Combinatorial Methodologies for Advanced Materials: Federal Assistance

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http://www.atp.nist.gov/www/ccmr/ccmr_off.htm

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Agenda

- The Global Business Environment
- The Technology Environment
- Why Combinatorial Methods (aka HTS/HTE)
- Some U.S. government opportunities
- Conclusions

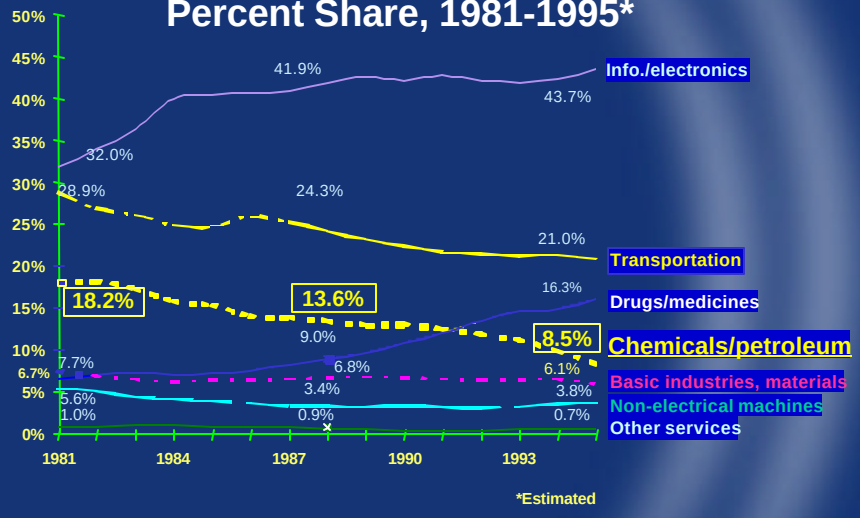
NIST National Institute of Standards and Technology • Technology Administration • U.S. Department of Commerce

Competitive Environment

- Advances in technology account for more than ***50 % of U.S. economic growth***
- Industry has chosen a focus on ***short-term return*** on investment
- Now more than ever, our nation's economic well being depends on ***rapid development and commercialization*** of technology

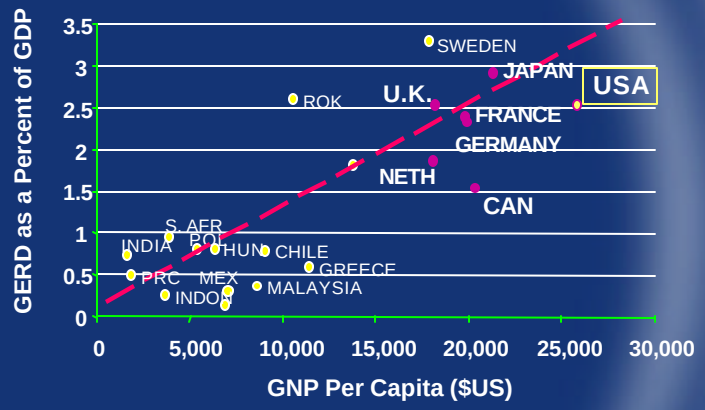
Industry R&D Expenditures

Percent Share, 1981-1995*



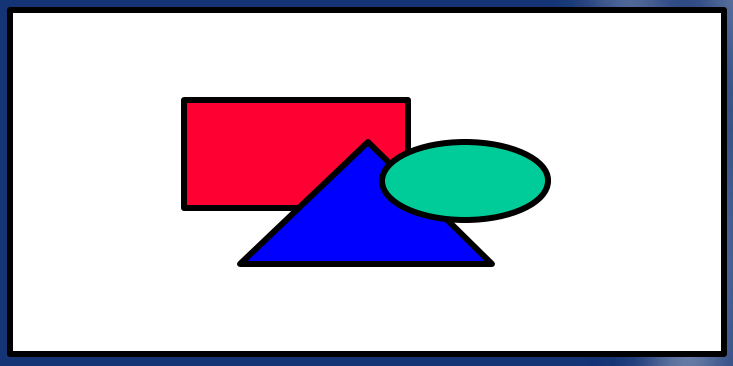
National R&D Spending

Percent of GDP Compared to GNP per Capita (1994)



