Federal Agency (NSF) View of Simulation-Based Engineering and Science

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Presentation Outline

- “Historical” (~5 year) perspective on SBE&S at NSF
  - Oden blue ribbon panel and report (SBES)
  - Glotzer international panel and report
  - Cummings strategic research directions workshop and report
  - OSTP-sanctioned FTAC on M&S for materials and climate science
- Current activities
- Prospects/plans for future directions and investments

Oden (SBES) Report, May 2006

- Blue Ribbon panel commissioned by John Brighton of NSF
- Panel composed of Tinsley Oden, Ted Belytschko, Jacob Fish, Thomas Hughes, Chris Johnson, David Keyes, Alan Laub, Linda Petzold, David Srolovitz, and Sidney Yip
- Study focused on modeling and simulation for prediction of physical events and behavior of complex engineered systems
- “Advances in mathematical modeling, in computational algorithms… competitiveness of our nation may be possible”
- “… advances… require basic research...”
- “Competitors in Europe and Asia… are making major investments in simulation research… much concern that the US is rapidly losing ground.”

SBE&S Study - Structure

- Intended to build on Oden report and expand breadth to include both science and engineering
- Focused on three thematic pillars: materials, energy and sustainability, and life sciences and biomedicine
- Initiated July 2007
- US Baseline Workshop held in November 2007
- Bibliometric analysis performed to identify “hot spots”
- Panel visited 57 sites in Europe and Asia
- Sites included universities, national labs, industrial labs
- Public workshop on study findings held in April 2008
- Final report published in April 2009 (wtec.org/sbes)
- Followed by Strategic Research Directions Workshop in April 2009 (at NAS)

SBE&S Study – Major Findings

- Inadequate education & training threatens global advances in SBE&S
  - Insufficient exposure to computational science & engineering
  - Multicore/gpu architectures introduce significant challenges for algorithm and software paradigms
  - Insufficient training in HPC; educational gap between domain and computer science ~ treatment of codes by domain scientists as “black boxes”
- Investment in algorithm, middleware, software development lags behind investment in hardware
- Lack of support and reward for code development & maintenance
- Progress in SBE&S requires crossing disciplinary boundaries
- Talented students are choosing curricula that prepare them for lucrative careers in finance, for example, rather than in STEM disciplines

RDW – Major Goals Identified

Overarching goals for the next decade identified in SBE&S RDW:

- Enable **broad access to** and **adoption** of SBE&S in U.S. industry
- Institutionalize a **life-cycle** culture for **data** from short-term capture and storage to long-term stewardship
- Build the infrastructure needed for the creation, dynamic development and stewardship of **sustainable software**
- Grow, diversify, and strengthen the SBE&S **workforce**, and identify core competencies and new approaches to modern **teaching** and lifelong **learning**

Other Relevant Workshops/Studies

- Computation-Based Engineering (CBE) Summit: Transforming Engineering through Computational Simulation (September 2008 at NAS; http:/www.sandia.gov/tecs/TECSsummit.html)
- Integrated Computational Materials Engineering (NAS study; http://www.nap.edu/catalog.php?record_id=12199)
- OSTP-sanctioned Fast Track Action Committee on Computational Modeling and Simulation (slides to follow)

FTAC on M&S for Materials and Climate Science

OSTP established a Fast Track Action Committee on Computational Modeling and Simulation (NSTC/CoT)

- Brainstorming 09/09 at WHCC; FTAC kickoff at NIST 03/10/10
- Co-chairs David Dean (DOE), Charles Romine (NIST), Clark Cooper (NSF)
- Charter signed 1 April 2010

<u>Purpose</u>

Provide advice on policies, priorities, and plans for computational science

- Focus on two areas: climate science, and materials science with an emphasis on manufacturing capabilities
- Identify challenges (and solutions) common to both

<u>Functions</u>

- Analyze current state of the art (challenges, emerging technologies, opportunities for tech transfer)
- Analyze current Federal landscape (opportunities for rapid progress, gaps, opportunities for public/private partnerships with impact
- Identify factors promoting/inhibiting collaborations
- Identify ideas for rapid progress in both disciplines

Computational Modeling and Simulation

- A tool in science and engineering
- An enabler of discovery and innovation
- A vital component of decision making
- A performance differentiator for (some!) US industry
  - Automotive tire design (reduced time to market)
  - Automobile power train design (robustness and reduced testing and development time)
  - Consumer container design (optimization)
  - Golf equipment (reduced design cycle)

