ATP Fall Meeting, Atlanta, GA
November 18, 1998

Workshop Agenda

- Introduction: Combinatorial @ ATP
- Presentations
- Breaks at 10:30 and 2:30
- Lunch at 12:30 - 1:30
- Break-out Session: Why ATP?

ATP Agenda

- The ATP Process
- Technology challenges
- Economic benefits to the US
- The Opportunity for ATP
- Conclusions

Workshop Goal: Develop highest quality proposals for the FY 1999 Open Competition

What is the NIST ATP?

- Opens new opportunities for U.S. industry in global markets
- Different from other government programs
  - ✓ *Intellectual Property retained by awardees*
  - ✓ *~50% cost-share*
  - ✓ *Proposals & project results are co. confidential (except for non-proprietary summaries)*

First-year funding for FY1999 Competition is $66M

High Technical Risk

- Technical challenges which display **significant recognized** uncertainty of successes
- Success will **dramatically change** the future direction of technology and its market impact
- Risk may be high in developing single innovations and/or in integrating technologies

No Proposal will be Funded That Does Not Have High Scientific and Technical Merit

Potential Economic Benefit

- Effects of the ATP
  - Would it happen without ATP?
  - Accelerates R&D and commercialization?
  - Increases/broadens opportunities for new products and processes?
  - Collaboration and synergies likely?

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Market Needs and Technologies Collide

- Markets demand higher performance/price ratios
- Globalization of markets increases *pace* of change

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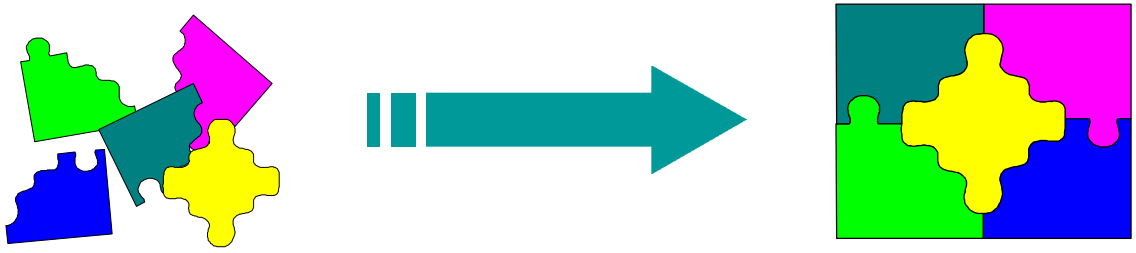
- Convergence of hardware and software technologies
- Lower cost, generic solutions increase availability



Combinatorial Discovery of Chemicals and Materials

An ATP Project Portfolio for 1999

Program Development Team
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Industry input to ATP:

Chemicals and advanced materials mfr.'s want to use high throughput R&D methodologies

BUT..... Large entry barriers exist:

Expensive to most non-pharmaceutical sectors

- Won't invest in non-core technologies or businesses
- Requires new base technologies and their integration
- Long pay-back of (high) R&D capital investment (ROI)
- Won't displace installed assets (ROA)

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Vision: Combinatorial Methods

ATP project portfolio of ‘99 Open Competition will implement, within U.S. chemical industries, new research tools and methodologies that will significantly and positively impact the breadth of innovation and cycle times.

