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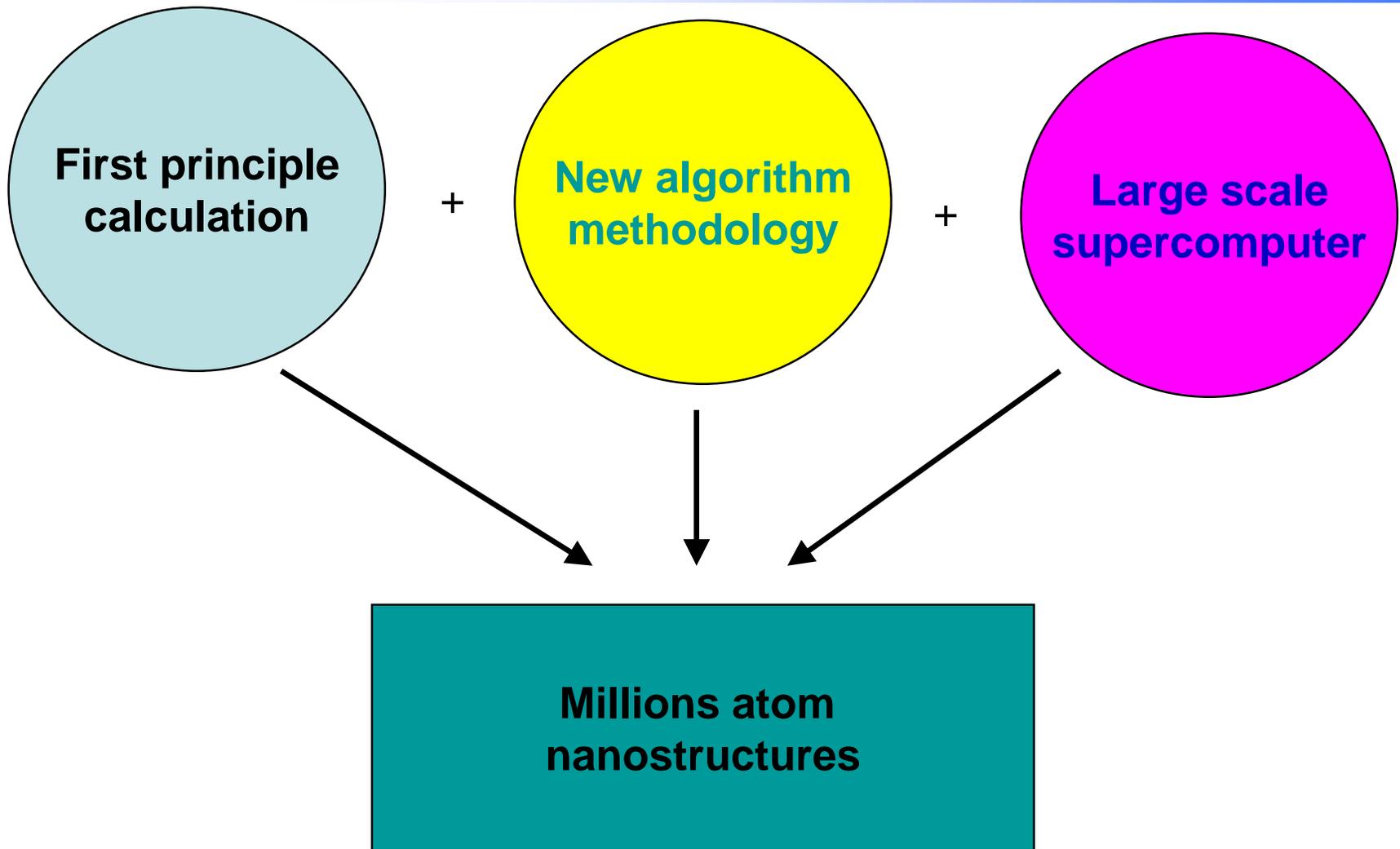
# Computational Nanoscience Activities at Berkeley Lab and at NERSC

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and Lin-Wang Wang  
November 18, 2003  
<http://www.nersc.gov/~simon>





