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Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine

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Paper 225b: Innovation and Insight via High-Fidelity Simulation and Large-Database Studies of Micro, Macro and Multi-Scale Phenomena

American Institute of Chemical Engineers Annual Meeting

Salt Lake City, UT November 7-12, 2010

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Outline

- Introduction
  - *Simulation-based engineering and science (SBE&S)*
  - *Timeline of workshops and reports*
- International Assessment of Research and Development in Simulation-based Engineering and Science
  - *Methodology*
  - *Outcomes*
- Vision for Research and Development in Simulation-Based Engineering and Science in the Next Decade
  - *Workshop*
  - *Report*
- NSF Advisory Committee for Cyberinfrastructure
  - *Structure and Workshops*
  - *Reports*

Follows path of National Nanotechnology Initiative

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Introduction

- Simulation-Based Engineering and Science
  - *Our definition*
    - *Use of computer modeling and simulation to solve mathematical formulations of physical models of engineered and natural systems*
  - *SBE&S today*
    - *Level of predictive capability that it firmly complements the traditional pillars of theory and experimentation/observation*
      - *"Three-legged stool of science"*
      - *Experiment, theory, and simulation/computation*
    - *Many critical technologies cannot be understood, developed or utilized without simulation*
      - *Climate*
      - *New energy technologies*
      - *Life sciences, medicine and healthcare*
      - *Materials*
      - *…..*

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SBE&S: Why now?

- A tipping point in SBE&S
  - *Computer simulation is more pervasive today, and having more impact, than ever before - hardly a field untouched*
  - *Fields are being transformed by simulation*
  - *Reached a useful level of predictiveness*
  - *Remarkable increase in hardware speed*
    - *Gigaflop achieved ~1998*
    - *Petaflop achieved in ~2008*
    - *Exaflop expected in ~2018*
  - *International competitiveness in computational facilities*
    - *US, Japan shared leadership in recent decades*
    - *China now major player*
      - *#1 in top 500 list, to be released next week at SC 2010*
  - *New massively multi-core computer chip architectures will allow unprecedented accuracy and resolution, as well as the ability to solve the highly complex problems that face society today*
    - *Programming models are major issue*
    - *Potentially disruptive*

Introduction

- Building on previous SBE&S reports such as
  - *Revolutionizing Engineering Science through Simulation (NSF)*
    - http://www.nsf.gov/pubs/reports/sbes_final_report.pdf
  - *Integrated Computational Materials Engineering (National Academies)*
    - http://www.nap.edu/catalog.php?record_id=12199
  - *Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security (DOE OASCR)*
    - http://www.er.doe.gov/ascr/ProgramDocuments/Docs/TownHall.pdf
  - *President's Information Technology Advisory Committee Report on Computational Science: Ensuring America's Competitiveness (PITAC)*
    - http://www.itrd.gov/pitac/reports/20050609_computational/computational.pdf
  - *Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering (National Academies)*
    - http://www.nap.edu/catalog.php?record_id=12451
- …and many workshops, such as
  - *Computation-Based Engineering Summit: Transforming Engineering through Computational Simulation*
    - http://www.sandia.gov/tecs/TECSsummit.html

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International Assessment of Research and Development in SBE&S

- Study designed to:
  - *Gather information on the worldwide status and trends of SBE&S research*
    - *State of the art, regional levels of activities*
    - *US leadership status*
    - *Opportunities for US leadership*
  - *Disseminate this information to government decision makers and the research community*
  - *Findings, not recommendations*

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International Assessment of Research and Development in SBE&S

- Structure of Study
  - *Primary thematic areas*
    - *Life sciences and medicine*
    - *Materials*
    - *Energy and sustainability*
  - *Core cross-cutting issues*
    - *Next-generation algorithms and high performance computing*
    - *Multiscale simulation*
    - *Simulation software*
    - *Validation, verification, and quantifying uncertainty*
    - *Engineering systems*
    - *Big data and data-driven simulations*
    - *Education and training*
    - *Funding*

International Assessment of Research and Development in SBE&S

- Panelists
  - *Sharon Glotzer (Chair), U Michigan*
  - *Sangtae Kim, NAE (Vice-chair), Purdue*
  - *Peter Cummings, Vanderbilt/ORNL*
  - *Abhi Deshmukh, Texas A&M*
  - *Martin Head-Gordon, UC Berkeley*
  - *George Karniadakis, Brown U*
  - *Linda Petzold, (NAE) UC Santa Barbara*
  - *Celeste Sagui, NC State U*
  - *Matsunoba Shinozuko, (NAE) UC Irvine*
- Advisers
  - *Tomas de la Rubia, LLNL*
  - *Jack Dongarra, (NAE) UTK/ORNL*
  - *James Duderstadt (NAE), U Michigan*
  - *David Shaw, D.E. Shaw Research*
  - *Gilbert Omenn (IOM), U Michigan*
  - *J. Tinsley Oden (NAE), UT Austin*
  - *Marty Wortman, Texas A&M*

International Assessment of Research and Development in SBE&S

- Study Process and Timeline
  - *US Baseline Workshop November 2007*
  - *Bibliometrics analysis*
  - *Panel visited 57 sites in Europe, Asia*
    - *Universities, national labs, industrial labs*
    - *Also: conversations, reports, research papers, bibliometric analysis provided basis for assessment*
  - *Public workshop on study findings in April 2008*
  - *Final report releases April 22, 2009*
    - *Coincided with research directions planning workshop*

International Assessment of Research and Development in SBE&S

Peking Univ./CCSE, Tsinghua Univ./DEM, ICCAS, ICMSEC/CAS, IPE/CAS,

Dalian Univ. of Technology

SSC, Shanghai Univ., Fudan Univ.