Explore digitally, confirm physically

FTAC Findings/ Recommendations

- Develop a permanent CS&E infrastructure to support SBE&S as a National asset
- Invest in development of new theoretical models of key physical phenomena, including realization in reusable software
- Invest in new computational methodologies and tools, including parallel algorithms, languages, software, esp. for multicore and cloud computing platforms
- Invest in methodology and tools for V&V and UQ
- Support…community-based algorithms, data platforms, cloud-based portals and services, *etc*.
- Develop an integrated curriculum at BS and MS levels in Computational Engineering that combines computer science and different engineering disciplines

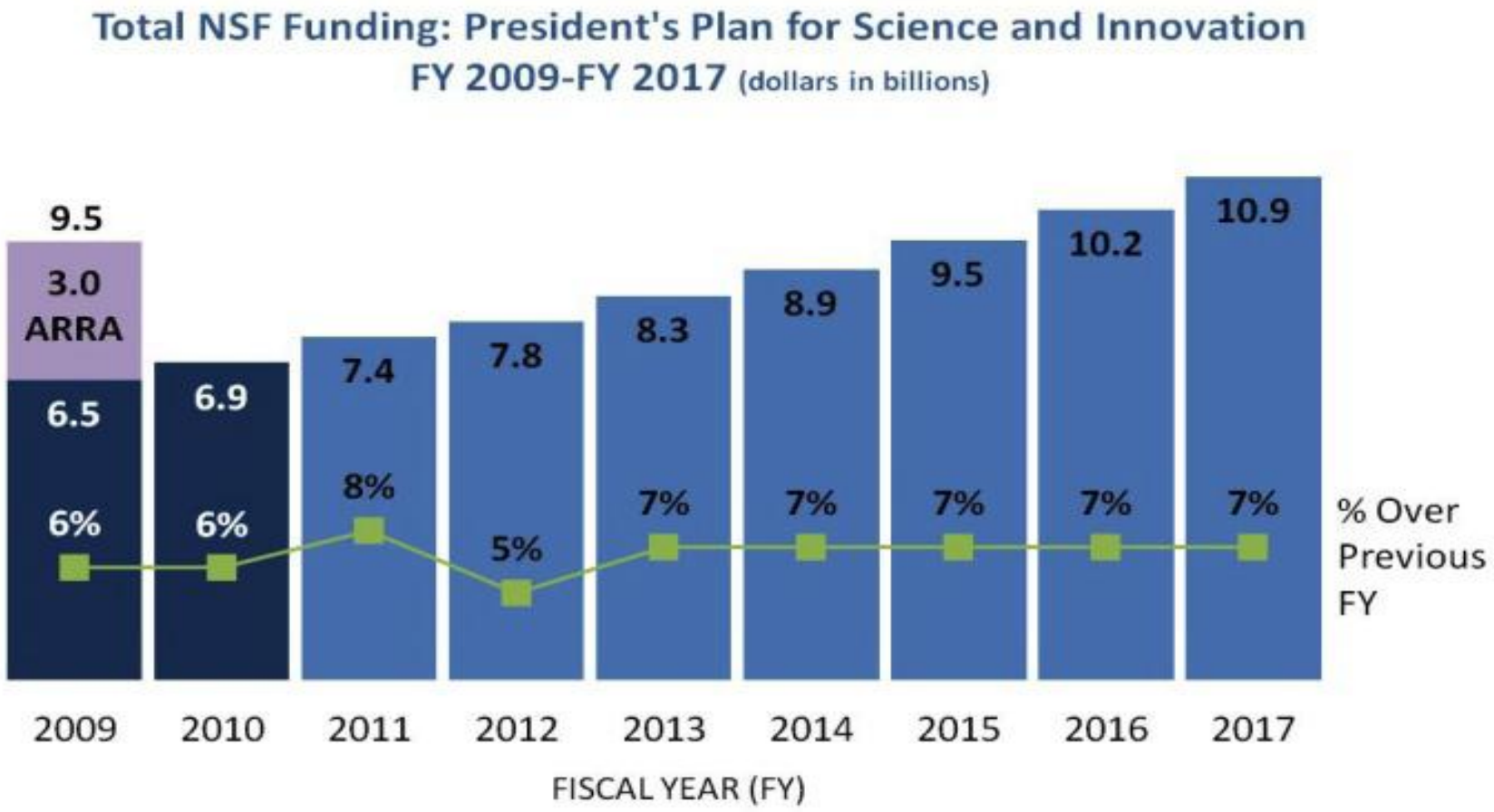
National Science Foundation

- Office of Inspector General
- Office of the Director
  - National Science Board
  - Staff Offices
  - Directorate for Biological Sciences
  - Directorate for Mathematical and Physical Sciences
  - Directorate for Computer and Information Science and Engineering
  - Directorate for Social, Behavioral, and Economic Sciences
  - Directorate for Education and Human Resources
  - Office of Cyberinfrastructure
  - Directorate for Engineering
  - Office of International Science and Engineering
  - Directorate for Geosciences
  - Office of Polar Programs

FY 2011 NSF Budget Request

$M	2009 Omni	2009 ARRA	2010	2011	% over 2010
Research	5152	2062	5564	6018	8.2%
Edu & HR	845	85	873	892	2.2%
TOTAL NSF	6469	2401	6873	7424	8.0%

NSF Funding Profile



FY'11 NSF Investments/ Scientific Opportunities

- Broadening Participation [NSF: 3% increase to $788M]
- Cyber-enabled Discovery and Innovation (CDI) [NSF: 3% increase to $106M]
- CAREER Awards [ENG: increase by 7% to $50M]
- Graduate Research Fellowships (GRF) [NSF: 16% increase to $158M]
- Science and Engineering Beyond Moore's Law (SEBML) [NSF: 1.5X increase to $70M; ENG: 2X increase to $20M]

CDI: Cyber-Enabled Discovery and Innovation

National Science Foundation
WHERE DISCOVERIES BEGIN

SEARCH
NSF Web Site

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Email Print Share