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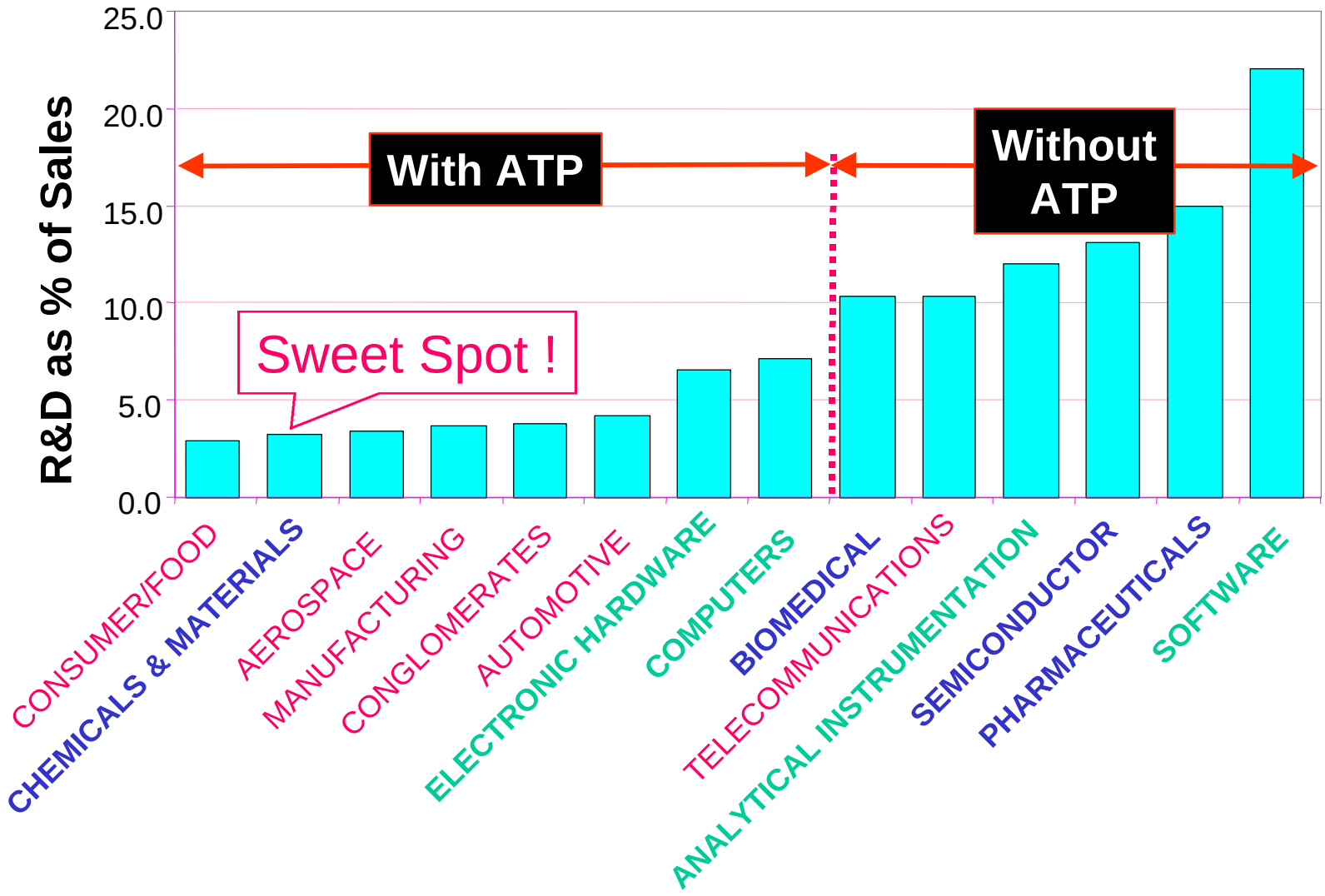
Where can ATP make a difference?