# NANOSCIENCE COMPUTATION



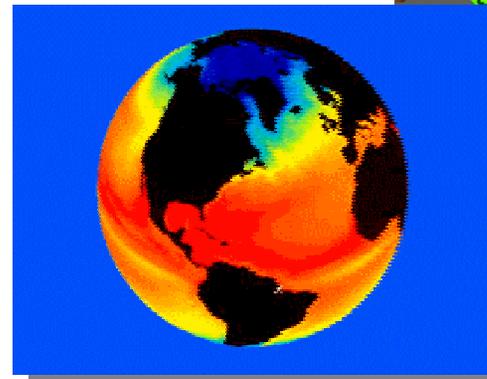
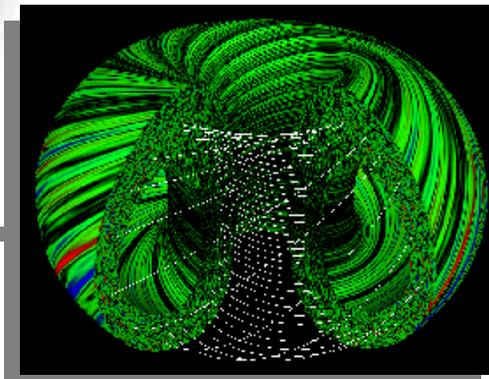
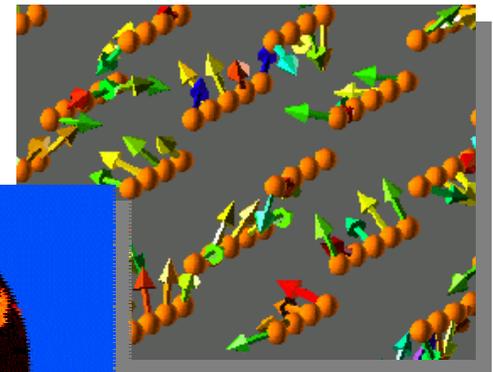
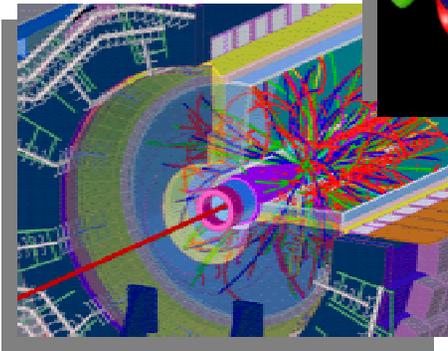
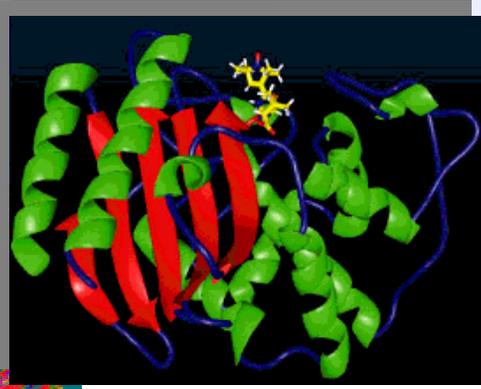


# National Energy Research Scientific Computing Center

- Serves all disciplines of the DOE Office of Science

• ~2000 Users in ~400 projects

- Focus on large-scale computing





## Upgraded NERSC 3 (Seaborg) Characteristics

- The upgraded “Seaborg” system has
  - 416 16-way IBM Power 3+ nodes with each CPU at 1.5 Gflop/s
    - 380 for computation
  - 6,656 CPUs – 6,080 for computation
  - Total Peak Performance of 10 Tflops
  - Total Aggregate Memory is 7.8 TB
  - Total GPFS disk will be 44 TB
    - Local system disk is an additional 15 TB
  - Combined SSP-2 is greater than 1.238 Tflop/s
  - NERSC 3E is in full production as of March 1, 2003



