Simulation-Based Engineering Science

Report of the NSF SBES Panel
to the
NSF Engineering Advisory Committee

National Science Foundation

May 3, 2006

Preliminaries

Purpose of the BRP:

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.

Blue Ribbon Panel:

J. Tinsley Oden (Chair) - UT Austin

Jacob Fish - Rensselaer Polytechnic Institute

Chris Johnson – University of Utah

Alan Laub - UCLA

David Srolovitz - Princeton

Ted Belytschko - Northwestern

Thomas J.R. Hughes - UT Austin

David Keyes – Columbia University

Linda Petzold - UCSB

Sidney Yip - MIT

SBES – A National Priority

The Promise:

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.

Why Engineering Science?

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. For this reason, we refer to the discipline as simulation-based engineering science: SBES.

SBES – A National Priority

SBES

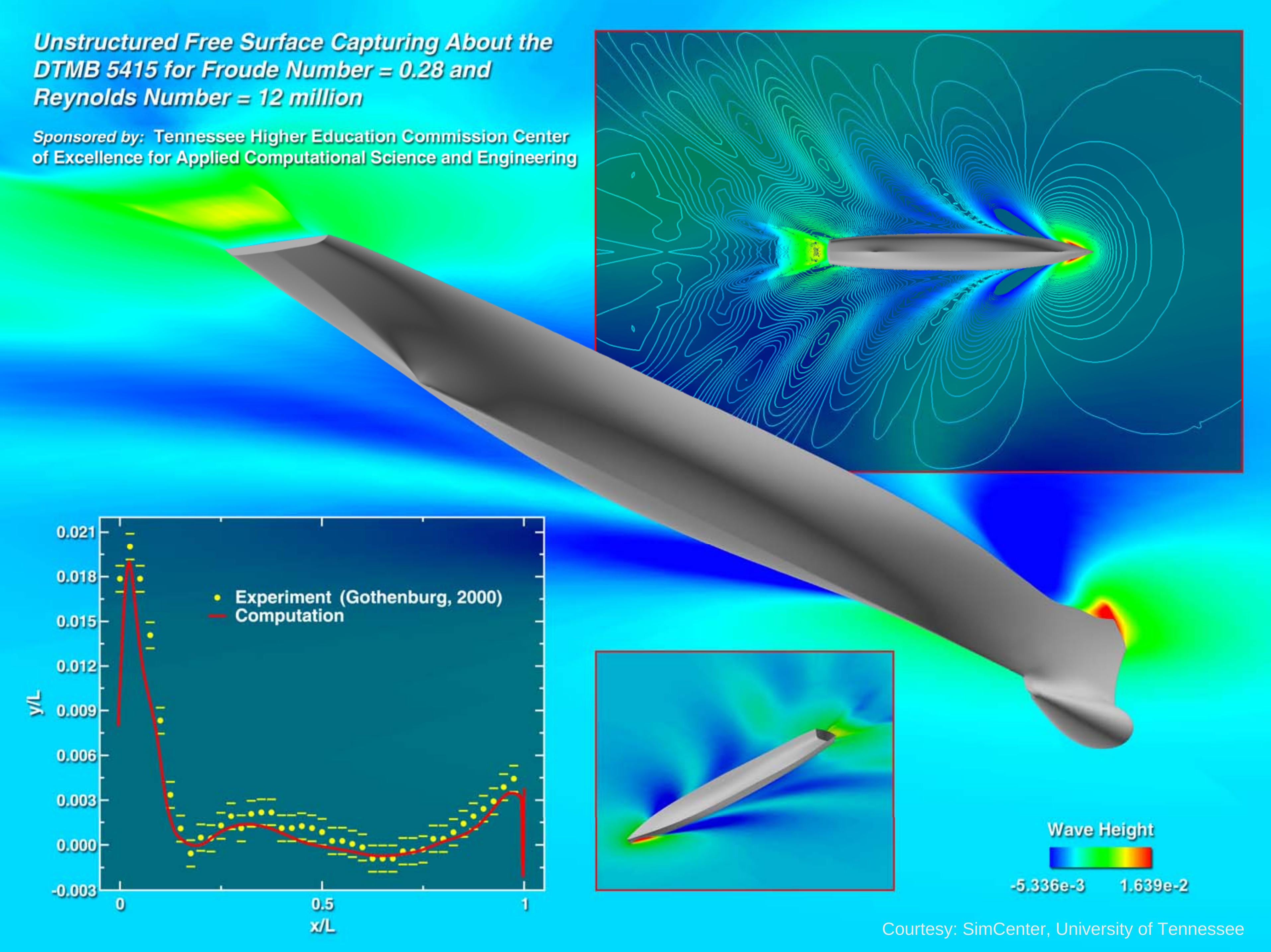
- Focuses on modeling and simulation for prediction physical events and behavior of complex engineered systems.
- Also address methods, devices, processes, and planning.
- Draws on advances in optimization, multiscale modeling, control, uncertainty quantification, inverse analysis, verification and validation, interactive visualization, and real-time response modeling.
- Addresses the most difficult aspects of modeling, engineering design, manufacturing, and scientific discovery.

