The Role of Large-Scale Computation and Cyber-Enabled Discovery in Multi-scale Simulations of Nanostructured Materials

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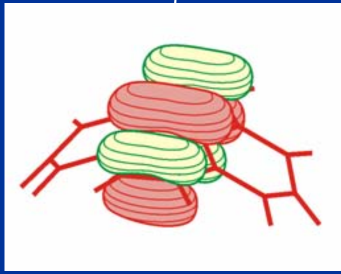
Outline

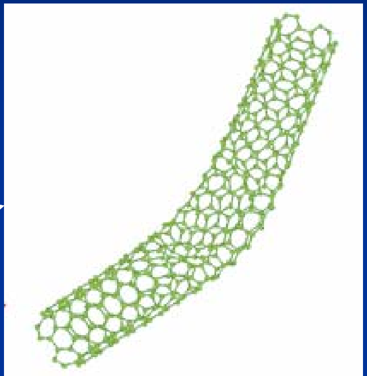
- Introduction to Computational Technology
- Classification of Multiscale Model
  - H-M, C-M, BDCM
  - Examples:
    - nanoscale materials: nanotubes and nanocomposites;
    - nanoscale devices: nano-oscillators
  - H-C-M
- HPC Technologies
- Cyberinfrastructure-enabled computing resource
- Integrated, logical, self-control, computational systems

Physical Multiscales in Spatial Dimensions

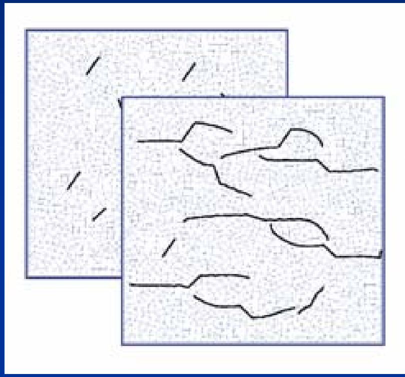


Molecular scale

(10^{-12}m)

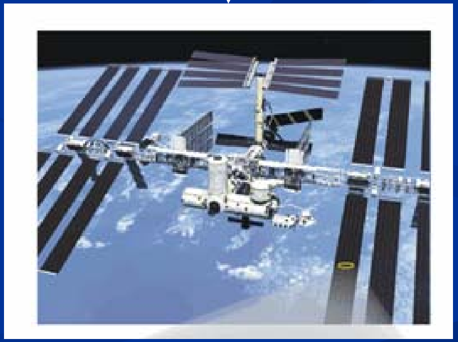


Nanoscale
(10^{-9}m)



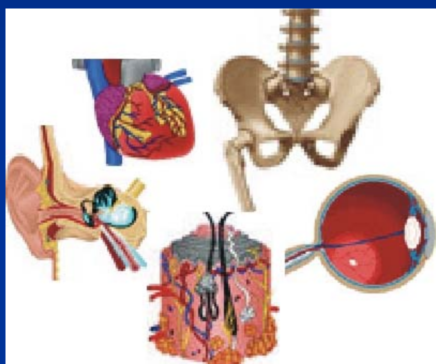
Microscale
(10^{-6}m)

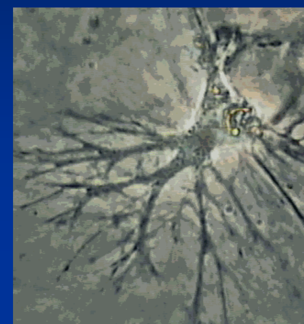
Mesoscale
(10^{-3}m)

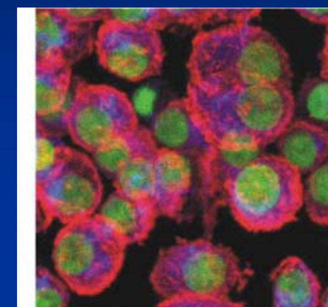


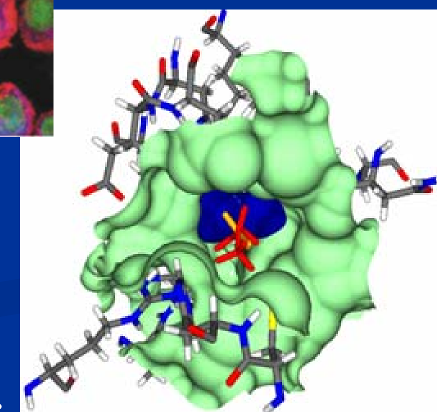
Macroscale
(>1 m)