Sites visited in China in December, 2007

http://www.lonelyplanet.com/maps/asia/china/

International Assessment of Research and Development in SBE&S

RIKEN/ACCC

Kyoto Univ.

NIMS/CMSC, RICS/AIST

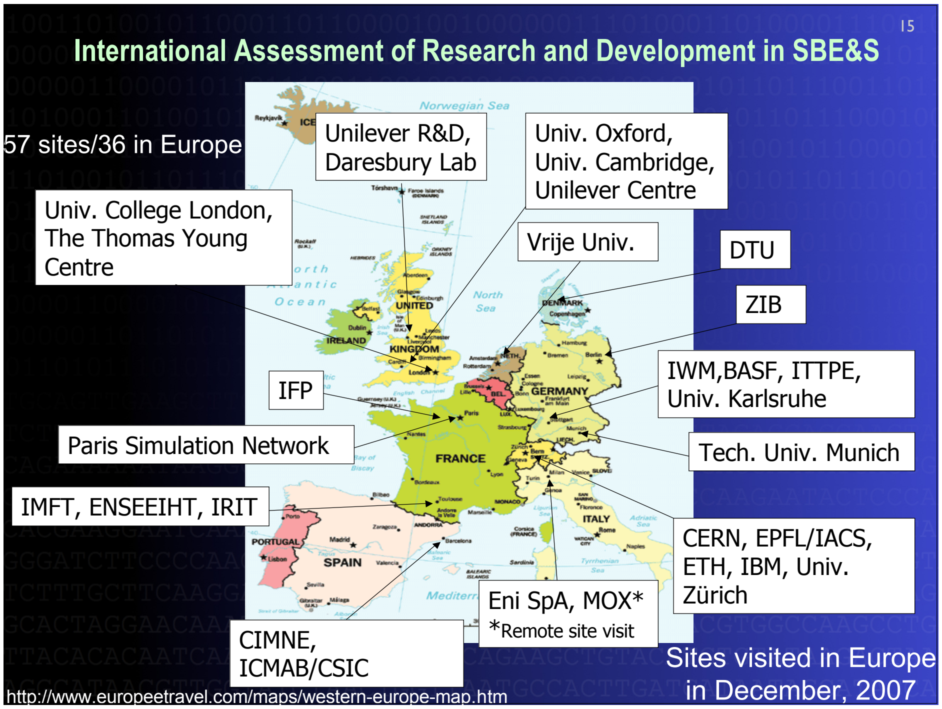
CRIEPI, SBI, Univ. Tokyo

Japan Agency for Marine-Earth S&T (ESC), Nissan Research Center, Mitsubishi Chemicals

Toyota Central R&D Labs., IMS

Sites visited in Japan in December, 2007

http://www.ease.com/~randyj/japanmap.htm



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International Assessment of Research and Development in SBE&S

- Life sciences & medicine, materials, and energy & sustainability are among most likely sectors to be transformed by SBE&S
  - *SBE&S is changing the way disease is treated, the way surgery is performed and patients are rehabilitated, the way we understand the brain*
  - *SBE&S is changing the way materials & components are designed, developed, and used in all industrial sectors*
    - *E.g. ICME (National Academies Report 2008, T. Pollock, et al)*
  - *SBE&S is aiding in the recovery of untapped oil, the discovery & utilization of new energy sources, and the way we design sustainable infrastructures*

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International Assessment of Research and Development in SBE&S

- Findings: Top Four Major Trends in SBE&S Research
  - *Data-intensive applications (especially Switzerland and Japan)*
    - *Integration of (real-time) experimental and observational data with modeling and simulation to expedite discovery and engineering solutions*
  - *Millisecond timescales for proteins and other complex matter with molecular resolution*
  - *Science-based engineering simulations (US slight lead)*
    - *Increased fidelity through inclusion of physics and chemistry*
    - *Better predictiveness through inclusion of V&V, UQ, risk assessment*
  - *Multi-core for petascale and beyond: not just faster time to solution - increased problem complexity*
    - *Cheap GPUs today give up to 200x speed up on some scientific applications*

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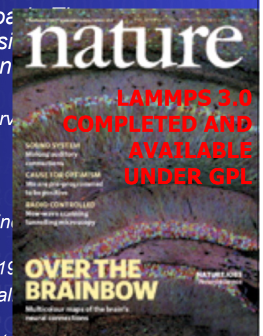
International Assessment of Research and Development in SBE&S

