WTEC International Assessment of Simulation-based Engineering and Science

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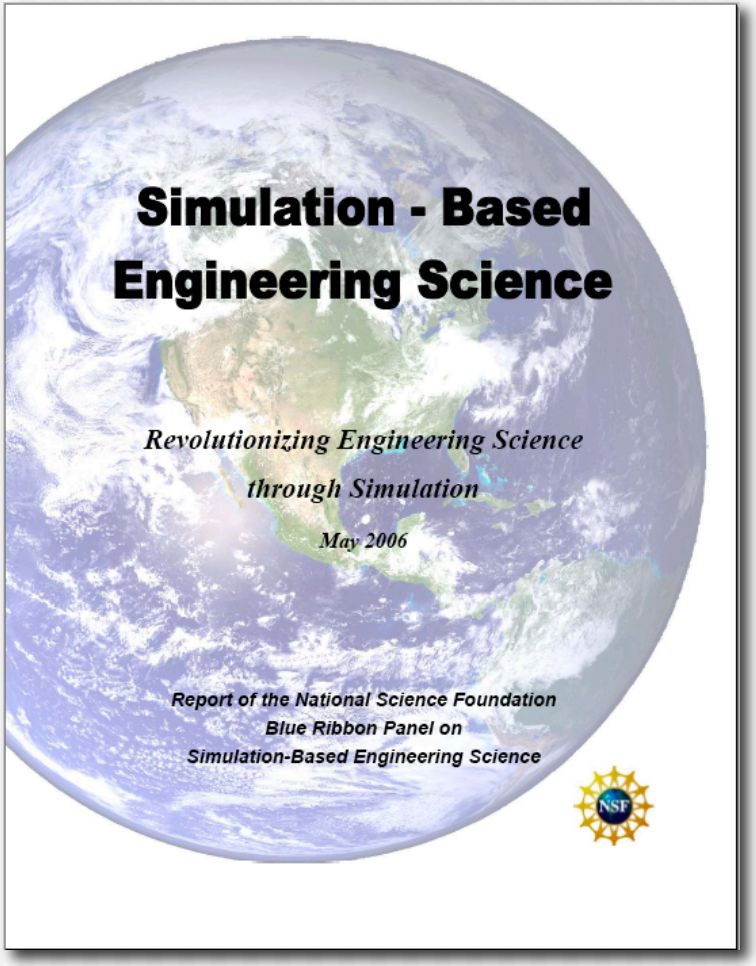
Background

- Workshops run by NSF Engineering Directorate (originated within mechanical engineering division)
- NSF Blue Ribbon Panel report chaired by J. Tinsley Oden
- Final report completed May 2006



http://www.nsf.gov/pubs/reports/sbes_final_report.pdf

Oden Blue Ribbon Panel Report on SBES

- Purpose: "To explore the emerging discipline of Simulation-Based Engineering Science, its major components, its importance to the nation, the challenges and barriers to its advancement, and to recommend to the NSF and the broader community concerned with science and engineering in the United States, steps that could be taken to advance development in this discipline."
- Scope: Medicine, Predictive Homeland Security, Energy & Environment, Materials, Industrial & Defense Applications, and core pervasive issues

Major findings of Oden report

- "Advances in mathematical modeling, in computational algorithms, in the speed of computers, and in the science and technology of data intensive computing have brought the field of computer simulation to the threshold of a new era, an era in which unprecedented improvements in the health, security, productivity, and competitiveness of our nation may be possible. A host of critical technologies are on the horizon that cannot be understood, developed, or utilized without simulation methods."
- "The great benefits of these advances are in the realm of engineering, but they will require basic research in the scientific components of modeling, simulation, computing, and other areas."

Oden report: SBES education & funding models

- Finding: "Educating tomorrow's engineers and scientists in SBES will require that the student acquire substantial depth in computational and applied mathematics and underlying scientific disciplines. This must be made possible through multidisciplinary programs. This will require dramatic changes in science and engineering educational systems."
- Finding: There is a need for "…changes in organizational structures and a new parallel program in SBES"
- Finding: "Long-range core funding of SBES will require changes in organizational structures."