Biological Multiscales in Spatial Dimensions









Organ systems

Organ (1m)

Tissue (10^{-3}m)

Cell (10^{-6}m)

(10^{-9}m) Protein

(10^{-12}m) Atom

Peter Hunter, University of Auckland

Common Computational Methods:

- Quantum mechanical calculations:
  - First principle calculation
  - Ab initio
  - Etc.
- Molecular methods:
  - Molecular dynamics/mechanics
  - Monte Carlo methods
- Multiscale methods:
  - Hierarchical multiscale modeling
  - Concurrent multiscale modeling

Hierarchical Modeling

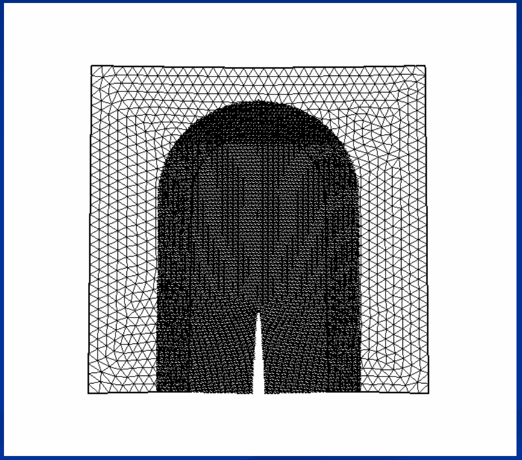
- The continuum approximation is used to model a large group of atoms
  - (Cauchy-Born rule)
- The major drawback is that it is only static without temperature effect
- Examples:
  - Ortiz and Philips of Caltech
  - Klein of Sandia National Laboratory
  - …

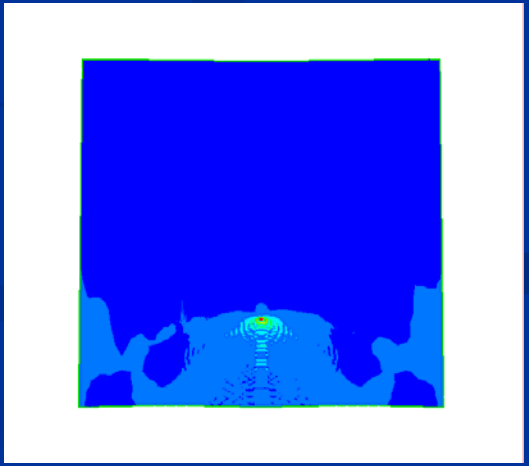
Concurrent Modeling

- Introduced at each length scale simultaneously
- Smooth coupling is implemented between different scales
  - continuum mechanics – for macro elastic media
  - molecular dynamics – for large groups of atoms
  - quantum mechanics – for bonds breaking
- Example:
  - MAAD, Abraham and co-workers at IBM
  - Bridging scale, Liu and co-workers, Northwestern University
  - Bridging domain coupling method
    - Belytschko (Northwestern University) and Xiao (U of Iowa)

Simulation of Crack Propagation in a Nanoplate Using C-M

- The crack is in the molecular domain surrounded by a continuum domain.
- Branching
- Evolution of kinetic energy during crack propagation.
- Since temperature is related to the average kinetic energy at the microscale, the move illustrates that the temperatures around crack tips are high.