- Threats to US leadership in SBE&S
  - *Finding 1: The world of computing is flat, and anyone can do it (except, for now, at the bleeding edge). We must do it better, and exploit new architectures before those architectures become ubiquitous.*
    - *Japan has an industry-university-govt roadmap out to 2025 (exascale)*
    - *Germany investing nearly US$1B in new HPC push, also with EU*
    - *Cheap to start up, hire in SBE&S (e.g. India)*
  - *Finding 2: Inadequate education and training of the next generation of computational scientists threatens global as well as US growth of SBE&S. This is particularly urgent for the US, since unless we prepare these researchers to use the next generation of computer architectures we are developing, we will not be able to exploit their game-changing capabilities.*
    - *Insufficient exposure to computational science & engineering and underlying core subjects at high school and undergraduate level*
    - *Increased topical specialization beginning with graduate school*
    - *Insufficient training in HPC – an educational "gap"*

International Assessment of Research and Development in SBE&S

- Threats to US leadership in SBE&S
  - *Finding 3: A persistent pattern of subcritical funding overall for SBE&S threatens US leadership and continued needed advances amidst a recent surge of strategic investments in SBE&S abroa... reflects recognition by those countries of the role of si... advancing national competitiveness and its effectiven... mechanism for economic stimulus.*
    - *US funding agencies and universities have typically underv...*
      - *Publication impact vs experimental discovery*
      - *Contrast with industry*
    - *China: SBE&S "footprint" changing rapidly*
    - *Strategic change towards innovation, and recognition by in... innovation requires simulation*
      - *China's S&T budget has doubled every 5 years since 19...*
        - *70% to top 100 universities (4/5 all PhDs, 2/3 al... international,1/3 all undergraduates)*
      - *Recognition of need to train new generation of "computationally-savvy" students, and new State money*
        - *Project 211: US$1B/year, all projects must have integrated simulation component* http://en.wikipedia.org/wiki/Project_211



International Assessment of Research and Development in SBE&S

- Additional details in report
  - *Specific findings in thematic areas*
    - *Life sciences & medicine, materials, and energy & sustainability*
  - *Specific findings in core cross-cutting issues*
    - *Next-generation algorithms & high performance computing, multiscale simulation, simulation software, validation+verification, & quantifying uncertainty, engineering systems, big data & data-driven simulations, education & training, funding*
  - *See report at* http://wtec.org/sbes/
    - *Proceedings of April, 2008, report-out-to-sponsors workshop also available at this site*

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Vision for Research and Development in SBE&S in the Next Decade

- Strategic Directions Workshop
  - *April 22-23, 2009 at National Academies building and GWU*
    - *Organized by Peter Cummings, Chair; Sharon Glotzer, co-Chair; Phil Westmoreland (NSF, now NCSU), Clark Cooper (NSF); other NSF program managers*
    - *Breakout leaders: John Allison, Ford; Brian Athey, U. Michigan;Jim Davis, UCLA; Sangtae Kim, Morgridge Institute; Padma Raghavan, PSU*
- Goal
  - *To develop community-driven report on future of SBE&S research in U.S. responsive to findings of international comparative study*
- Answer the questions
  - *Why are advances in SBE&S crucial to the future success of U.S. science,engineering, and industry, and how will they contribute to U.S. economic competitiveness? (Day 1)*
  - *What strategic investments in SBE&S are needed in order to achieve the promise of SBE&S? (Day 2 breakouts)*
  - *How (over what time frame) and in what format can these investments be most productive? (Day 2 breakouts)*

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Vision for Research and Development in SBE&S in the Next Decade

- Presentations
  - *Introduction*
    - *Peter Cummings: Welcome and Introduction to the Workshop*
    - *Phil Westmoreland: Objectives and Expected Outcomes*
    - *Ed Seidel: Cyberinfrastructure and Computational Science for Research and Education*
    - *J. Tinsley Oden: Revolutionizing Engineering Science through Simulation: Summary of NSF Blue Ribbon PanelStudy*
    - *Sharon Glotzer: International Assessment of R&D in Simulation-Based Engineering and Science*
  - *Overview of recent reports and workshops*
    - *John Allison: Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security*
    - *Horst Simon: Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security*
    - *Dan Reed: President's Information Technology Advisory Committee Report on Computational Science: Ensuring America's Competitiveness*
    - *John Lyons: Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering*
    - *Arthur Ratzel: Computation-Based Engineering Summit: Transforming Engineering through Computational Simulation*

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Vision for Research and Development in SBE&S in the Next Decade

- Presentations
  - *Science and Technology Drivers*
    - *Jim Hack: Projections of climate change consequences: A scientific and computational grand challenge*
    - *Greg Beroza: Simulating the big one: How we try to anticipate the effects of future earthquakes*
    - *Mary Wheeler: Modeling and simulation of subsurface grand challenges*
    - *Loren Miller: Competitive advantage for industry using simulation-based engineering and science*
    - *Rex Reklaitis: Successes and challenges for simulation and modeling in process systems engineering*
    - *Gene Stanley: Large-scale simulations of complex systems: predicting large economic events*

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Vision for Research and Development in SBE&S in the Next Decade

- Presentations
  - *Science and Technology Drivers (cont'd)*
    - *Brian Athey: Data explosion and complexity in bioinformatics*
    - *Larry Nagahara: Prospects for simulation-based engineering and science approaches applied to cancer*
    - *Phil Colella: Software requirements and software frameworks for using simulation-based engineering and science*
    - *Thomas Schulthess: Petascale computing: Opportunities in materials and nanoscience*
    - *Jackie Chen: Petascale simulations of turbulent combustion*
    - *Teresa Head-Gordon: Challenges in molecular theory, models and simulation*
    - *Paul Avery: The challenge of petascale distributed computing in high energy physics*
    - *Peter Cummings: Summary and charge to breakout sessions*

