Cyberinfrastructure-Enabled Petascale Computing for Nanotechnology (cPCN)

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CI-driven Computing in Multi-disciplines

- Exciting field with many potential applications
- Significant potentials
- Great opportunities and funds
- Broader impacts in not only in materials science, but also in engineering, electronics, medicine and other disciplines.
- Challenge in multi-disciplinary knowledge

Definition

- Used to create novel nano-scale materials and devices (nano-systems) with special structures, functions, computation, and/or simulations are extremely important.
- Large-scale computations play an important role in mathematical modeling and the simulation of nano-systems.

Definition

- There are many numerical approaches.
  - For example, Molecular Dynamics (MD) is one of remarkable and effective numeric methods for elucidating complex physical phenomena, simulating nano-devices, studying nanostructures' physical/chemical/mechanical properties, and predicting materials' properties
  - Spatial size with a cubic volume of 1 μm^3 contains trillions of atoms (10^{12})
  - Temporal time-step in an MD simulation is about one femto-second ($\sim 10^{-15}$s)

Remain Unsolved Issues

- The current HPC-based computations for nanotechnology are only at the status of
  - Applications to the principle design of nano-devices
  - Primary exploration of homogeneous nanostructure materials
  - Property predictions
- Complete modeling and simulation of heterogeneous nano-materials <u>have yet to be employed and integrated</u> into enterprise CAD systems due to the insufficient power of computing.

Why CI?

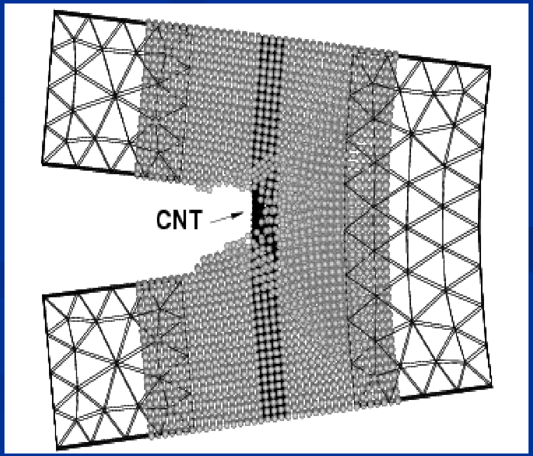
- The cyberinfrastructure-enabled computing will be crucial to the research and development and education in this scientific domain of great potential
- Cyberinfrastructure guides the contemporary scientific and engineering computing
- Stimulates the unprecedented computations in the near future in order to implement a complete multi-scale modelings
- Conduct the corresponding large-scale simulations for 21th century discoveries in nanotechnology

Examples

- There are two examples selected from the current studies of computational nanotechnology and applications at the University of Iowa, which can be used to demonstrate the urgent need of petascale computing systems.

Computing to Couple Different Physical Domains

- Large-scale Parallel Bridging Domain Multi-scale (PBDM) algorithm by decomposing the physical domain into different computational domains
- each of which use different methods, such as an atomic-level MD, for a small cracking region and the Finite Element Method (FEM) for a large-scaled region.
- The computations for Carbon-Composite Nanotube (CNT) (aluminum and carbon atoms) cracking predictions were conducted on NCSA's TeraGrid computing platform to study the CNT's feasibility, applicability and high performance.

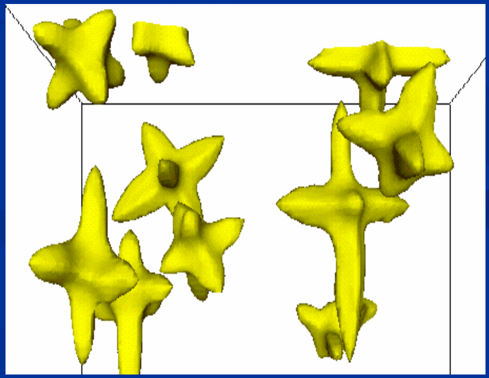


Petascale computing needed

- Although the method is very promising, applying it to practical nano-composites requires up to trillions of atoms.
- Even with a multi-scale model, it is impossible to simulate in any available system at the NCSA.
- This defect raises the demand for a petascale computing system.
- The present primary study will significantly influence the R&D's future in engineering, especially in material science and mechanical engineering systems.

