Computational Aspects of Multi-scale Modeling

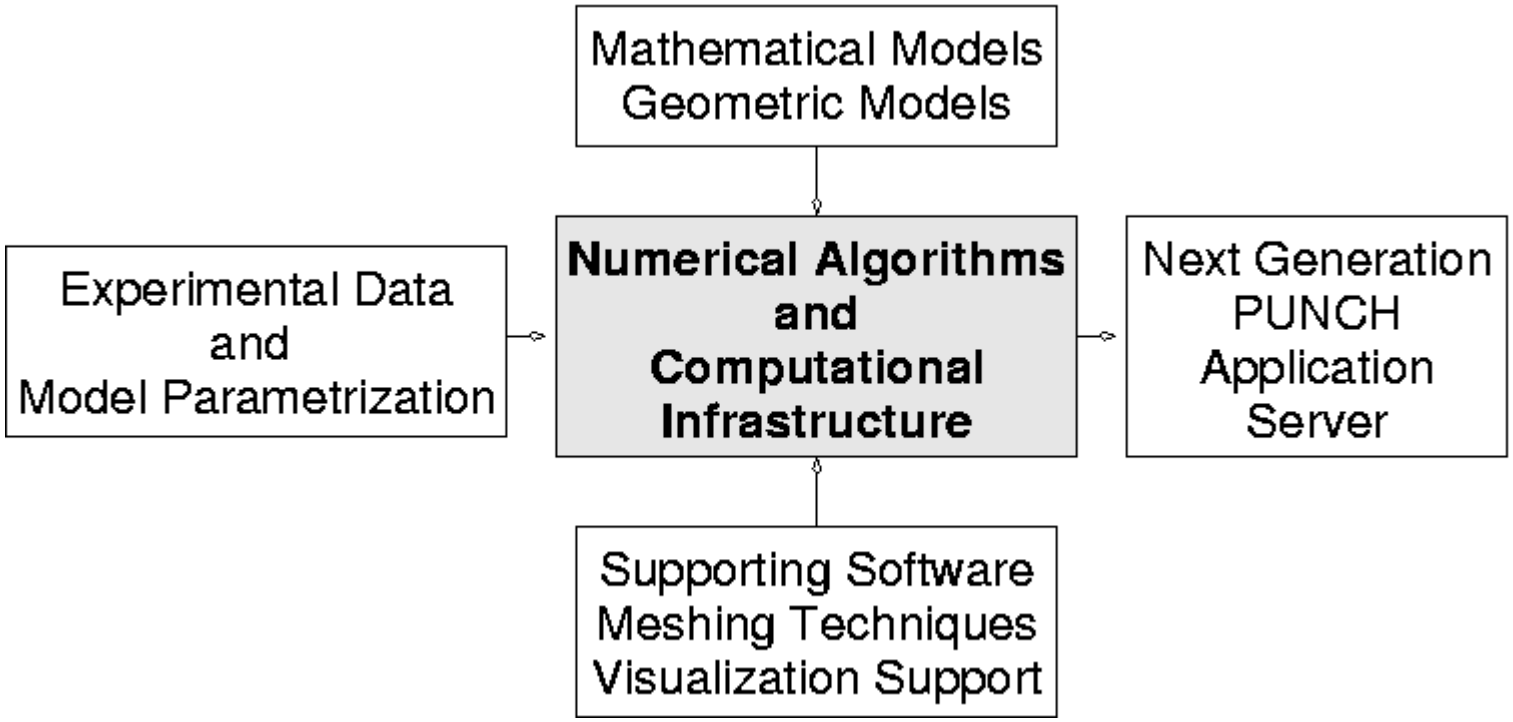
Ahmed Sameh, Ananth Grama
Computing Research Institute
Purdue University.

Technical Objectives

- Efficient Numerical Algorithms
- Parallel and Distributed Computing
- Software and Libraries
- Interfaces to Experimental Data Acquisition and Design Components
- Interfaces to Application Servers

The overall goal is to develop a comprehensive simulation environment built upon novel algorithms and parallelism for multi-scale modeling of NEMS.

