Innovation: From Pure to Applied Chemistry – The U.S. Perspective

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US Chemical Industry in the U.S.

- $400 Billion in shipments- nearly 2% of GDP
- 50% of output to other manufacturing industries
- an “enabling industry”
- US plants provide 24% of world chemical production
- One of the top exporters
- R&D intensive in the past

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Wealth from New Technology

- A great run for the chemical industry
- Source: new technology
- Technology created from a sophisticated science base
- Industry understood how to take products of science and create value

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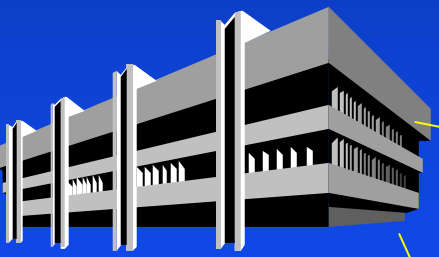
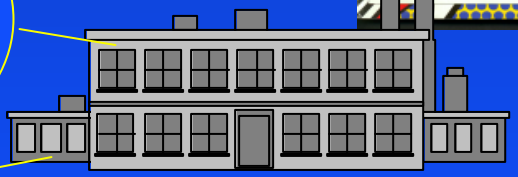
Science and Technology Network

- Helped create the industry
- Sustains it
- Offers opportunities for growth

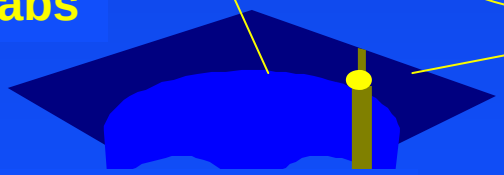


rnment Labs

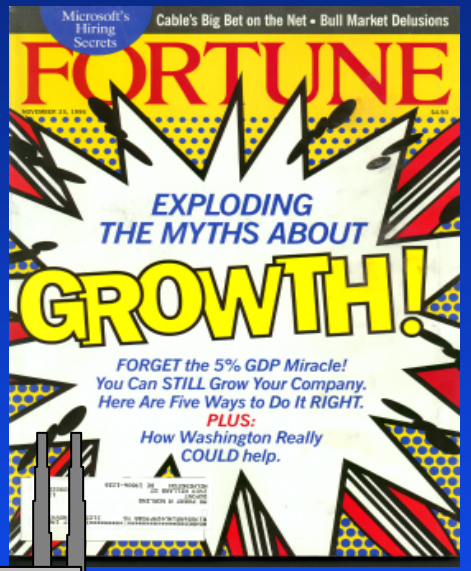
Global Network of Science and Technology



Other Companies



Universities



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Impact of Scientific Discoveries

- Growth of the chemical industry
- Scientific discoveries from discovery research have had great impact on technology development.
- Formation of entire industries from research in magnetic resonance, superconductivity, lasers, antibiotics to name a few


NATIONAL MEDAL OF TECHNOLOGY WI

On behalf of the American people, the President of the United States and the U.S. Dep salute the winners of the National Medal of Technology, the nation's highest honor fo vation and leadership. Since 1985, the Medal has been awarded to individuals, team exemplify the American spirit of innovation. Through their creative energy and accom fortified the nation's economic prosperity and quality of life, and inspired future gene

STEPHANIE K

STEPHANIE KWOLEK
THE DUPONT COMPANY

"For her contributions to the discovery, development and liquid crystal process- ing of high-performance aramid fibers which provide new products worldwide to save lives and benefit humankind."

The National Medal of Technology is not only a great honor for the individuals, teams and compa- nies that receive it, but a symbol of the country's continued value and support for technology and all the benefits that "we the people" derive from it.

Stephanie Kwolek's pioneering work is just such an example. Her initial discoveries in the area of liquid crystalline polymer solutions ultimately became the world's strongest fiber, Kevlar®. It's in the brakes of trains, planes and automobiles. It's in skis, helmets, protective clothing and most anyplace else requiring a unique combination of light weight and strength. In bullet-resistant vests, it has saved the lives of some 2000 law enforcement officers.

"I am honored to receive the 19 Technology for myself as well as ees of the DuPont Company wh the successful development of th fiber. Science and technology ar behind the economic growth an country. In addition, they have l through advances in medicine, t communication and so forth. Fo country, science and technology of all of us."