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Vision for Research and Development in SBE&S in the Next Decade

- Report
  - *Available at*
    - *http://www.nsf.gov/mps/ResearchDirectionsWorkshop2010/RWD-color-FINAL-usletter_2010-07-16.pdf*
- Recommendations
  - *Overarching goals for next decade to guide growth and development of SBE&S*
    - *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*
  - *Specific recommendations by area*
    - *Building the National SBE&S Infrastructure for Innovation, Resource Management, and Decision Support*
    - *Revolutionizing Discovery through Simulation-Based Engineering and Science*
    - *Transforming Data into a Critical National Asset through SBE&S*
    - *Ensuring Sustainable Software for Simulation-Based Engineering and Science*
    - *Educating, Training and Diversifying the SBE&S Workforce*

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Vision for Research and Development in SBE&S in the Next Decade

- Recommendations (cont'd)
  - *Multi-tiered national-level investment strategy to ensure that researchers, laboratories, and institutions have sufficient resources to continue to be the global leaders in SBE&S*
    - *Provide long-term (5+ years) single and small group grants*
    - *Create long-term team grants that support interdisciplinary collaborations among domain scientists, computational scientists, and mathematicians*
    - *Build large-scale virtual institutes/centers tasked with developing and stewarding community codes for specific SBE&S domains*
    - *Provide 10 long-term (10-year) grand challenge public-private partnership grants*
    - *Provide grants for curriculum development and dissemination, and new programs and approaches to foster a highly skilled SBE&S workforce*

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Vision for Research and Development in SBE&S in the Next Decade

- Recommendations (cont'd)
    - *Support graduate students and postdoctoral fellows with traineeship grants, including portable awards that support the transition of exceptionally talented individuals to permanent industrial, academic, or government SBE&S research positions*
    - *Establish leveraged investment programs to promote partnerships between academia and industry*
    - *Establish 20+ multi-investigator SBE&S interdisciplinary research institutes, with broad research programs in specific SBE&S problem domains, data and software*
    - *Establish 40+ multi-investigator SBE&S interdisciplinary research centers, with more focused research efforts in SBE&S problem domains, data and software*
    - *Award several hundred innovator grants to individuals or small teams conducting high-risk, high-reward transformative research in data and software*

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NSF Advisory Committee for Cyberinfrastructure

- Six CI Task Forces established in 2008
  - *Grand Challenges and Virtual Organizations (J. Tinsley Oden, UT Austin; ENG)*
  - *Software (David Keyes, Columbia/KAUST; MPS)*
  - *High Performance Computing (Thomas Zacharia, ORNL/UTK; DOE)*
  - *Data and Visualization (Shenda Baker, Harvey Mudd College; MPS; Tony Hey, Microsoft; CISE)*
  - *Campus Bridging (Craig Stewart, Indiana U; BIO)*
  - *Learning & Workforce Development (Alex Ramirez, Hispanic Association of Colleges and Universities; CEOSE)*
- Activities
  - *14 workshops; 5 "birds of a feather" meetings (BOFs); more than 30 phone conferences*
  - *3 more workshops and 1 more BOF before Dec*
  - *Over 1230 researchers involved to date*
- Final reports are being published
  - *Interim results and recommendations being provided*

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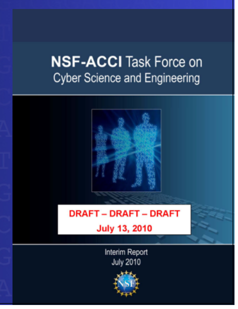
NSF Advisory Committee for Cyberinfrastructure

- Grand challenges
  - *Advanced New Materials**
  - *Prediction of Climate Change**
  - *Quantum Chromodynamics and Condensed Matter Theory*
  - *Semiconductor Designs and Manufacturing*
  - *Assembling the Tree of Life**
  - *Drug Design and Development*
  - *Energy through Fusion*
  - *Water Sustainability*
  - *Understanding Biological Systems**
  - *New Combustion Systems*
  - *Astronomy and Cosmology**
  - *Hazard Analysis and Management**
  - *Cardiovascular Engineering*
  - *Virtual Product Design**
  - *Cancer Detection and Therapy*
  - *CO2 Sequestration**



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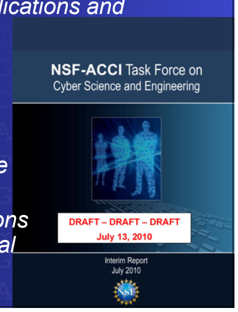
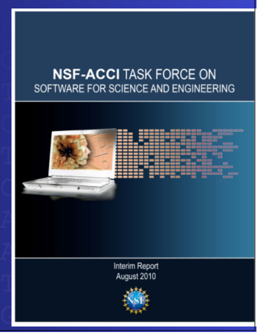
NSF Advisory Committee for Cyberinfrastructure