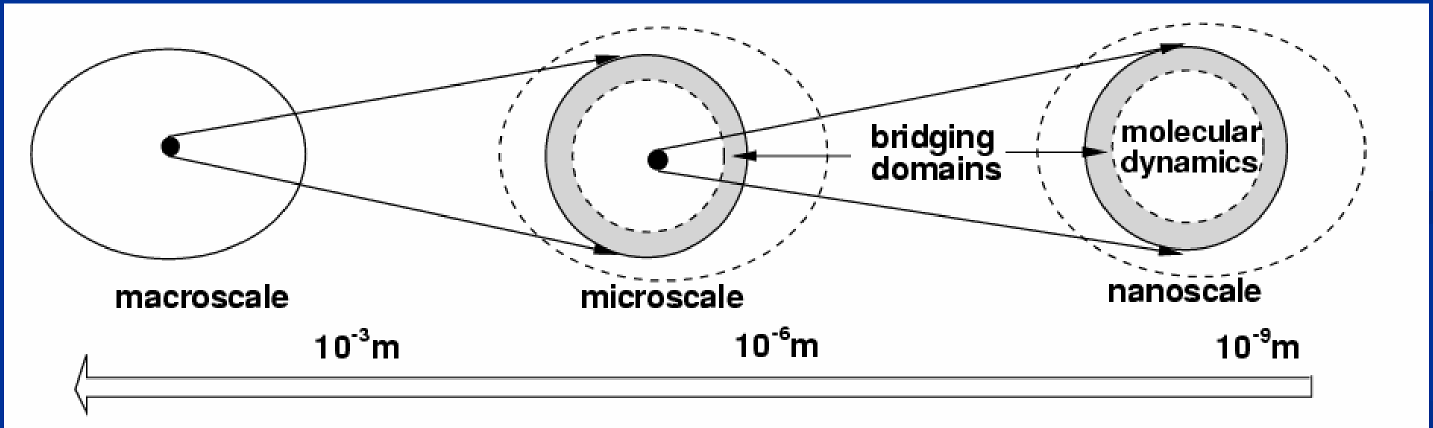
HPC-enabled Multiscale Simulations

- A cubic volume of 10-3 μm^3 contains billions of atoms
- A nano second needs millions of time steps

- Prompt:
  - High-end computing resources
  - Innovative algorithms
  - System computations
    - Robotic computations with logical thinking
    - Resource Rescheduling
    - Monitoring
    - Control
    - Feedback
    - Workflow

HPC-enabled Multiscale Simulations

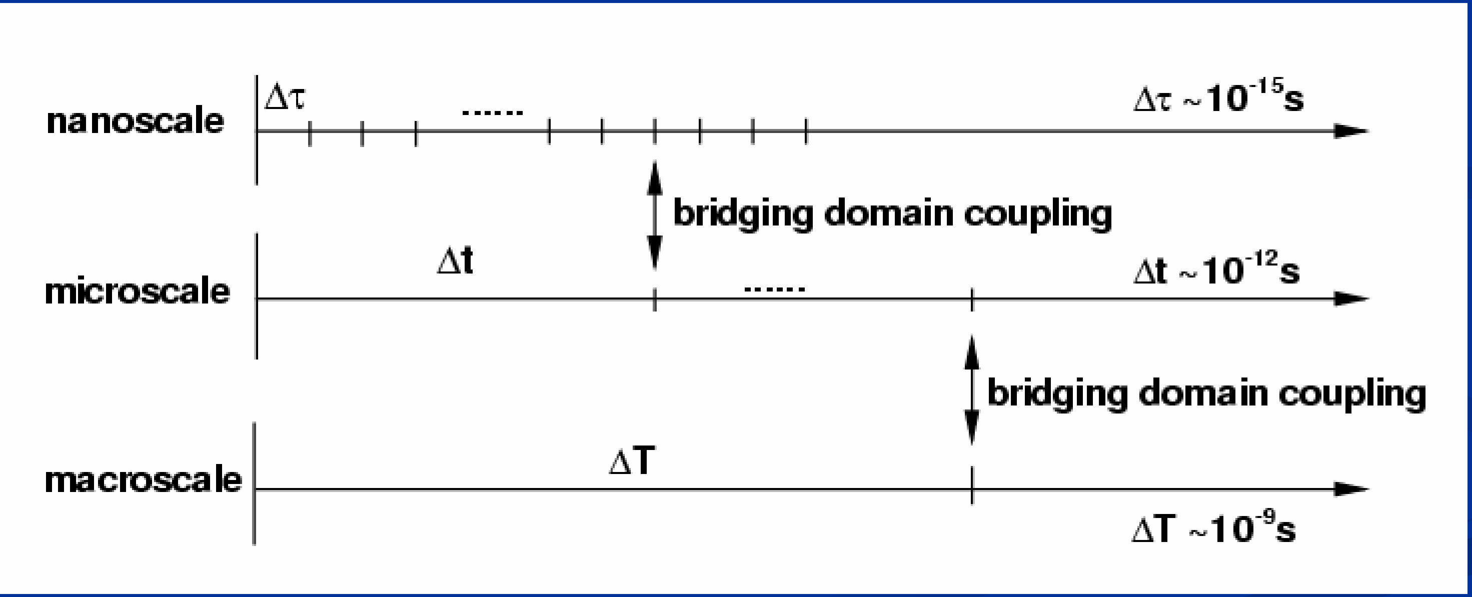
- HPC-based bridging domain multiscale method:
  - Multiple-length-scale model



Macroscale: Linear finite element methods
Microscale: Meshfree particle methods
Nanoscale: Molecular dynamics