Source: The Global Competitiveness Report, 1996, World Economic Forum, Geneva, Switzerland
WORLD BANK, From Plan to Market: World Development Report 1996, NSF, Science and Engineering Indicators, 1996

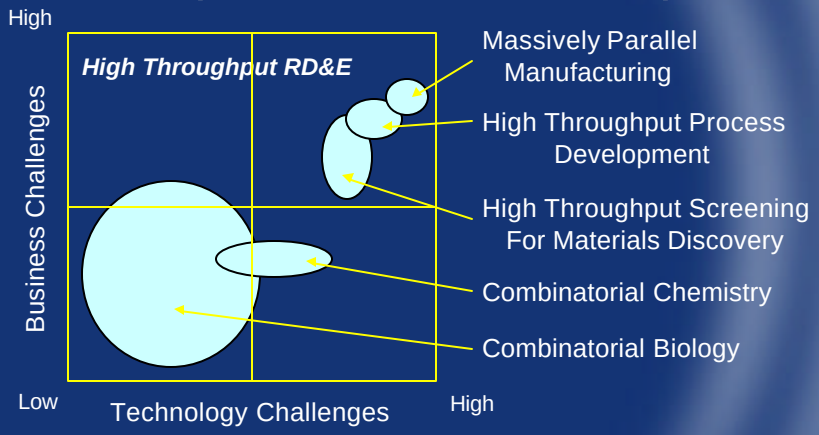
Why Government Support of R&D?



- Procurement of services, technologies, etc.
- Broad-based social and economic benefits to U.S. society

Ref.: National Science Board, *Science & Engineering Indicators – 1998*, Arlington, VA: National Science Foundation, 1998 (NSB 98-1).

What are Combinatorial Methods (aka HTS, HTE, etc.)



Target Applications for HTE

Catalysts	
Electronic Materials	Polymers/Chemicals Phosphors Magnetic Materials Ceramics Semiconductors
Polymers	Membranes Encapsulants/packaging Adhesives Coatings
Biomaterials	Bio-sourced polymers Bio-compatible materials Bio-degradable polymers
Optical materials	Coatings Photo-refractives Opto-electronics Non-Linear Optical materials
Structural materials	Metals and alloys Composites Ceramics/metal oxides
Glasses	Fibers Electronic Magnetic Optical
Smart Materials	
Advanced Ceramics	Specialty Optical & Electronic Super-conducting Structural Coatings

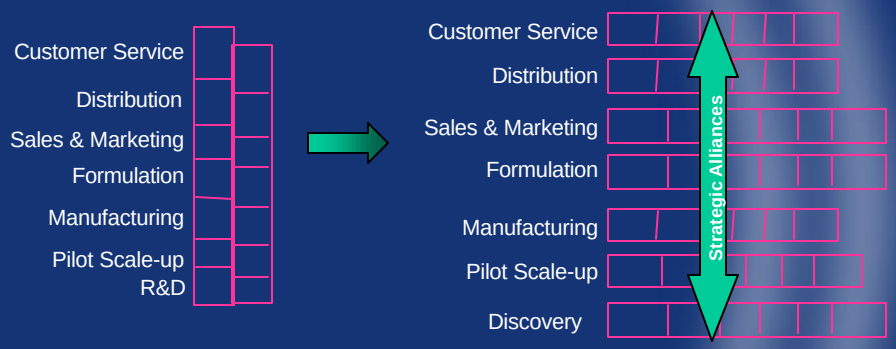
Profit Margin, R&D Budget, and Cost/Benefit Define Entry

Competitive Threats

- Reverse engineering of intellectual property
- First-to-market, first-to-follow market positioning
- Faster response to customer needs
- Lower R&D cost structures, higher-performance
- Leverage of government funding