NSF-wide

Cyber-Enabled Discovery and Innovation (CDI)

CONTACTS

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Drs. Misawa, Russell, and Whang are being assisted by a multidisciplinary team of Program Officers drawn from throughout NSF. CDI team members include: Kile Baker (GEO/ATM), Beverly Berger (MPS/PHY), Maria Burka (ENG/CBET), William Chang (OD/OISE), John Cherniavsky (EHR/OAD), Fahmida Chowdhury (SBE/OAD), Arlene Garrison (OD/OIA), Ping Ge (EHR/DGE), Anita La Salle (CISE/CNS), Dan Lubin (OD/OPP), Manish Parashar (OD/OCI), David Rockcliffe (BIO/MCB), Nigel Sharp (MPS/AST), Carl Taylor (BIO/DBI), Rita Teutonico (SBE/OAD), Susan Winter (OD/OCI), William Wiseman (OD/OPP), and Eva Zanzerkia (GEO/EAR).

PROGRAM GUIDELINES

Solicitation 10-506

Please be advised that the NSF Proposal & Award Policies & Procedures Guide (PAPPG) includes guidelines implementing the mentoring provisions of the America COMPETES Act (ACA) (Pub. L. No. 110-69, Aug. 9, 2007.) As specified in the ACA, each proposal that requests funding to support postdoctoral researchers must include a description of the mentoring activities that will be provided for such individuals. Proposals that do not comply with this

- Multi-disciplinary research seeking contributions to more than one area of science or engineering, by innovation in, or innovative use of computational thinking
- Two types currently funded:
  - Type I:
    ~2 PIs, 2 graduate students, 3 years; proposals due January 19, 2011
  - Type II:
    ~3 PIs, 3^+ grad students, 4 years; proposals due January 20, 2011

CDI: Cyber-Enabled Discovery and Innovation

Program Information:

- Five year program, initiated in FY 2007
- Cross-NSF; all directorates participating

Program Goals:

- To support multi-disciplinary research for advancing more than one field of science or engineering as they become increasingly computational (referring to computational concepts, methods, models, algorithms, tools, as applied to all fields of science/engineering)
- To produce paradigm shifts in our understanding of science and engineering phenomena and socio-technical innovations.