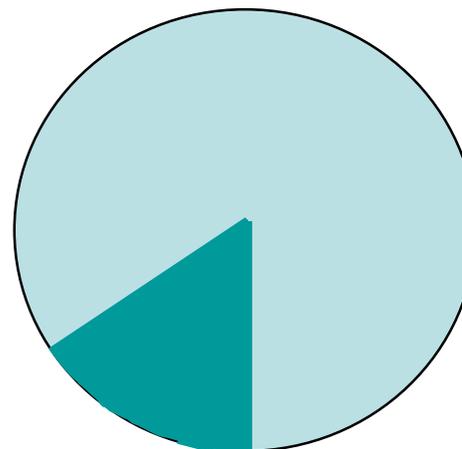


# Material Science Computer Time Allocation at NERSC

**NERSC computer time allocation**

~16% for material science

~ 6Million hours for FY02

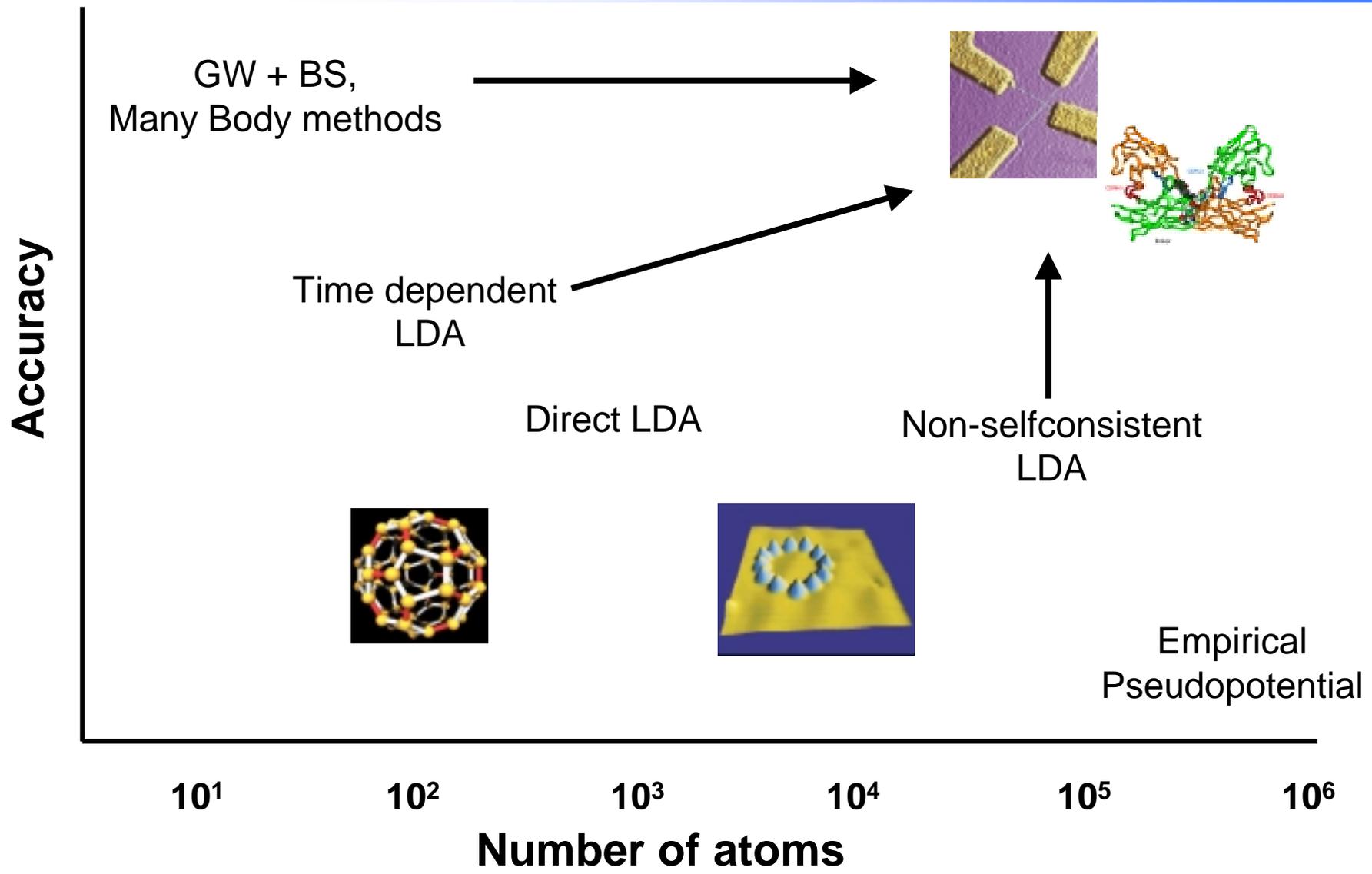


## MPP allocation breakdown

	Num	time	percentage
<b>total</b>	<b>46</b>	<b>5.92M</b>	
<b>DFT electronic structure</b>	<b>34</b>	<b>5.06M</b>	<b>85%</b>
<b>classical MD or MC</b>	<b>8</b>	<b>0.74M</b>	<b>13%</b>
<b>other</b>	<b>4</b>	<b>0.12M</b>	<b>2%</b>

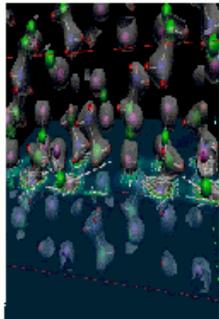


# Methods Landscape

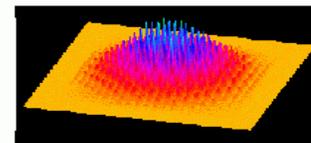
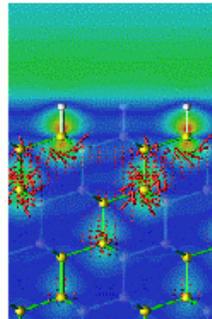




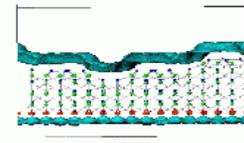
# Software at NERSC: Paratec and PEtot planewave LDA codes



## PARAllel Total Energy Code



## PEtot's Homepage



### What is PEtot ?

PEtot stands for parallel total Energy (Etot). It is a parallel plane wave pseudopotential program for atomistic total energy calculation based on density functional theory. It is designed for large system simulations to be run on large parallel computers like Cray T3E and IBM SP machines at NERSC. It is developed under U.S. Department of Energy fundings and it is a freely distributed public source code. It has a GNU license, which means that you can use it and change it for noncommercial purposes. However, we will not be responsible for any potential problems it might cause directly or indirectly due to the running of this code.