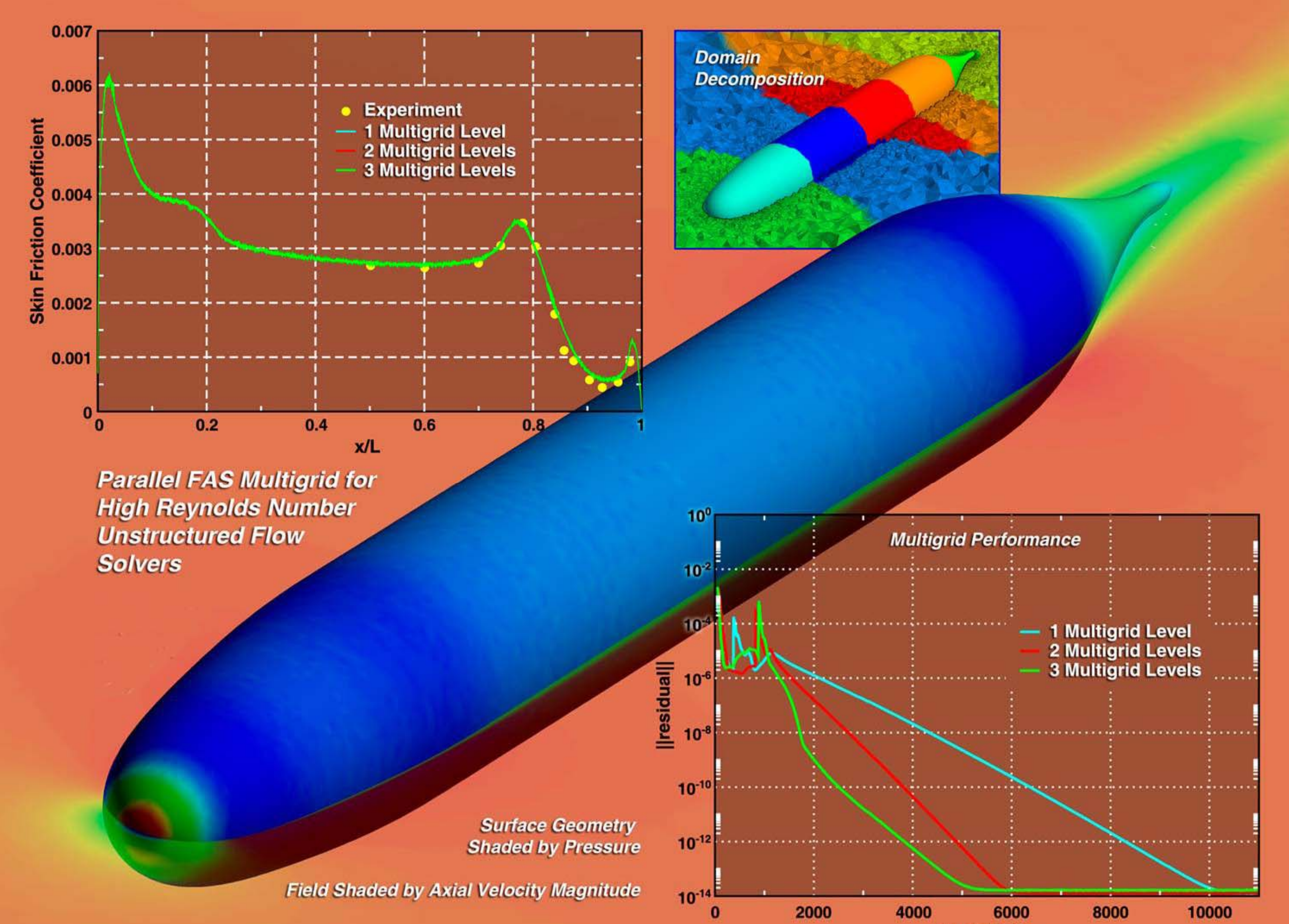
Why Now?

1. The remarkable developments in computational and computer sciences, in computing equipment and infrastructure over the past decade have brought simulation theory and technology to the brink of a new era, one that can have a dramatic impact on all areas of engineering science.
2. A host of critical technologies are on the horizon that cannot be understood, developed, or utilized without simulation methods.

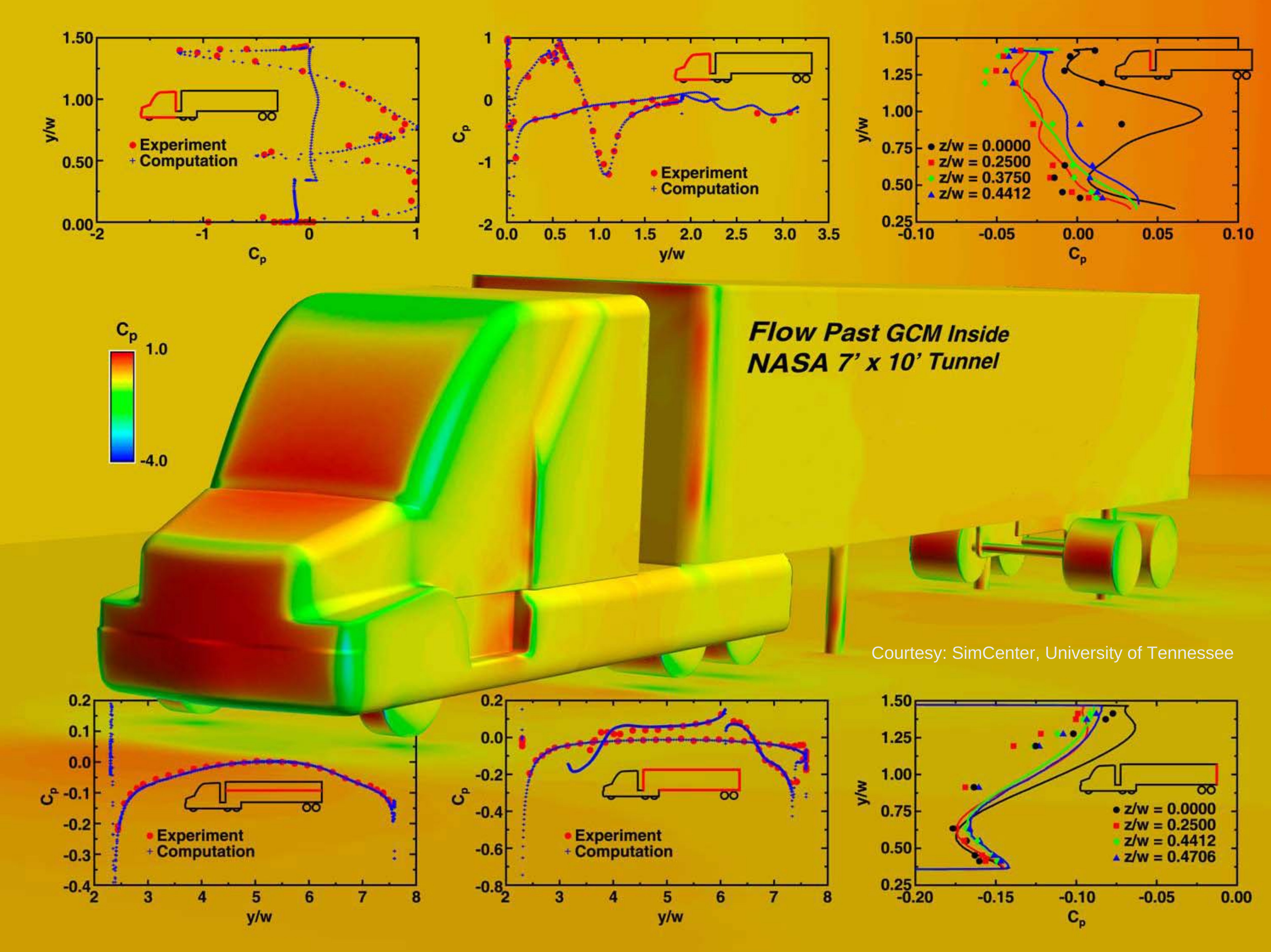
Recent Simulation Advances

- **Industrial Applications**
- **Medical Planning**
- **Weather Prediction**
- **Homeland Security**
- **Astrophysics**
- **Micro and Nano Devices**