- Grand Challenges and Virtual Organizations Task Force
  - *Recommendations*
    - *Creation of an Interagency Working Group on CS&E*
    - *Broad-based, comprehensive, long-term, and vigorous research program in advanced computational methods supporting interdisciplinary teams*
    - *Support the creation of reliable, robust science and engineering applications and data analysis and visualization applications and the professional staff needed*
    - *NSF should support research infrastructure and robust persistent cyberinfrastructure to empower data-driven science and data-intensive computing*
    - *NSF should support education, training, and workforce development using educational excellence grants, transition grants …*
    - *NSF should invest in research on Virtual Organizations that includes study of VO's, connecting smaller virtual organizations to large-scale infrastructure …*



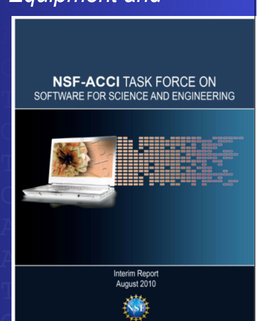
NSF Advisory Committee for Cyberinfrastructure

- Software for Science and Engineering Task Force
  - *Findings*
    - *Software is a critical and pervasive component of the cyberinfrastructure for science and engineering*
    - *Software is a tool for new knowledge discovery in many disciplines and often also itself serves as a representation of knowledge – "new language of science"*
    - *NSF does not adequately support software evolution and lifecycle costs*
    - *Software needs to address questions of open access, portability, reuse, composability and dissemination*



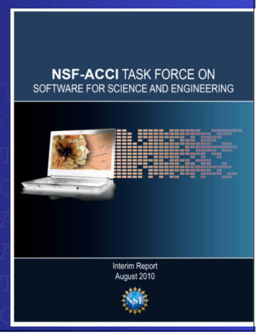
NSF Advisory Committee for Cyberinfrastructure

- Software for Science and Engineering Task Force
  - *Recommendations*
    - *NSF should develop a multi-level (individual, team, institute), long-term program of support of scientific software elements (SSE) ranging from complex applications to tools of use in multiple domains. Such programs should also support extreme scale data and simulation and the needs of Major Research Equipment and Facilities*
    - *NSF should take leadership in promoting verification, validation, sustainability and reproducibility of software developed with federal support*
    - *NSF should develop a uniform policy on open source that promotes science and encourages innovation*
    - *NSF support for software should entail collaborations among all of its divisions, related federal agencies and private industry*



NSF Advisory Committee for Cyberinfrastructure

- Software for Science and Engineering Task Force
  - *Recommendations*
    - *SSE project budgets should accommodate senior software engineers. Student and post-doctoral participation will be restricted to research aspects*
    - *NSF should encourage reproducibility in all computational research it sponsors requiring the preservation of software and data*
    - *NSF should develop criteria for evaluating software projects that are complementary to the intellectual merit and broader impact criteria*
    - *NSF should promote a healthy software industry through support of university-industry partnerships, acquisition of commercial tools and support for translation of research software into commercial tools*
      - *Today's research codes form the basis for tomorrow's computer-aided design tools*



OSTP Recommendations for FY12

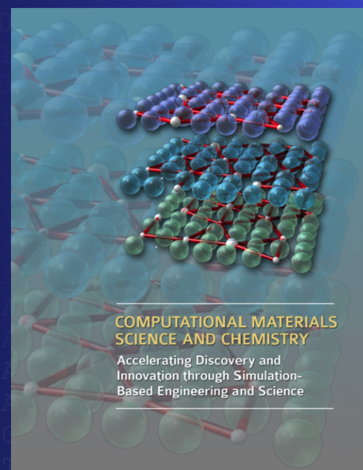
This document is a draft version of "Simulation-Based Engineering and Science for Discovery and Innovation," a report being produced by the National Science and Technology Council's Fast Track Action Committee on Computational Modeling and Simulation. As discussed in this blog post, the subcommittee is seeking feedback on several aspects of this document. With participation from individuals across economic sectors and areas of expertise, we hope to improve upon this draft and sharpen our recommendations while achieving the Administration's Open Government goals of enhancing transparency, participation, and collaboration. For more information about this project and how to participate, please go to: http://opennstc.ideascale.com/

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

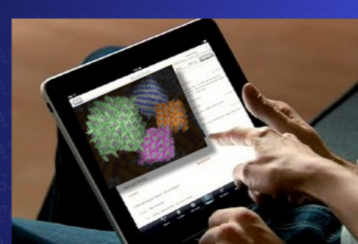
DOE Office of Science SBE&S Report

- ❑ DOE Office of Science Response to Report by FTAC on Computational Modeling and Simulation – report of a workshop in Bethesda, MD July 2010



Continued investments in HPC have produced computing platforms that are now fast enough to go beyond insight and understanding, to prediction.

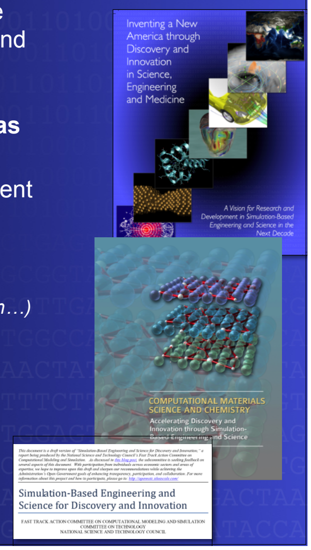
Exascale



- ❑ But, despite many successful examples of the use of SBE&S, we have only just begun to exploit its full capabilities and promise for discovery and innovation.

