Combinatorial Methodologies for Advanced Materials: An ATP Technology Cluster

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

Agenda

- The NIST Advanced Technology Program
- ATP and Combinatorial Methods
- The FY1999 Combinatorial Methods Cluster
- Plan Forward: FY '00 Open Competition
- The ATP Selection Criteria

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

NIST is…..

Measurements and Standards Program

Advanced Technology Program

Manufacturing Extension Partnership

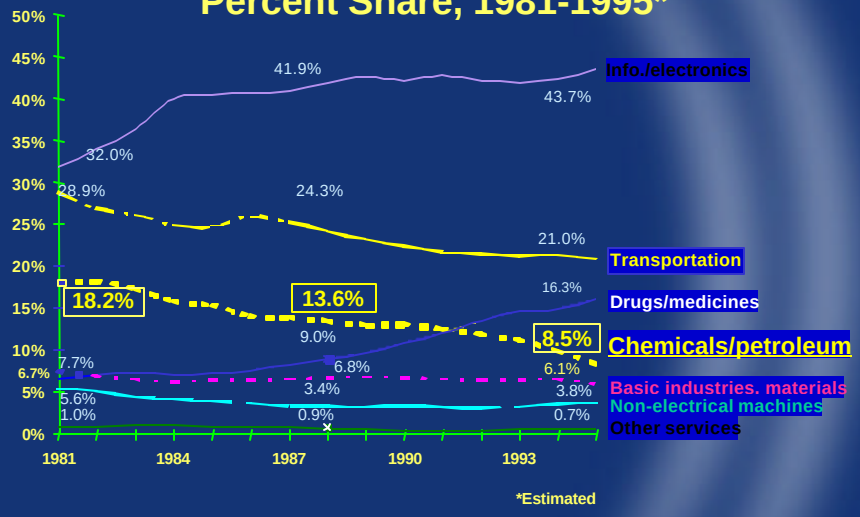
National Quality Program

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

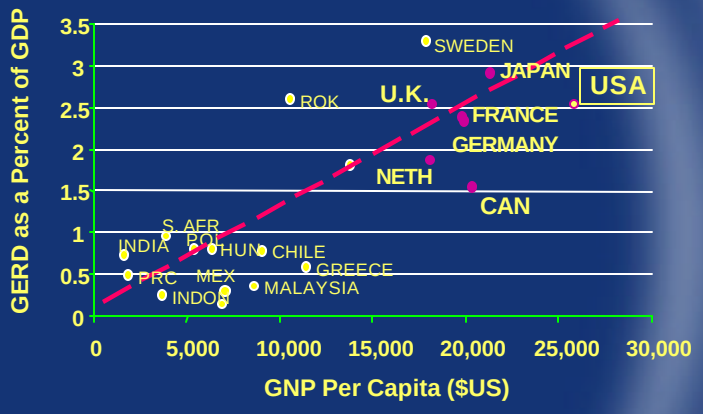
Percent Share, 1981-1995*



*Estimated

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

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What ATP Looks For…

ATP Cost-Shares High Risk, Enabling Technology

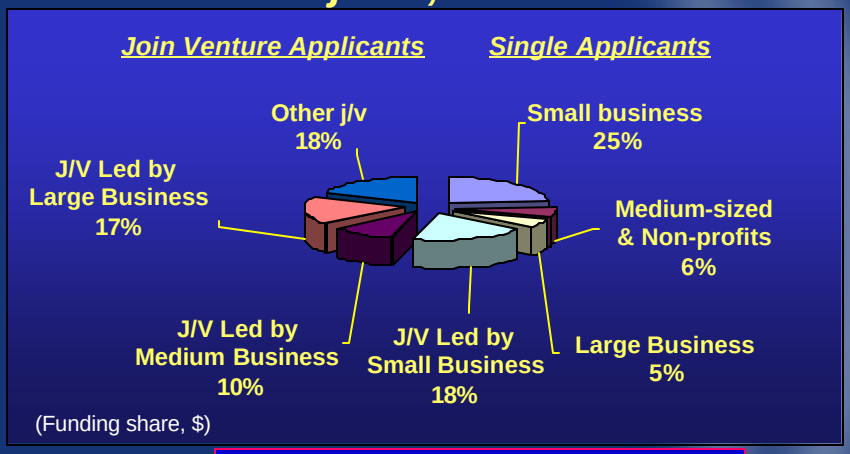
- Path-breaking technology
  - ✓ *Opens up new possibilities*
  - ✓ *Revolutionary in nature*
- Infrastructural technology
  - ✓ *Supports an entire industry*
- Multi-use technology
  - ✓ *Many distinct applications*

ATP Ground Rules:

- Confidential reviews by Federal employees
- Companies retain patent rights
- Projects in *all* technology areas are considered

$1,496M to ATP Awardees

468 Projects, 1990 - 1999



Substantial University Participation

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

The Chemical Industry

Technology Clusters	Program Managers
Catalysis & Biocatalysis Technologies	Robert Bloksberg-Fireovid, Ph.D
Selective-Membrane Platforms	Robert Beyerlein, Ph.D
Combinatorial Methods for Advanced Materials	John Hewes, Ph.D

ATP Technology Clusters

1993-1999

	Catalysis & Biocatalysis Technologies	Membrane/ Separations Technologies
Active or completed projects:	20	18
Estimated ATP funding:	$ 87.8M	$ 35.5M
Industry cost-share funding:	$ 94.4M	$ 45.0M
Total Impact:	$182.2M	$ 80.5 M

Why Combi @ ATP?