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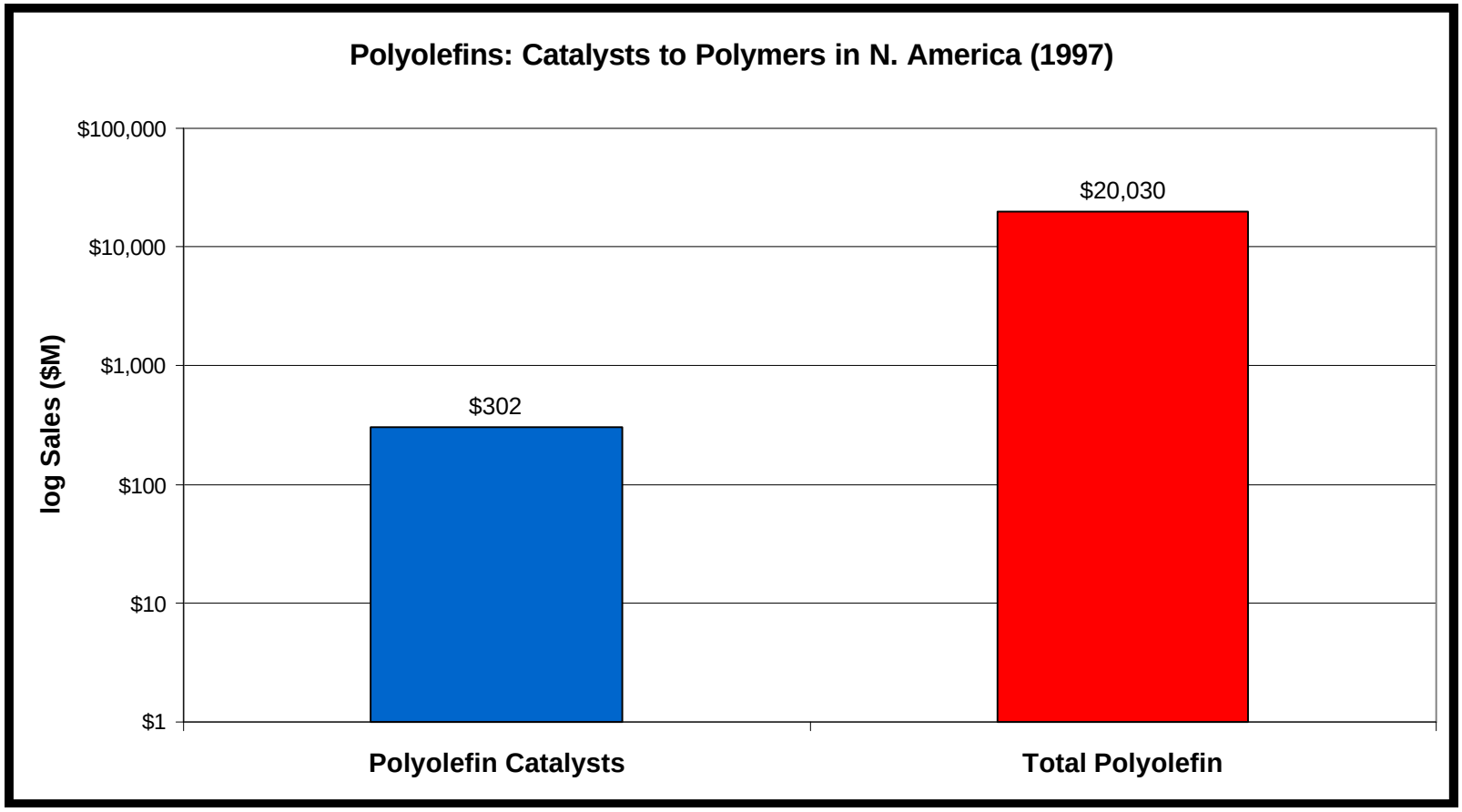
An Example: Polyolefin Catalysts