### Download the PEtot Package (source files)

Double click to download PAR.ETOT.tar.gz (0.5MB)



#### History and features of PEtot

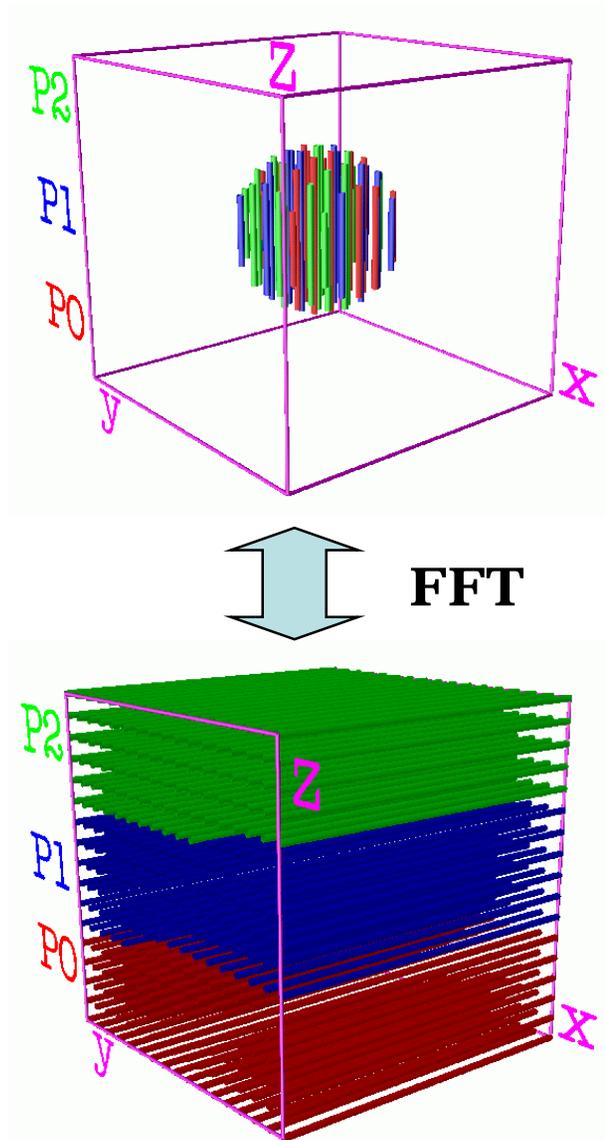
- How to run PEtot
- Basic concepts for DFT calculations
- Basic program flowing chart

[www.nersc.gov/projects/paratec](http://www.nersc.gov/projects/paratec)

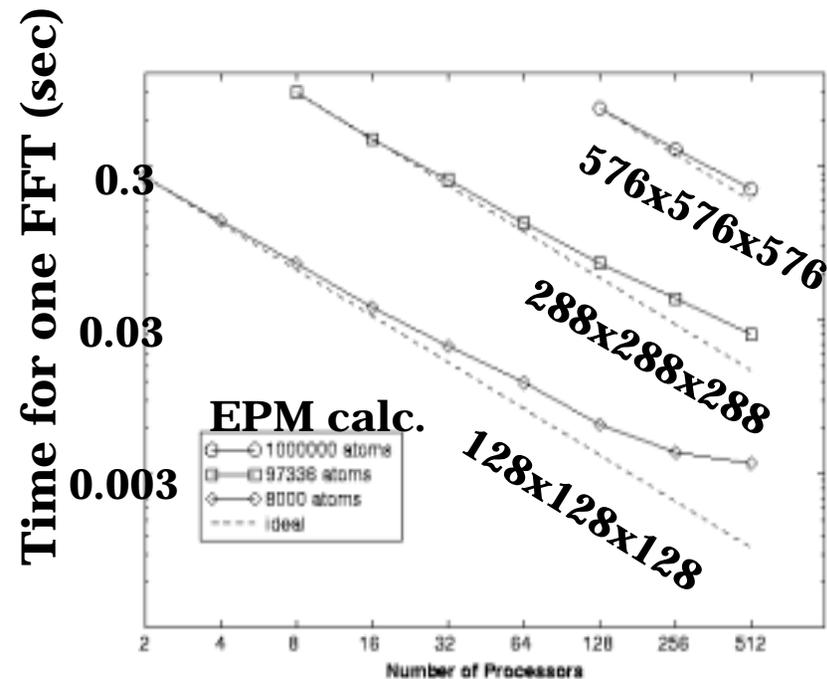
[crd.lbl.gov/~linwang/PEtot/PEtot.html](http://crd.lbl.gov/~linwang/PEtot/PEtot.html)