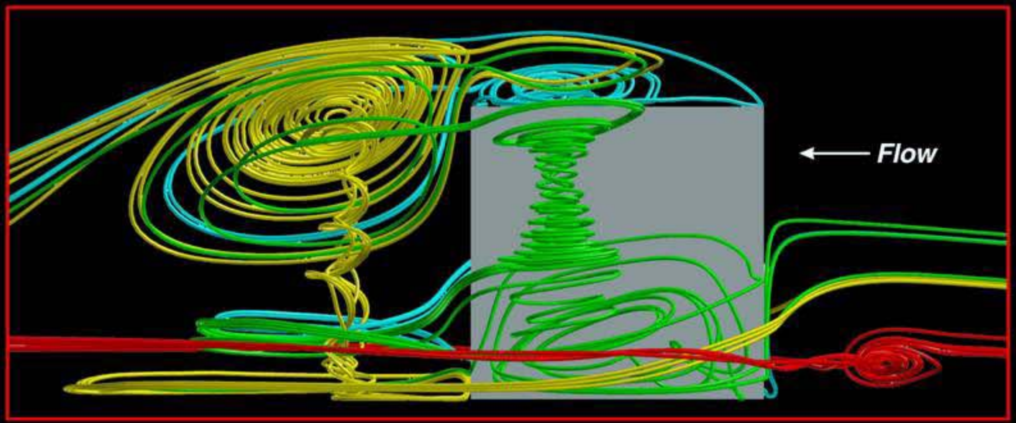

Unstructured Free Surface Capturing About the DTMB 5415 for Froude Number = 0.28 and Reynolds Number = 12 million
Sponsored by: Tennessee Higher Education Commission Center of Excellence for Applied Computational Science and Engineering
Experiment (Gothenburg, 2000)
Computation
y/L
x/L
0.021
0.018
0.015
0.012
0.009
0.006
0.003
0.000
-0.003
0
0.5
1
Wave Height
-5.336e-3
1.639e-2
Courtesy: SimCenter, University of Tennessee

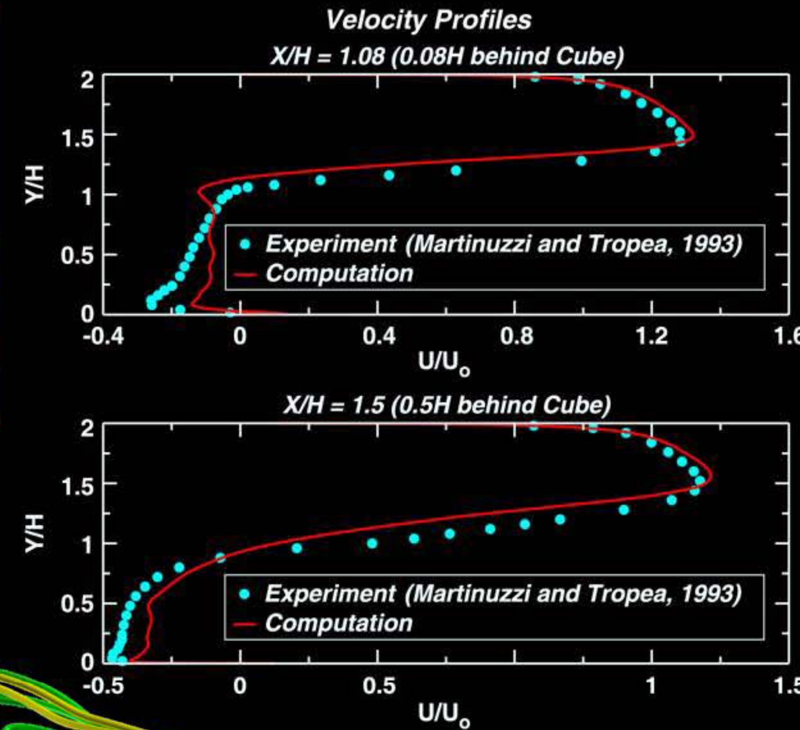


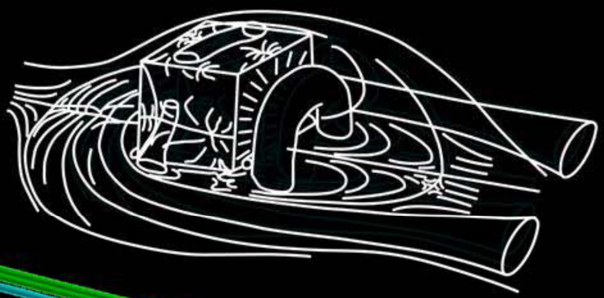
Courtesy: SimCenter, University of Tennessee