- Stimulate convergence of technologies
- Focus infrastructure development toward advanced materials applications
- Leverage leading-edge capabilities to lower-margin, less R&D-intensive industries
  - ✓ *Timing is critical*
  - ✓ *Benefits firms of all sizes, with many alliances possible*
  - ✓ *Multi-Skill Center effort (broad synergies)*
  - ✓ *New tools for research and development*
  - ✓ *Large spill-over benefits to/from basic science*

ATP can help U.S. industry implement!

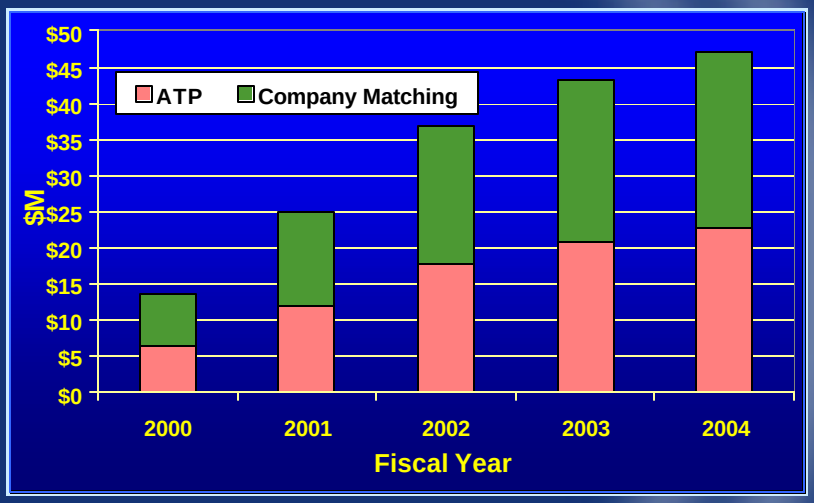
ATP Technology Cluster

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



Target Applications-Combi

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

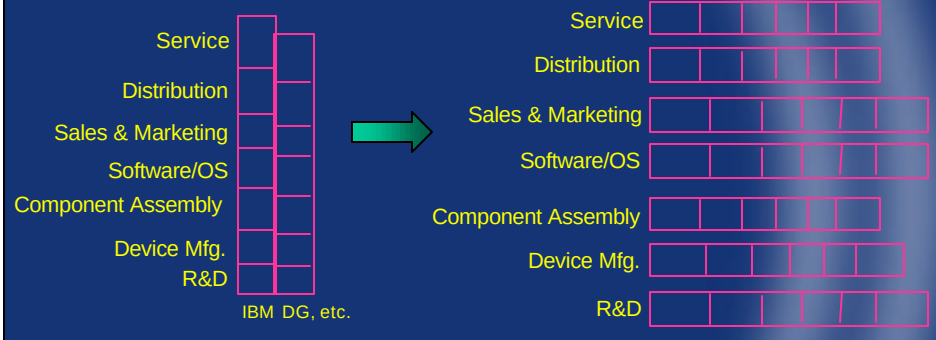
Profit Margin, R&D Budget, and Cost/Benefit Define Combi Entry

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

"Horizontalization" of industry sectors



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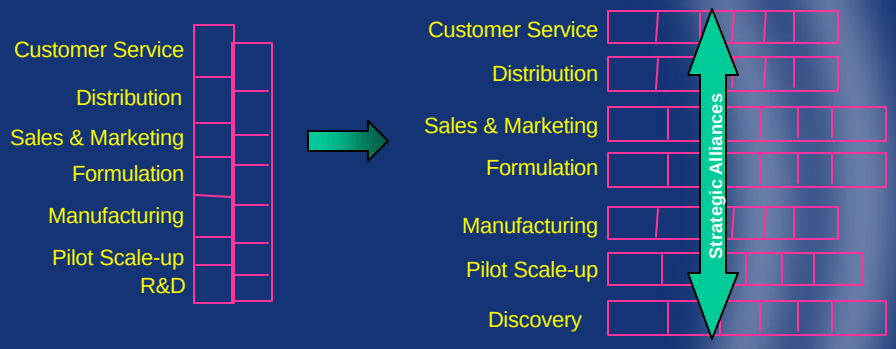
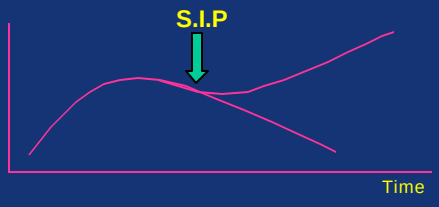
"Horizontalization" of Industry



