Software on the Discovery Cluster

Discovery cluster uses “modules” to control all software available to users. Modules enables software to be independent of the Linux kernel on every node across the cluster, allowing software to use its own specialized and optimized libraries and provides performance and configuration flexibility in an “object-oriented” manner not possible otherwise. Information on using modules and the software on the cluster is on the Research Computing (RC) web-site at http://www.northeastern.edu/rc in the “Software on Discovery Cluster” tab. Further information is also available in the “Submitting Jobs on Discovery Cluster” tab on the RC website.

List of some Software on Discovery Cluster

- Scheduler – SLURM 14.11.8
- GNU 4.4.7, 4.8.1, 4.9.3, 5.2.1 (OpenACC 2.0/CUDA 7.0), and Intel 13.1
- Cuda SDK 5.5 to Cuda SDK 7.5 with OpenCL and AMD-APP-SDK-v2.9
- IBM Platform MPI 9.1 with HPCTSTRIT and PAPI (hpcrun, hpcstruct, hpcprof, hpcviewer, hpctraceviewer)
- mpich 3.0.4 and OPENMPI 1.8.3, TotalView Debugger 8.14.1 (8 core license)
- Platform MPI, mpich and OPENMPI are TCP/IP, IOPIB and RDMA mode enabled depending on queue used
- Python 2.7.5 with SAGE, BioPython and MPI4PY, and PERL 5.20.0 with BioPerl, CANTERA 2.2.1, PACBIO-2.3.0, Python 3.3.2
- SPARK 1.2.0, 1.3.1, 1.4.1 with HADOOP 2.4 series, Julia 0.3.5 and 0.4.6
- Oracle Java SDK 1.7u40, 1.8u60 and ant 1.9.3, Eclipse (on login nodes only – load Java SDK module to use)
- R 3.0.2 compiled with GNU Compiler with Rmpi and SNOW, and all BioConductor packages (recommended R to use as kernel is built with GNU), R 3.0.1 compiled with Intel Compiler
- GUROBI 6.5, ITK 4.7.0 (Insight Segmentation and Registration Toolkit), ANTs (Advanced Normalization Tools v78931aa), c3d 1.1.0, IBM CPLEX 12.6.1, c3d_caffe
- Matlab 2016a with all toolboxes released by Matlab including Parallel Computing and GPU Toolbox and Distributed Computing Server integrated with SLURM 14.11.8 (Older Matlab 2013b was integrated with IBM Platform LSF)
- Mathematica 10, SAS 9.4 and STATA 14.1
- NAMD-2.9 with VMD 1.9.1 and ATSAS 2.7.0, and ORCA 3.0.2
- GROMACS (single and double precision both Intel and GNU versions with/without GPU)
- LAMMPS (single and double precision both Intel and GNU versions with/without GPU)
- GAUSSIAN 09.b.1 / 09.e with GaussView5 and NWChem 6.5, OpenBabel 2.3.2, MOPAC, EIGEN 3.2.4, AMBER-12
- openfoam 3.2.1, openfoam 3.0+, foam-extend-3.2, Ansys/Fluent 14, Schrodinger 2016
- ROOT 5.34.14
- DATABASES: RCSB (Protein Data Bank), NR (NCBI)
- kdevelop, htcp, cfunick-2.1.1, abinit-7.4.3, lemon-1.3, root-5.34.14, afni, samtools-0.1.19, sundials-2.5.0, dnaclust, blat_branch_hmmer_lemon, satscan, boost-1.55.0, scons-2.3.0, bowtie-1.0.0, bowtie-2.1.0, tophat-2.0.9, ncbi-blast-2.2.28, trinity_rna_seq_2013_08, clang LLVM_3.4, clang LLVM_3.7, cmake-2.6.4, cmake-2.8.1, cmake-3.3.2, octave-3.6.4, vtk-5.10.1, vtk-6.2.0, petsc-3.4.3-debug, petsc-3.4.3-opt, checkmate-1.1.6, gaussview5, fftw-3.3.3, fftw-3.3.3-single-thread, fftw-3.3.3-single-thread, fftw-3.3.4, AMD-APP-SDK-v2.9, freesurfer-5.3.0, carma-1.3, catcdcc-4.0, protobuf, OpenCV, caffe, ImageMagick-6.9.0, cdco-1.6.8, VisIt-2.8.2, opencv-4.4.4, tachyon-0.98.9, paraview-4.3.1 and 4.4.0 (in openfoam-3.0+), vaa3d-2.921, avogadro-1.1.0, pdsh-2.29, Lumerical ftdt_solutions-8.11.422, GLPK-4.55, ginac-1.5.6, cln-1.3.4, trng-4.17, 3d-rism (reference interaction site model), multi2sim-4.2, openmm-6.3.0, mafft-7.273, emboss-6.6.0, plumed-2.2.1, raxml, FSL for FMRI, MRI and DTI, TPP-4.8.0, sketchmap-0.2, igraph-0.7.1, LuaJIT/TORCH, TANDEM Spectral Modeler
- User requested: Several modules exist that are compiled from user’s code or code they modified from available software e.g. Rkkr005_Rcpa005_Ccp1d005, gromacs-4.0.5_single_intel_TMD_HARMONIC_v3, gromacs-4.0.5_double_intel_TMD_HARMONIC_v3, cciedg, cciedg-gpu

You can request software and modules for your own code by emailing researchcomputing@neu.edu.

Related Links
Northeastern Research Computing: http://www.northeastern.edu/rc
Software on Discovery Cluster: http://nuweb12.neu.edu/rc/?page_id=16
Submitting Jobs on Discovery Cluster: http://nuweb12.neu.edu/rc/?page_id=18

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