CDI: Cyber-Enabled Discovery and Innovation

CDI seeks ambitious, transformative, multidisciplinary research proposals within or across the following areas:

- **From Data to Knowledge: enhancing human cognition and generating new knowledge from heterogeneous digital data**
- **Understanding Complexity in Natural, Built, and Social Systems: deriving fundamental insights on systems comprising multiple interacting elements**
- **Building Virtual Organizations: enhancing discovery and innovation by bringing people and resources together across institutional, geographical, and cultural boundaries**

CF21/CIF21: Cyber Infrastructure for the 21st Century

National Science Foundation
4201 Wilson Boulevard
Arlington, Virginia 22230

NSF 10-015

Dear Colleague,

Today, every discipline of science and engineering is being revolutionized by the widespread use of comprehensive cyberinfrastructure (CI). Computing power, data volumes, and network capacities are all on exponential growth paths, collaborations are growing dramatically, and all forms of CI---and multiple communities spanning multiple agencies and international domains---often must be brought to bear to address a single complex grand challenge problem, such as climate change. All of these developments are part of a revolutionary new approach to scientific discovery in which advanced computational facilities (e.g., data systems, computing hardware, high speed networks) and instruments (e.g., telescopes, sensor networks, sequencers) are coupled to the development of quantifiable models, algorithms, software and other tools and services to provide unique insights into complex problems in science and engineering.

NSF has, for over two decades, been providing the scientific community with open access to high performance computing facilities and the associated user support so that those facilities could be used to enable state-of-the-art, often transformative, scientific investigations. The support began in the 1980's with the initial funding of the NSF supercomputer centers, followed by the Partnerships for Advanced Computational Infrastructure (PACI) program and finally the TeraGrid program. Along with these programs, there have been other important developments in cyberinfrastructure such as the Open Science Grid, the National Virtual Observatory, data activities, major collaborative projects such as Network for Earthquake Engineering Simulation (NEES), The National Ecological Observatory Network (NEON), Ocean Observatories Initiative (OOI), Large Hadron Collider (LHC) and many others too numerous to list here.

As a logical next step, it is imperative that NSF develop a strategic long term vision of what is being called a *Cyberinfrastructure Framework for 21st Century Science and Engineering (CF21).*

- **Contact Information:**
  - **(703) 292-8970**
  - **Office of Cyberinfrastructure**

Dear Colleague Letter: 10-015

Campus Bridging: Craig Stewart, Indiana U

Data & Viz: Tony Hey, Microsoft & Dan Atkins, U Michigan

6 ACCI* Task Forces

- Advising NSF – to inform CF21 programs & NSF CI Vision
- Engaging broader academic community through workshops

Software: David Keyes, Columbia U/KAUST

Computing: Thomas Zacharia, ORNL/UTK (DOE)

***ACCI = Advisory Committee for Cyberinfrastructure**

Education & Workforce: Alex Ramirez, HACU

Grand Challenge Communities/VOs: Tinsley Oden, U Texas - Austin

Cyberinfrastructure Ecosystem (CF21)

Organizations
Universities, schools
Government labs, agencies
Research and Medical Centers
Libraries, Museums
Virtual Organizations
Communities

Expertise
Research and Scholarship
Education
Learning and Workforce Development
Interoperability and operations
Cyberscience

Scientific Instruments
Large Facilities, MREFCs,,telescopes
Colliders, shake Tables
Sensor Arrays
- Ocean, environment, weather, buildings, climate. etc

Discovery
Collaboration
Education

Data
Databases, Data repositories
Collections and Libraries
Data Access; storage, navigation
management, mining tools, curation, privacy

Computational Resources
Supercomputers
Clouds, Grids, Clusters
Visualization
Compute services
Data Centers

Networking
Campus, national, international networks
Research and experimental networks
End-to-end throughput
Cybersecurity

Software
Applications, middleware
Software development and support
Cybersecurity: access, authorization, authentication

Maintainability, sustainability, and extensibility

Software Infrastructure for Sustained Innovations (SI^2) - Mechanisms

- Create a software ecosystem that scales from individual or small groups of software innovators to large hubs of software excellence
- 3 interlocking/interdependent levels of funding