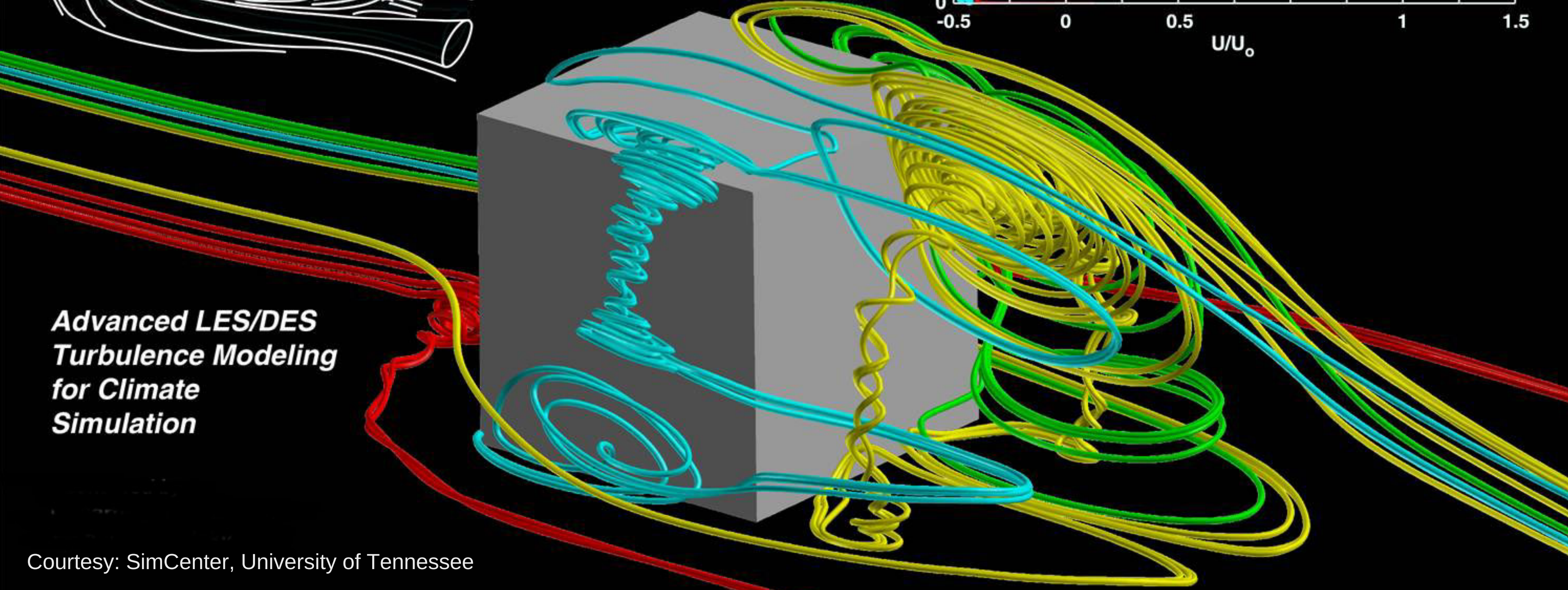


Flow Past GCM Inside
NASA 7' x 10' Tunnel
Courtesy: SimCenter, University of Tennessee
Cp
1.0
-4.0
Experiment
Computation
y/w
Cp
z/w = 0.0000
z/w = 0.2500
z/w = 0.3750
z/w = 0.4412
z/w = 0.4706





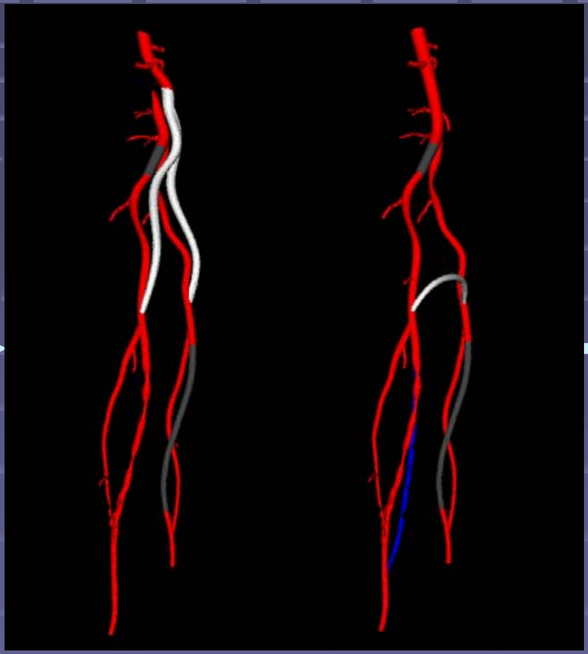




Advanced LES/DES Turbulence Modeling for Climate Simulation

Courtesy: SimCenter, University of Tennessee

Computer-Aided Medical Planning



Patient-specific models constructed from diagnostic imaging data

Computer simulations of blood flow to evaluate alternate treatments

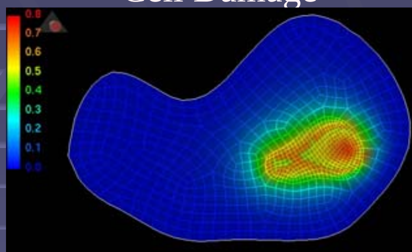
Blood Flow Simulation of Heart-Vein-Artery System

- 3D MR Image of heart and aorta of healthy 46 year old man.
- Computational analysis of 3D pulsatile aortic flow field.

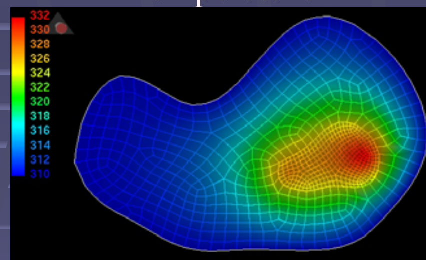
Courtesy: CvE, University of Texas at Austin

Cancer Research and Laser Surgery

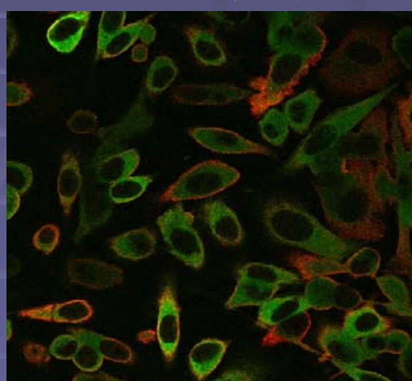
Cell Damage



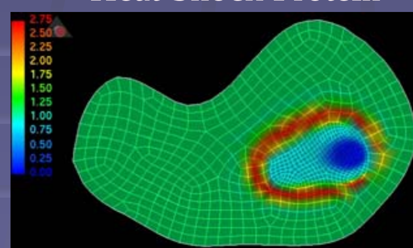
Temperature

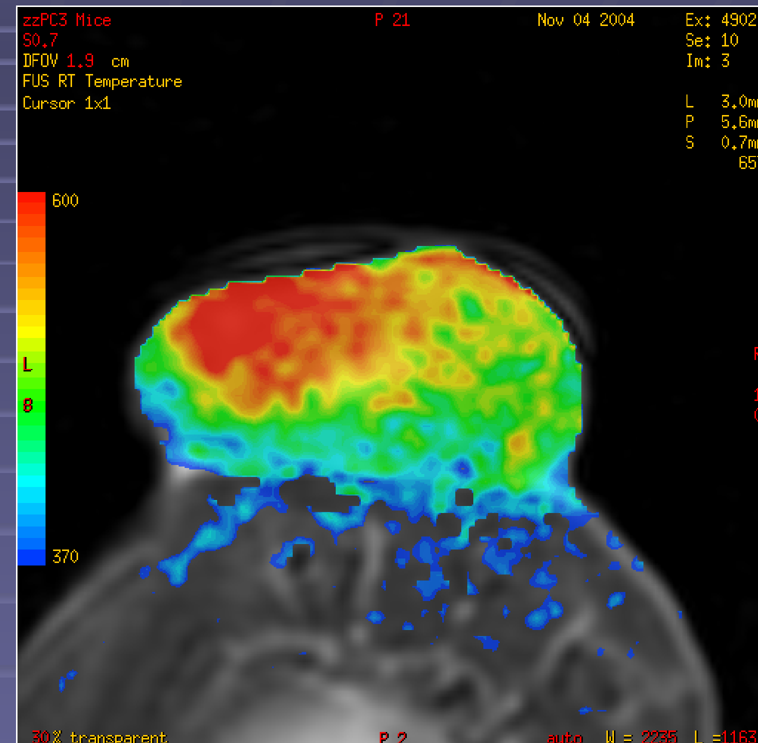


HSP27(Green),
HSP70(Red)