Oden report

- "Our competitors in Europe and Asia are building on U.S.-pioneered developments of the 20th century and are making major investments in simulation research."
- "There is much concern that the US is rapidly losing ground to Western Europe, East Asia, and Japan …."

Background: Next steps

- NSF planning for major initiative in SBE&S (note ampersand), joint between ENG and MPS directorates
- Potential for multi-agency joint initiative like NNI
- Next steps: perform international comparative study of SBE&S, followed by a Research Directions workshop (like NNI)
  - Study done through World Technology Evaluation Center (WTEC)
  - Nearly 30 program managers from six agencies on board (NSF, DOE, NIH, NASA, DOD, NIST)
  - Over $750K raised for this study; more than for any previous study

WTEC study: Goals

- Gather key data needed to assess:
  - where US is leading, trailing, or in danger of losing leadership in SBE&S
  - where critical investments in SBE&S needed to maintain or gain US leadership, and how those investments will impact R&D in strategic areas for US (materials, energy, life sciences/medicine)
- Provide sufficient analysis and guidance to inform and shape development of multi-agency federal initiative in SBE&S

WTEC study: Strategy

- US baseline workshop
  - 1.5 days in June
- Solicit input from colleagues in US and abroad
- Bibliometrics study
  - Trends in publication, funding & organizational structures, new programs, doctorates awarded, etc.
- Two international trips to Europe and Asia
  - Visits to companies, national labs, universities
- Research directions workshop
- Final report with interim report-outs, and standalone executive summary.

Technical scope of WTEC study

- 3 thematic pillars
  - Will serve as very broad, key encompassing themes, to be refined by panel and available data as study develops.
- Crosscutting core issues (as in Oden report)
- Education & training
- Funding & organization structures

Technical scope: application areas/thematic pillars

- Materials
  - SBE&S critical for next-generation materials design, innovation and engineering from building blocks to function.
- Energy & sustainability
  - SBE&S critical in discovering and developing alternative energy solutions and in designing sustainable infrastructure.
- Life sciences
  - Computational science has made inroads in many biomedical domains, especially genomics and proteomics. Current challenge is application of SBE&S to clinical medicine & bio systems at cellular, tissue and organ scales. We will focus on intersection of life sciencess and materials and informatics.

Crosscutting themes: nano, complex systems, predictive design

...where CI meets SBE&S

Technical scope: Core issues

WTEC study will assess and quantify progress & investment in the following core issues identified by Oden report:

- Tyranny of scales: multiscale simulation
- Validation, verification and uncertainty quantification
- New vistas in simulation software
  - Including open source codes, commercial packages, computational steering, dynamic data driven simulation systems, etc.
- Big data and visualization
- Next generation algorithms & computational performance
- Education & training of the next generation of simulators

Committee structure

- Chair (SCG)
- ~ 8 panelists (including deputy or co-chair)
  - Scientists, engineers, applied mathematicians
  - Coverage of thematic areas, core issues (e.g. V&V, HPC, software)
- ~ 4-8 advisory committee members
  - Avail ourselves of visionaries, architects of initiatives at "arms length" from study (i.e. non-simulators)
  - Sounding board; provide guidance to panel to develop a report of highest possible impact

Timeline

- March 07 - Chair confirmed; meeting with sponsors
- Spring 07 - Panelists confirmed. Meeting with panel & sponsors.
- Summer 07 - US baseline workshop, some US trips, bibliometrics analysis: prelim report to sponsors; planning of int'l trips
- Fall 07 - Two international trips
- Late Fall 07 - Public workshop to report findings to sponsors
- Winter 08 - Research Directions Workshop and report
- Spring/Summer 08 - Full report completed

NATIONAL MATERIALS ADVISORY BOARD

CICME

Committee on Integrated Computational Materials Engineering

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What is CICME?