Zone into much small scales

- Study of multi-scale (atomic-microscopic-meso-scopic, macroscopic) mathematical modeling and simulations of nanostructure materials' formation and processing.
- Extension of Ni and Backmann's multi-phase micro-/macroscopic model
  - Developed in the early 1990s



Zone into much small scales

- Considerations of couplings
  - Atomic interactions for nucleation using molecular dynamics
  - Crystallization using nano-scale kinetics
  - Microstructure topology, formation
    Dynamic crystal growth using thermal and species non-equilibrium and interfacial theorems
  - Nano-crystal formations and micro- /macroscopic coupling using thermal sciences and computational fluid dynamics
  - Nano-particles embedded for composing nano-materials using particulate dynamics
  - Final material property predictions based on final microstructure (nano-particle grain size and distribution) such as physical and chemical, mechanical properties

Zone into much small scales

- Very complex and challenging
  - A large number of physical and chemical variables and quantities;
  - Form a huge set of system equations to be solved numerically
  - Such an outstanding simulation requires
    - Petascale-based HPC systems
    - Data intensive computing and other resources
    - Experimental data and data analysis, data mining
- Bottom line is "CI" is a catalyst to ensure the success of this such model and simulation

Conferences

- Recent efforts to promote HPCs for nanotechnology have been made through a couple of – several conferences and workshops, listed here:
  - Computational Nano-Science and Technology (CNST'05) in ICCS05, organized by Jun Ni (UI), Shaoping Xiao (UI), and Jack Dongarra (UTK)
  - HPCNano05, in SC|05, (http://www.hpcnano.org/HPCNano05/), organized by Jack Dongarra (UTK), Jun Ni (UI), Deepak Srivastava (NASA)
  - HPCNano06, in SC|06 (http://www.hpcnano.org/HPCNano06/), organized by Thom Dunning (NCSA), Rupak Biswas (NASA), Jun Ni (UI), Andrew Canning (LBNL)
  - HPCNano07, in SC|07 (http://www.hpcnano.org/HPCNano07), organized by Michael Stopa (Harvard), Gerhard Klimeck (Purdue), Andrew Canning (LBNL), Jun Ni (UI)

Snapshots

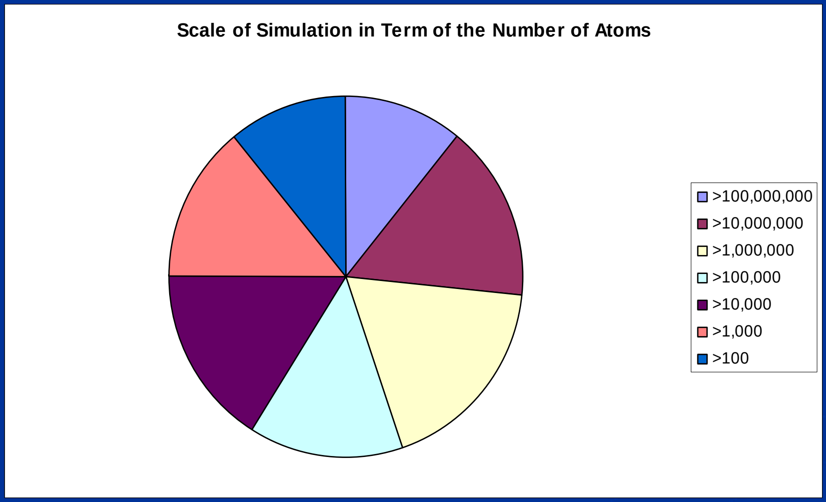
Charlie Catlett of TeraGrid enthusastically explained NSF cyberinfrastructure and NSF TeraGrid resources to support future computing for nanotechnology

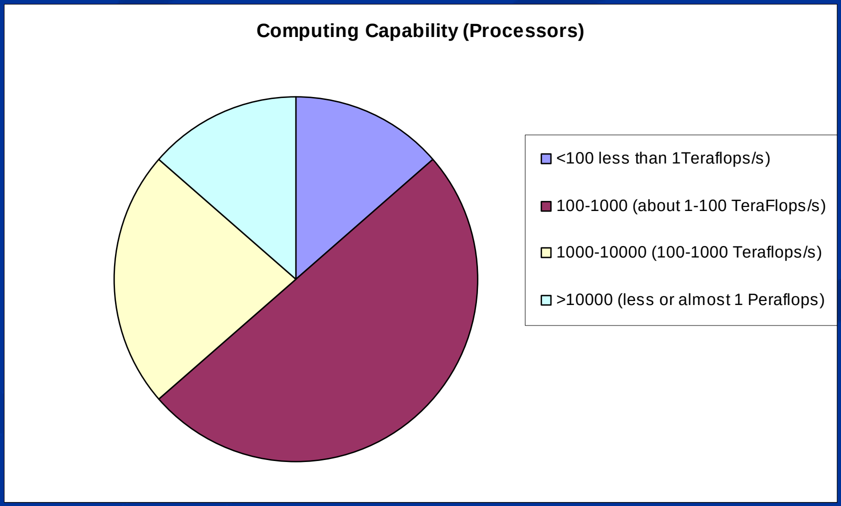
Gerhard Klimeck of Purdue University energetically presented NNI's operation and NanoHub project at Purdue

HPC Survey at SC06

- Message I
  - Survey, conducted by Univ. of Iowa, Boeing, and SGI
  - Results from the survey: that a lack of a petascale computing system creates a major roadblock for researchers.