# Paratec Kernel: A parallel Fast Fourier Transformation code



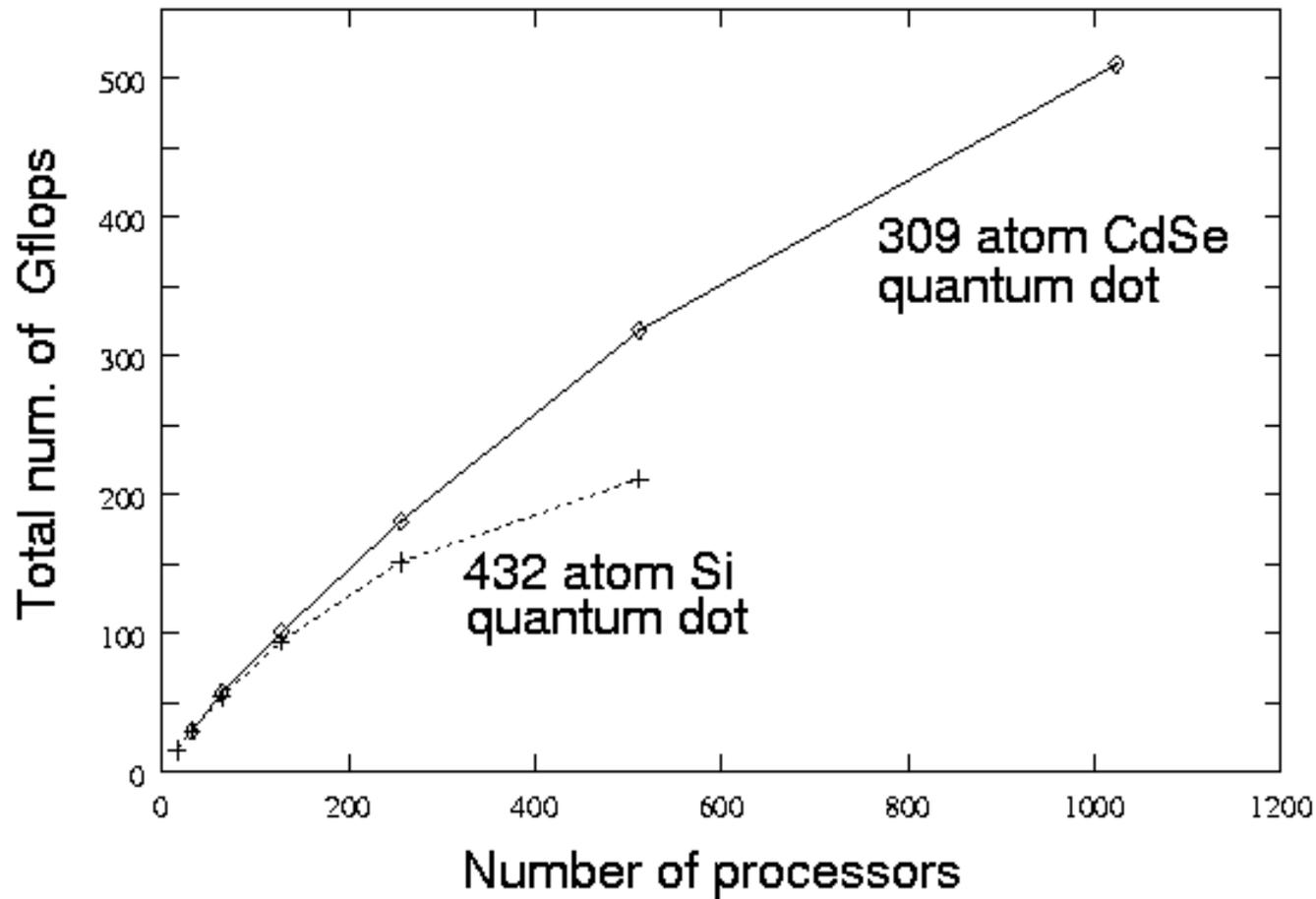
- Specially designed for PW elec. structure calculation.
- Work load balance
- Memory balance
- Minimum communication





