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NSF PROGRAMS

WITH EMPHASIS ON NANO MECHANICS AND MATERIALS

by

Ken P. Chong

PhD, PE, Hon. M.ASCE, F.AAM

Director of Mechanics & Materials

National Science Foundation

www.nsf.gov

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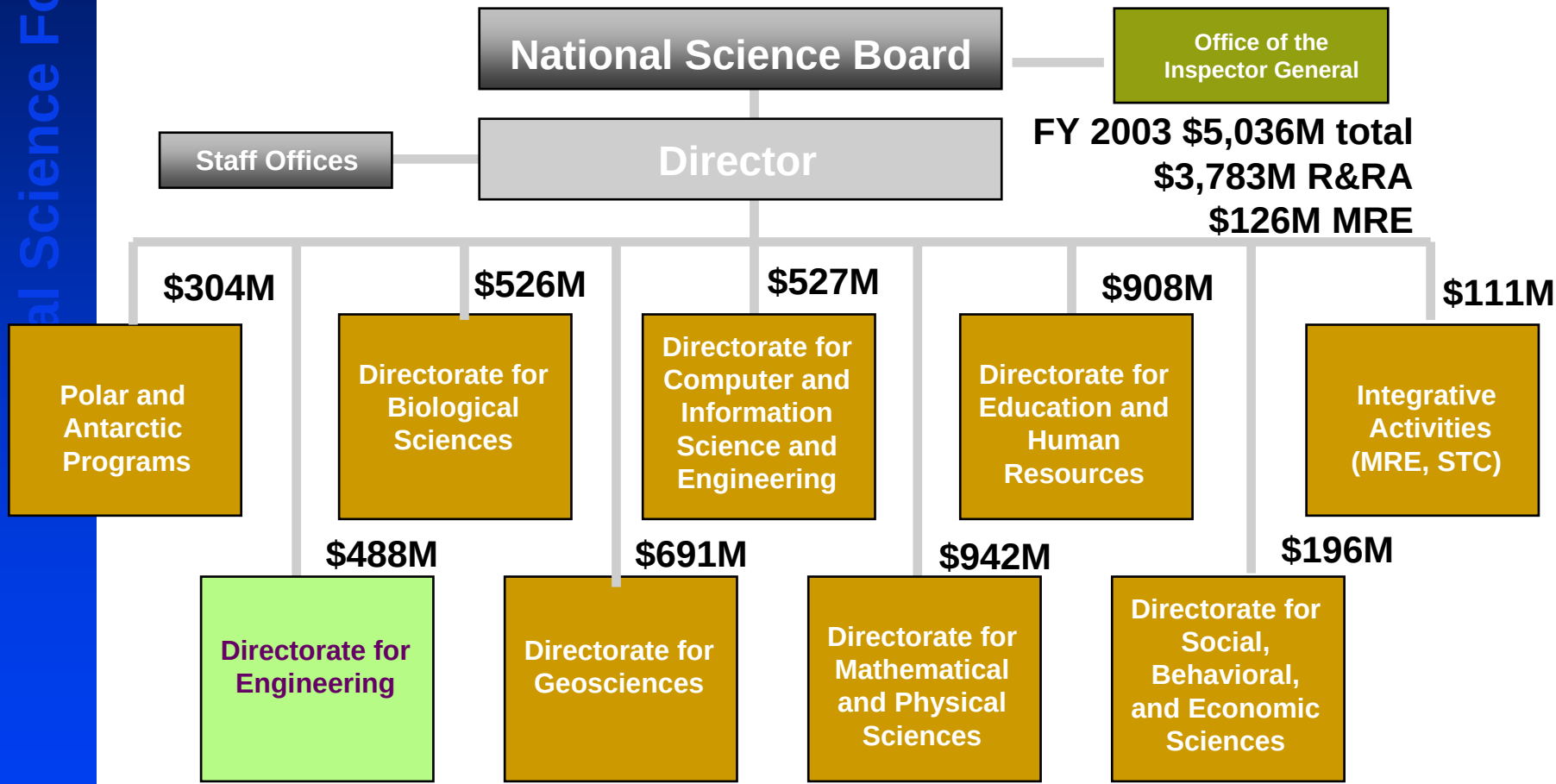
FY2003 Budget Request



