Legacy Cluster - Archived Documentation

32 Node Xeon processor cluster

These pages archive the documentation for the original CNF Cluster install. The new CNF Cluster install has its own series of pages. The original CNF Cluster was taken offline on Monday, April 3, 2017 for an extended maintenance period. The cluster is targeted to be brought back online by end of fall 2018.

- Accessing the CNF Computing Cluster
- Scientific Codes Available on the Nanolab Cluster - Archived

The CNF Cluster is self-supported and available on an as-is basis. CNF IT staff can provide help with navigating UNIX/LINUX. Contact cluster-admin (at) cnf.cornell.edu .
CNF Computing staff may also install additional software upon request as time allows.
The below documentation is archived for your convenience.

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Description:

The Nanolab cluster provides users of the CNF the opportunity to use a wide range of modeling software tailored for nanoscale systems. The cluster consists of dual Xeon E5620 and dual Xeon E5-2620 processors. All nodes are linked via Gigabit Ethernet. The cluster runs Red Hat Linux Enterprise 5.

The CNF Cluster was made possible by donations from Intel Corp. in 2004, 2005, and 2007. In 2010, we also expanded the capability of the cluster with the additional of 20 new Xeon nodes with a large amount of RAM to handle memory intensive calculations.

Capabilities:

We have a wide range of scientific libraries available for code development including ATLAS, GSL, and FFTW. In addition, we have Intel compilers (Fortran, C/C++) and MKL math libraries available. These Intel products are designed to optimize performance on the Xeon architecture. The cluster is currently capable of running parallel programs based on the MPI message passing protocol using LAM-MPI. Please contact cluster-admin (at) cnf.cornell.edu if you are interested in getting an account on the cluster.

Applications:

The cluster provides a high performance computing environment for modeling nanoscale systems with existing codes. It is also an ideal site to test and develop new codes for nanoscale research.

Installed Codes:

ABINIT (www.abinit.org): Abinit is an open source first principles code based on pseudopotentials and a plane wave basis. This code can be used to model systems ranging from molecules to crystals. It provides the ability to calculate a wide range of material properties including total energy, relaxed crystal structure, phonon dispersion, and charge distribution.

PWscf (www.pwscf.org): PWscf is an ultra-soft pseudopotential electronic structure that can calculate a variety of physical properties. In addition, since this code takes advantage of ultra-soft pseudopotentials, it is also one of the fastest plane-wave codes available. Some of the properties that can be calculated include ground-state energy, atomic forces, molecular dynamics, nudged elastic band, phonon frequencies, and electron-phonon interaction coefficients for metals.

LM Suite: This all-electron first principles code, developed primarily by Mark van Schilfgaarde (ASU), describes systems using a linear muffin tin orbital approach. For closed packed systems, this leads to very efficient calculations for large systems (> 100 atoms). In addition this code has the ability to include spin-orbit coupling and noncollinear spins, making it ideal for calculations of magnetic systems. The addition of a fully non-equilibrium Green's function branch of the code now makes it possible to study electronic transport in nanoscale devices. A GW branch of the code is also available.

CPMD (www.cpmd.org): This code can be used to perform ab-initio molecular dynamics. It provides a wide range of features include time-dependent DFT, wavefunction optimization, and path integral molecular dynamics.

MIT Photonics Bands (ab-initio.mit.edu): The program allows you to calculate the photonic band structure of periodic dielectric structures. This is ideal suited for modeling photonic crystals, wave guides, and resonant systems.
Calculations can be performed in both serial and parallel modes on the cluster.

UTQUANT: This program is a quasi-static CV simulator for one-dimensional silicon MOS structures.

PARSEC (PARSEC website): This program provides users with ability to solve the electronic structure of confined systems such as clusters, molecules, and quantum dots by using a real space approach. The current version can calculate forces and is capable of performing ab-initio molecular dynamics studies, including simulated annealing

A more comprehensive listing is available on this page.

Loading Environments for Using Codes:

The Cluster makes use of the Modules package for loading and unloading environment variables allowing use of the various installed codes. Modules can have dependencies on other modules. Depending on how you fire off your cluster job, you may wish to include the module loading commands either in your cluster script or in your shell environment.

Submitting Jobs to the Cluster:

Information on the new job submission system for the cluster can be found here.

DO NOT RUN JOBS OUTSIDE OF THE BATCH SYSTEM

Additional Resources:

- NNIN/C Pseudopotential Virtual Vault