Staff estimates, The Catalyst Group

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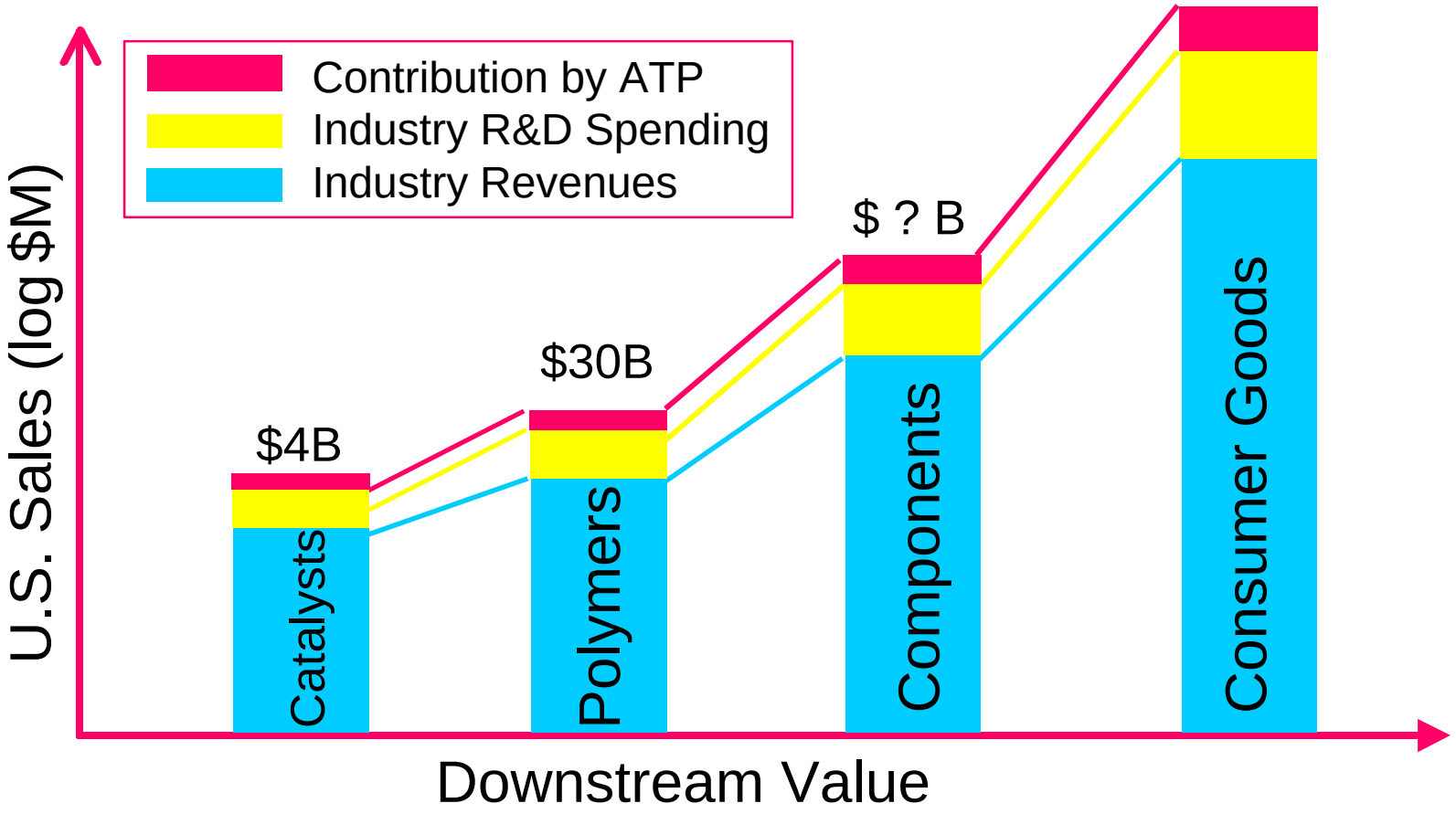
Widespread economic benefits estimated



* Staff estimates, Freedonia, SRI, Frost & Sullivan

Technical Issues to Address

- What is the technology roadmap ?
  - Emerging technologies
  - Enabling technologies
- Hardware/software integration
- Software integration
- Scalability (micro- to bulk properties)
- Generic technology vs. specialized

Basic as well as applied research is needed--NOW!