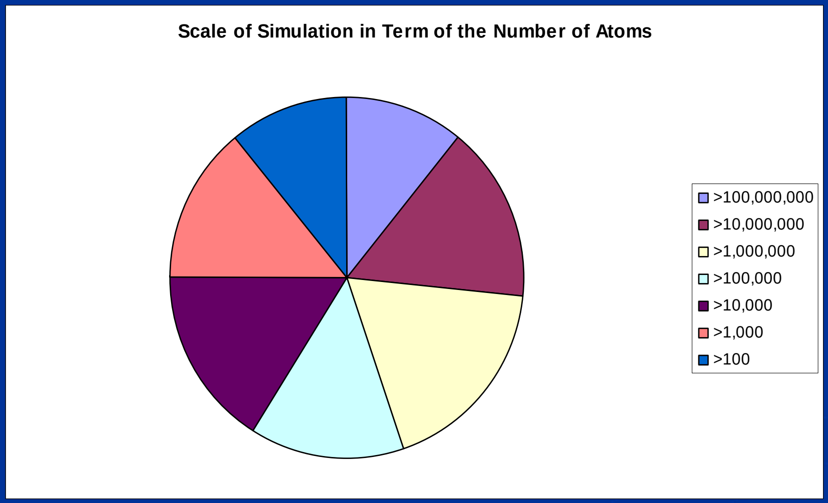
  - According to the results of survey, today's nano-simulations have atoms generally in the 10^2 to 10^9 range. The 22.73% of research institutions require a 100 teraflops to 1.0 peraflops system, while 13.64% of research institutions strongly demand a system bigger than the petascale one.

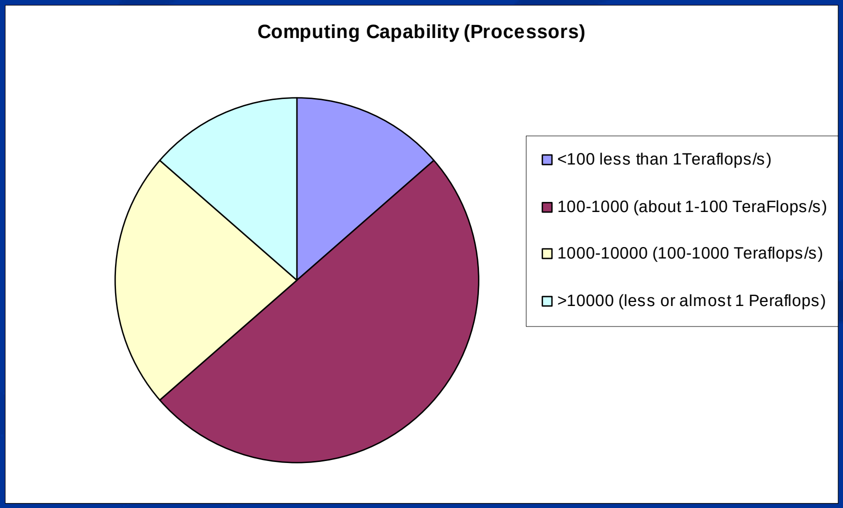




HPC Survey at SC06

- Message II
  - Raise an issue to initiate community to promote HPC computing for nanotechnology in terms
    - New theory
    - Smart and scalable algorithm
    - Parallel implementation and test-ends
    - System architecture and resources
    - Software development
    - Workgroups





Proposal

- Consider to establish a cross-institutional, multi-disciplinary community in petascale computing for nanotechnology
- CI must play a catalytic function to develop a petascale computing capacity for the next-generation of nano explorations
- The brainstorms to form the cPCN

Organization Considerations

- Organizational structure of cPCN
- Affiliation with the GLC organizational dependency;
- Kept its technical independency and close relationship with National Nanotechnology Initiative (NNI)
- The potential, institutional participants (Purdue, NCSA, Cornell, Harvard U., PSC, UTK, NBL, U Iowa, Arizona St. Univ., Louisiana State University, ANL, MIT, Arizona State University, Univ. of Georgia, W. Virginia University, USC, CalTech, Texas A&M University, Virginia Tech., NASA Ames, Penn State University, Brown University, UIUC, University of Kentucky, Georgia Tech., …)
- 5 Committees (computational nanotechnology; parallel computing and computational science; computing facility, and education committee, industrial outreach); define committee's role and functions

Scopes to discuss

- Define major urgent needed large-scale algorithms, test-beds, and benchmark standards.
- Initiate collaborative grant proposals (nano-structured device, nanomaterials formation and processing, bio-nano research and applications, …) to NSF, NIH, DOE, NASA
- The petascale computing facility will be at NCSA's petascael system. NCSA provide system support and consultation servicves
- Organize national conferences and workshops in this domain, like HPCNano05, HPCNano06, HPCNano07, etc.

Scopes to discuss

- Each GLC colleges, universities and research laboratories are involved and participate in the cPCN's activities
- Publish journal papers and books related to petascael computing in nanotechnology
- Develop a network to bridge NNI and GLC through NSF's cyberinfrastructure mission
- Provide training program and workshops around GLC colleges and cPCN members.

Yours?