Priority Areas

	Millions of Dollars		
	FY 2002 Plan	FY 2003 Request	Percent Change
Nanoscale S&E	$199	$221	11%
Information Technology Research	$278	$286	3%
Mathematical Sciences	$30	$60	100%
Social, Behavioral & Economic Sciences	$0	$10	N/A
Biocomplexity in the Environment	$58	$79	36%
Learning for the 21st Century Workforce	$145	$185	27%

creation of new materials, devices and systems at the molecular level

phenomena associated w/ atomic & molecular interactions strongly influence macrospic mat'l properties [I. Aksay, Princeton]

significantly improved mechanical, optical, chemical, electrical... properties

"there is plenty of room at the bottom"
[Richard Feynman, 1959]

"nanoscale technology will have an impact equal to the Industrial Revolution"
[Rita Colwell, 2002]

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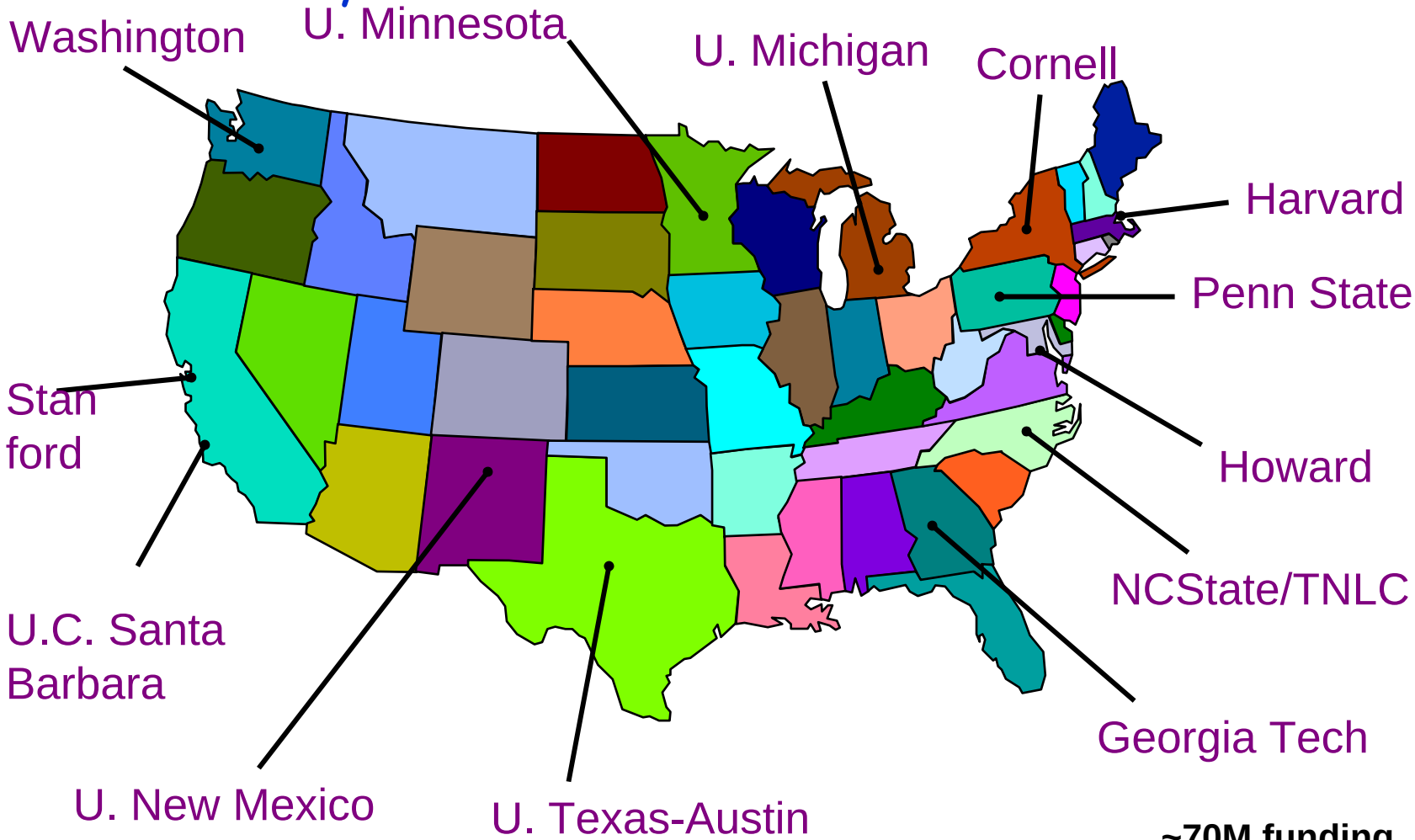
Changing R&D focus in 2004

