Research in Mechanics and Nano S&E
by
Ken P. Chong
PhD, PE
Director of Mechanics & Materials Engineering Directorate
National Science Foundation

www.nsf.gov
NSF Engineering Directorate
FY2005 Request

Assistant Director
John A. Brighton
Deputy Assistant Director
Michael Reischman

($10.3M) $471.8M

Bioengineering & Environmental Systems
BES
($-1.3M) $49.8M
Bruce Hamilton

Civil & Mechanical Systems
CMS
($18.3M) $85.5M
Ken Chong*

Chemical & Transport Systems
CTS
($-1.7M) $67.2M
Richard Buckius

Design, Manufacture & Industrial Innovation
DMII
($-0.1M) $65.9M
Warren DeVries

Electrical & Communications Systems
ECS
($-1.9M) $72.7M
Vasu Varadan

Engineering Education & Centers
EEC
($-3.3M) $130.7M
Gary Gabriele

SBIR/STTR**
($0.5M) $104.1M
Kesh Narayanan

**NSF-wide program – now changed to Office of Industrial Innovation; * now Adnan Akay
Microelectronics – Moore’s Law: doubling the capabilities every two years for the last 30 years; unlimited scalability; nanotechnology is essential to continue the miniaturization process.

Information Technology – NSF backbone project in the 1980s was instrumental in launching the Internet revolution; confluence of computing and communications.

Biotechnology – molecular secrets of life with advanced computational tools as well as advances in biological engineering, biology, chemistry, physics, including mechanics and materials.
“I was close to a breakthrough when the grant money ran out.”
Nanotechnology
Definition on www.nano.gov/omb_nifty50.htm (2000)

- Working at the atomic, molecular and supramolecular levels, in the length scale of approximately 1 – 100 nm range, in order to understand, create and use materials, devices and systems with fundamentally new properties and functions because of their small structure

- NNI definition encourages new contributions that were not possible before.
  - novel phenomena, properties and functions at nanoscale, which are nonscalable outside of the nm domain
  - the ability to measure / control / manipulate matter at the nanoscale in order to change those properties and functions
  - integration along length scales, and fields of application
NNI FY 2006 Budget Request
Total = $1,054 million
Infrastructure Outcomes of 2001-2005: NSF R&D Networks and User Facilities

- **Network for Computational Nanotechnology (NCN)**
  7 universities (Purdue as the central node)
  Nanoelectronic device simulation/modeling

- **National Nanotechnology Infrastructure Network (NNIN)**
  13 universities with user facility
  Development measuring & manufacturing tools, including
  NEPM Education and societal implications

- **Oklahoma Nano Net (EPSCoR award)**

  **Centers:**
  16 Nanoscale Science and Engineering (NSEC) - 6 (2001); 2 (2003); 6 (2004); 2 (2005)
  1 Nanotechnology Center for Learning and Teaching (NCLT)
  6 new Materials Research Science and Engineering Centers (MRSEC)
Areas of investment in FY2006 (Program Component Areas)

1. Fundamental Nanoscale Phenomena and Processes
2. Nanomaterials
3. Nanoscale Devices and Systems
4. Instrumentation Research, Metrology, and Standards for Nanotechnology
5. Nanomanufacturing
6. Major Research Facilities and Instrumentation Acquisition
7. Societal Dimensions
Simulation - Based Engineering Science

Revolutionizing Engineering Science through Simulation
February 2006

Report of the National Science Foundation
Blue Ribbon Panel on Simulation-Based Engineering Science

TINSLEY ODEN, CHAIR; UT-AUSTIN

POC: KEN P. CHONG, NSF
Preliminaries

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.

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

Homeland Security
Mod. & Simu. at Nanoscale
MSM BBB
Energy & Env.
Multi-Phenomena-Physics-Scale Systems
Global Enterprises
Healthcare
Mfg. Supply Chain & Transport
Simulation Software
Next Generation Algorithms
Big Visualization Data

V&V and UQ
DDDAS
CRCNS

HP mat’ls/devices

Modern Computation
Applied Math
HPC, CI
Computer Science
Engineering Sciences
Others
Overarching Framework for Multiscale Modeling:
atomistic $\rightarrow$ micro $\rightarrow$ meso $\rightarrow$ macro

Key: interfaces between models at different scales

Questions:

- What are the *information* that needs to be transferred from one model to another?
- What are the *correct* ways to achieve such transfer of information?
- What physical principles must be satisfied during the transfer of information or simulation results?