New compositions, faster, at lower R&D cost

Business Models are Evolving



"Horizontalization" of Industry

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Technical Challenges

Drug Discovery	vs.	Solid State Materials
• Discrete molecules of C, H, F, N, O, P		• Extended structures of many elements potentially in metastable states
• Finite number of active sites, can be characterized and modeled computationally		• Ill-defined distribution of active sites and structures
• Synthesis usually leads to substances of >85% purity; parallel purification techniques employed before characterization		• "Pure" solids are meaningless especially with small samples having interfacial effects with the library substrate
• Structures reproducible (*a priori*)		• Reproducible structures hard, if not impossible, to create *a priori*
• Chemical characterization, biological activity well developed for rapid or parallel, methods • Descriptors for diversity		• Characterization of properties and composition not straightforward • No ideas exist about how to do it
• Registration of library samples straightforward		• No ideas exist about how to do it
• Synthetic building blocks available		• A few building blocks available

NIST is…..

Measurements and Standards Laboratory

Advanced Technology Program

Manufacturing Extension Partnership

National Quality Program

Total ATP Investment

Electronics and Photonics ($329M)

- Microelectronics
- Optics Technologies
- Power Technologies
- Wireless Electronics
- Organic Electronics

Biotechnology ($254M)

- DNA Technologies
- Tissue Engineering
- Drug Discovery Methods
- Proteomics
- Medical Devices & Imaging

Information Technology ($389M)

- Advanced Learning Systems
- Component-Based Software
- Digital Video
- Information for Healthcare
- Electronic Commerce
- Dependable Computing Systems
- Integration of Manufacturing

Chemistry and Materials ($344M)

- Catalysis & Biocatalysis
- Combinatorial Methods
- Separations/Membranes
- Nano-technology
- Engineered Surfaces
- Sensors
- Composites

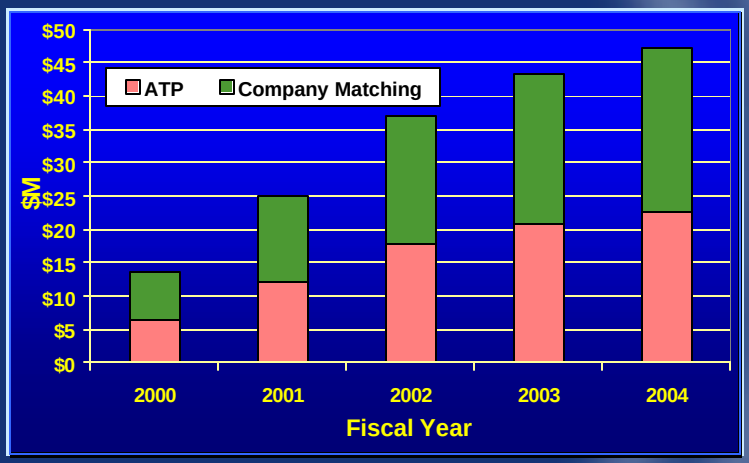
ATP Technology Cluster

Combinatorial Methods for Advanced Materials R&D
FY 1999 Projects: $23M from ATP over 5 years

Nonlinear Dynamics/UOP LLP	**"Combinatorial Tools and Advanced Data Analysis Methods for Heterogeneous Catalysts"** **$14,715K (ATP) + $15,186 (j/v) (5 yrs.)**
GE/Avery-Dennison	**"Combinatorial Methodology for Coatings Development"** **$3,127K (ATP) + $3,200K (j/v) (3 yrs.)**
Catalytica/CombiChem/Exxon	**"A Strategy for Reclaiming U.S. Leadership in High Value Polymers (Polyolefins)"** **$4,861K (ATP) + $6,049K (j/v) (3 yrs.)**

ATP Combi Methods Cluster

Cumulative Project Expenditures, 1999 - 2004



Plan Forward—FY '00

Chemical/Materials industry identified two challenges for Discovery and Product & Process Development Processes