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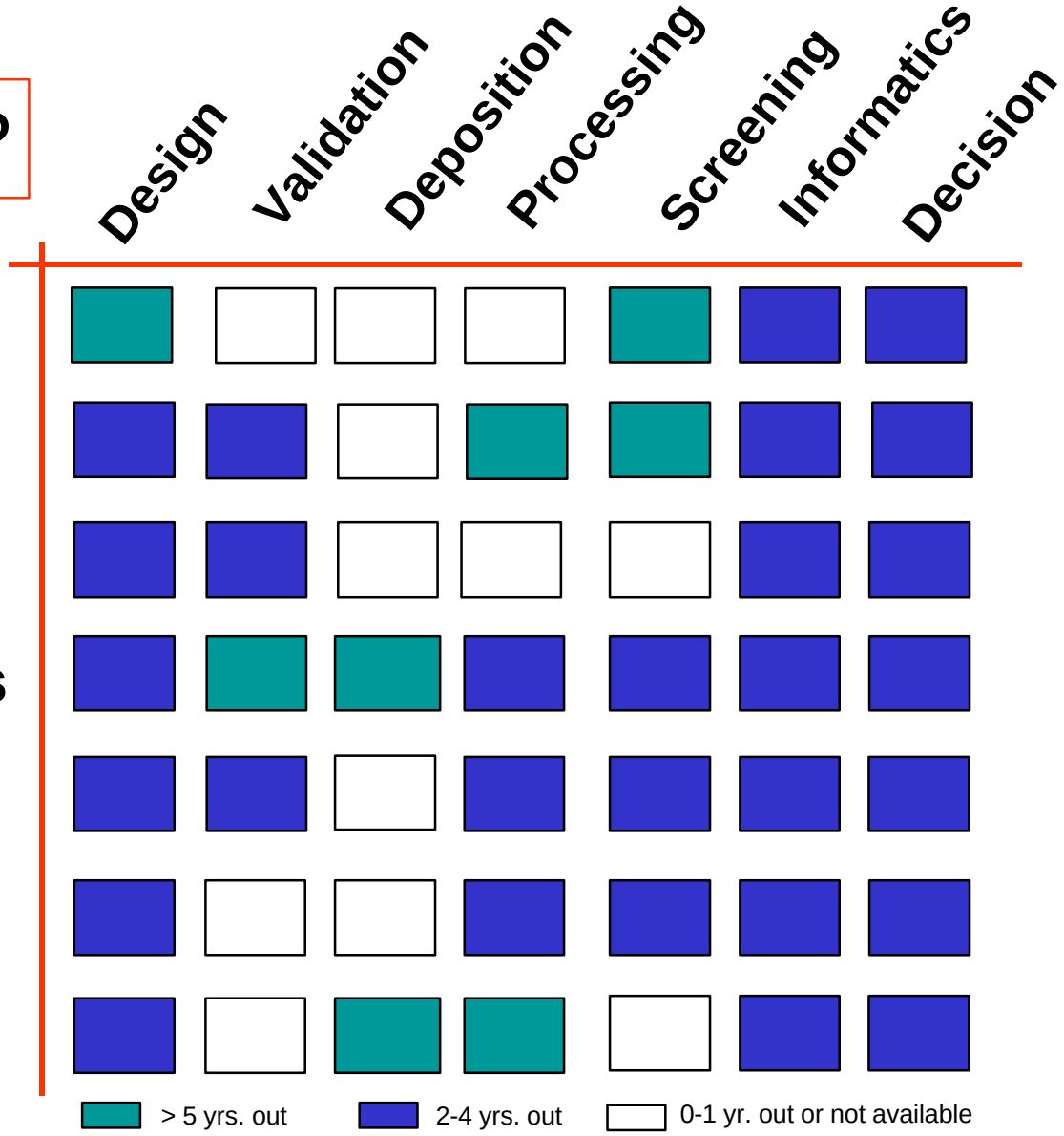
Where's the Risk?