The National Materials Advisory Board has formed the Committee on Integrated Computational Materials Engineering (CICME) to

- Identify critical paths forward and propose a strategy to facilitate innovation in the interdisciplinary field of computational materials engineering;

- Improve knowledge sharing among researchers, developers, and designers across the research programs supported by the federal government; and

- Identify the challenges associated with gaps in knowledge and understanding.

Statement of Task for ICME

The focus of this study is very much on the I and E of ICME – that is on the development of a comprehensive, integrated suite of verified computational materials models linked to models for simulating manufacturing processes and engineering design.

Such a suite of tools in a robust, user-friendly computational environment would enable simultaneous optimization of manufacturing process and component design, material selection or rapid materials development.

In summary the committee is charged with the following tasks:

- **1. The exploration of the benefits and promise of integrated computational materials engineering (ICME) to materials research through a series of case studies of compelling materials research themes that are enabled by recent advances and accomplishments in the field of computational materials.**
- **2. An assessment of the benefits of a comprehensive ICME capability to the national priorities.**
- **3. The establishment of a strategy for the development and maintenance of an ICME infrastructure, including databases and model integration activities. This should include both near-term and long-range goals, likely participants and responsible agents of change.**
- **4. Making recommendations on how to best meet the identified opportunities.**

Who is CICME?

Tresa M. Pollock, University of Michigan *Chair*
John Allison, Ford Research Laboratory *Vice-Chair*

Daniel Backman, Worcester Polytechnic Institute
Mary Boyce, Massachusetts Institute of Technology
Anthony G. Evans, University of California, Santa Barbara
Mark Gersh, Lockheed Martin Space Systems Company
Elizabeth A. Holm, Sandia National Laboratories
Richard LeSar, Iowa State University
Mike Long, Linux Networx Inc
Adam Powell, Veryst Engineering, LLC
Jack J. Schirra, Pratt & Whitney
Deborah DeMania Whitis, GE Aircraft Engines
Christopher Woodward, Air Force Research Laboratory

When will CICME be done?

Meeting Schedule

First Meeting:	November 30 – December 1, 2006 in Washington, DC
Second Meeting	March 13 – March 14, 2007 in Washington, DC
Third Meeting	May 29 – May 31, 2007 in Irvine, CA
Final Meeting	October 18 – October 19, 2007, in Irvine, CA (closed)

First meeting focused on hearing from the study's sponsors and other government agencies:

- Sponsors: DOD, DOE-EERE, DOE-NNSA
- Government: NSF-DMR, DARPA, DOE-Nuclear
- Other: iNEMI

Second and third meetings -- focus on hearing from ICME practitioners and other speakers from fields relevant to the charge.

Fourth and final meeting will be closed and will focus on finalizing the committee's report.

Report is due by about March 2008

Web Resources for CICME

http://www.nationalacademies.org/icme

More detail and copies of the presentations from the first two CICME meetings can be found on the web site.

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Committee on Integrated Computational Materials Engineering: Developing a Roadmap for a Grand Challenge in Materials

Summary

The National Materials Advisory Board has formed the Committee on Integrated Computational Materials Engineering to identify critical paths forward and propose a strategy to facilitate innovation in the interdisciplinary field of computational materials engineering; improve knowledge sharing among researchers, developers, and designers across the research programs supported by the federal government; and identify the challenges associated with gaps in knowledge and understanding.

Background

Closely coupling computational models for manufacturing process and engineering design has many important benefits, including decreased time and reduced cost to develop new products and enhanced durability. The missing link, however, has been lack of the robust materials models required to bridge these disciplines. Because of its complexity and broad scope, materials engineering is a decade or more behind other engineering disciplines in developing a core set of computational tools available to practicing engineers. Finite element analysis and computational fluid dynamics are central to undergraduate curricula in mechanical engineering and are routinely used by practicing engineers in manufacturing and engineering design. There is no analogous computational tool available to materials engineers despite major accomplishments in computational materials science.