Need: A set of logic, mathematical, and physical rules to govern information transfer across the interfaces

JIMMY HSIA, NSF
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
Cutting edge activities are at the interfaces

- **Solid and Bio Mechanics**
  - Contact mechanics, biomimetic materials, thin film mechanics

- **Nano- and Micro Mechanics**
  - MEMS reliability, strength, lubrication; nano-biomechanics

- **Materials and Surface Engineering**
  - Nanotribology, ultra thin film behavior, AFM mechanics, nano-structured surfaces

- **Multiscale modeling**
Mechanics and Materials

Adv. Solid Mechanics
- Constitutive relations
- Analytical, theoretical
- Experimental methods
- Numerical methods
- Damage mechanics
- Advanced Simulation

Micro-Mechanics
- Defects
- Micro-Structure
- Fracture, fatigue
- Deformation
- Theoretical methods
- Numerical, Exptal, analytical

Meso-Mechanics
- Interfacial mechanics
- Constitutive models
- Structural states
- Transformation, evolution
- Numerical, Exptal, analytical
- Simulation, modeling

Macro-Mechanics
- Damage mechanics
- Advanced Composites
- Thermal stresses
- Durability, performance
- Numerical, Exptal, analytical
- Simulation, modeling

Multi-scale Mechanics
- Multi-phenomena
- Multi-physics
- Thermal, env. forces
- Numerical, Exptal, analytical
- Simulation, optimization

Engineering Materials
- Electronic materials
- Wet/dry; smart materials
- Self-healing, Self-cleaning

Frontiers in solid mechanics and engineering materials
Grand Challenges & The Great Payoff: Applications and Benefits of SBES

- Medicine
- Homeland Security
- Energy and Environment
- Materials
- Industrial Applications
- ...
NSF Press Release 06-049
Supercomputer Maps One Million Atoms of a Complete Virus in First Simulation of a Life Form
Virtual virus takes 100 days on supercomputer, 35 years on a desktop for 50ns

Credit: University of Illinois at Urbana-Champaign's Theoretical and Computational Biophysics Group.
Composites of Carbon Nanotubes (CNT)

- Baseline Material, available today
- Best available under development
- Emerging material, carbon nanotubes

Specific Modulus, GPa/(g/c^3)

Specific Strength, GPa/(g/c^3)

- Single Crystal bulk material (CNT)
- CNTFRP Composite
- CFRP Composite
- Aluminum 2219

Long-term potential of CNT material

from NASA-larc
Systems Analysis Results for a Reusable Launch Vehicle (RLV)

Predicted Weight Savings from Polymer Matrix Composites
(Primary Structure and Cryogenic Fuel Tanks)

Vehicle Dry Weight

1.0

55% reduction

82% reduction

Aluminum  CFRP Composite  CNTFRP Composite

from NASA-larc
EDUCATION

• $10^{-12}$ m QUANTUM MECHANICS [TB, DFT, HF…]

• $10^{-9}$ MOLECULAR DYN. [LJ…]; NANOMECHANICS; MOLECULAR BIOLOGY; BIOPHYSICS

• $10^{-6}$ ELASTICITY; PLASTICITY; DISLOCATION…

• $10^{-3}$ MECHANICS OF MATERIALS

• $10^{-0}$ STRUCTURAL ANALYSIS

MULTI-SCALE, MULTI-PHENOMENA ANALYSES & SIMULATIONS…

TB = TIGHT BINDING METHOD; DFT = DENSITY FUNCTIONAL THEORY; HF = HATREE-FOCK APPROX.; LJ = LENNARD JONES POTENTIAL

• NSF SUMMER INSTITUTE OF NANOMECHANICS & MAT’LS, NORTHWESTERN UNIVERSITY –contact: PROF. W.K. LIU
NSF Summer Institute on Nano Mechanics and Materials *

Co-sponsored by: ASME, the Northwestern University NASA URETI BIMat Center, NU Nanoscale Science and Engineering Center, Northwestern University, and the CSET, NSF IGERT on Virtual Tribology and AVS Science & Technology Society

Professor Wing Kam Liu (Director)
Professor Ted Belytschko (Co-Director)
Professor Q. Jane Wang (Co-Director)

Northwestern University, Robert R. McCormick School of Engineering and Applied Science, 2145 Sheridan Rd. Evanston, IL 60208

* Funded by the Civil and Mechanical Systems Division, monitored and guided by Dr. Ken P. Chong.
Scales in Plasticity

size effects: 0.1 \( \mu m \) – 0.1 mm

discrete dislocation models  \( \Rightarrow \) plasticity

classical plasticity theories

Dislocation-based plasticity theories?