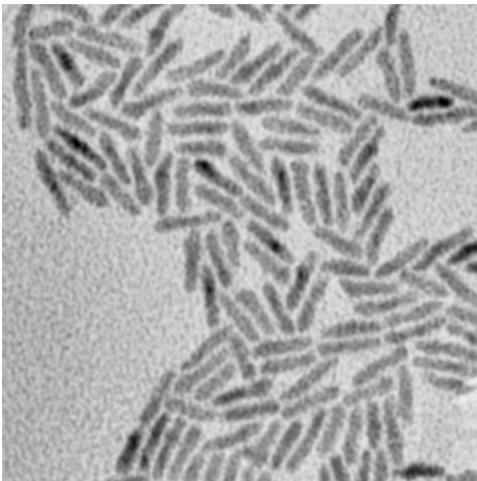
# PARATEC performance

PARATEC performance on Seaborg

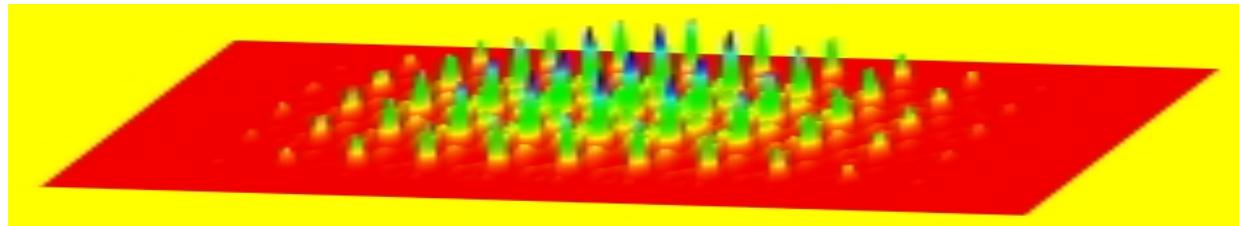
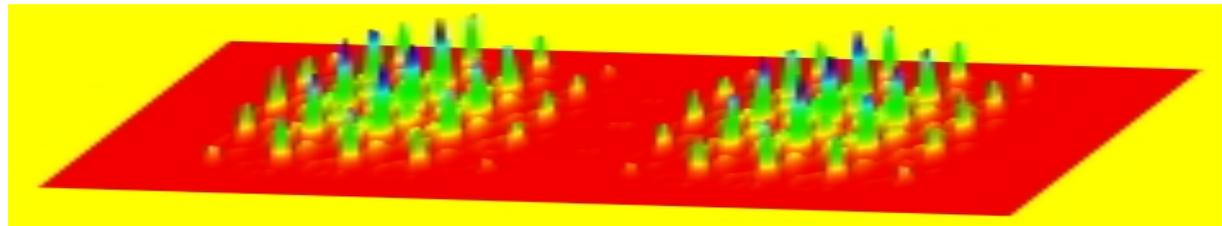




## Polarization of CdSe quantum rods



**CdSe quantum rods**

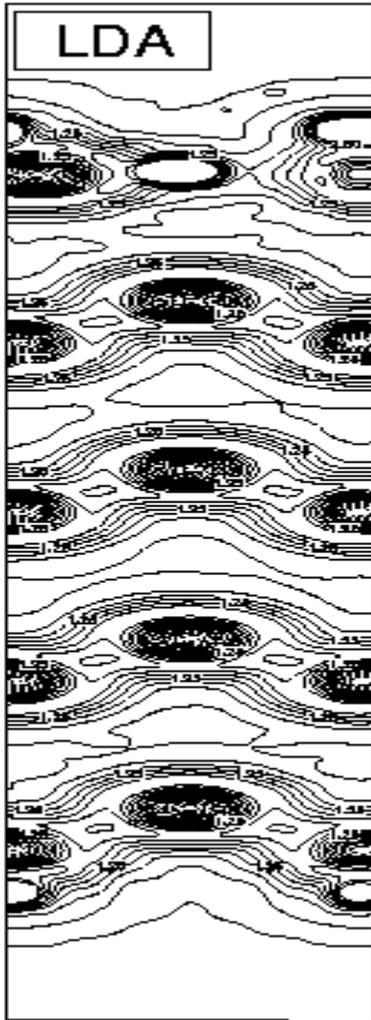


**The electron wavefunctions of a quantum rod**

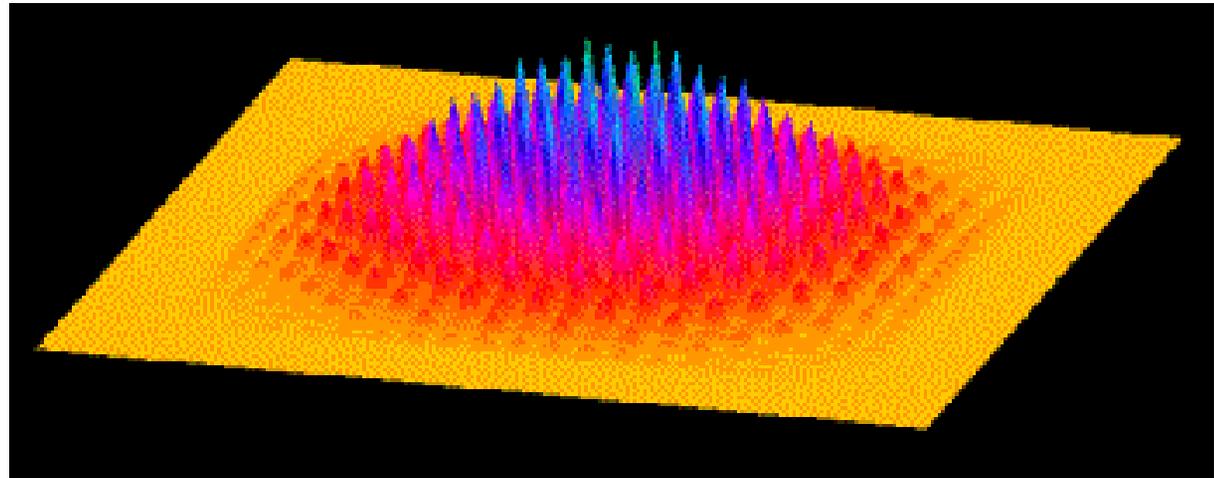
- The electronic structures and optical properties change with the shape of the quantum rods.
- The thousand atom quantum rods can be calculated using the planewave pseudopotential method and the NERSC supercomputers.
- Programs exist at NERSC to calculate such nanosystems and compare with experimental electronic and optical results.



