Applied Mathematics Research

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Contributions to Overall ASCR Strategic Goal

- "Forefront computational capabilities" to "extend the frontiers of science" ***requires***
  - Well-posed mathematical models (e.g., PDEs)
  - Mathematical analysis of model behavior
  - Solvable discrete versions (grid generation and discretization)
  - Efficient algorithms for solving the discretized models
  - Predictability analysis and uncertainty quantification for model reduction and to determine levels of confidence in the results
  - Engineering design optimization, discrete optimization problems, constrained optimization problems
  - New areas*: dynamical systems, multiresolution analysis, multiscale mathematics, scalable algorithms*

Extends the Frontiers of Science

- Chemically reacting flows / Combustion
- Climate Dynamics
- Materials Science
- Fundamentals of turbulence
- Subsurface flow
- Particle accelerator design
- Fusion reactor design and analysis
- Plasmas & MHD
- Astrophysics
- Defense applications
- Biology
- Infrastructure (e.g., power grids, transportation)
- …

Investment Areas

- PDEs
- CFD
- Meshing
- Adaptive Mesh Refinement
- Solvers (linear, nonlinear, eigenvalue)
- Optimization (continuous and discrete, constrained)
- Dynamical Systems
- High Performance Computation
- Automated Reasoning
- Boundary Integral Methods'
- Interface tracking methods (e.g., FronTier, Level Set)
- Statistics
- Multiscale Math
- Predictability Analysis / Uncertainty Quantification
- Fast methods (e.g., FFTs, Fast Multipole, multigrid)
- Scalable methods
- Software tools (e.g., PETSc, TAO, EBChombo, MPSalsa, LOCA, Trilinos, Hypre, SuperLU, FronTier, …)
- Nanoscience
- Future star development
  - Named fellowships at National Laboratories
  - Early Career Principal Investigator (ECPI) Program
  - Computational Sciences Graduate Fellowship (CSGF) Program

History & Activities

- Over 50 years: started with von Neumann's suggestion to AEC
- Program in Labs & Universities
- Two components: Base & SciDAC (ISICs/CETs & Institutes)
- Activities
  - Linear Algebra, Optimization, Predictability
  - PDEs, High Performance Computing
  - CFD, Advanced meshing, & Other
  - Multiscale Mathematics
  - SciDAC

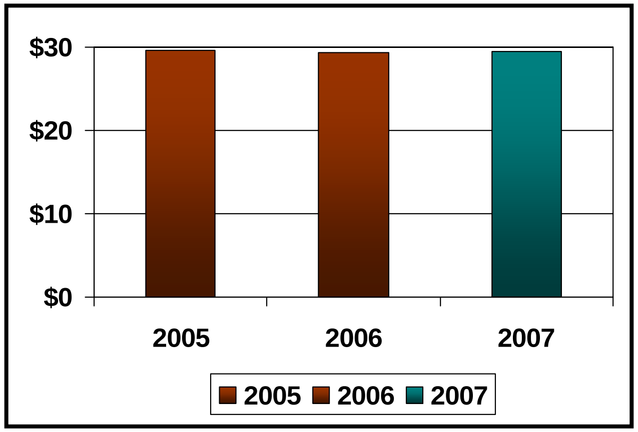
U.S. Department of Energy

Office of Science

Advanced Scientific Computing Research

Budget for Applied Math

- **Base:**
  - FY 05 - $29,577
  - FY 06 - $29,354
  - FY 07 President's Budget Request - $29,495
  - Lab/Univ = 53%/47% in FY 05



- **SciDAC FY 05 - $9,921**
- **Continue support of new initiatives such as MultiScale Math**
- **Broaden SciDAC to include Institutes**

Recent Accomplishments - SciDAC

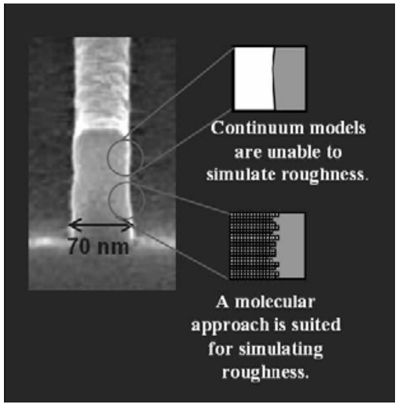
- **Integrated Software Infrastructure Centers (ISICs)** - partnerships between DOE national laboratories and universities focused on research, development, and deployment of software to accelerate the development of SciDAC application codes

- **Three Mathematics ISICs were begun under SciDAC1**:
  - Terascale Optimal PDE Simulations Center (TOPS) : create fast algorithms
  - Terascale Simulation Tools and Technologies Center (TSTT): framework for coupling different types of grids
  - Applied Partial Differential Equations Center (APDEC): structured adaptive grids for simulation

- **Significant improvements in performance, modeling and analysis capabilities, e.g. doubling the performance on 64 processors of the Community Atmosphere Model component of the SciDAC climate modeling activity; Adaptive Smoothed Aggregation (ASA) method to QCD: scalable convergence behavior and shown to be faster than existing methods**

Multiscale Mathematics

- **Across the Office of Science, applications involve multiscale physics / biology / chemistry**
  - Climate: Regional effects on global climate
  - Biology: Timescales from vibrational frequencies to ligand transport time
  - High-Energy Physics: supernova modeling involves many length/time scales
  - Combustion: fast chemical reaction rates to slow-moving flame fronts
  - Fusion: From the electron gyroradius to the connection length

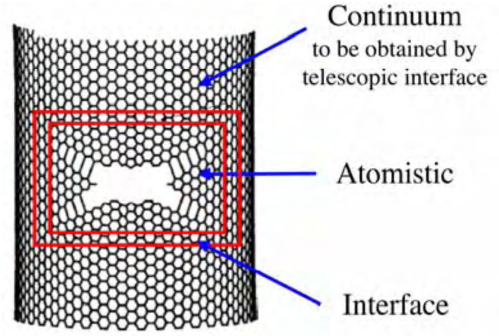


Materials: T. Oden/ Texas

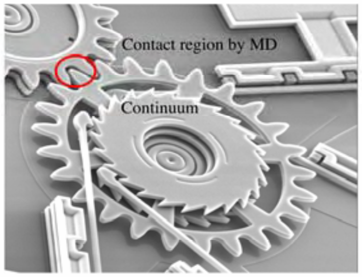
- **Current models assume separation of length/time scales, which fails in practice**

Multiscale Mathematics

- Each involves transfer of information across scales
  - Coupled equations are not known to be well-posed
  - Data are frequently unreliable
  - Current solution techniques are not adequate to handle multiple scales
  - Greater demand on computational power



Fracture of nanotubes



SNL nanomachine

2005 Multiscale Math awards

- 13 Collaborative Projects
- Projects: Atomistic-to-Continuum, Biological Systems, Climate, Materials, Reacting Flow, Plasmas, …

Future of AMR

- **Maintain balance between short-term (1-3 year) and long-term (3-10+ year) horizons**
  - Alignment with ASCR priorities
    - Petascale Computing: scalable libraries & algorithms
    - GNEP
    - SciDAC
  - Target future barriers to scientific progress (e.g., application specific algorithms, multiphysics, multiscale, ultrascalable algorithms, asymptotically optimal methods, model reduction techniques, applications of discrete methods, hybrid methods, …)