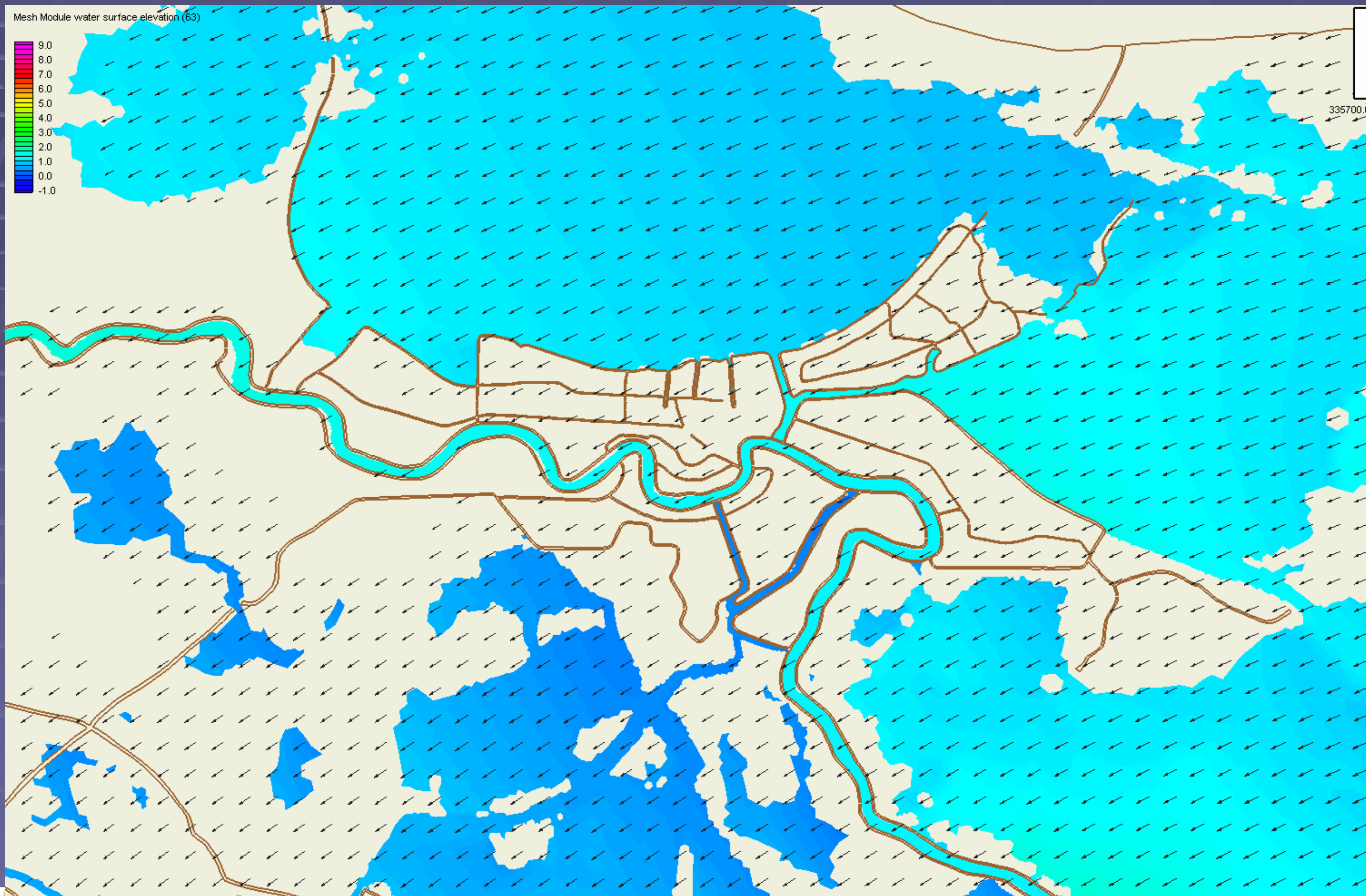
Heat Shock Protein



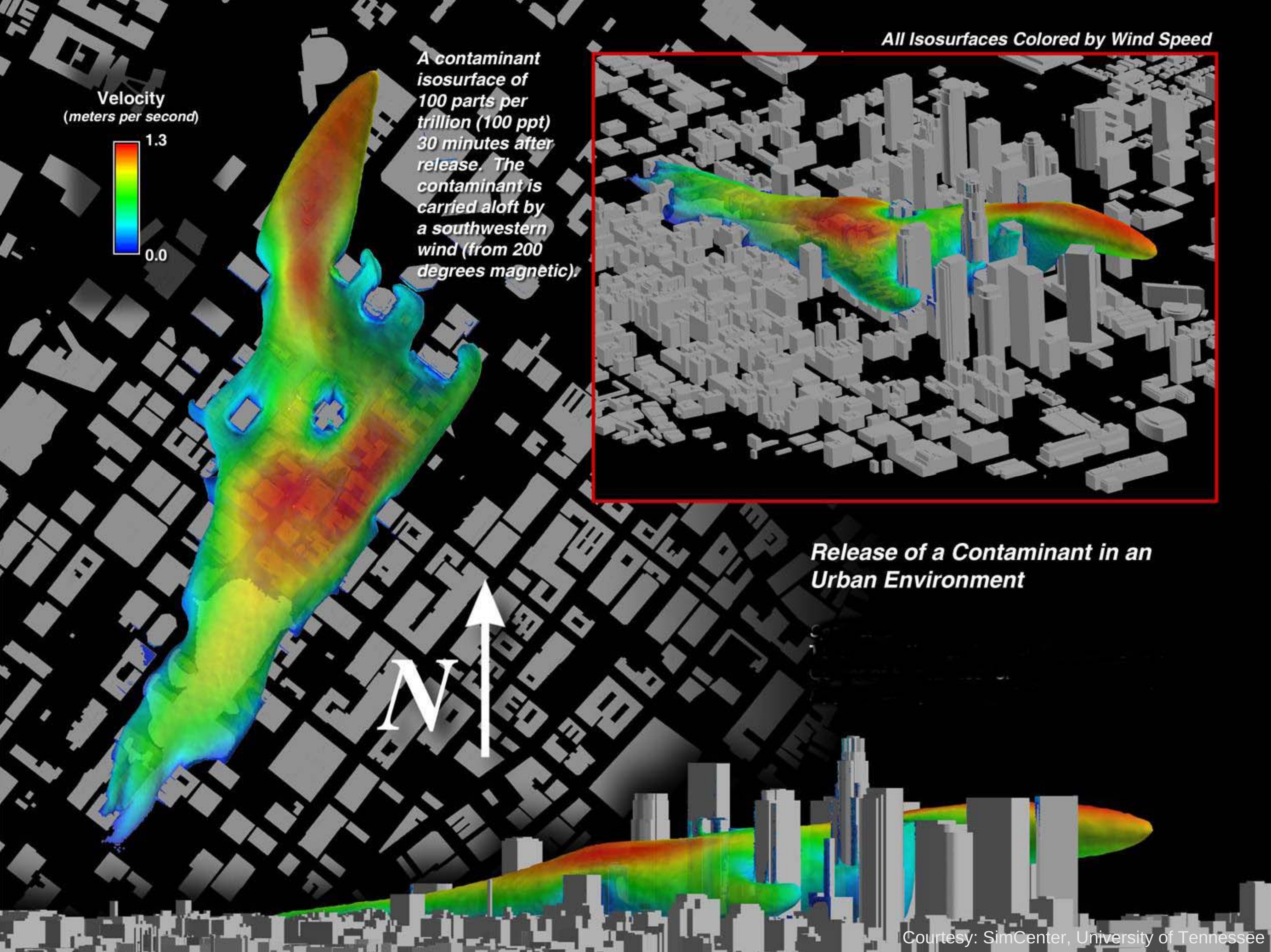


Laser surgery promises to treat clusters of cancerous tumors as well as isolated tumors. However, accurately predicted HSP distribution and cell damage will lead to a better treatment planning to prevent cancer recurrence.

Hurricane Katrina Hindcast

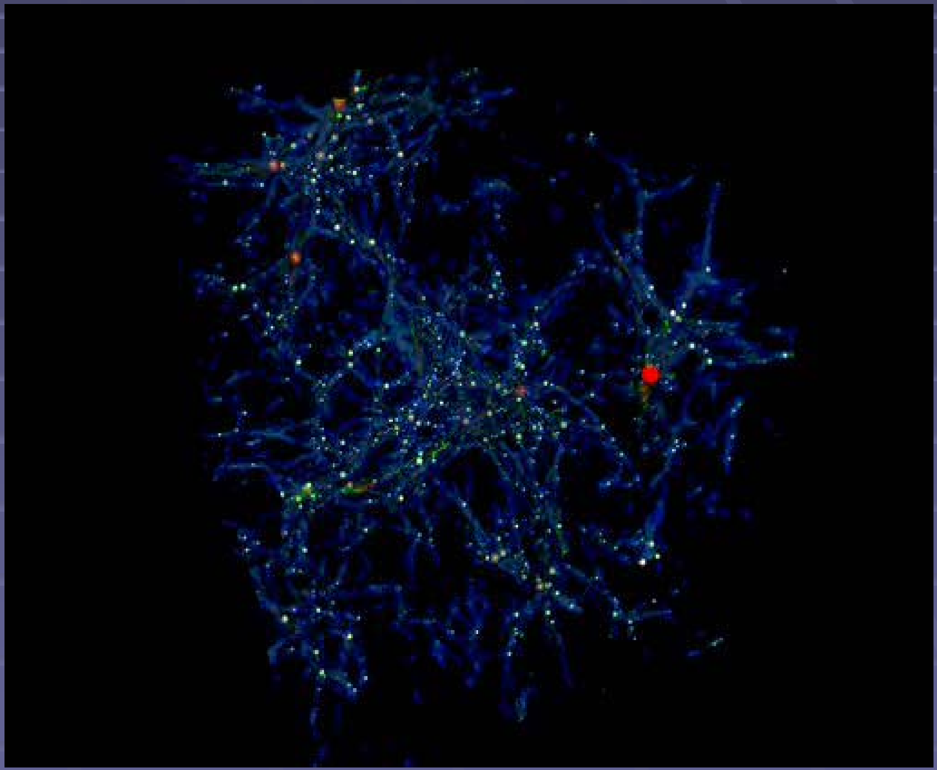


Courtesy: CSM, University of Texas at Austin


Velocity
(meters per second)
1.3
0.0
A contaminant isosurface of 100 parts per trillion (100 ppt) 30 minutes after release. The contaminant is carried aloft by a southwestern wind (from 200 degrees magnetic).
All Isosurfaces Colored by Wind Speed