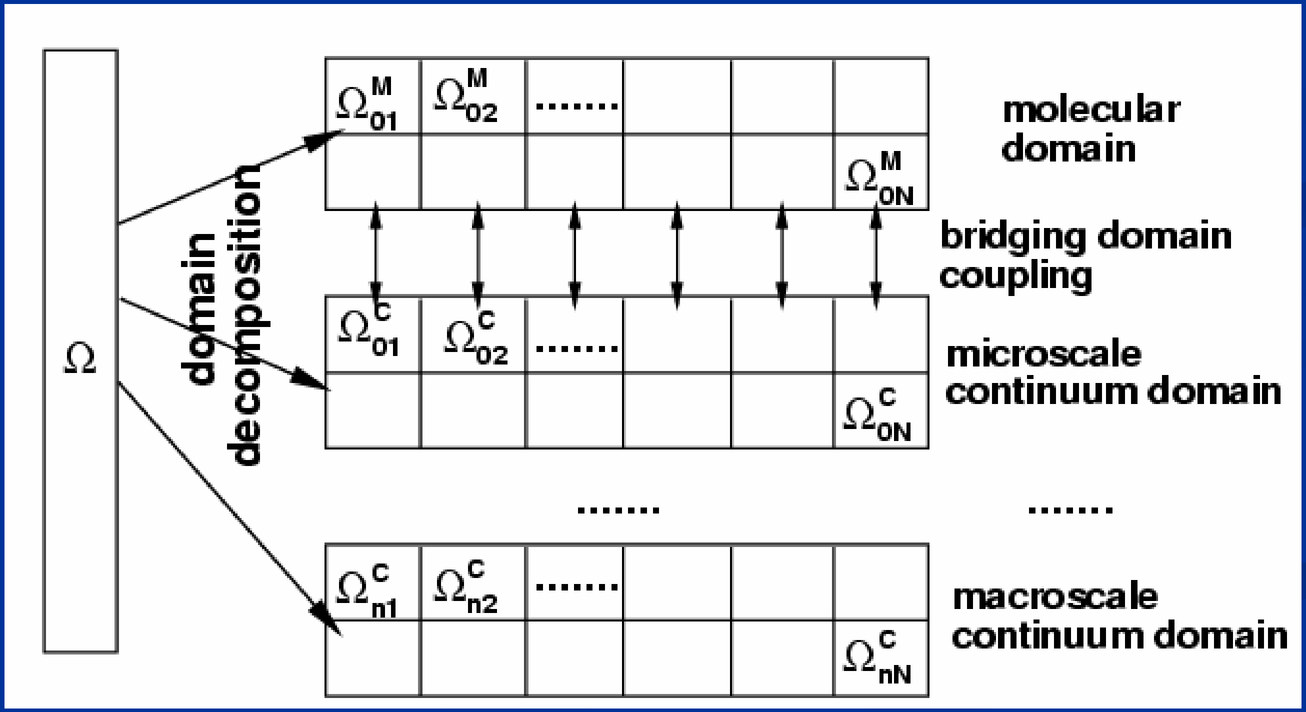
HPC-enabled Multiscale Simulations

- **HPC-based bridging domain multiscale method:**
  - Multiple-time-scale model



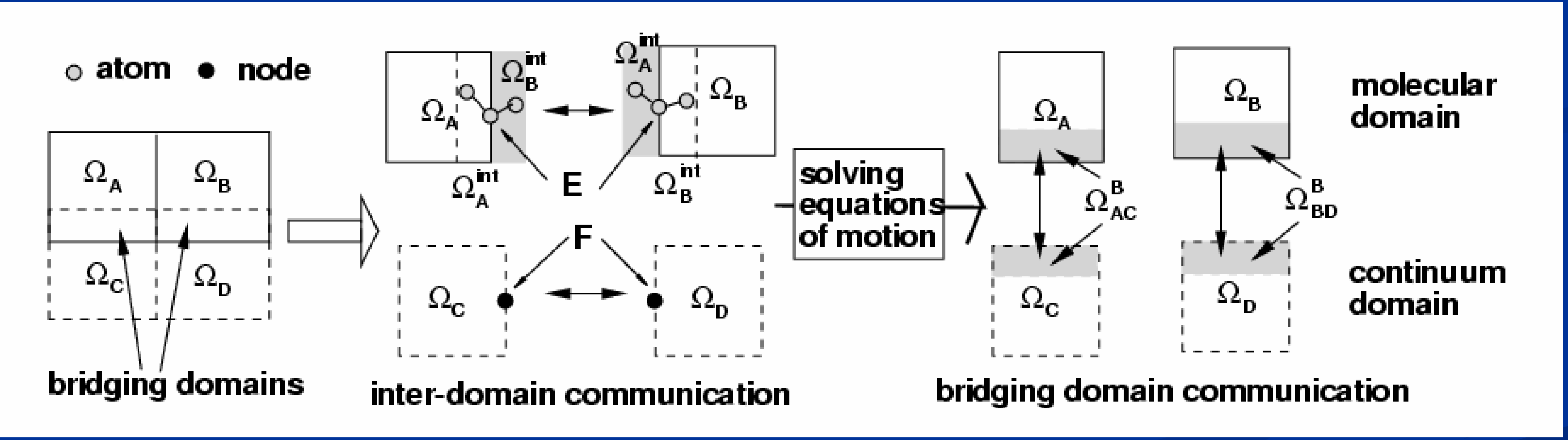
HPC-enabled Multiscale Simulations

- HPC-based bridging domain multiscale method:
  - Domain Decomposition



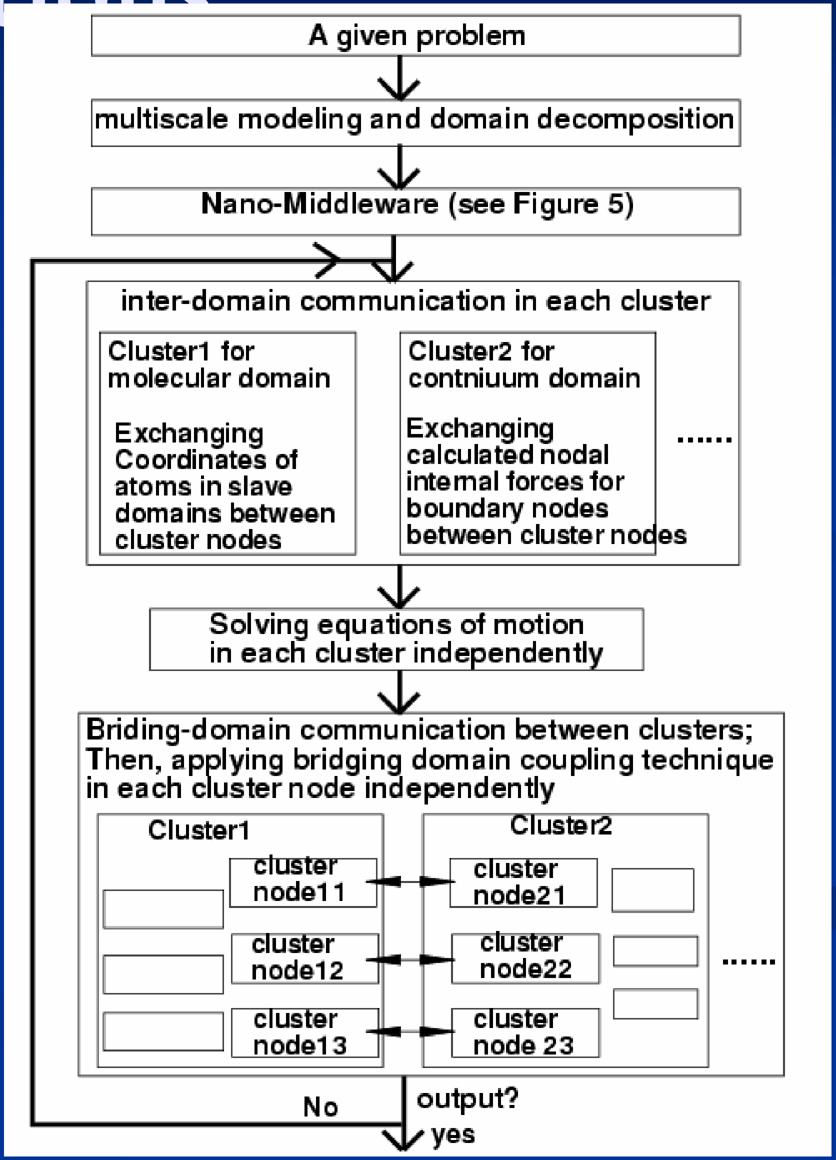
HPC-enabled Multiscale Simulations

- HPC-based bridging domain multiscale method:
  - Communication



HPC-enabled Multiscale Simulations

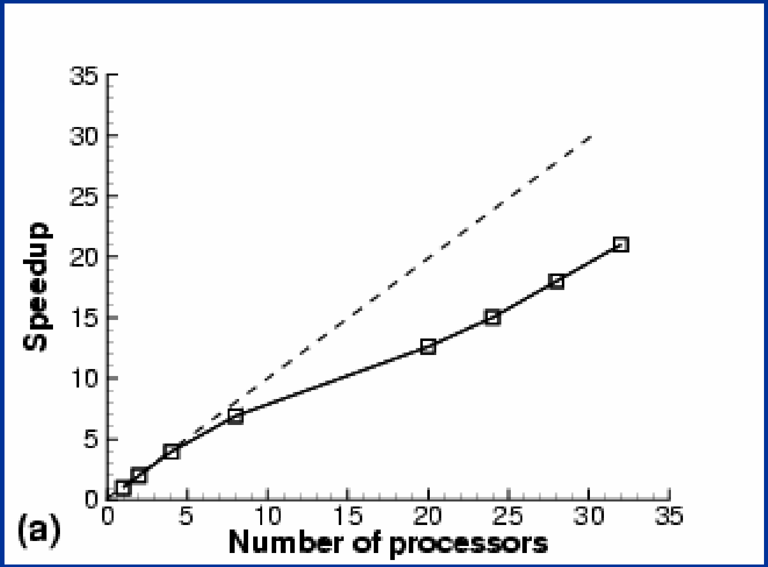
