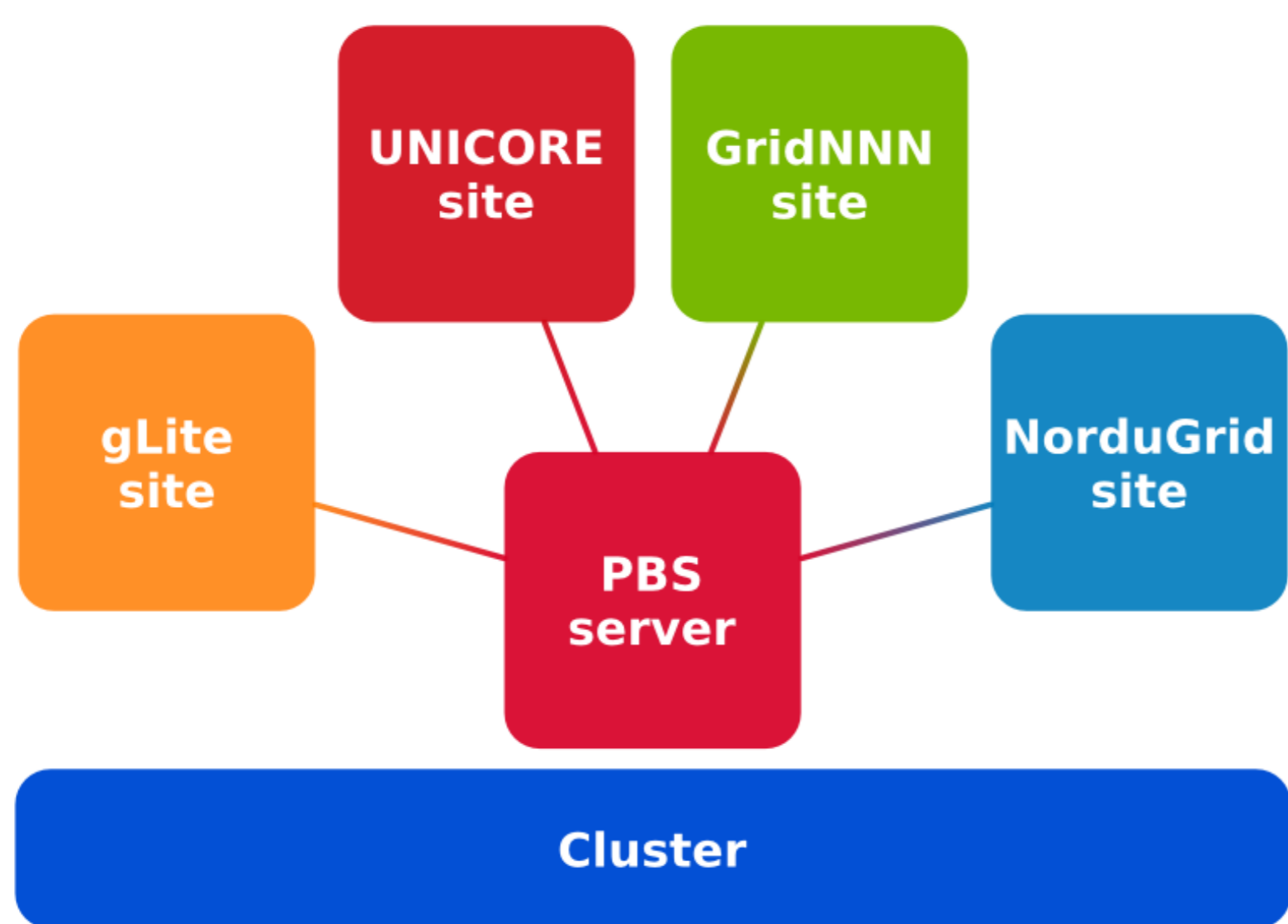


UNICORE testbed of Physics Faculty of Saint-Petersburg State University

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Introduction

The activities in the area of distributed computing that have been carried out at our department since 2005 are aimed at application of grid technologies in education and science, as well as at study and experimental verification of new technological solutions [1]. One of the directions of our work is development and support of a multifunctional computational system based on cluster resources of the physics faculty. The system is used mainly in educational activities on parallel and distributed computation technologies, but the resources are also granted to students that perform computations for their scientific work.