Simulation-based engineering and science (SBE&S) as a critical and sustainable national infrastructure

- ❑ The investments we have made as a nation in the field of computing and in computational science and engineering provide the foundation for the next essential **step—the integration and full-scale deployment of computational methodologies as community tools for predictive simulation**.
- ❑ This step requires a long-term, sustained investment in simulation software as infrastructure, and the creation of an innovation ecosystem as a national infrastructure
  - *Today: science first, software second (or third….or fourth…)*



Elements of CS&E underpinning an SBE&S innovation ecosystem

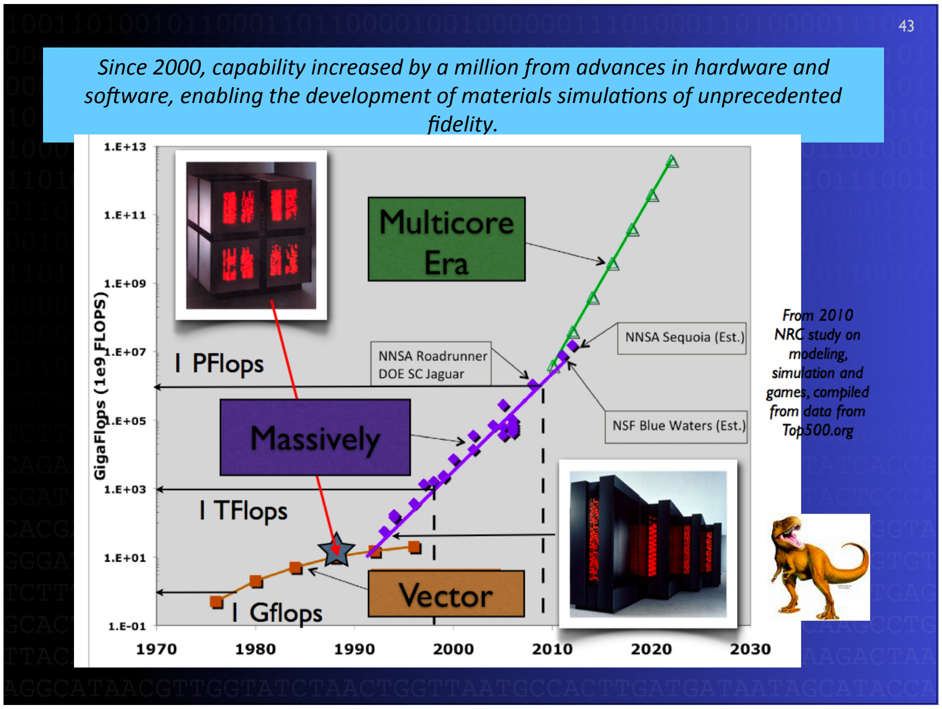
- ❑ Developing and sustaining this capability requires a long-term commitment that is at the same time *financial, intellectual, and programmatic*, requiring:
  - *Ongoing investment in all aspects of computational science and engineering—from theory, models, and algorithms to languages and compilers, to faster computers, to software and open-source databases, to workforce.*
  - *Ongoing support of the **software communities and the codes they develop**.*
    - *Development, dissemination, and long-term support of materials models, codes, and simulation platforms, with particular attention to code maintenance, interoperability, sharing, and reuse*
  - *Close partnership between experiment, theory, and simulation to advance fundamental scientific understanding, validate and verify codes and models, and to quantify the uncertainty inherent in any prediction, which is required for risk assessment and decision-making (open data considerations, etc.).*
  - *Expediting and facilitating the transformation of scientific research codes to design tools suitable for the industrial laboratory setting and manufacturing floor (partnerships).*
  - *Training a future workforce sufficiently expert to both develop and use these tools, and assess their usefulness and role within a company.*
- ❑ Together, these elements of computational science and engineering form the foundational infrastructure for the predictive capability afforded by SBE&S.

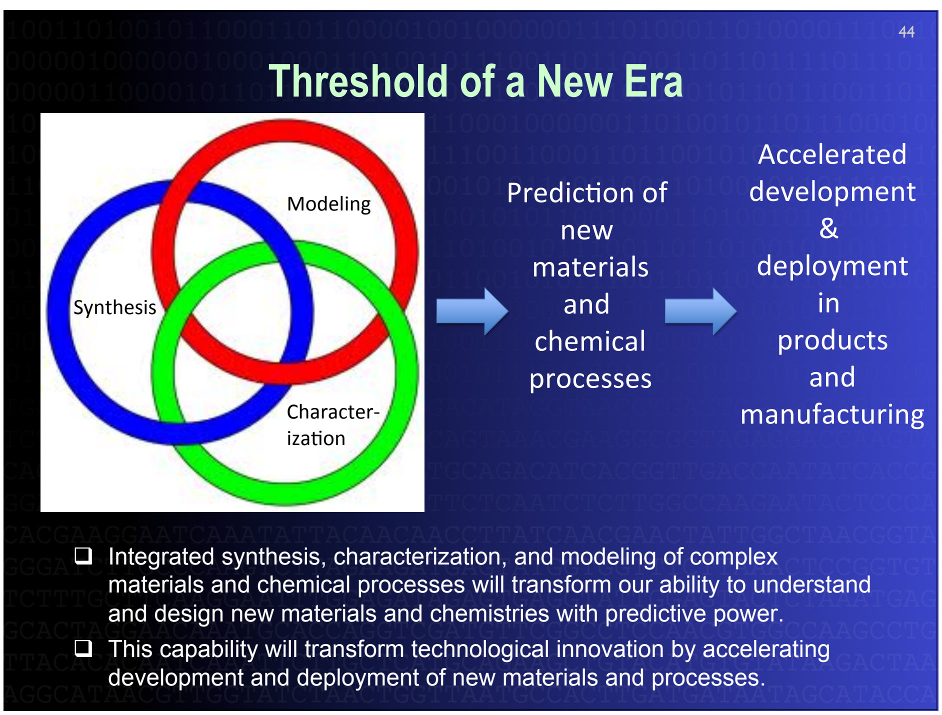
Creating an innovation ecosystem for materials and chemical process design through SBE&S