- HPC-based bridging domain multiscale method:
  - Workflow

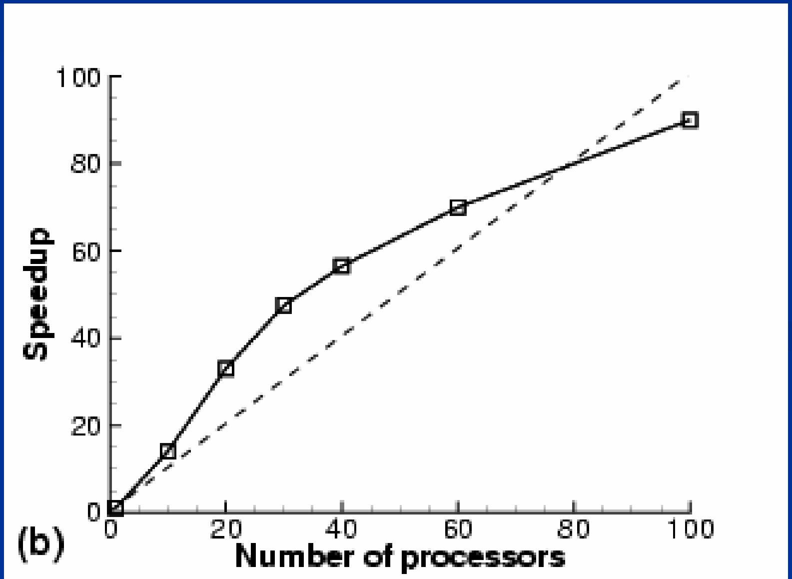


S. W. Wang, ***S. P. Xiao*** *and J. Ni, "A Grid-based Bridging Domain Multiple-Scale Method for Computational Nanotechnology",* *Lecture Notes in Computer Science**, Vol 3516, 2005, pp 326-333*

