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Integration of the computing cluster into the information system of facility

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The experience of integration of the computing cluster into the information system of facility is described. The cluster is comprised of one control node (2×CPU Intel Xeon E5-2670, 64 Гб RAM) and two compute nodes (1×CPU Xeon E5-2670, 64 Гб RAM, 1×GPU Nvidia Tesla M2090).

The following problems had to be solved during cluster configuration.

Integration of the cluster authentication system with faculty's local network authentication system.

Setting the consistent software updates on the cluster's control node and the compute nodes.

The centralized initial cluster setup with help of xcat utility.

Installing additional software with CUDA technology support.

Creating the local software repository for specific software support (for example, PBS / Torque with CUDA support).

The following software were to be installed on the cluster: GNU Compiler Collection (gcc) [2], with gfortran version 4.4.7 c OpenMP [3], Julia language compiler [4], Python interpreter version 2.7. Oslo following libraries have been installed: OpenMPI [5], MPICH [6], BLAS [7], LAPACK [8], GSL (GNU Scientific Library) [9], GAMESS (US) (General Atomic and Molecular Electronic Structure System) [10], Python NumPy and SciPy [11].

All the software listed above is widely known and a good account of itself in the field of scientific computing. However, it may be useful to give a little bit more details about Julia programming language —the new open source programming language that is in the stage of active development. Julia language has created to achieve following goals: multiparadigmality, focus on scientific computing, the possibility of interactive language constructions execution (like iPython), achieving the performance close to C/C++ and Fortran, built-in support of parallel computing, easy integration of an external Fortran and C/C++ libraries.

Литература

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2. GCC, the GNU Compiler Collection —<http://gcc.gnu.org/>
3. OpenMP API specification for parallel programming —<http://openmp.org/wp/>
4. The Julia Language —<http://julialang.org/>
5. Open MPI: Open Source High Performance Computing —<http://www.open-mpi.org/>
6. MPICH: High-Performance Portable MPI —<http://www.mpich.org/>
7. BLAS (Basic Linear Algebra Subprograms) —<http://www.netlib.org/blas/>
8. LAPACK — Linear Algebra PACKage —<http://www.netlib.org/lapack/>
9. GSL - GNU Scientific Library —<http://www.gnu.org/software/gsl/>
10. The General Atomic and Molecular Electronic Structure System (GAMESS) —<http://www.msg.ameslab.gov/games/games.html>
11. SciPy/NumPy —<http://scipy.org/>

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