- Growing area, from discovery to technological innovation
  - **Materials, including bulk, coating, dispersed systems**
  - **Chemicals, including catalysts**
  - **Pharmaceuticals**
  - **Electronics**
- Emerging areas in 2003 (support in FY 2004)
  - **Nanomedicine**
  - **Energy conversion and storage**
  - **Agriculture and food systems**
  - **Molecular architectures**
  - **Realistic multiphenomena/multiscale simulations**
  - **Environmental implications**
  - **Converging technologies from the nanoscale**

National Nanotechnology Infrastructure Network (NNIN)

13 University User Facilities to Advance R&E in NSE



~70M funding

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M. ROCO, ~2002

Table 3. Potential Global Economic Impact of Nanotechnology in 15-20 Years [1]

Materials; Materials Processing	$340B
Information Technology Devices	$300B
Pharmaceuticals/Biotechnology	$180B
Chemical Manufacturing, Catalysis	$100B
Aerospace	$70B
Tools, Automation, Life Cycle Costs	$20B
Healthcare - Diagnostics, Prosthetics	$30B
Sustainability - Agriculture, Water, Energy	$45B
Total	**~$1T**

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Organizations that have prepared and contribute to the National Nanotechnology Initiative (**NNI**)

Presidential Council of Advisors in Science and Technology (PCAST)

White House

Office of Management and Budget (OMB)

Office of Science and Technology Policy (OSTP)

National Science and Technology Council (NSTC)

IWGN (October 1998-August 2000)

NSET (August 2000 - continuing)

Departments

DOC/NIST, DOD, DOE, DOJ, DOS, DOT, DOTreas, DHS, USDA

Independent Agencies

EPA, FDA, NASA, NIH, NRC, NSF, USG

Est.:	Federal Government R&D funding	NNI (~$700M in 02)
	Industry (private sectors)	~ NNI funding
	State and local (universities, foundations)	~ 1/2 NNI funding

Fundamental nanoscale science and engineering
Principal Areas of Investigation – core programs

(FY 2002)

- **Biosystems at the Nanoscale** ~ 14%

  biostructures, mimicry, bio-chips
- **Nanostructure 'by Design', Novel Phenomena** **45%**

  physical, biological, electronic, optical, magnetic
- **Device and System Architecture** 20%

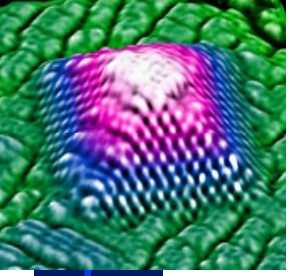
  interconnect, system integration, pathways
- **Environmental Processes** 6 %

  filtering, absorption, low energy, low waste
- **Multiscale and Multiphenomena Modeling** 9 %
- **Manufacturing at the nanoscale** 6%
- **Education and Social Implications** (distributed)

Grand Challenges (NNI, FY 2002)

• Nanostructured materials "by design"	~ 22%
• Nanoelectronics, optoelectronics and magnetics	**39%**
• Advanced healthcare, therapeutics, diagnostics	8%
• Environmental improvement	4%
• Efficient energy conversion and storage	5%
• Microcraft space exploration and industrialization	3%
• CBRE Protection and Detection (revised in 2002)	7%
• Instrumentation and metrology	6%
• Manufacturing processes	5%

(details in the NNI Implementation Plan, http://nano.gov)

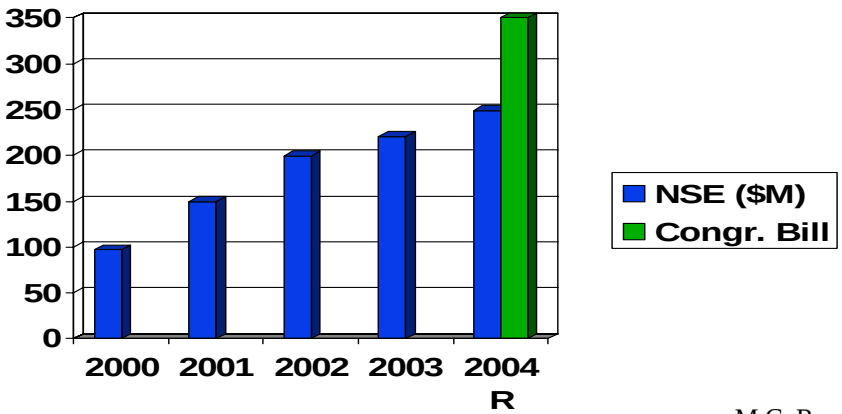


NSF - a pioneer among Federal agencies and at the international level in Nanoscale Science and Engineering (NSE)