The vision for Integrated Computational Materials Engineering (ICME) is the development of a comprehensive, integrated suite of verified computational materials models linked to models for simulating manufacturing processes and engineering design. Such a suite of tools in a robust, user-friendly computational environment would enable simultaneous optimization of manufacturing process and component design, materials selection or rapid materials development. A strategy to develop ICME could include initiatives in several areas: Methods and Tools; Databases and Informatics; Dissemination and Infrastructure.

Study Plan

In carrying out this study the committee will identify critical paths forward and propose a strategy to facilitate innovation in this interdisciplinary field; improve knowledge sharing among researchers, developers, and designers across the research programs supported by the federal government; identify the challenges associated with gaps in knowledge and understanding. Issues that might be considered include: workforce and educational needs for progressing the identified goals for the field; the separate roles of professional societies, software firms and academic institutions in development and maintenance of the infrastructure, and identifying the connections between research in computational materials engineering and other fields, in particular, emerging software and web-based technologies.

In summary the committee's statement of task involves:

1. Exploration of the benefits and promise of integrated computational materials engineering (ICME) to materials research through a series of case studies of compelling materials research themes that are enabled by recent advances and accomplishments in the field of computational materials. To be included in these case studies is an examination of the Return on Investment of computational science and simulation in the materials engineering arena.

2. Assessment of the benefits of a comprehensive ICME capability to the national priorities including the processing-structure-properties relationships of materials.

3. Establishment of a roadmap for the development and maintenance of an ICME infrastructure, including databases and model integration activities. This should include both near-term and long-range goals, likely participants and responsible agents of change.

4. Suggest strategies to best meet the identified opportunities

Membership

- Tresa M. Pollock, University of Michigan, Chair
- John Allison, Ford Research Laboratory, Vice Chair
- Daniel Backman, Worcester Polytechnic Institute
- Mary Boyce, Massachusetts Institute of Technology
- Anthony G. Evans, University of California, Santa Barbara
- Mark Gersh, Lockheed Martin Space Systems Company
- Elizabeth A. Holm, Sandia National Laboratories
- Richard LeSar, Iowa State University
- Mike Long, Linux Networx Inc
- Adam Powell, Veryst Engineering, LLC
- Jack J. Schirra, Pratt & Whitney
- Deborah DeMania White, GE Aircraft Engines
- Christopher Woodward, Air Force Research Laboratory

The biographies of the committee can be viewed at the NRC Current Projects System.

potential study title/scope:

"Computation for Next Generation Devices"

• study should dovetail with developing initiative on simulation-based science and engineering (NSF-run or NSF-lead initiative, possibly for FY09)

• to focus on new opportunities for computational materials science and materials physics

• not length scale or method driven, goes beyond quantum mechanics

• highlight intersections with other fields (energy [solar, hydrogen, biofuels], medicine/biology, electronics [eg, devices, batteries, post-CMOS])

• identify the fundamental advances that are needed in computation to enable the development of next generation devices

•committee formed by both theorists and some experimentalists.

• sample topics: patterned materials, self-organization, oxide heterostructures and electronics, force fields, kinetics, multiscale modeling, integrating statistical mechanics, interfaces between organics/inorganics/hydrogen, optimizing materials structure at the nano/micro-scale for efficient electronic transport, multilayer materials, molecular conductors, quantum dots.

  •Crystalline as well as disordered materials, polymers, macromolecules, nanostructures and systems of reduced dimensionality.

  •Additional challenges include efforts and algorithms to properly model molecules on varying scales, quantum decoherence, qbits, accurate time dependence, understanding transport across hard/soft material interfaces.

  •Emphasis will be on prediction via simulation.

  •Find from experimentalists what it is that they badly need (eg, the modes of oscillation for a molecule acting as a bridge between leads).

• could focus on the intersection between the National Nanotechnology Initiative and the developing simulation-based science and engineering initiative

• focus on nanoscale and some mesoscale but not beyond mesoscale

• integration of nanostructures into functional devices