Informatics

- **Design of the Library**
  - ✓ *Computational/Modeling: QSPR*
  - ✓ *Statistics and control of error*
  - ✓ *Design of Experiments*
- **Informatics**
  - ✓ *Increasing Information/Bandwidth*
  - ✓ *Experimental complexity*
  - ✓ *Data integration/analysis*
  - ✓ *Hardware control*
  - ✓ *Expert systems for data analysis*

Micro-Characterization

- **Screening**
  - ✓ *MEMS: Lab-on-chip, Sensors*
  - ✓ *Deposition/library fabrication*
  - ✓ *Process control*
    - ▪ *Temperature/pressure*
  - ✓ *Scalability Predictions*
    - ▪ *Interfacial properties*
- **Synthesis and Processing**
  - ✓ *Automation: 10^3 -10^4 samples*
  - ✓ *Reproducibility*
  - ✓ *Validation*

Contact Information

www.atp.nist.gov

To Get on the ATP Mailing List:

Call toll-free:	800-ATP-FUND (800-287-3863)
Fax your name and address to:	(301) 926-9524
Send an e-mail message to:	atp@nist.gov

Defense Advanced Research Projects Agency DARPA

"Fundamental Research at the [Bio:Info:Micro] Interface," is to create interdisciplinary teams of researchers drawn from the fields of biology information technology and microsystems technology at institutions of higher education. disciplines contributing to the development of senso materials, microfluidics, micromechanics, microphotonics, microelectronics and large-scale systems created from such components. Defen Sciences Office (DSO) A typical budget is expected to be between $500,000 and $2,000,000 per year.

SENSOR INFORMATION TECHNOLOGY SOL BAA00-25 DUE 020700 POC S. Kumar, DARPA/ITO, FAX: (703) 522-7161 SENSOR INFORMATION TECHNOLOGY SOL BAA 00-25 DUE 02/07/00 POC DR. SRI KUMAR, DARPA/ITO, FAX: (703) 522-7161. PROGRAM GOALS: The goal of the Sensor Information Technology (SensIT) program is to create a new class of innovative and effective software for distributed micro sensor networks.

R&D -- SMALL BUSINESS INNOVATION RESARCH (SBIR) PROGRAM DUE 011200 POC SBIR Support Services -- phone number: 800-382-4634 DEPARTMENT OF DEFENSE (DOD) SMALL BUSINESS INNOVATION RESEARCH (SBIR) PROGRAM. (For further information, call 800/382-4634.) Small firms apply first for a six-month phase I award of $60,000 to $100,000 to test the scientific, technical, and commercial merit of a particular concept. If phase I proves successful, the firm may be invited to apply for a two-year phase II award of $500,000 to $750,000 to further develop the concept, usually to the prototype stage.

MICROELECTRONICS, OPTO-ELECTRONICS AND/OR PHOTONICS TECHNOLOGY SOL 99-X-6904 POC Maureen Battern (619) 553-4489 e-mail battern@spawar.navy.mil E-MAIL: BAA Administrator, battern@spawar.navy.mil. BROAD AGENCY ANNOUNCEMENT (BAA): The Space and Naval Warfare Systems Center, San Diego (SPAWARSYSCEN) in support of the Defense Advanced Research Projects Agency (DARPA) Microsystems Technology Office (MTO) is seeking proposals (technical and cost) for research and development of microelectronics, micro-electromechanical systems (MEMS), opto-electronics and/or photonics technology. Also of interest are proposals for research and development of technologies for heterogeneous integration of electronics, photonics, MEMS, and other components.

Defense Advanced Research Projects Agency DARPA

MicroFluidic Molecular Systems (MicroFlumes)

•BAA 97-39: MicroFluidic Molecular Systems and Design for Mixed Technology Integration

NEXT GENERATION INTERNET (NGI) SOL BAA00-21 DUE 020200 POC M. Maeda, DARPA/ITO, Fax: (703) 522-7161 NEXT GENERATION INTERNET (NGI). SOL BAA 00-21. DUE 02/02/00. POC DR. MARI MAEDA, DARPA/ITO, FAX: (703) 522-7161. The goal of the NGI Program is to develop key networking technologies that will accelerate the development of revolutionary applications with capabilities vastly beyond the web-centric applications that are being built today.