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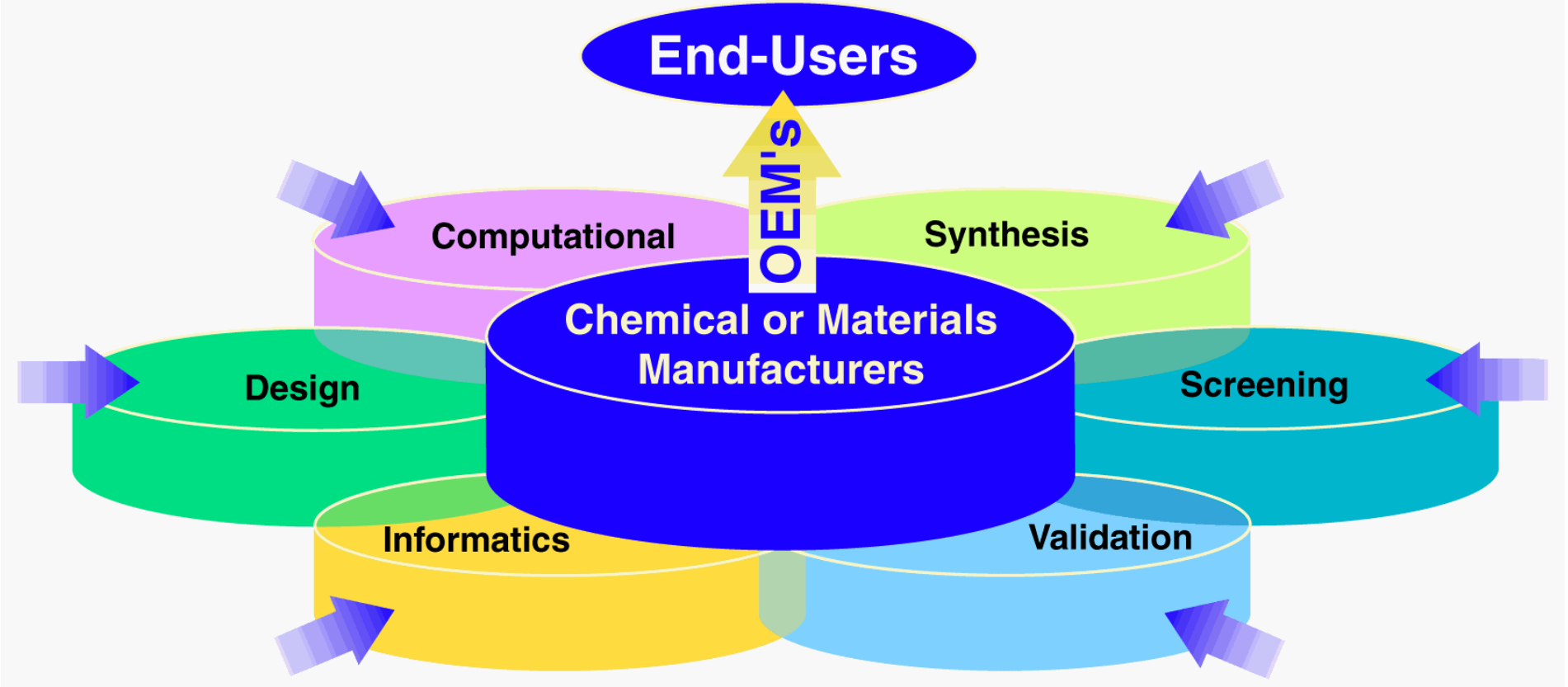
ATP Portfolio Strategy



Focused infrastructure on specific applications

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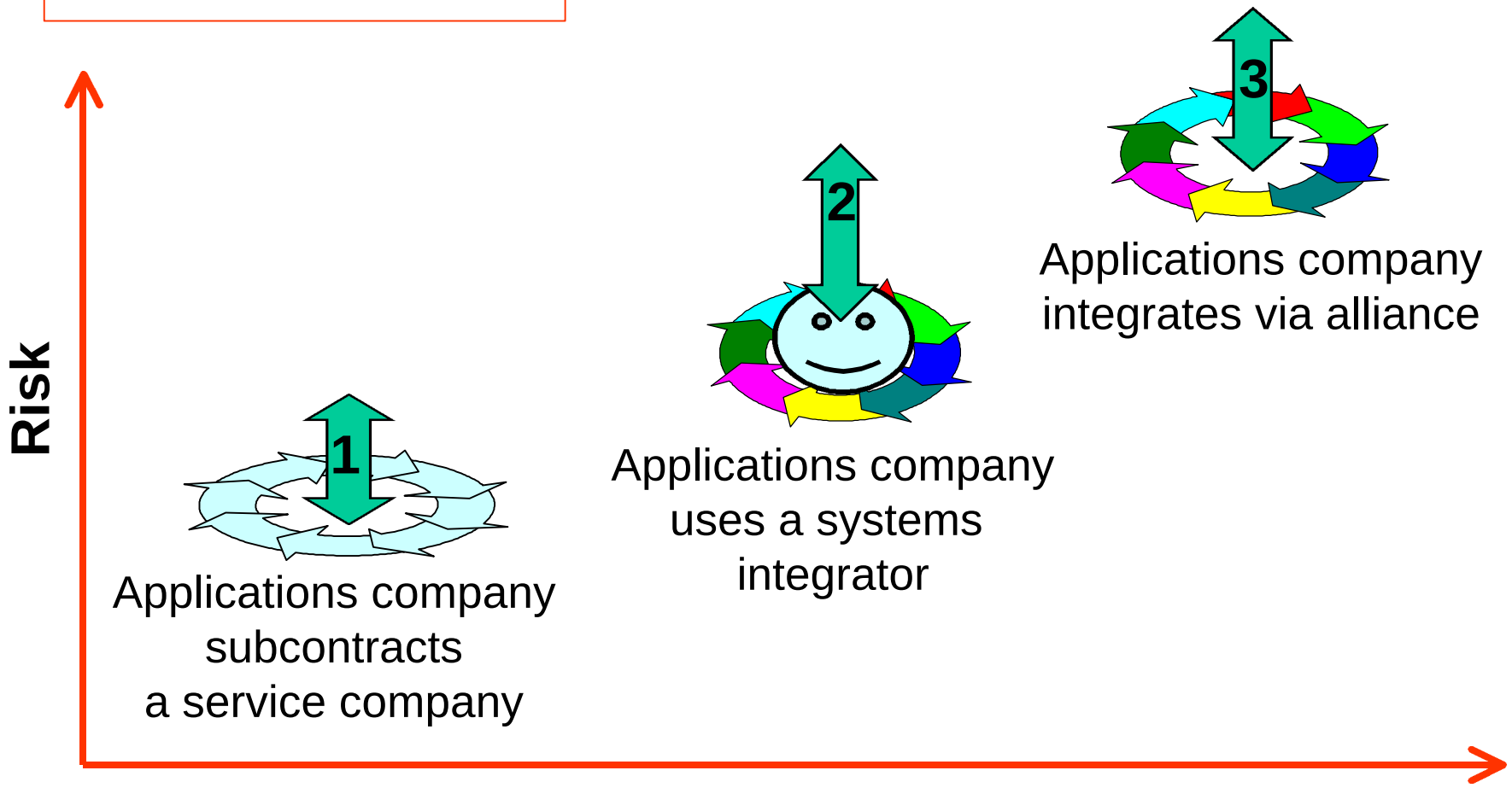
Risk Scenarios