- Any continuum plasticity theories apply only above 0.1\( \mu m \)!
  
  less than 0.1\( \mu m \)  \( \Rightarrow \) individual dislocations  \( \Rightarrow \) plasticity
  
  (analogy: less than 1 nm  \( \Rightarrow \) individual atoms  \( \Rightarrow \) elasticity)

Y. HUANG, UIUC
Size Effect in Plasticity

Torsion of thin wires

Fleck et al., 1993

Bend of thin beams

Soboyejo et al., 2003

Al matrix with SiC particles

\( V_f = 15\% \); Particle diameter:

\( d = 16\mu m \) and \( 7.5\mu m \)

Smaller is harder!
Nano-mechanics

-- A continuum theory based on the interatomic potential

Interatomic Potential
(nonlinear, multi-body springs)

Molecular Dynamics

Atomistic-based Continuum Theory

Y. HUANG, UIUC
Principle of AFM

http://www.di.com/app_notes/spmtechnology_appnotes.htm

MEASURE FORCE  \( F = F(d) \)
GERD BINNIG
1986 NOBEL PRIZE [STM]
CHALLENGES

multi-scale
Map of Deformation-Measurement Techniques

K.-S. Kim, Nano & Micromechanics Laboratory, Brown University

Field of View (Gage Length in m)

<table>
<thead>
<tr>
<th>Field Projection Method</th>
<th>Equilibrium Smoothing</th>
</tr>
</thead>
<tbody>
<tr>
<td>HRTEM-CFTM</td>
<td>AFM/SEM DIC</td>
</tr>
<tr>
<td>Interferometric Gain of Resolution</td>
<td>AFM/SEM DIC</td>
</tr>
<tr>
<td>LDLM</td>
<td>LSI</td>
</tr>
<tr>
<td>SRES</td>
<td>FGLM &amp; LSI</td>
</tr>
<tr>
<td>Fringe Density Limit</td>
<td>Optical Diffraction Limit</td>
</tr>
<tr>
<td>DEC</td>
<td>Adaptive Reference Grating</td>
</tr>
</tbody>
</table>

Strain Resolution

<table>
<thead>
<tr>
<th>HRTEM</th>
<th>CFTM</th>
<th>LDLM</th>
<th>FGLM</th>
<th>LSI</th>
</tr>
</thead>
<tbody>
<tr>
<td>High Resolution Transmission Electron Microscopy</td>
<td>Computational Fourier Transform Moire</td>
<td>Large Deformation Laser Moire</td>
<td>Fine Grating Laser Moire</td>
<td></td>
</tr>
<tr>
<td>AFM</td>
<td>SEM</td>
<td>SRES</td>
<td>DIC</td>
<td></td>
</tr>
</tbody>
</table>

NSF Award No. CMS-0070057, Engineering Directorate (Program Manager: Dr. K.P. Chong & Jorn Larsen-Basse)
Techniques:

Nano-\(\text{nm}\) → Micro-\(\mu\text{m}\) → (Meso-) → Macro-\(\text{mm}\)

- AFM
- Optical Microscopy
- Laser Scanning Confocal Microscopy
- Light Scattering
- Neutron Scattering
  - SANS
  - USANS

L. SUNG, NIST
<table>
<thead>
<tr>
<th>MATERIALS</th>
<th>STRUCTURES</th>
<th>INFRASTRUCTURE</th>
</tr>
</thead>
<tbody>
<tr>
<td>nano-level ((10^{-9}))</td>
<td>micro-level ((10^{-6}))</td>
<td>meso-level ((10^{-3}))</td>
</tr>
<tr>
<td>Molecular Scale</td>
<td>Microns</td>
<td>Meters</td>
</tr>
<tr>
<td>*nano-mechanics</td>
<td>*micro-mechanics</td>
<td>*meso-mechanics</td>
</tr>
<tr>
<td>*self-assembly</td>
<td>*micro-structures</td>
<td>*interfacial-structures</td>
</tr>
<tr>
<td>*nanofabrication</td>
<td>*smart materials</td>
<td>*composites</td>
</tr>
</tbody>
</table>

Fig. 1. Physical scales in materials and structural systems
Why Multiple Temporal Scales?