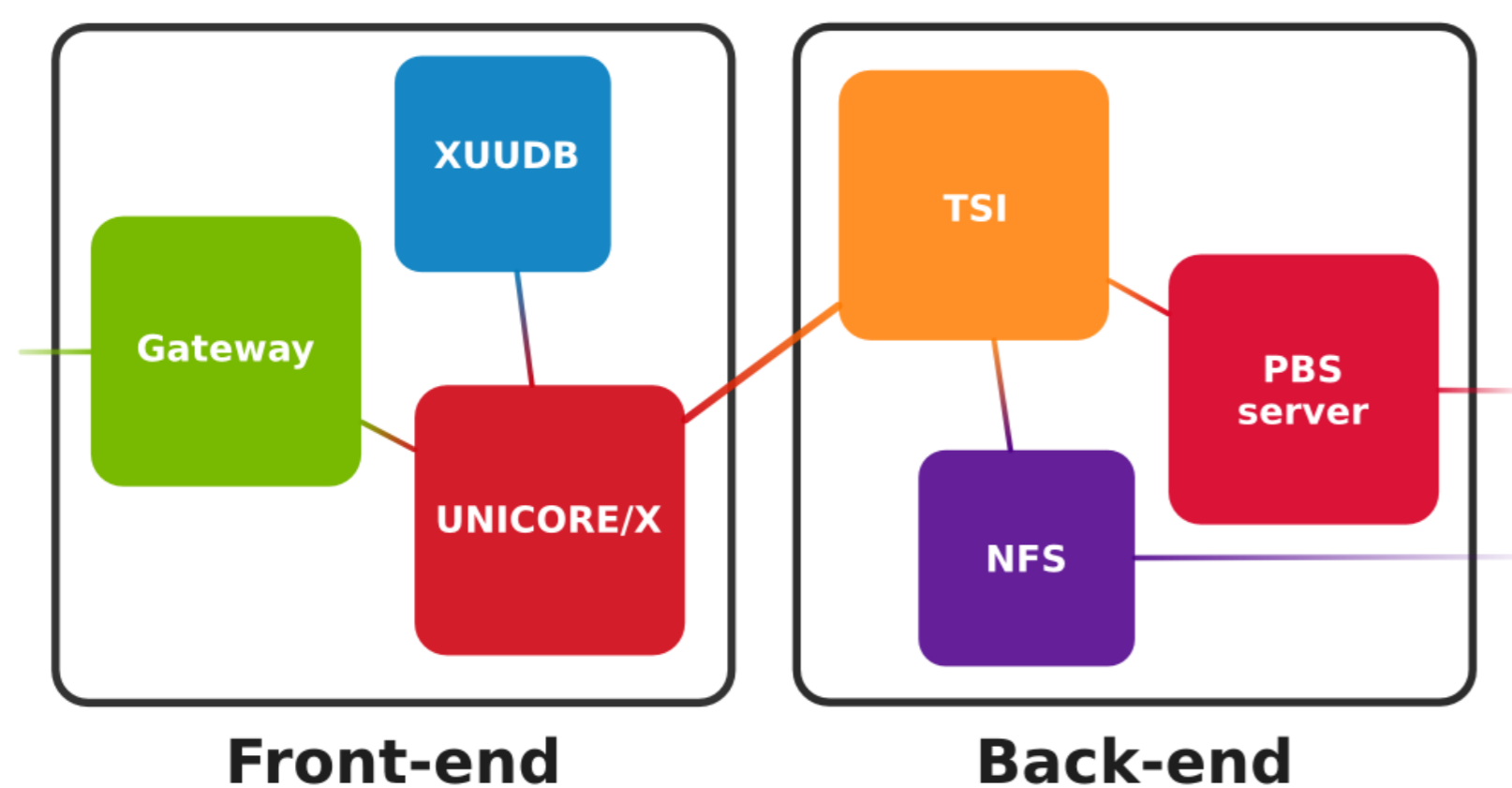
We have created an integrated grid system that provides simultaneous access to a single computational cluster from various grids (GridNNN, Nordugrid ARC, gLite and UNICORE based). Such configuration makes it possible not to follow a typical scheme, according to which available hardware resources are divided into several clusters with their own settings, each serves up one site. The proposed solution provides high mobility and utilization efficiency of computational resources and enables students to gain wide practical experience with extensive set of modern grid software. Access to user jobs and scientific software packages can be granted via both a batch system and grid sites.