- ❑Modeling and simulation is today a key tool throughout science and engineering.
- ❑However, while models and methods are well understood in some engineering fields, and modeling tools are embedded within several related industry sectors, SBE&S capabilities for materials research are much less mature.
- ❑Although scientific models and algorithms are in hand for many materials applications, critical information is missing for others, and there are only a handful of simulation-based materials design tools sufficiently predictive and robust for industrial use.
- ❑As a result, despite many successful examples of the use of SBE&S, we have only just begun to exploit its full capabilities and promise for discovery and innovation when it comes to the critical pacing technologies of new materials.

A Tipping Point

- ❑ Over the past two decades, the US has developed and deployed – through x-ray and neutron sources, nanoscale science facilities, and high-performance computers - the world's most powerful collection of tools to make, interrogate, and model materials and chemical systems at nanometer scales.
  - *Unprecedented view of the atomic-scale structure and dynamics of materials and the molecular-scale basis of chemical processes.*
  - *For the first time in history, we can make, interrogate, and model materials and chemical behavior at the length scale – the nanoscale - where this behavior is controlled.*

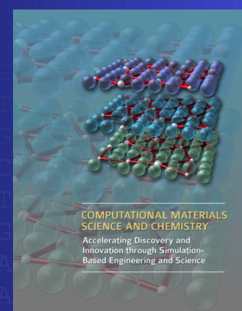

43
Since 2000, capability increased by a million from advances in hardware and software, enabling the development of materials simulations of unprecedented fidelity.
GigaFlops (1e9 FLOPS)
1.E+13
1.E+11
1.E+09
1.E+07
1.E+05
1.E+03
1.E+01
1.E-01
1970
1980
1990
2000
2010
2020
2030
Multicore Era
1 PFlops
NNSA Roadrunner
DOE SC Jaguar
NNSA Sequoia (Est.)
NSF Blue Waters (Est.)
Massively
1 TFlops
Vector
1 Gflops
From 2010 NRC study on modeling, simulation and games, compiled from data from Top500.org


44
Threshold of a New Era
Modeling
Synthesis
Character-ization
Prediction of new materials and chemical processes
Accelerated development & deployment in products and manufacturing
❑ Integrated synthesis, characterization, and modeling of complex materials and chemical processes will transform our ability to understand and design new materials and chemistries with predictive power.
❑ This capability will transform technological innovation by accelerating development and deployment of new materials and processes.

Foundational Predictive Capabilities

DOE Office of Science Workshop Report on Computational Materials Science and Chemistry: Accelerating Discovery and Innovation through Simulation-Based Engineering and Science

- Breakouts/chapters
  - *Materials for extreme conditions: Controlling microstructures*
  - *Designing and engineering materials at the nanoscale: Understanding and controlling self-assembly*
  - *Light harvesting: Photons to energy*
  - *Controlling chemical reactions: Combustion and catalysis*
  - *Designer fluids: Separations and carbon capture*
  - *Designer interfaces: From interfacial materials to advanced batteries*
  - *Controlling electronic structure: Modeling strongly correlated electrons*