- Multiple temporal scales
- Single Physical Process
- Induced by Multiple Physical Processes

Global Scale
Component Scales
Material Scales

Induced by Multiple Spatial Scales

Deformation
Fatigue
Creep

Electro Magnetism
Chemical Reaction
Heat Transfer
Multiple Temporal Scales for Fatigue

- Multiple time scales:
  \[ \zeta = \frac{r}{\phi} \]
  
  \( \zeta \): scaling parameter determined by load frequency and material parameters
  
  \( r \): characteristic length of macro-chronological time
  
  \( \phi \): characteristic length of micro-chronological time

- Two-scale model:
  
  response fields (e.g., displacement, stress, strain, etc...)

J. FISH, RPI
Multi-Scale Multi-Phenomena Modeling of Structure / Property / Function

Multi-Scale Composite

Epoxy Matrix

Carbon Fiber

Nanocomposite

Carbon Nanotubes

Atomic Interactions

Stretching

Bending

Torsion

van der Waals

Modeling Hierarchy – Bridging the Scale from Nano to Macro

T.W. CHOU, U. DEL.
Multiscale Atomistic-to-Continuum Simulations

Finite Element

Molecular Dynamics

Density Functional

Continuum Elasticity away from Nonlinearities

Nonlinear Regions Atomistic Simulations

Bond Breaking Quantum Mechanics

RAJIV KALIA, LSU
Validation of Interaction Potential

- **Static structure factor** of amorphous Si$_3$N$_4$ (Misawa et al, '79)
  \( q = \text{scattering wave vector} \)

- **Phonon density of states** of \( \alpha - \text{Si}_3\text{N}_4 \) crystal (Loong et al, '95)

- **Elastic moduli of \( \alpha \)-crystal** (Cartz & Jorgensen, '81)

<table>
<thead>
<tr>
<th>Material</th>
<th>MD</th>
<th>Expt.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si$_3$N$_4$ at 3.2 g/cc</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Bulk modulus</td>
<td>289 GPa</td>
<td>282 GPa</td>
</tr>
<tr>
<td>Young's Modulus</td>
<td>419 GPa</td>
<td>456 GPa</td>
</tr>
</tbody>
</table>
Scalable Scientific Algorithm Suite

On 1,024 IBM SP3 processors:
- 6.44-billion-atom MD of SiO₂
- 444,000-electron (111,000-atom) DFT of GaAs
DISCUSSIONS OF COMMON MODELING METHODS

• FIRST PRINCIPLE CALCULATIONS - TO SOLVE SCHRODINGER’S EQ. AB INITIO, e.g. HATREE-FOCK APPROX., DENSITY FUNCTIONAL THEORY,…
  - COMPUTATIONAL INTENSIVE, \( O(N^4) \)
  - UP TO ~ 3000 ATOMS

• MOLECULAR DYNAMICS [MD] - DETERMINISTIC, e.g. W/ LENNARD JONES POTENTIAL
  - MILLIONS TIMESTEPS OF INTEGRATION; TEDIOUS
  - UP TO ~ BILLION ATOMS FOR NANO-SECONDS

• COMBINED MD & CONTINUUM MECHANICS [CM], e.g. MAAD; LSU; BRIDGING SCALE; …
  - PROMISING…
Bio-inspired Mechanics and Materials
Hierarchical Structure of Human Bone

- Macrostructure
  - Trabecular bone
  - Cortical bone
- Microstructure (10 – 500 µm)
  - Single osteons (cortical bone)
  - Trabeculae (trabecular bone)
- Sub-microstructure (1 – 10 µm)
  - Lamellae
- Nanostructure (below 1 µm)
  - Collagen fibrils
  - Hydroxyapatite (HA) crystals
  - Crystal-Collagen structure

I. Jasiuk, GA Tech
The Mechanical Performance of Nacre from Seashells – Superior Toughness through Microstructural Design

H.D. Espinosa

NORTHWESTERN UNIVERSITY

National Science Foundation
Award No. CMS-0301416
Ken Chong
Motivations

Nacre (95 % aragonite): A tough bio-composite
\[ K_{IC} = 8-10 \text{ MPa.m}^{1/2} \]