UNICORE site

Our interest in the middleware has arisen because of several reasons.

- First of all, UNICORE is an original project and does not rely on side components.
- Secondly, we believe UNICORE not to be widespread and well-studied in Russia as compared to the other middleware, e.g. Globus Toolkit.

We have accomplished installation of a basic UNICORE 6.3.1 bundle and configuration of a site. The following services have been installed: Gateway, UNICORE/X, XUADB and TSI. All services use valid certificates from Russian Data Intensive Grid (RDIG) CA. User certificates solely from RDIG CA are supported.



The site comprises:

- a front-end node with Gateway, UNICORE/X and XUADB services
- and a back-end node with TSI service and an instance of PBS server connected to a cluster

Such placement of the services meets our needs in the best way.

A cluster comprises 12 2xIntel Xeon 3GHz Dual Core HT / 4GB RAM / Scientific Linux 5.4 nodes and is operated by PBS Torque 3.0.0. Special

measures have been taken in order to improve the control of resources:

- PBS has been built with `cpuset` Linux kernel feature patches enabled [2]
- OSC Mpiexec utility, which supersedes `mpirun` and `mpiexec`, is used [3]

A dedicated queue with 32 CPUs for UNICORE jobs is available.

Educational activities

On the basis of the integrated grid system, seminars are held. These seminars are the part of a special course on grid technologies for students of the physics faculty and the mathematics faculty. The course enables students to learn modern computational systems and tools, to put into practice their theoretical knowledge and to acquaint themselves with the ways grid technologies can be applied in their research work. Special attention is paid to launching of scientific applications. During the course students have to accomplish their self study that includes development of their own applications with the use of MPI and OpenMP technologies and compilation with the necessity to run those applications on grid sites. This spring, the UNICORE site was used in the course for the first time. Students have learnt about the command-line client, job description language and also rich client.

Scientific packages

The underlying cluster is used not only in education, but also for scientific computations. The main part of load is molecular dynamics and quantum chemistry simulations that are performed by various professional scientific packages.

Using the IDB mechanism we have made the LAMMPS [4] and Firefly (PC GAMESS) [5] packages available on the UNICORE site. The packages can be launched in both serial and parallel modes. Parallel mode is available by means of an MPI execution environment.

Here is an example of LAMMPS job description:

```
1 {
2   "ApplicationName": "LAMMPS",
3   "ApplicationVersion": "10Sep10",
4   "Arguments": [
5     "-echo log"
6   ],
7   "Environment": [
8     "INPUT=in.pour",
9     "LOG=log.pour"
10  ],
11  "Imports": [
12    { From: "in.pour", To: "in.pour" }
13  ],
14  "Exports": [
15    { From: "log.pour", To: "log.pour" },
16    { From: "dump.pour", To: "dump.pour" }
17  ],
18  "Resources": {
19    "Nodes": 2,
20    "CPUsPerNode": 2
21  },
22  "Execution environment": {
23    "Name": "MPI",
24    "Options": [ Verbose ]
25  }
26 }
```

References

- [1] M. M. Stepanova, A. N. Makarov, S. L. Yakovlev. Grid-systems in process of research and teaching at faculty of physics of SPbSU. Distributed Computing and Grid-Technologies in Science and Education: 3rd Intern.Conf. (Dubna, June 30–July 4, 2008). — Dubna: JINR, 2008, pp. 113–114.
- [2] Linux cpuset support in Torque, last visited: June, 2011, <http://www.adaptivecomputing.com/resources/docs/torque/3.5linuxcpusets.php>
- [3] Mpiexec home page, last visited: June, 2011, <http://www.osc.edu/~djohnson/mpiexec/>
- [4] LAMMPS Molecular Dynamics Simulator home page, last visited: June, 2011, <http://lammps.sandia.gov/>
- [5] Firefly home page, last visited: June, 2011, <http://classic.chem.msu.su/gran/gamess/>

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