HPC-enabled Multiscale Simulations

- Parallel Performance





Microway 64-bit AMD Opeteron 32 processors

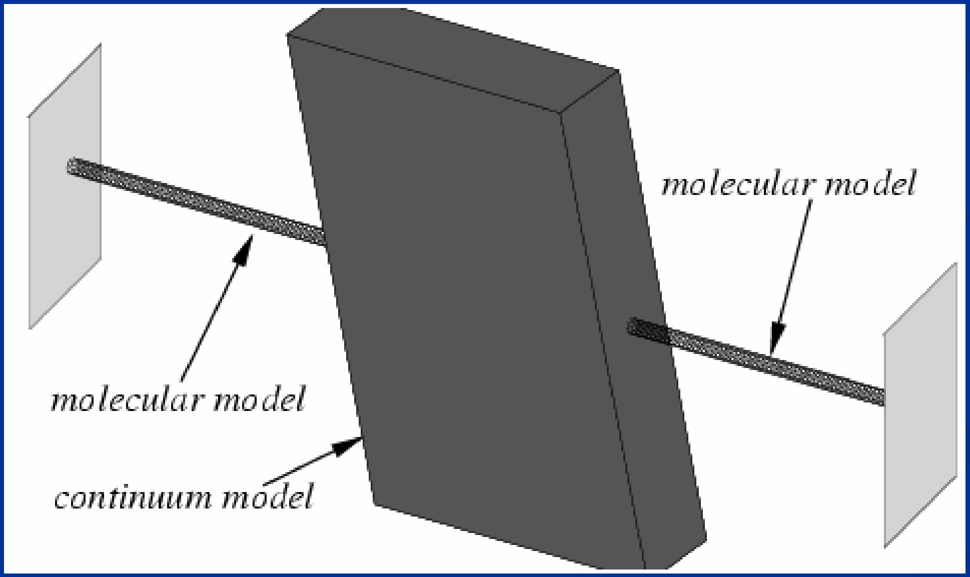
NSF's TeraGrid (NCSA) 100 processors

Nanoscale Devices

- **Nanotube-based resonant oscillators**

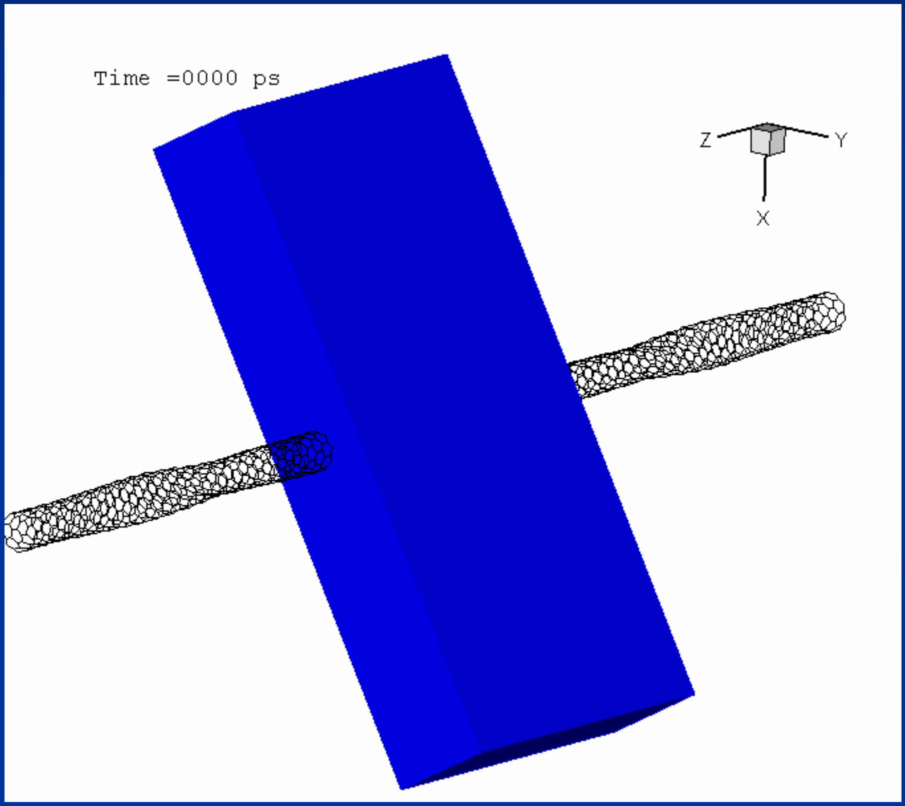
Multiscale modeling of nanotube-based resonant oscillators:

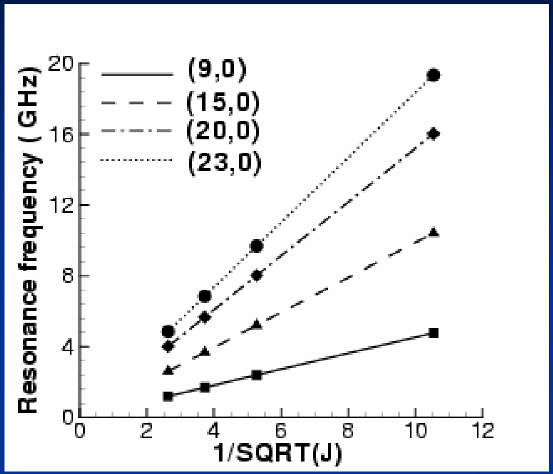
- The nanotube is modeled via molecular dynamics
- The block is modeled as a continua (rigid body)
- The molecular domain and the continuum domain are attached with each other
- Torsion of the nanotube results in torque on the block