- Nacre is 20-30 times tougher than aragonite
- How does the microstructure make nacre tough?
- This is still unclear (see G. Mayer in *Science*, 2005) but it is much sought after, because it may open the way to synthetic mimics of nacre with superior properties (biomimetics)

Geological Aragonite: A brittle ceramic
\[ K_{IC} = 0.3 \text{ MPa.m}^{1/2} \]
Gecko: nano-scale attachment (K. Autumn et al. 2002)

Gecko Foot Structure

Rows of Sticky Leaves (Lamellae)

Lamellae

↑ Rear of animal

(From: Cesario 1975)
Mechanics of a Mosquito Bite
- Design of a Bio-mimetic Painless Needle
(Supported by NSF Grant Number CMS 0402857)
M. K. Ramasubramanian, PI
J.F. Tu, Co-PI
Charles Apperson (Entomology)
Mosquito Skin Penetration Mechanics

- Non-conservative force application for significant increase in bucking load (Beck’s Column).
- Labium provide lateral support and keep the fascicle moist and lubricated.
- The head oscillates between .5 to 5 Hz horizontally, maintaining the force application direction tangential to the fascicle, and prevent buckling.
- Increase in buckling load is sufficient for skin penetration.
**What’s special about spider silk?**

<table>
<thead>
<tr>
<th>Material</th>
<th>Strength (N m$^{-2}$)</th>
<th>Elasticity (%)</th>
<th>Energy to Break (J kg$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dragline Silk</td>
<td>4 x 10^9</td>
<td>35</td>
<td>1 x 10^5</td>
</tr>
<tr>
<td>Minor Silk</td>
<td>1 x 10^9</td>
<td>5</td>
<td>3 x 10^4</td>
</tr>
<tr>
<td>Flagelliform silk</td>
<td>1 x 10^9</td>
<td>200+</td>
<td>1 x 10^5</td>
</tr>
<tr>
<td>KEVLAR</td>
<td>4 x 10^9</td>
<td>5</td>
<td>3 x 10^4</td>
</tr>
<tr>
<td>Rubber</td>
<td>1 x 10^9</td>
<td>600</td>
<td>8 x 10^4</td>
</tr>
<tr>
<td>Tendon</td>
<td>1 x 10^9</td>
<td>5</td>
<td>5 x 10^3</td>
</tr>
</tbody>
</table>

**TABLE 1.** Various biological and manmade materials are listed with their strengths, elasticities, and energies to break. Note the over ten-fold increase in the energy to break of dragline silk compared to KEVLAR. This dramatic increase is due to the elasticity of dragline silk. Also note the differences in elasticity among dragline, flagelliform and minor ampullate silks.

*Randy Lewis, et al*
Defining the vision and implementation plan

National Nanotechnology Initiative

1999: 10-year vision

Planning with feedback after each: 5 years, 1 year, 1 month; and various levels: national/NSET, agency, program

In preparation: Topical reports; new 2004:10 year vision
Defining the vision for the second strategic plan (II)

National Nanotechnology Initiative

2004

2004: 10-year vision/plan

Agriculture and Food

Energy

Societal Implications 2004

Government Plan (annual)

Nanomaterials by Design: From Fundamentals to Function

Survey manufacturing

Reports

Chemical Industry R&D Roadmap for Nanomaterials By Design: From Fundamentals to Function

2004: Update 10 year vision, and develop strategic plan

Other topical reports on www.nano.gov

MC Roco, 3/16/05
www.nsf.gov

chaired by J. Tinsley Oden, 2006 report on “Simulation-Based Engineering Science”:

www.asme.org/nanowebcast


NSF SUMMER INSTITUTE ON NANO MECHANICS & MATERIALS
http://tam.northwestern.edu/summerinstitute/Home.htm
SUMMARY & DISCLAIMER
An overview of major advances, challenges and research concerning mechanics and materials are presented. The author would like to thank his colleagues and many members of the research communities for their comments and input during the writing of this presentation.

Information on NSF initiatives, announcements and awards can be found in the NSF website: www.nsf.gov. The opinions expressed in this article are the author’s only, not necessarily those of the National Science Foundation [NSF]. Any commercial products identified are for illustrations only, do not imply any endorsement.