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How can ATP Help ?

- Applications mfr.'s have <u>some</u> combi. capabilities
  - ***Awaiting one or more enabling technologies***
- Technology infrastructure can provide solutions
  - ***Focus on specific applications***
  - ***Develop alliance***
  - ***Integrate systems***

<u>Without ATP</u>	***<u>With ATP</u>***
Resource-rich sectors	Resource-limited sectors
Methodologies diffuse slowly	Methodologies diffuse faster

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Benefits to U.S. Industry

- **Reduced innovation cycle times and time-to-market**
  - **Bench-scale discovery**
  - **Process development**
  - **Customer service and flexible manufacturing**
- **Productivity impacted: reduced costs of development**
- **New products, new technologies = new markets**
- **Allows for “out-of-box” experimentation**
  - **Broadens spectrum of materials in development**

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The ATP Opportunity

- Bring leading-edge, generic technologies to lower-ROI sectors
  - Spur discontinuous innovation in industrial R&D
  - Help develop lower-cost hardware and software tools
- Focus base technology innovation toward applications
- Facilitate systems integration (hardware and/or software)
- Improve competitive stance in portfolio industries
  - Challenge threats to intellectual property
  - Reduced commercialization cycle times
  - Permit discovery with “out-of-box” ingredients

Break-out Session

3:45 to 5:00 PM

The ATP Selection Criteria

1. Potential <u>Broad-Based</u> Economic Benefit

2. High Technical Risk

3. Commercialization Plans

4. Organizational Commitment/Organizational Structure

Break-out Session Goals

4:00 to 5:00 PM

Agenda

Force Field Analysis: without ATP vs. with ATP

1. Technology challenges facing industry entry
2. Economic benefits if hurdles are overcome
3. Therefore, why does industry need ATP ?
4. Present results

Results will be compiled and put on ATP web page

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New Paradigms and Issues in R&D

- Cycle time reduced to hours/days from months/years
- Hardware/software/enterprise-wide integration
- Statistical design and expert systems become key
- Grow from discovery to process development
- Threat of re-engineering composition of matter IP
- Intangible returns for chemical industry