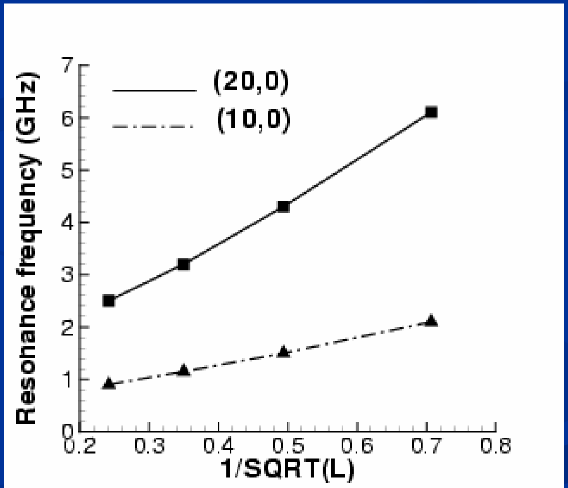


Nanoscale Devices

- **Nanotube-based resonant oscillators**



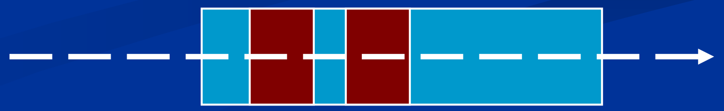




***S. P. Xiao** and W. Y. Hou, "Multiscale modeling and simulation of nanotube-based torsional oscillators", <u>Nanoscale Research Letter,</u> 2(1): 54-59, 2007*

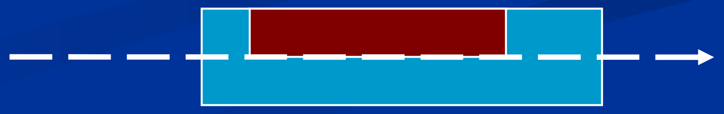
Classification of Multiscale Models

- Hierarchical Model (H-M)
  - Intrinsic properties of nanostructured materials are determined at the atomic level (using MD embedded in a continuum model)
  - Sequentially process the workflow of model simulation
  - Only applicable to homogenous structure or processing
  - At different time-scales
  - Coupling continuum model through either physical properties or time-space.
  - It belongs to task-decomposition



Classification of Multiscale Models

- Concurrent Model (C-M)
  - Divided into multiple sub-region or sub-domains in spatial dimension
  - Simultaneously process each domain.
  - It processes in spatial dimension.
  - It belong to data decomposition in simulations.
  - Coupling continuum model with atomic level through a common boundary or overlapped common domain.



Classification of Multiscale Models

- H-C Model (HCM)
  - Hybrid Combination of HM and CM
  - Statically and dynamically decompose tasks and domains
  - Sequentially and/or process in parallel on tasks and domains.
  - It processes in spatial and time dimensions.
  - It belong to integrated task decomposition and data decomposition in an overall simulation.
  - Logically coupling continuum model with atomic model through both time and geometrical dimensions.
  - Need computational thinking during model simulations.

Classification of Multiscale Models

	H-M	C-M	H-C-M
Time (T-space)	Yes	No	Yes
Spatial (L-space)	No	Yes	Yes
Decomposition	Task	Domain	Task/Domain

Cyber-enabled, large-scale computing resources

- Cyberinfrastructure
  - Unprecedented computing power (petascale computing) and networked distributed computing resources (grid computing)
  - Data Intensive Computing for data storage and acquisition, data processing and mining, etc
  - Virtual Organization to accelerating cross boundaries collaboration and resource sharing.
  - Develop workforce, education, and training

Cyber-enabled, innovative and creative computational process

- Computational Thinking
  - Logical computation
  - Focus on an integrated computation system with multiple well-established application software and algorithms
  - System engineering embedded computing
    - Workflow in simulations
    - Computational check points
    - Application switch during simulation
    - Simulation process control system (monitoring and controls)
    - Feedback adjustment
    - Inverse problem solving strategies using intensive data
    - Visualization embedded in simulation, rather than post-processing
    - …

Cyber-enabled, innovative and creative computational process

- Towards to real-time simulation in both time and space dimensions
- Establish integrated computational systems
- Reconsideration of models and simulations in multi-disciplinary research
- Education of logical thinking for computational science to foster new generation who can use today’s computational technology to solve global challenge problems.

Acknowledgements

- NSF
- USA Air force
- DOE

- Intel Corporation
- Microsoft
- Boeing

Question

- Should be approaching to Petascale computing for multiscale nanotechnology modeling and simulations?
- If yes,
  - What are the new algorithms?
  - How the existing algorithms should be turned to be scalable enough for unprecedented computing in the future?

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Thorm Dunning, Director of NCSA