BIO-FLUIDIC CHIPS SOL 00-11 DUE 012500 POC Dr. Abraham P. Lee, DARPA/MTO, FAX (703) 696-2206 WEB: http://www.darpa.mil, http://www.darpa.mil. E-MAIL: baa00-11@darpa.mil, baa00-11@darpa.mil. PROGRAM OBJECTIVES AND DESCRIPTION: The Defense Advanced Research Projects Agency (DARPA) is soliciting research proposals in the area of Bio-Fluidic Chips (BioFlips) and Simulation Tools for Chemical/Biological Microsystems. Proposed research should investigate innovative approaches that enable revolutionary advances in science, devices or systems. Awards totaling approximately $30 million over three years are expected to be made during the first half of calendar year 2000.

NETWORK MODELING AND SIMULATION (NMS) SOL 00-18 DUE 020100 POC Dr. Sri Kumar, DARPA/ITO, FAX: (703) 522-7161 WEB: http://www.darpa.mil/ito/solicitations.html, http://www.darpa.mil/ito/solicitations.html. E-MAIL: baa00-18@darpa.mil, baa00-18@darpa.mil. PROGRAM GOALS: ADMINISTRATIVE NOTE: NEW REQUIREMENTS/PROCEDURES HAVE BEEN IMPLEMENTED, EFFECTIVE AS OF SEPTEMBER 1999. The Network Modeling and Simulation (NMS) program solicits innovative research and development leading to the creation of modeling and simulation tools that are trustworthy to predict, with known and characterizable accuracy, network behavior over a broad range of time scales, network sizes and technology composition.

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NSF

Information Technology for the Twenty-First Century (IT^2)

- Proposed $366 million FY 2000 multi-agency Federal information technology R&D initiative.
- Long term IT research
  - -- Software
  - -- Human computer interfaces and information management
  - -- Scalable information infrastructure
  - -- High end computing

- Advanced computing for science, engineering, and the Nation
  - -- Acquisition of high end systems for research
  - -- Scientific and engineering simulation software and tools
  - -- Multidisciplinary science and engineering research teams

- Research on economic, social, and workforce implications of the Information Revolution

NSF

Knowledge and Distributed Intelligence

- **Knowledge Networking**
- **Learning and Intelligent Systems**
- **New Computational Challenges**

- **Automated Design and Discovery of Novel Pharmaceuticals using Semi-Supervised Learning in Large Molecular Databases,** M.J. Embrechts, K.P. Bennett, C. M. Brenema **(**Rensselaer Polytech Inst, 9/199 – 8/31/02, $1,200,000 Est.)

- **Multi-scale Simulation Including Chemical Reactivity in Materials Behavior Through Integrated Computational Hierarchies,** R.J. Bartlett, H.-P. Cheng, J.H. Simmons, S.B. Trickey, M.C. Zerner (University of Florida 9/15/99 – 9/31/02, $2,200,000 Est.)

NSF

Knowledge and Distributed Intelligence

KDI: Accessing Large Distributed Archives in Astronomy and P article Physics, A.S. Szalay, H.B. Newman, E.T. Vishniac, M.T. Goodrich, A. Pevsner 9/15/ 99 – 8/31/02, (Johns Hopkins University) $2,500,000 (Estimated)

KDI: Simulation and Modeling of Organic and Inorganic Non-cr ystalline Semiconductors P. Clancy, G.G. Malliaras,E.C. Kan, M.P. Teter, M.O. Thompson (Cornell University-Endowed) 9/15/99 – 9/31/ 02 $1,700,000 (Estimated)