FY 2003: ~ **1/3 of Federal** and **1/10 of World Investment**

- **Seven themes**: Biotechnology, Nanostructures 'by design' and novel phenomena, Device and system architecture, Environmental Processes, Multiscale modeling, Nanoscale manufacturing; Societal implications and Improving human performance
- **Establishing the infrastructure**: over 1,600 active projects; 20 large centers, 2 user facilities (NNIN, NCN), multidisciplinary teams
- **Training and education** over 7,000 students and teachers

Fiscal Year	NSF	HR766
2000	$97M	
2001	$150M	
2002	$199M	
2003	$221M	
R 2004	$249M	$350M



Nanotechnology R&D Funding by Agency

Fiscal year (all in million $)	*2000*	*2001* Enacted/actual	*2002* Enacted/actual	*2003* Requests	2004
National Science Foundation	97	150 /150	199 / 204	221	249
Department of Defense	70	110 /125	180 /180	243	222
Department of Energy	58	93 /88	91.1 /89	133	197
National Institutes of Health	32	39 /39.6	40.8 /59	65	70
NASA	5	20 /22/	35 /35	33	31
NIST	8	10 /33.4	37.6 /77	69	62
Environmental Protection Agency	-	/5.8	5 /6	6	5
Homeland Security (TSA)	-		2 /2	2	2
Department of Agriculture	-	/1.5	1.5 /0	1	10
Department of Justice	-	/1.4	1.4 /1	1.4	1.4
TOTAL	270.0	422.0 /464.7	~ 600 /653	~ 774	~ 849

Other NNI participants are:
OSTP, NSTC, OMB, DOC, DOS, DOTreas, FDA, NRC, DHS, Intel

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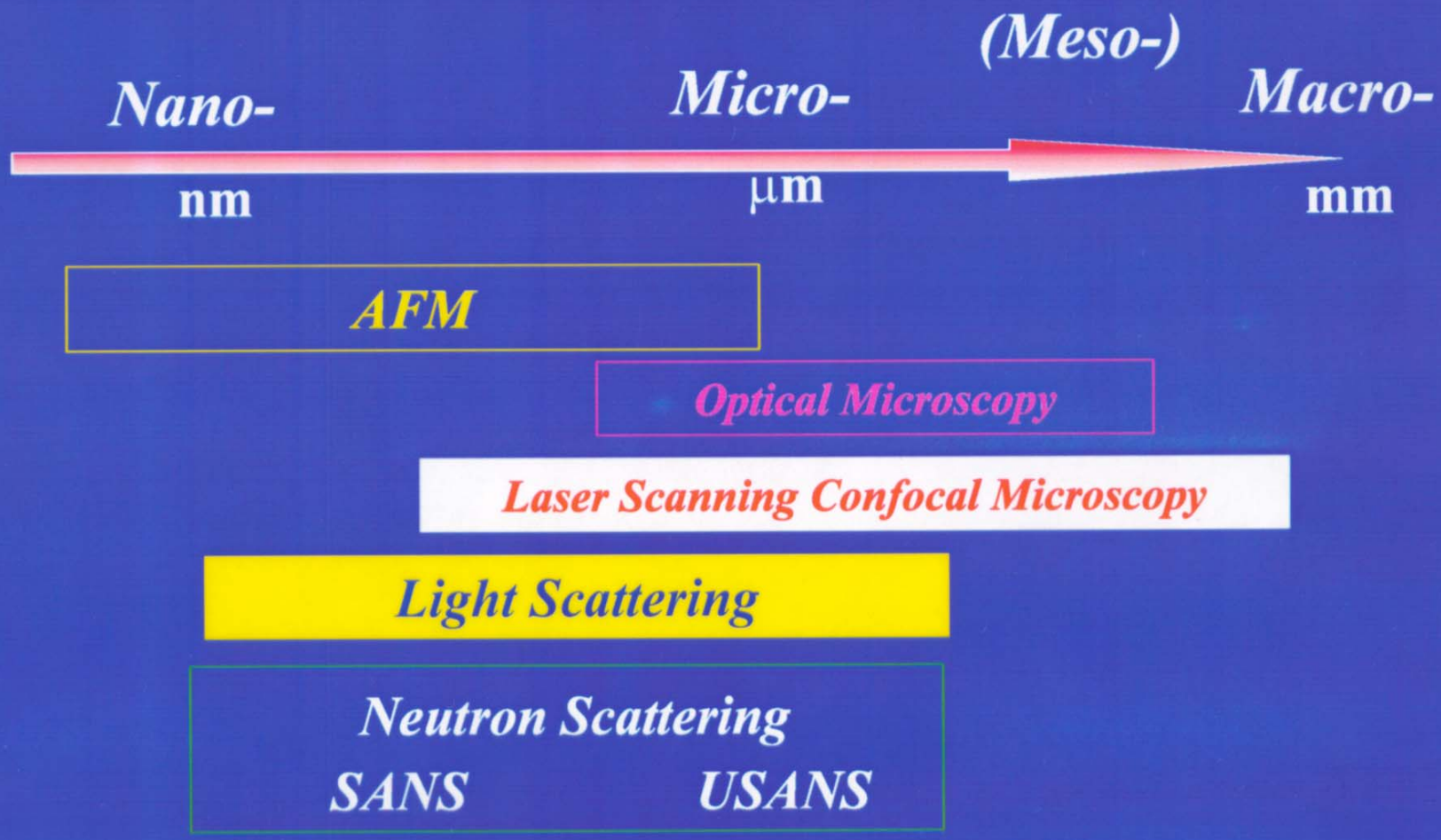
Bio-mechanics/materials
Simulations/modeling
Thin-film mechanics/materials MEMS
Wave Propagation;
NDT Smart materials/structures
Nano-mechanics/materials
Scale effects
Designer materials
Virtual modeling and testing