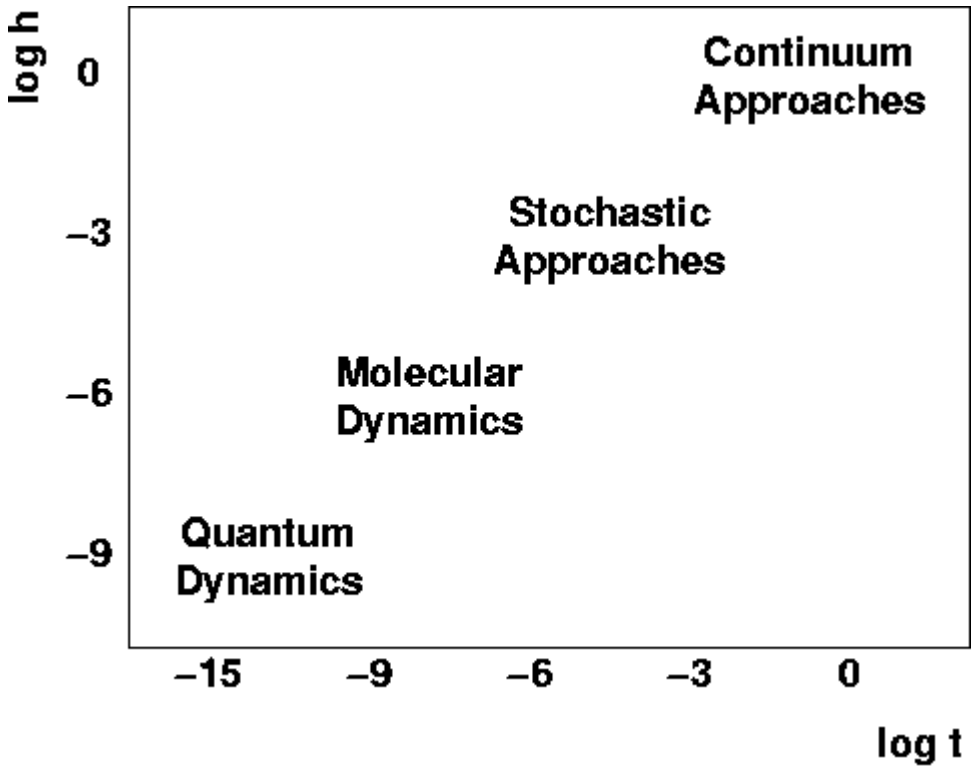
Technical Objectives



Technical Challenges

- Diversity of phenomena - multiphysics
- Variance in spatial scales - nm to cm
- Variance in temporal scales - fs to s
- Variety of modeling phenomena
- Self consistency between scales and phenomena

Technical Challenges



Technical Challenges

- Making software tools available to applications researchers - next generation PUNCH
- Portable, efficient parallel software development using in-house tools such as the Polaris compiler and Ursa Minor performance profiler

Computational and Mathematical Challenges

- Novel problems in linear algebra
- Special functions and approximations
- Self consistency between scales and phenomena
- Highly dynamic geometries and interfaces
- Extremely large number of degrees of freedom
- Need for scalable parallelism

Quantum Simulations

- Five to six orders of magnitude more expensive than classical MD
- Typical simulations limited to few hundred atoms
- Ab-initio methods solve complex many-body Schrodinger equation
- A number of packages such as VASP and ABINIT have been developed

Quantum Simulations

- Iterative matrix diagonalization schemes based on conjugate gradients, block Davidson methods (and our own Trace Minimization Scmeme), and residual minimization are at the core
- Preconditioning is critical for accelerating this procedure
- We have extensive experience in iterative schemes, eigenvalue problems, and developing parallel preconditioners.

Molecular Dynamics

- Describe atomic-scale phenomena
- Particles move as rigid bodies in many-body potential
- A variety of potentials describe pair-wise interactions, local potential (using e.d.f.), and long-range atomic interactions
- Short-range potentials are typically truncated and long-range potentials are evaluated using particle-particle-particle-mesh methods.

Molecular Dynamics - Prior Results

- Error control in hierarchical approximation techniques
- Parallel formulations - high efficiency and scalability to hundreds of processors
- Use in iterative boundary element solvers with multipole-based matrix vector products
- Preconditioners for boundary element solvers
- Use of multipole operators as preconditioners for sparse matrices

Outstanding Challenges in Molecular Dynamics

- Approximations for long range potential functions
- Efficient algorithms for integrating long-range and short-range potentials in a parallel framework
- Self-consistent handshake with quantum simulations
- Software development

Meso-scale Models

- 1 - 100 micron scales
- Defect-interface interactions and defect dynamics become significant
- Models for dynamics of defect ensembles (interacting cracks, dislocations)
- Statistical approaches (Kinetic Monte Carlo Methods)

Continuum Models

- Space and time scales in excess of defects (100 microns or more)
- Finite difference and finite element approaches are most commonly used
- In addition to classical problems in FE/FD modeling of highly unstructured domains, NEMS pose novel problems for continuum models.