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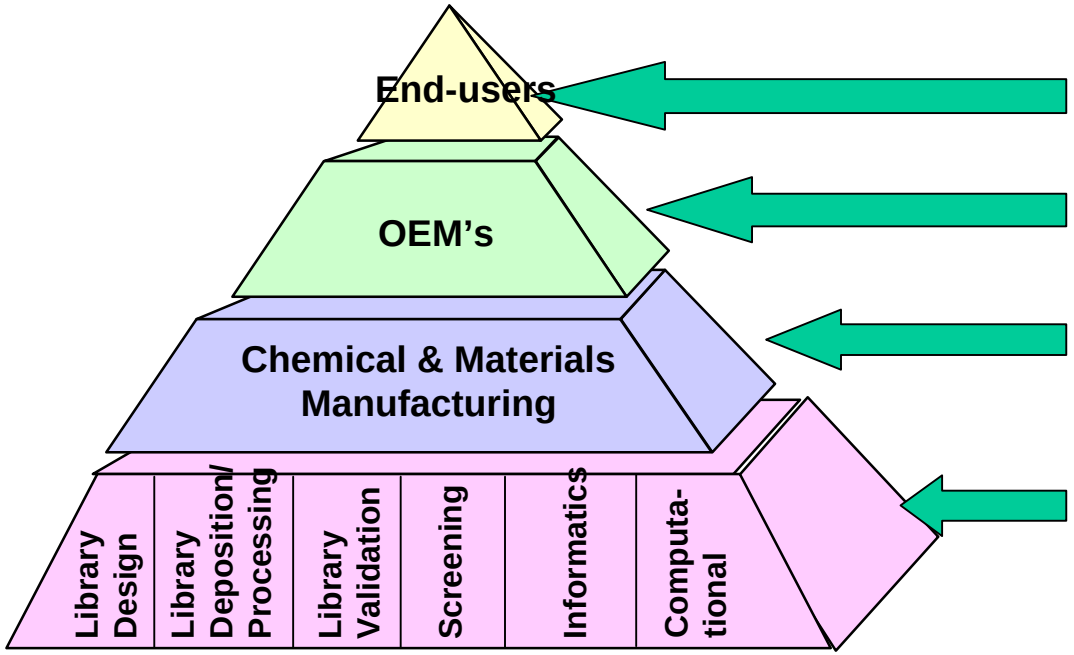
Hierarchy of Benefits



- **Faster/lower-cost R&D**
- **Lower-cost processes**
- **Sales of higher value products**

- **Network development**
- **Sales of tools**

Most diffusion from end-users and infrastructure

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Weaknesses

- doesn't fully address synthesis hurdles
- high entry costs
- technology stretch // high risk
- long lead time to fully integrated system
- cultural backlash (technical & business communities)
- requires strength in multiple disciplines (very difficult for small companies)
- difficult to protect intellectual property
- no guarantee of success
- lose serendipity aspects of current research

Threats

- Needs demo to prove worth
- Coordination to integrate all efforts quickly
- US leadership could change face of innovation
- First generation stage of the technology -- need to focus on how future generations will look
- Creation of automation experts
- International (esp. Japan & Germany)
  - Empirical approach fits core competencies
  - Material science core expertise
  - Miniaturization, automation, databases

Why ATP?

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Technology Base Needs

Synthesis and Processing
- Automation
- Sensors

Design of the library
- Statistics
- AI/expert systems

Scalability Predictions
Interfacial vs. bulk properties

Screening (HTS)
- Sensors
- MEMS
- Robotics

Cheminformatics
- Samples control
- Information flow
- Data integration
- Data analysis
- Hardware support

Leverage developments from pharmas

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Hardware Issues

SENSORS

- Catalytic Selectivity
- Catalytic Turn-over
- Chemimetrics
- Degradation
- Electrical properties
- Luminescent properties
- Mechanical Properties
- Optical characterization
- Polymer architecture/morphology
- Thermal properties

PROCESS CONTROLS

- Control of interfacial, diffusion, mass transport
- Control of physical (e.g., temperature, time, stress)

DEPOSITION EQUIPMENT

- Chemical Vapor Deposition
- Laser ablation
- Ink jet
- **Thermally-driven transport (e-beam, LEED, laser, etc.)**

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Software Issues

Computational

- Diversity analysis/clustering/analysis
- Computational: Molecular Modeling QSAR, QSPR
- Reagent Building Block Analysis
- Statistics, modeling, design of experiments

Informatics

- Indexing
- Entity Inventory
- Electronic Laboratory Notebook (ELN)
- Search engines/Inferential Engines
- Patent and prior art reviews
- Literature/Patent Databases

Validation

- Micro-Inspection/Error Identification

Decision/Analysis

- Neural Net
- Fuzzy Logic
- Prediction Tools

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