## Potential $V(r)$

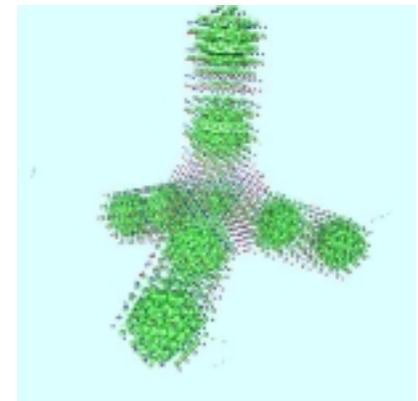
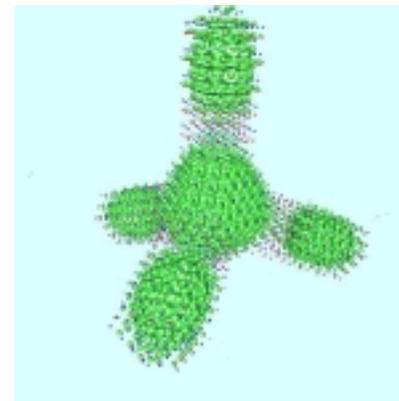
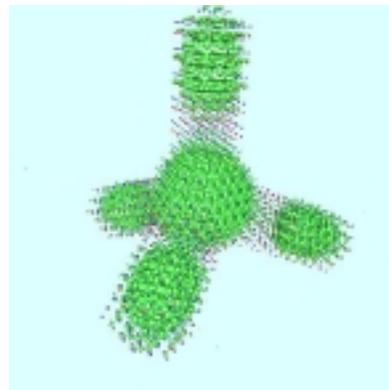
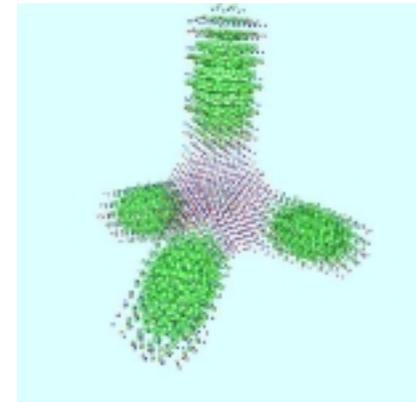
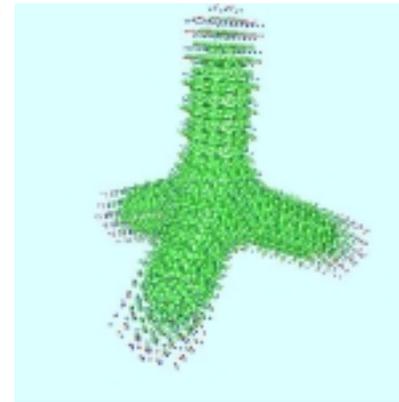
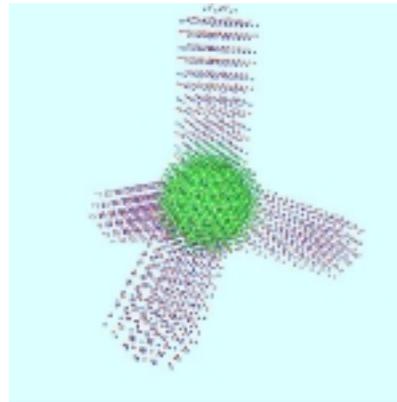
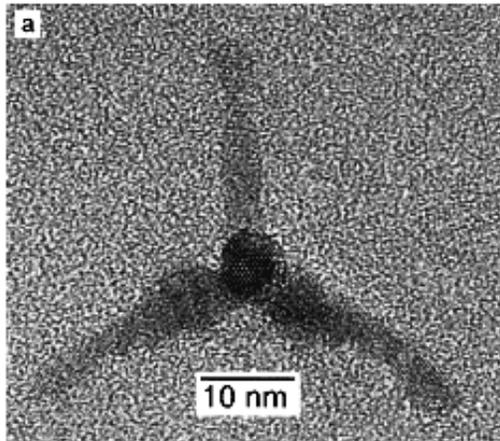