Scientific Software Elements (SSE): 1–2 PIs

- $0.2 – 0.5M, 3 years

Scientific Software Integration (SSI): Focused Groups

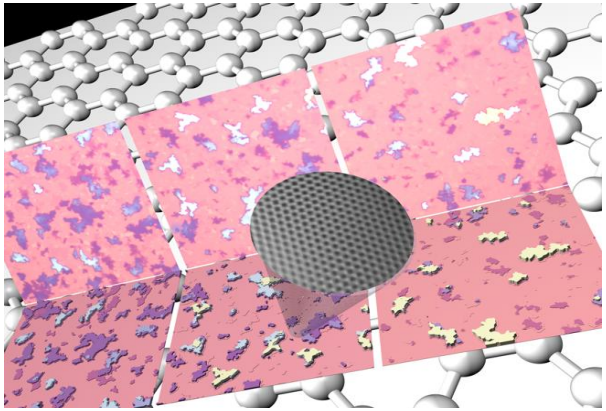
- ~$1M per year, 3 – 5 years

Scientific Software Innovation Institutes (S2I2): Large Multidisciplinary Groups

- ~$4–8M per year, 5 (+) years
- Planning Activities
- FY 11 and beyond only

Focus on innovation → **Focus on sustainability**

Science and Engineering Beyond Moore's Law (SEBML)



- NSF-wide commitment of $70M (incl. $20M from ENG for:
  - Devices
  - Systems and architecture
  - Materials, such as graphene, for ultra-fast computing
  - Multi-scale modeling and simulation research
  - Quantum information science and engineering
  - Design of efficient and sustainable manufacturing equipment, processes, and facilities

(Selected) DOE follow-on activities in Modeling and Simulation

Simulation-Based Engineering and Science for Discovery and Innovation

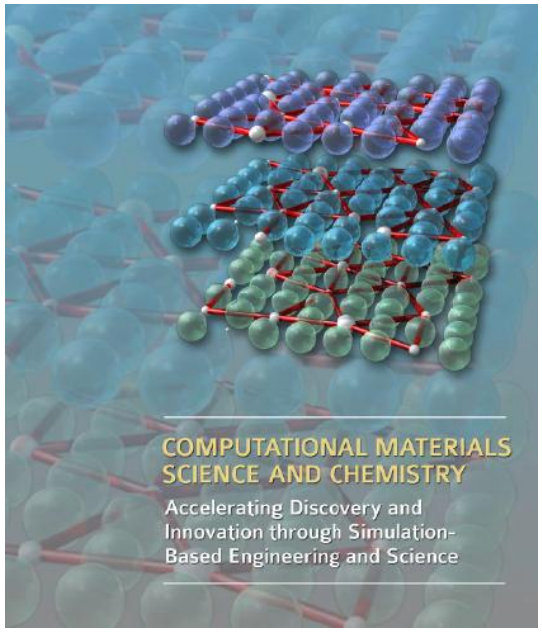
FAST TRACK ACTION COMMITTEE ON COMPUTATIONAL MODELING AND SIMULATION
COMMITTEE ON TECHNOLOGY
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

Actively considering how to implement FTAC rec's; held workshop (July) and "simulations summit" (October)

ON THE ECONOMIC FUTURE OF THE U.S.

Why the U.S. must lead in supercomputing

June 14, 2010 | By Steven E. Koonin



A EXASCALE CSRC

FY12 Cross Cut Budget Justification exercise

DOE Simulations Summit

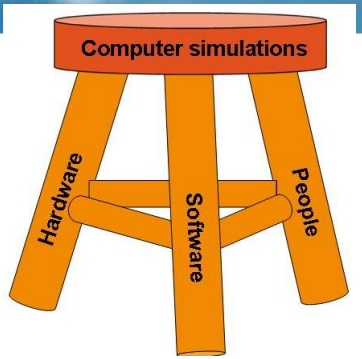
The DOE strategy should be to make simulation part of everyone's toolbox. At first simulation requires immense parallelism. With the new approaches you have to build software and new hardware concurrently (we learned that at Nvidia) or the software guys won't know what to do with the hardware. --*Steven Chu*

http://www.science.doe.gov/bes/reports/abstracts.html#CMSC
http://www.science.doe.gov/ascr/WorkshopsConferences/DOESimulationsSummit.html

Questions/ Discussion

Backup Slides

SBE&S Summary



- Interoperability of software and data are major hurdles
- Use of simulation software by non-simulation experts is limited
- In most S&E applications, algorithms, software and data are primary impediments
- Visualization of simulation outputs remains a challenge
- Treatment of uncertainty (UQ) is inadequate
- Links between physical and system level simulations are weak
- Training of scientists and engineers is inadequate to address simulation and modeling needs