Strategic Inflection Points



The New SIP: Combinatorial Methods

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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		• Characterization of properties and composition not straightforward
• Descriptors for diversity		• 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

Plan Forward—FY '00

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

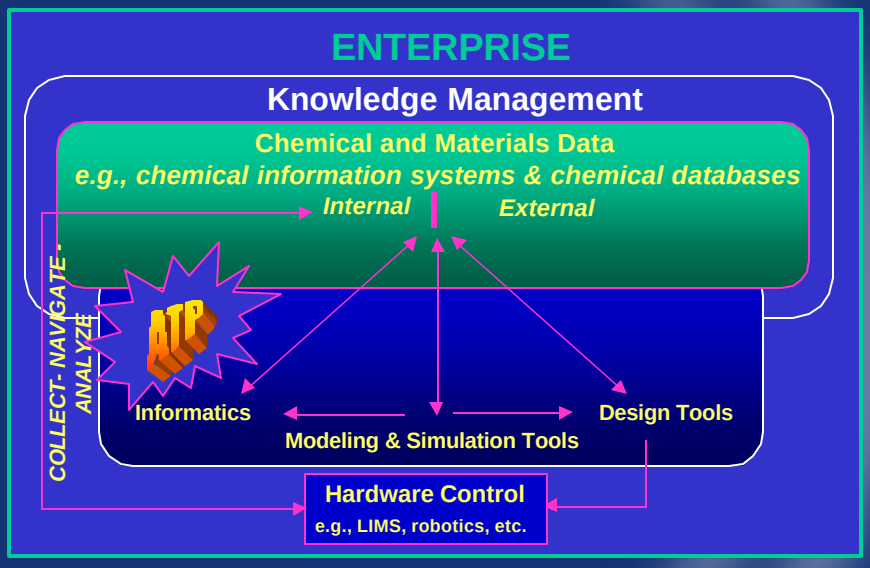
Informatics

- **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*

Issues--Informatics



Issues--Characterization

- Miniaturization/parallelization of reaction, processing, and testing apparatus
- Micro-sensors (*in situ* analysis)
- High-level Integration
- Clear understanding of "scalability"
  - ✓ Validation of micro- vs. bulk properties
- Deposition of samples
  - ✓ Ink jet, PVD, CVD, etc…..

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Rules for Participation ...

- Must produce U.S. economic benefits
  - ✓ R&D and manufacturing in the U.S.
  - ✓ Increase U.S. employment
  - ✓ Promote U.S. supplier infrastructure
- Companies incorporated in the U.S.
- Keep intellectual property rights
- Confidentiality (not subject to FOIA)
- Universities and non-profit research organizations may receive share of return from royalties but cannot own title to intellectual property

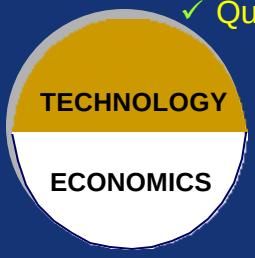
How to apply

- Pre-proposals--Year-round submission
- Full Proposals—Annual Competition
  - ✓ *Announced late Fall, due early Spring*
- Obtain and ***read*** the Preparation Kit
  - ✓ *Hardcopy, online or CD-ROM*
- Assemble Proposal
  - ✓ *Commercialization **and** Technical Plans are evaluated by experts for feasibility*
  - ✓ Multi-functional team highly recommended

Most Common Error is Lack of Detail in Proposal

Critical Proposal Elements

- **Scientific and Technological Merit (50%)**
  - ✓ Innovations in the Technology
  - ✓ High Technical Risk & Feasibility
  - ✓ Quality of R&D Plan



- **Broad-Based Economic Benefits (50%)**
  - ✓ Economic Benefits
  - ✓ Need for ATP Funding
  - ✓ Pathway to Economic Benefits

Common Weaknesses

- Proposals lack of sufficient detail for peer review
  - ✓ *How you will reach technical and commercial objectives*
  - ✓ *What's innovative about the approach*
  - ✓ *Why a risky technical approach is needed*
- Proposals have unsupported assertions that project meets ATP's criteria
- Proposals miss ATP's window of opportunity
  - ✓ *Low risk - product development (too late)*
  - ✓ *Lacks demonstrated feasibility (too early)*

Some helpful hints …

- Proposals due at **3:00 p.m. (Eastern)** on the specified date -- ***no fax or electronic transmittal***
- Late proposals rejected. ***NO EXCEPTIONS!***
- Overnight mail companies sometimes *don't* deliver overnight
- Send your proposal in early
- **Read the Proposal Prep Kit**

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