KDI: 3D Knowledge: Acquisition, Representation and Analysis in a Distributed Environment, A. Razdan, G.E. Farin, D. L. Collins, M.R. Henderson, A.W. Simon **(**Arizona State University) 9/01/99- 8/31/02 $2,100,000 (Estimated)

NSF

Other Opportunities

- **NSTC Interagency Working Group on Nanoscience, Engineering and Technology**
- **Small Business Innovation Research (SBIR)**
- **Small Business Technology Transfer (STTR)**
- **Materials Research Science and Engineering Centers (MRSECs)**

U.S. Government R&D Funding Agencies

ARO

ARL

NIST

Case Study: Symyx Technologies

•Phase II grant from a Small Business Innovative Research (SBIR) Program funded by the U.S. Department of Energy, and two grants from the Defense Advanced Research Projects Agency (DARPA) through the Office of Naval Research (ONR),

•first DARPA/ONR contract will support the discovery of novel permanent magnet materials.

•DARPA/ONR grant will fund the use of Symyx's combinatorial methodologies to discover improved thermoelectric materials.

•DOE Phase II SBIR grant is directed toward accelerating the search for novel anode materials for use in a direct methanol fuel cell (DMFC).

•Totaling approximately $4.5 million

-- April 7, 1999

NRL and ONR

SIMULATIONS OF CONDENSED PHASE CHEMISTRY (BAA 929) (NRL)
- Theoretical Chemistry Section of the Naval Research Laboratory
- To perform molecular dynamics simulations of solid-state and materials-related chemistry

DEVELOPMENT OF MICROMACHINED SENSORS FOR PHYSICAL, CHEMICAL AND BIOCHEMICAL APPLICATIONS BAA 928(1)

Developing new micromachined sensors to measure physical phenomena such as magnetic and electric fields, pressure, electromagnetic radiation, temperature, humidity, and other meteorological parameters; (2) developing new micromachined sensors to detect chemical species with high selectivity and sensitivity; and (3) developing new micromachined sensors to detect biochemical species with high selectivity and sensitivity.

SUPERCONDUCTING MATERIALS (BAA 932)

Proposals for research and development of devices, components and circuits fabricated from materials with superconducting transition temperatures below 30K will be considered for funding if deemed suitable for potential Naval applications.

NRL and ONR

Engineering, Materials, and Physical S&T Department

Five divisions comprise this department: Physical Sciences Science and Technology; Materials Science and Technology; Mechanics and Energy Conversion Science and Technology; Ship Structures and Systems Science and Technology; and Biomolecular and Biosystems Science and Technology. The divisions contribute to naval strengths in the areas of chemistry, physics, biotechnology, structural materials, functional materials, structural mechanics, solid mechanics, fluid mechanics, propulsion and energetics. Ideas and techniques developed in these areas are applied to surface ship, submarine, and other undersea weapons systems and improve naval warfighting effectiveness and opportunities for environmental amelioration in all aspects of Fleet operations.

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Industrial and Corporate Programs Department

Because affordability is a top priority for the Navy and Marine Corps, ONR's integrated science and technology program interests include consideration of the manufacturing methods used to build naval warfighting systems. With affordability and the delivery of quality naval combat technologies in mind, ONR's Industrial and Corporate Programs Department stimulates advantageous government-industry partnerships and promotes the development in manufacturing of innovative, cost-efficient, and cost-reducing processes.
In addition, its Corporate Programs Division manages ONR's cross-disciplinary education and research infrastructure programs to increase the numbers and improve the capabilities of engineers and scientists working on issues of concern to the Navy, now and in the future.

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NRL and ONR

The commercial MEMS industry is expected to grow at an extraordinary rate into the next millennium. Market studies project a twelve to fourteen times rate of growth reaching $12-14 billion by the year 2000. Currently, pressure and acceleration sensors represent the largest commercial market for MEMS products (demand has been almost entirely driven by the automobile industry). Even though the MEMS sensor market will continue to grow, a substantial portion of the growth is projected to be in the non-sensing, actuator-enabled applications (i.e., displays, scanners, fiber-optic switches, flow regulators, etc.).