## Wavefunction $\psi(r)$





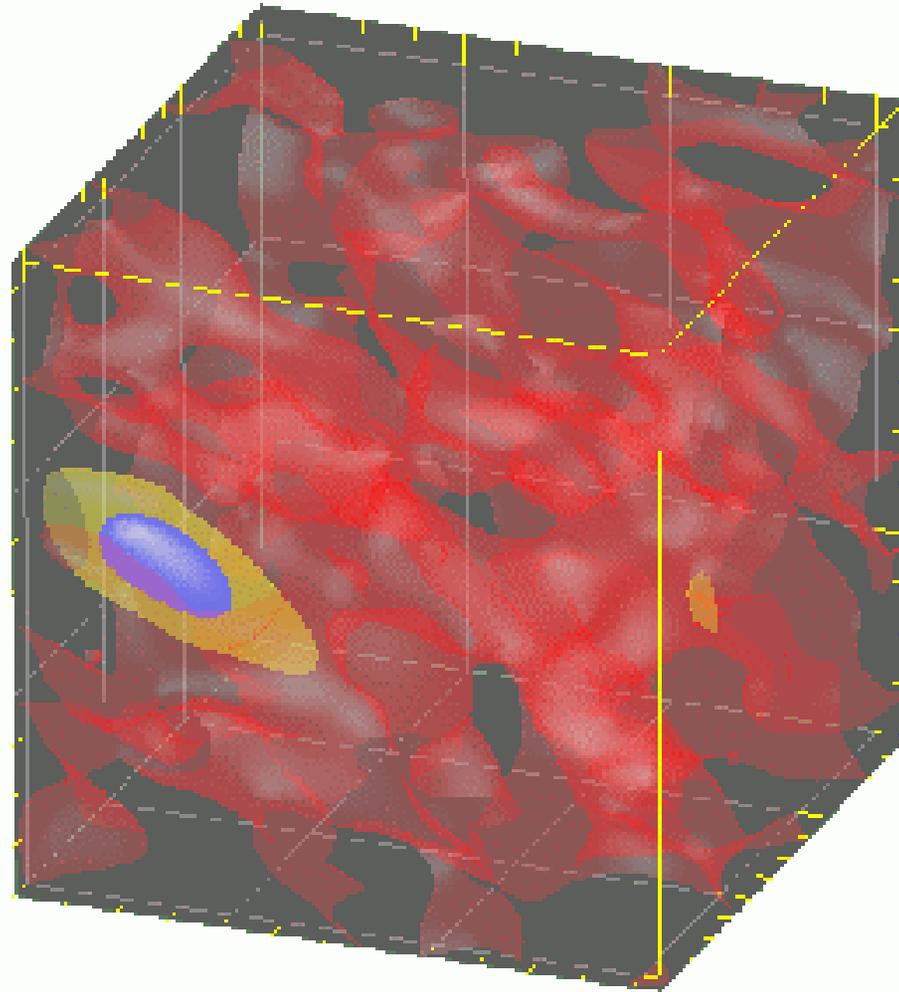
# CdSe tetrapod conduction band wavefunctions





ERSC

# 2 million atom GaAlAs alloy wavefunction





# Computer requirement priorities

- (1) Fast memory access**
- (2) Communication band width (for large processor count)**
- (3) Communication latency**
- (4) Vectorization**
- (5) Homogeneous architecture (don't want too many layers, most people just use MPI)**
- (6) Synchronous calculation**

**Processor speed and the total number of processors**



# Mathematical challenges in nanoscience

- **Numerical Linear Algebra**
  - Scalable linear solvers
  - Large eigenvalue problems
  - Interior eigenvalue problems
- **Global and Local Optimization**
  - Misfit between experimental (noisy) data and a computer model
  - Geometric potential energy surfaces: minima, saddle points, reaction paths
  - Expensive cost functions with many local minima - derivatives not usually available analytically
- **Multiscale algorithms**
  - Need to span many spatial and temporal scales



# Molecular Foundry Status

- Design approved by Regents, April 2003
- Successful independent external review completed, June 2003
- Budget:
  - \$6.8M for FY 2003
  - Total project cost: \$85M



# Molecular Foundry

2003

2004

2005

2006

2007

2008

2009

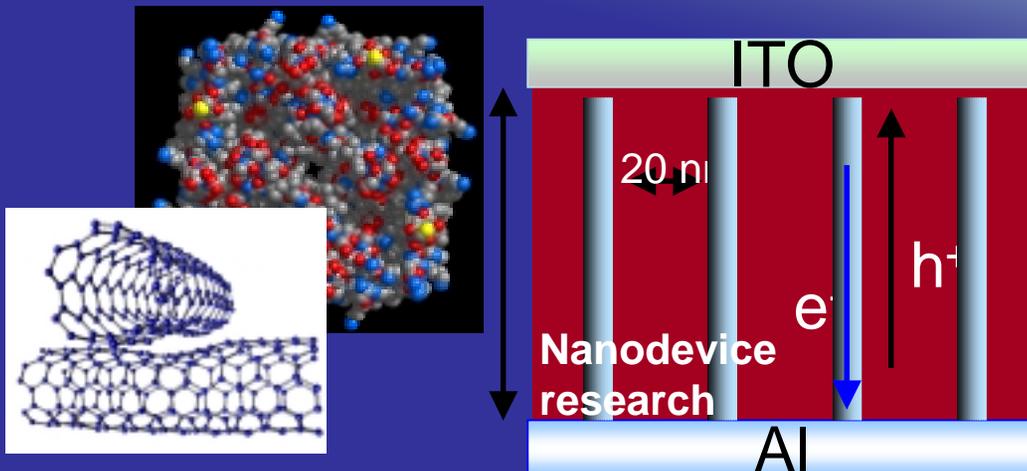
Engineering design  
and start construction

Conventional  
facilities  
complete

Molecular  
Foundry  
begins  
operation

Nanomaterials  
and component  
design and  
fabrication

Hire scientific staff and ramp up user program





# Molecular Foundry and Computation

- **Theory and Simulation Program at MF**
  - **Large Scale Cluster for MF in 2005**
  - **NERSC access for MF users**



# NANOSCIENCE COMPUTATION

