

Computational Center for Nanotechnology Innovations

Rensselaer Polytechnic Institute




CCNI COMPUTATIONAL CENTER for NANOTECHNOLOGY INNOVATIONS

A computational and research center dedicated to nanotechnology innovations

A University/Industry/State Partnership







CCNI COMPUTATIONAL CENTER for NANOTECHNOLOGY INNOVATIONS

Computational Systems


- 100 teraflops of heterogeneous computing

Allocation of resources

- Founding partners receive 20% each
- 40% allocated for Industry Members

CCNI Locations

- Rensselaer Technology Park - main system
- Rensselaer Campus - CCNI machine room



Computing Systems

Blue Gene/L System

- 16 rack IBM Blue Gene/L - 32,768 cores
- 12 TB of memory total

Blade Server Cluster

- 462 IBM LS21 blades - 1,848 Opteron cores
- 5.5 TB of memory total
- 4X InfiniBand interconnect (10 Gbps)

File System



- 832 TB of raw disk storage - IBM General Parallel File System
- 52 IBM x3655 file server nodes

AMD and Intel SMP Servers

- 40 IBM x3755 servers - Each with 8 Opteron cores and 64 GB
- 2 IBM x3755 servers - Each with 64 Opteron cores and 128 GB
- 2 IBM x3950 servers with Xeon processors
 - One with 64 processor cores and 128 GB
 - One with 32 processor cores and 256 GB
- All with 4X InfiniBand interconnect


Power SMP Server IBM p590

- 16 Power 5+ processors and 256 GB

CCNI Rensselaer Tech. Park Facility

4500 sq. ft. machine room



CCNI Connectivity

Local fiber: CCNI/campus/NYSERNet

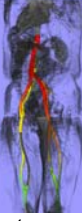
State

International

Modeling and Simulation at Rensselaer

Long history of collaboration with industry

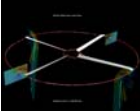
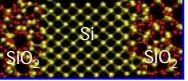
- Scientific Computation Research Center
- Center for Automation Technologies and Systems
- Rensselaer Nanotechnology Center
- Inverse Problems Center
- Center for Biotechnology and Interdisciplinary Studies
- Center for Integrated Electronics
- Center for Multiphase Research
- Multiscale Science and Engineering Center
- Center for Pervasive Computing and Networking



Current Rensselaer CCNI Research

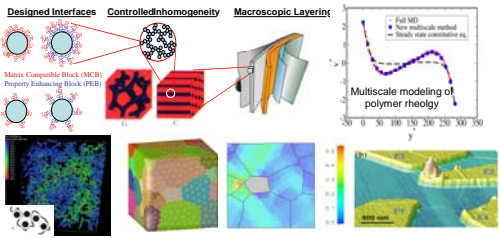
Partial List

- Nanoelectronics modeling and simulation
- Modeling of nano-material structure and behavior
- Quantum chemistry
- Modeling of complex flows
- Computational biology
- Protein engineering
- Biomechanical system modeling
- High energy physics
- Economic Dynamics
- Multiscale methods
- Parallel simulation technologies

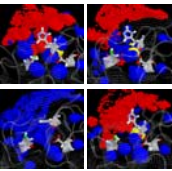
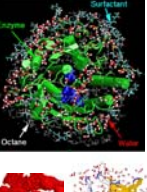
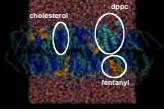
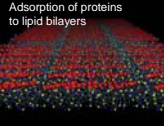
Nano-Material Structure and Behavior

- Mechanics and synthesis of nanostructures
- Modeling polycrystalline materials
- Modeling of nanostructured polymer rheology



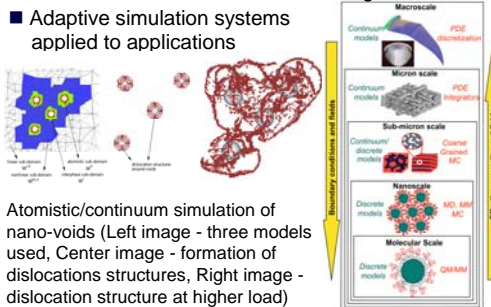
Computational Biology

- Protein structure and interactions with small molecules
- Modeling cellular processes and communities of cells
- Membranes and membrane protein structure and function

Multiscale Modeling

- Multiscale mathematics and modeling
- Adaptive simulation systems applied to applications



Atomistic/continuum simulation of nano-voids (Left image - three models used, Center image - formation of dislocations structures, Right image - dislocation structure at higher load)

CCNI Industrial Members Program

Benefits

- Use of the computing capabilities
- Access to the facilities and people
- Research activities and results

Focused on industry memberships

- Provide a full range of support for CCNI industry members
- Jointly defining IP policies

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