Release of a Contaminant in an Urban Environment
N
Courtesy: SimCenter, University of Tennessee

Simulation of Galaxy Formation

- Simulates the general expansion of comoves
- Redshift z = 9 corresponding to 3.26 million light years earlier in time
- Dark matter halos:
  - red = 100 million solar masses
  - blue = 400,000 solar masses

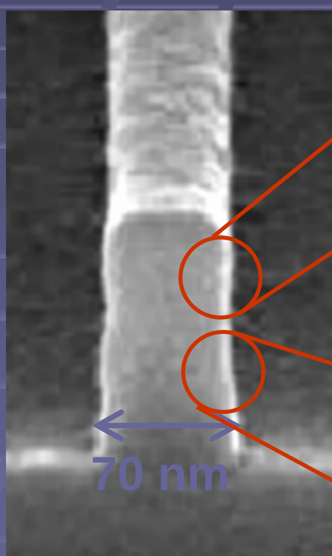


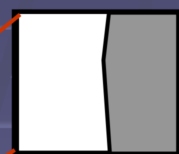
Courtesy: CVC, University of Texas at Austin

Micro and Nano-Mechanics

Nanofabrication – Simulation of Semiconductor Processes

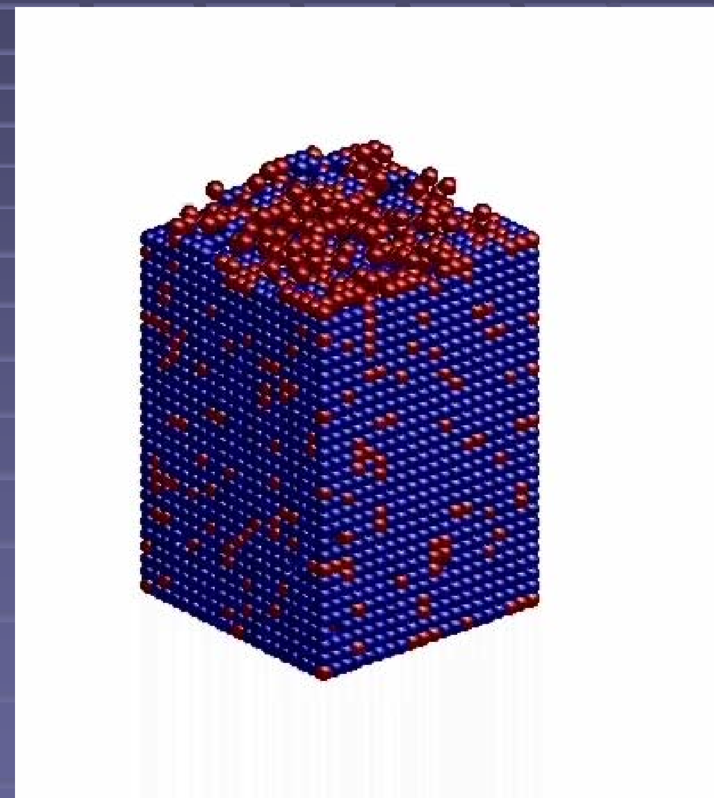
Dimensions of features are at a scale where the effects of individual molecules are important.