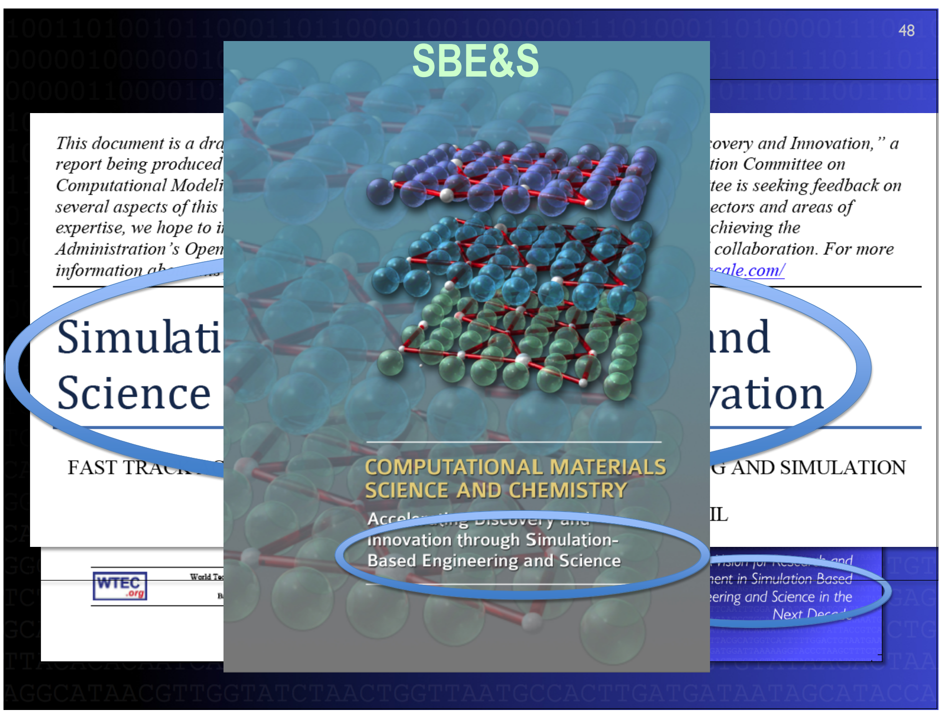
Preparing an SBE&S Workforce

SBE&S experts and just SBE&S-"savvy"

- Insufficient exposure to computational science & engineering and underlying core subjects in high school and undergraduate
- Increased topical specialization beginning with graduate school
- Insufficient training in HPC – *an educational "gap"*
  - *Gap b/t domain science courses and CS courses; insufficient "continued learning" opportunities related to* ***programming for performance***
  - *Gap b/t current CSE curricula and knowledge/skills needed for multicore, petascale, etc.*
- Students use codes as black boxes; who will be innovators?
- No real training in software engineering for sustainable codes
- Little training in UQ, V&V, risk assessment & decision making
- Institutions stove-piped and non-committal to CS&E (but graduate certificate programs abound), but faculty, students eager for structure.
  - *E.g. Virtual School of Computational Science & Engineering*
- New ideas, approaches, partnerships, commitment needed!

Data: Part of the SBE&S Ecosystem

- Open databases and digital libraries for broad classes of materials will be needed to expedite model and code validation
- Managing, storing, sharing, utilizing and visualizing data is a critical part of SBE&S
- Large data sets are increasingly important in materials research (experimental & simulational)
  - *Can easily generate 100's of terabytes of useful data overnite. How to adapt? How to think about research approach?*
- Data issues/opportunities involve:
  - *Integration of heterogeneous data from disparate sources (not like bioinformatics)*
  - *Sharing, reuse of, dealing with data "locally" (individual, group, team, community)*
  - *Data as a "public good"*
- Finding of SBE&S International Study (2009) – materials is behind
- Recommendation of SBE&S Vision Study (2010) – transform data into a critical national asset
  - *Institutionalize data life-cycle*
  - *Meet challenges of managing massive amounts of data from everywhere*
  - *Appreciate data as inextricable part of SBE&S*



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Exciting time for scientific computing!

Computational Science and Engineering

Simulation-Based Engineering & Science

Computational Modeling & Simulation

Scientific Computing

Computational & Data-Enabled Science and Engineering

★ ★ ★ ★ = $$$$

Predictive capability for discovery and innovation

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Conclusions

- Unanimity of findings throughout all reports
  - *SBE&S is critical to future of U.S. science and technology Education, training, but seriously underfunded at federal level*
  - *HPC world is flat*
  - *Multi-core revolution*
  - *Education and training are critical constraints*
- Unanimity of recommendations throughout all reports
  - *SBE&S should be elevated to much higher-profile, dramatically better-funded activity*
  - *Large group activities in addition to single-PI and small-group grants*
  - *University/industry/national lab coalitions*
- Chemical engineers
  - *Pioneers in use of modeling and simulation in fundamental research and industrial design*
    - *FLOWTRAN -> ASPEN Tech, PSE,…*
      - *Yet training of students in computation/simulation weakened in recent decades*
  - *Making SBE&S a national priority requires support/push*
    - *Industry groups and academia (e.g., Council on Competitiveness)*
    - *Professional societies (e.g., AIChE)*

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Report Links-Summary

- President's Information Technology Advisory Committee Report on Computational Science: Ensuring America's Competitiveness (PITAC) [2005]
  - http://www.itrd.gov/pitac/reports/20050609_computational/computational.pdf
- Revolutionizing Engineering Science through Simulation (NSF) [2006]
  - http://www.nsf.gov/pubs/reports/sbes_final_report.pdf
- Simulation and Modeling at the Exascale for Energy, Ecological Sustainability and Global Security (DOE OASCR) [2007]
  - http://www.er.doe.gov/ascr/ProgramDocuments/Docs/TownHall.pdf
- Integrated Computational Materials Engineering (National Academies) [2008]
  - http://www.nap.edu/catalog.php?record_id=12199
- Potential Impact of High-End Capability Computing on Four Illustrative Fields of Science and Engineering (National Academies) [2008]
  - http://www.nap.edu/catalog.php?record_id=12451
- International Assessment of Research & Development in Simulation-Based Engineering & Science (SBE&S) [2009]
  - http://www.wtec.org/sbes/
- Inventing a New America through Discovery and Innovation in Science, Engineering and Medicine [2010]
  - http://www.nsf.gov/mps/ResearchDirectionsWorkshop2010/RWD-color-FINAL-usletter_2010-07-16.pdf
- Computational Materials Science & Chemistry [2010]
  - http://www.er.doe.gov/bes/reports/files/CMSC_rpt.pdf