High Performance Modeling through the NNIN

http://www.nnin.org

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Modeling across the NNIN
The National Nanostructure Infrastructure Network (http://www.nnin.org)

- **Computational mission**: Develop modeling resources that complement and expand on the current experimental capabilities.
- Development of new computing clusters.
- Acquisition of commercial software packages.
- Construction of new codes to address user needs.
- Expansion and distribution of localized programs to user network.
- *Web based access – truly remote research*
Computational Resources available across the country

- **Computing Power**
  - **Cornell Nanoscale Facility**
    - 48 node dual processor Xeon (3.06 GHz) cluster
    - 16 AMD 64 bit Opteron workstations
  - **Harvard University**
    - 48 node dual processor Xeon (3.06 GHz) cluster
    - 4 4-way 32 GB Opterons from Sun Microsystems (coming soon!)
  - **University of Texas, Austin**
    - Access to 600 processor Xeon cluster
    - 224 (1.3 GHz) Power4 processor cluster
  - **Stanford and University of Michigan** (resources coming soon!)
A Platform for more than just computation…

Services to encourage collaboration and enhance existing tools.

- Web based discussion groups that allow new users to learn from existing users.
- A conduit for codes developed by localized groups to reach a larger audience (beta testing, optimizing, streamlining)
- Creation of input file libraries for different programs
The Right Tools for the Job
(developing high performance codes)

- **Scientific Libraries:**
  - **ATLAS:** self optimizing numerical library built on LAPACK and BLAS routines
  - **GSL:** Open source numerical routines for C/C++
  - **FFTW:** Fastest fourier transform in the West!
  - **MKL:** Intel’s LAPACK and BLAS libraries optimized for Xeons

- **Compilers**
  - Native Gnu compilers (gcc, g77, and g95 *(experimental)*)
  - Intel compilers for C/C++ and Fortran

- **Parallel Libraries**
  - **LAM-MPI:** message passing protocol ([http://www.lam-mpi.org](http://www.lam-mpi.org))
  - **PVM:** parallel virtual machine (to be installed)
Programs for everything nanoscale...

- **Electronic Structure**
  - Abinit
  - LM Suite
  - HARES
  - PARSEC

- **Quantum Chemistry**
  - NWChem
  - ANEBA

- **Device Design Tools**
  - Silvaco
  - Cadence
  - Cats
  - TOMCAT

- **Nano Transport**
  - LM Suite
  - SEMC-2D
  - SETE

- **Molecular Dynamics**
  - CPMD
  - EDIP

- **Nano photonics**
  - MIT Photonic-Bands

- **NNIN Network**
  - LM Suite
  - SEMC-2D
  - SETE
First principles pseudo-potential code (plane wave basis)

- Model molecules, crystals, surfaces, and interfaces.
- Optimize crystal geometry
- Find total energy, charge density, phonon dispersion, and more...
- Open project – source code freely available, large user community, and online resources
ABINIT – (10,0) Carbon Nanotube

Charge density cross-section of a (10,0) carbon nanotube.

Band diagram for (10,0) carbon nanotube.
LM Suite (Linear Muffin Tin Orbital)

- All electron first principles code (localized orbitals) developed by Mark van Schilfgaarde and many others.

- Features:
  - Full potential and atomic sphere approximation (ASA) versions available
  - Non-collinear spins and spin-orbit coupling
  - Non-equilibrium transport calculations
  - GW branch available to correct for the local density approximation (LDA) band-gap problem.
Spin Polarized Tunneling from Co surface (LM Suite)

- Tunneling from oxidized and unoxidized Co surfaces to Al probe.

- Oxygen monolayer on Co flips the spin polarization of tunneling from negative (minority carriers) to positive (majority carriers).

**Figure:** $k$ resolved transmission from clean (111) Co for (a) majority and (b) minority carriers and from oxidized Co for (c) majority and (d) minority carriers. Units $10^{-11}$ for (a,b) and $10^{-14}$ for (c,d).

Belashchenko et al., PRB, 69, 174408 (2004)
Molecular Electronics with the LM Suite

Benzene dithiol (BDT) between gold leads

Photonic Bands (MIT)

Calculates the band structure and EM modes for photonic crystals, waveguides, and resonator systems.

Collection of Dielectric Rods in Air

Electric Fields for TM fields in the photonic crystal (red high, blue low)

TM Band 1

TM Band 3

TM Band 5
Parallel Calculations with LAM-MPI

MIT Photonic Bands calculation –
triangular lattice of air holes in dielectric slab

![Graph showing calculation time vs. number of processors](image-url)
What programs do you need?
(Programs under consideration)

- **PWscf** — open source plane wave code that takes advantage of ultra-soft pseudopotentials

- **Transiesta-C** — well developed program for modeling transport in devices ranging from nanotubes to multilayers

- **ATAT** — automated cluster expansion package that generates phase diagrams from *ab-initio* calculations.

- **DFT++** — plane wave and wavelet first principles code, could wavelets help to model transport in open systems?
Getting Started!

- Become a NNIN user:
  - Contact a representative at one of our sites
    - Michael Stopa (Harvard) stopa@deas.harvard.edu
    - Derek Stewart (Cornell) stewart@cnf.cornell.edu
    - Zhiyong Zhang (Stanford) zyzhang@stanford.edu
    - Sanjay Banerjee (U. of Texas, Austin) anupam@uts.cc.utexas.edu
  - Get an account set up at your site.
  - Start running jobs.
    - Assistance is available for porting codes to the cluster.
    - In special cases, research staff can develop new code components to address user needs.
    - Web-based programs and tutorial sessions possible in the future to reduce the learning curve.
Conclusions

- Computational resources (cluster, workstations) at the NNIN are available to assist in your research.

- The NNIN will help in moving codes from a localized setting (i.e. single research group) to a network wide distribution.

- Training and tutorials will be available to help reduce the learning code
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