Continuum models are unable to simulate roughness.

A molecular approach is suited for simulating roughness.



Polymer dynamics simulation of solvent evaporation and shrinkage in semiconductor simulation

Courtesy: WRG, University of Texas at Austin

SBES: Complements Several Studies Pointing to the Urgency of Advancement in Simulation

- Lax Report (1982)
  - "Increased research in computational mathematics, software, and algorithms necessary to the effective and efficient use of supercomputer systems."
- SciDAC (2000) ; SCaLeS (2003-2004)
  - "It is time to take full advantage of the revolution in computational science with new investments that address the most challenging scientific problems…"
- Roadmap for Revitalization of HEC (2003); Federal Plan for HEC (2004)
  - "US capability in science and engineering is increasingly being called on to address urgent challenges in national and homeland security…health care, and environmental protection…current programs will neither maintain US leadership nor keep pace with accelerating growth of demand for HEC resources"
- Revolutionizing Science and Engineering Through Cyberinfrastructure (2003)
  - "This Panel believes that the National Science Foundation has a once-in-a-generation opportunity to lead the revolution in science and engineering…"
- PITAC Report (2005)
  - "Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such areas as national security, public health and economic innovation"
- Simulation-Based Engineering Science Report (2006)
  - "The present report enters a domain already reverberating with recent calls to increase the vigor in research and training in computation based simulation in the United States. It is in harmony with its predecessors and owes its brevity to their effective presentations, but it also sounds new notes, emphasizing additional and extremely important elements of simulation that have been overlooked, and adds the voice of engineering that has not been fully heard. "

Foreign Competition in Simulation

- 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.
- Overwhelming data suggests that the US is rapidly losing ground to Western Europe, East Asia, and Japan in producing science and engineering journal articles and in citations in scientific papers. (PITAC, 2005)
- "From 1980 to 2001, the U.S. share of global high-technology exports dropped from 31 percent to 18 percent, while the share for Asian countries rose from 7 to 25 percent" (PITAC, 2005). Since 2001, the trade balance in high-tech products has been negative.
- China is emerging as the chief global economic competitor of the US. In 2003 China graduated approximately 498,000 engineers at the bachelor's level, compared with 70,000 in the US. (Rising Above the Gathering Storm, 2006)

CORE ISSUES: Challenges, Barriers and Opportunities

- Tyranny of Scales
- Verification, Validation, and Uncertainty Quantification
- Dynamic Data Driven Simulation Systems
- Sensors, Measurements, and Heterogeneous Systems
- New Vistas in Simulation Software
- Big Data and Visualization
- Next Generation Algorithms

The Tyranny of Scales: The Challenge of Multi-Scale Modeling and Simulation

Many fundamental and important problems in science and technology involve events taking place over many spatial and temporal scales

- nanoscience and technology
- n
- c
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- a
- a

FINDING:

Formidable obstacles remain in linking highly disparate length and time scales and disciplines in many SBES applications. Fundamental discoveries are needed to surmount these obstacles.

In many … al univ… func… o scale. Tomorrow's technological advances cannot tolerate this partitioned view of nature.

V & V and UQ

Validation: "Are the right equations solved?"

Verification: "Are the equations solved right?"

V&V a … imulation –

the co …

UQ: U …

Data a … challenge

is to c … esults.

FINDING:

V&V and UQ will have a profound impact on the reliability and utility of simulation methods in the future. New theory and methods are needed for handling stochastic models and to quantify uncertainty.

V&V and UQ

Will require major innovations in data-intensive computing, stochastic pde's, statistics, decision theory, etc.

Dynamic Data Driven Application Systems - DDDAS

DDDAS: A new paradigm in computer simulation

involv … 6] in
which … interact
in rea … the
simul

- A c … noted in the
- Co
- Wi … nputing, anc
- Fo

FINDING:

Research is needed to effectively use and integrate data-intensive computing systems, ubiquitous sensors, imaging devices, and other data gathering devices, and to develop methodologies and theoretical frameworks for their integration in dynamic simulation systems.

New Vistas in Simulation Software

- The next generation of engineering problems cannot be supp… code…
- Entir… pment of th… d meth…
- Tom… on algo… throu… l and comp…

FINDING:

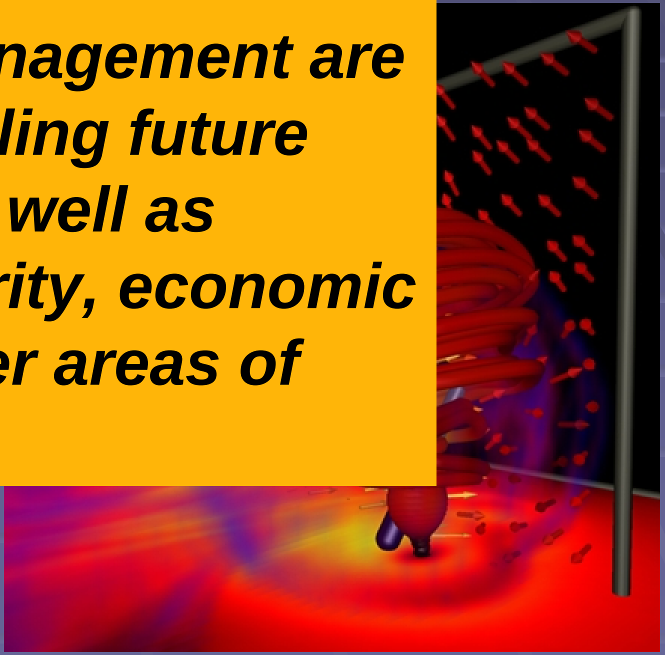
Much of our current software in computational engineering science is inadequate for dealing with multifaceted applications. New software tools, paradigms, and protocols need to be developed so that software is more transferable between application fields, are based on modern algorithms, and function on heterogeneous systems.

Big Data and Visualization

- In all of the SBES challenges, the use and generation of immense data sets is clearly an integral component of SBES
- Visualiza
of comple
human pl
multidime

FINDING:

Visualization and data management are key technologies for enabling future contributions in SBES, as well as scientific discovery, security, economic competitiveness, and other areas of national concern.