NEMS

Nano-photosynthesis

Cyberinfrastructure

Techniques:



L. SUNG, NIST

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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 ANALYSES & SIMULATIONS…

TB = TIGHT BINDING METHOD; DFT = DENSITY FTNAL THEORY;

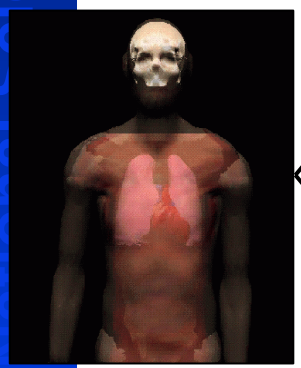
HF = HATREE-FOCK APPROX.; LJ = LENNARD JONES POTENTIAL

- **NSF SUMMER INSTITUTE OF NANOMECHANICS & MAT'LS, NORTHWESTERN UNIVERSITY – contact: PROF. W.K. LIU**

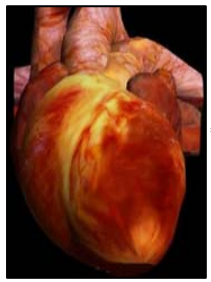
A Biology/Bioengineering Grand Challenge

Organism & organ systems (10^{-12}m) **Organ** (1m) **Tissue** (10^{-3}m) **Cell** **Protein** (10^{-6}m) **Atom** (10^{-9}m)

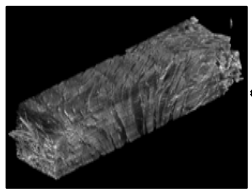
Systems-models



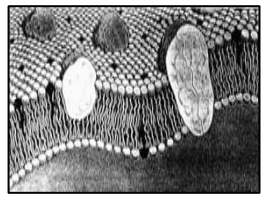
Continuum models (PDEs)



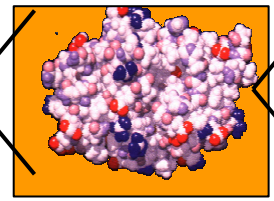
ODEs



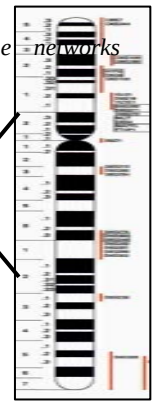
Stochastic models



Pathway models



Gene networks



Modeling, Simulation, Visualization, Software Frameworks, Databases, Networking, Grids

Peter Hunter, University of Auckland

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MATERIALS		STRUCTURES		INFRASTRUCTURE
nano-level (10^{-9})	micro-level (10^{-6})	meso-level (10^{-3})	macro-level (10^{+0})	systems-level (10^{+3}) m
Molecular Scale	*Microns*	*Meters*		*Up to Km Scale*
*nano-mechanics	*micro-mechanics	*meso-mechanics	*beams	* bridge systems
*self-assembly	*micro-structures	*interfacial-structures	*columns	* lifelines
*nanofabrication	* smart materials	*composites	*plates	*airplanes

Fig. 1. Physical scales in materials and structural systems

BORESI AND CHONG, *ELASTICITY IN ENGINEERING MECHANICS*, WILEY, 2000.