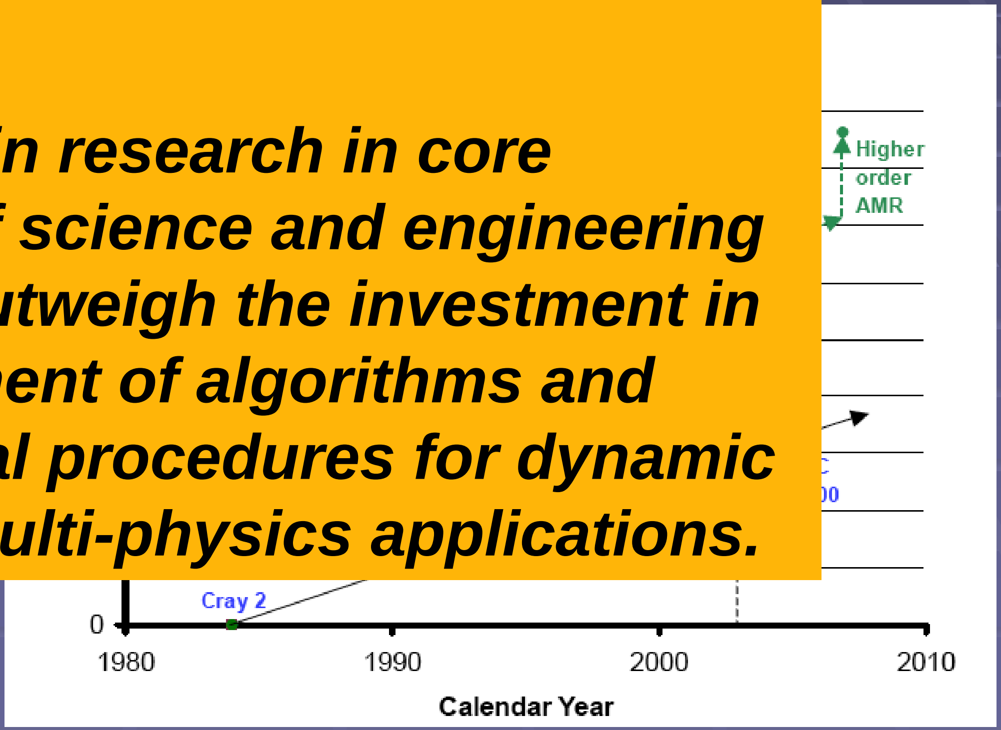


Courtesy: SCI, University of Utah

Next-Generation Algorithms and Performance

Performance Metrics

- Time
- A me
  confi



FINDING:

Investments in research in core disciplines of science and engineering should not outweigh the investment in the development of algorithms and computational procedures for dynamic multiscale, multi-physics applications.

Grand Challenges & The Great Payoff: Applications and Benefits of SBES

- Medicine
- Homeland Security
- Energy and Environment
- Materials
- Industrial Applications
- …

SBES in Medicine

Patient-specific models constructed from diagnostic imaging data

Core Technologies:

- Multiscale Modeling
- Complex Geometry
- Real Time Visualization
- Interacts with Sensors
- V&V, Calibration
- Uncertainty

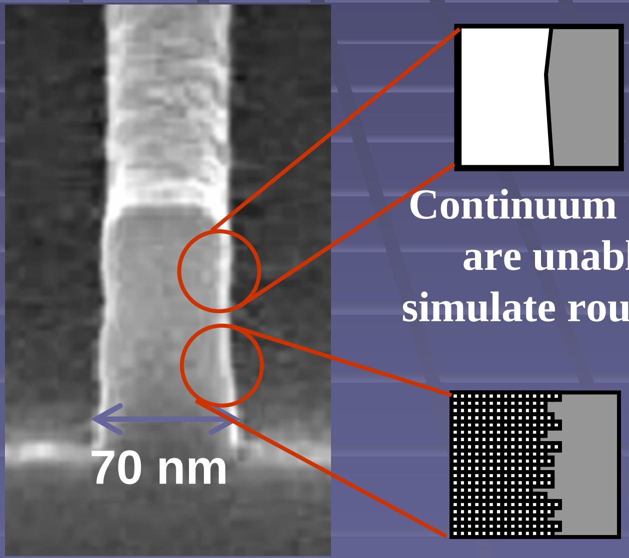
SBES in Materials

Nanofabrication – Simulation of semiconductor processes

Core Technologies:

- Multiscale Modeling
- Complex Geometry
- Real Time Visualization
- Interacts with Sensors
- V&V, Calibration
- Uncertainty

Dimensions of features are at a scale where the effects of individual molecules are important.



Continuum models are unable to simulate roughness.

Molecular models are needed for simulating roughness.

SBES Education for Tomorrow's Engineers and Scientists

- Restructuring of university-level engineering educational systems will be necessary to integrate simulation as a discipline and an engineering tool into the educational exper … for practi…
- Educ … SBES will re … oth in comp … rlying scien … throu…
- NSF … s to open the door for a new generation of multidisciplinary research.

FINDING:

Lasting SBES advances will require dramatic changes in science and engineering education. Interdisciplinary education in computational science and computing technology will be essential for tomorrows scientists and engineers.

Principal Recommendations

- Changes in Organizational Structures and a New Parallel Program in SBES
  - Long-range core funding of SBES will require changes in organizational structures.
  - The feasibility of developing an overarching program in SBES that interfaces multiple divisions of NSF parallel to and in concert with Cyberinfrastructure should be given serious consideration.
  - Realizing the full potential of SBES will require support across all divisions within the Engineering Directorate within NSF and from other Federal Agencies.

Principal Recommendations

- Maintaining Leadership in Engineering and Engineering Sciences
  - SBES is a key element to revolutionary advances in engineering.
  - Advances in computing speed alone or in networking or in measurement devices cannot meet the great challenges facing the nation. Substantial investments in core SBES components are needed.
  - To maintain leadership, a minimum six-fold increase in funding over the FY 05 levels of SBES-related disciplines is recommended.

Principal Recommendations

- Long-Term Program of High-Risk

A long-term program of high risk research will be needed to exploit the considerable promise of SBES. The Panel strongly supports the observation made in the PITAC report and elsewhere that short-term investments and limited strategic planning will lead to excessive focus on incremental research rather than on long-range sustained research with lasting impact. Progress in SBES will require the creation of interdisciplinary teams that work together on leading-edge simulation problems. The work of these teams should be sustained for a decade or more to yield the full fruits of the investment.

Principal Recommendations

- Education in SBES
  - A sweeping overhaul of current educational systems may be needed
    - – bridge or remove silo-structure
  - NSF underwrite the work of an NRC Committee on Interdisciplinary Education in Engineering and Science to explore this issue