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DISCUSSIONS OF COMMON MODELING METHODS

- **FIRST PRINCIPLE CALCULATIONS - TO SOLVE SCHRODINGER'S EQ. *AB INITIO*, e.g. HATREE- FOCK APPROX., DENSITY FUNCTIONAL THEORY,…**

  - *COMPUTIONAL 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...*

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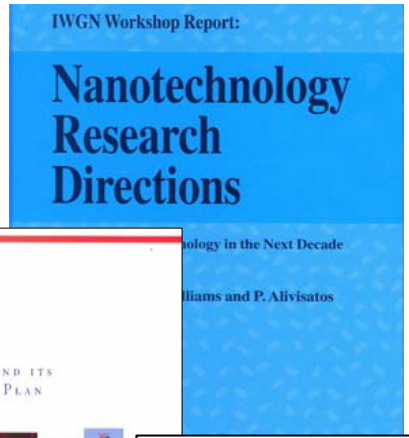
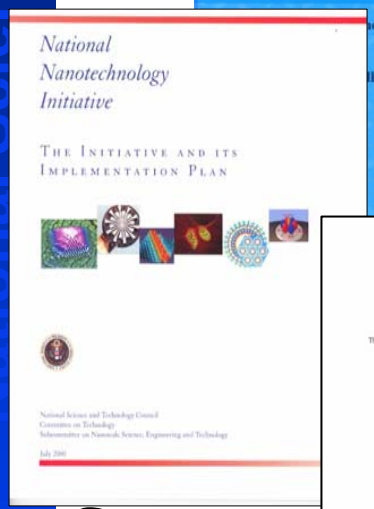
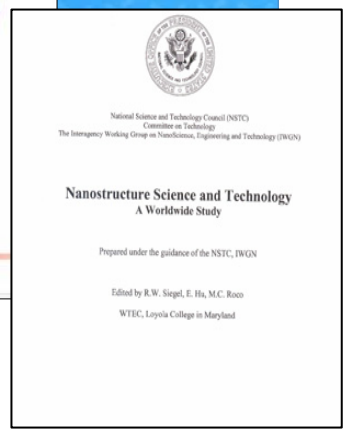
Defining the vision and implementation plan

National Nanotechnology Initiative

1999: 10-year vision



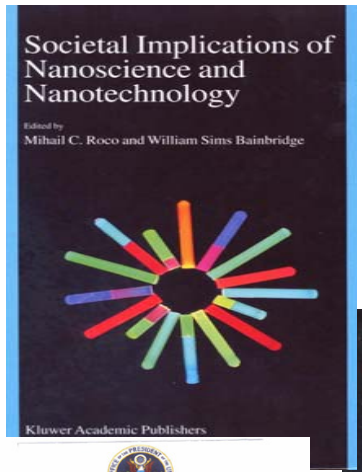




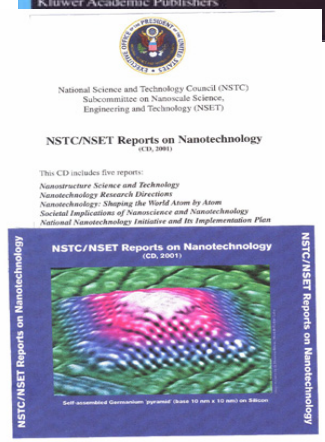
Govt plan

Reports

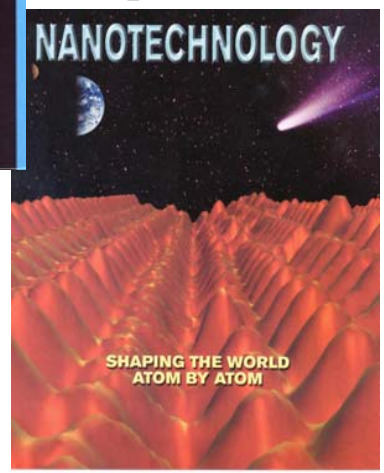
Worldwide benchmark



Societal implications



Brochure for public



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

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Chong, K. P., “Research and Challenges in Nanomechanics” 90-minute Nanotechnology Webcast, ASME, Oct. 2002; archived in *www.asme.org/nanowebcast*

NSF SUMMER INSTITUTE ON NANO MECHANICS & MATERIALS
http://tam.northwestern.edu/summerinstitute/Home.htm

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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.