DUPONT

Better things fo

The National Medal of Technology was created by Congress to foster technological innova

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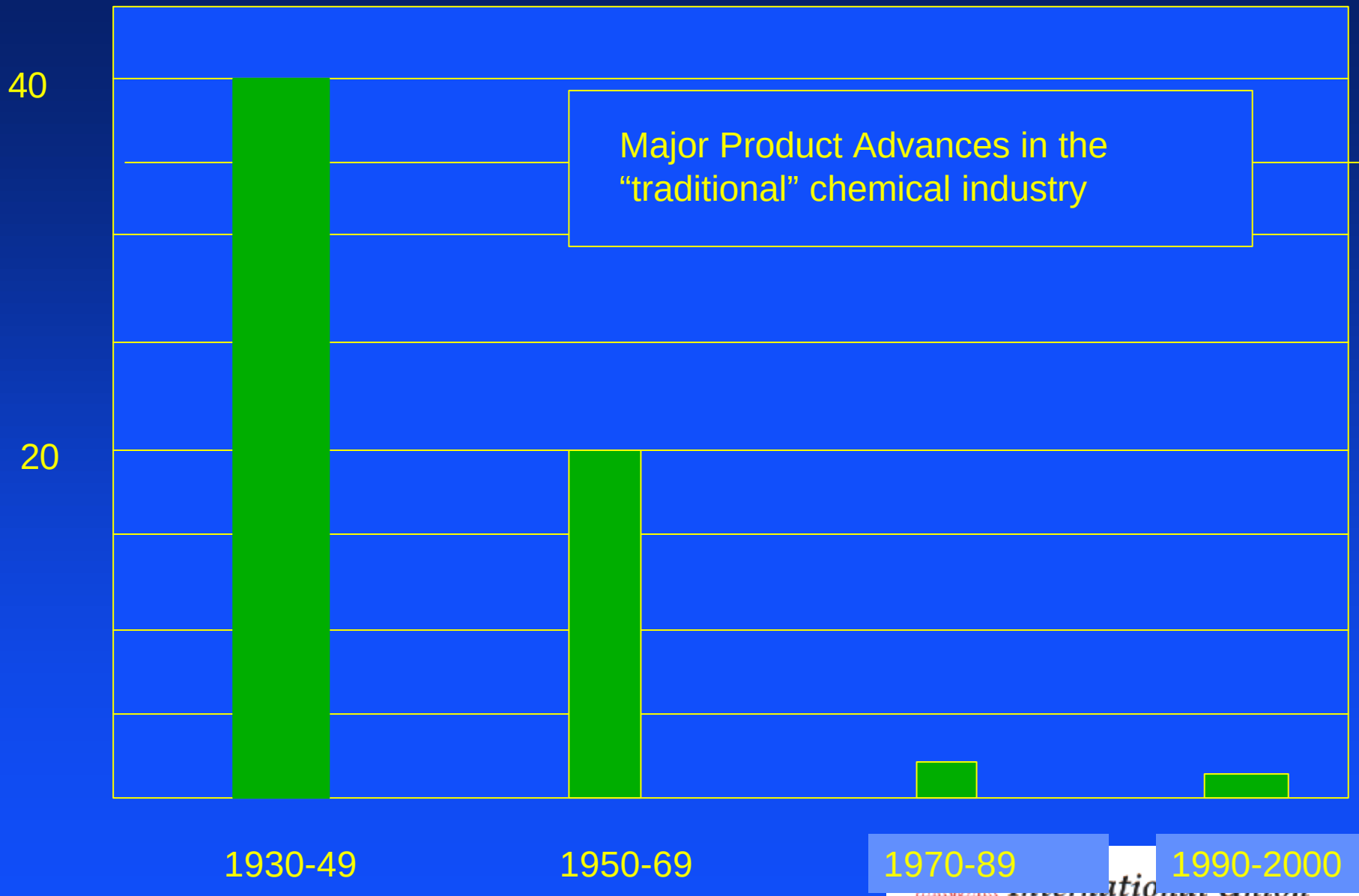
Concern Today

- Number of innovations in the “traditional” chemical industry has dropped considerably
- R&D Intensity is dropping

Innovation in the U.S. Chemical Industry has plummeted



mission on Industrial Productivity; AT Kearney;
Business July/August 2002 p. 20

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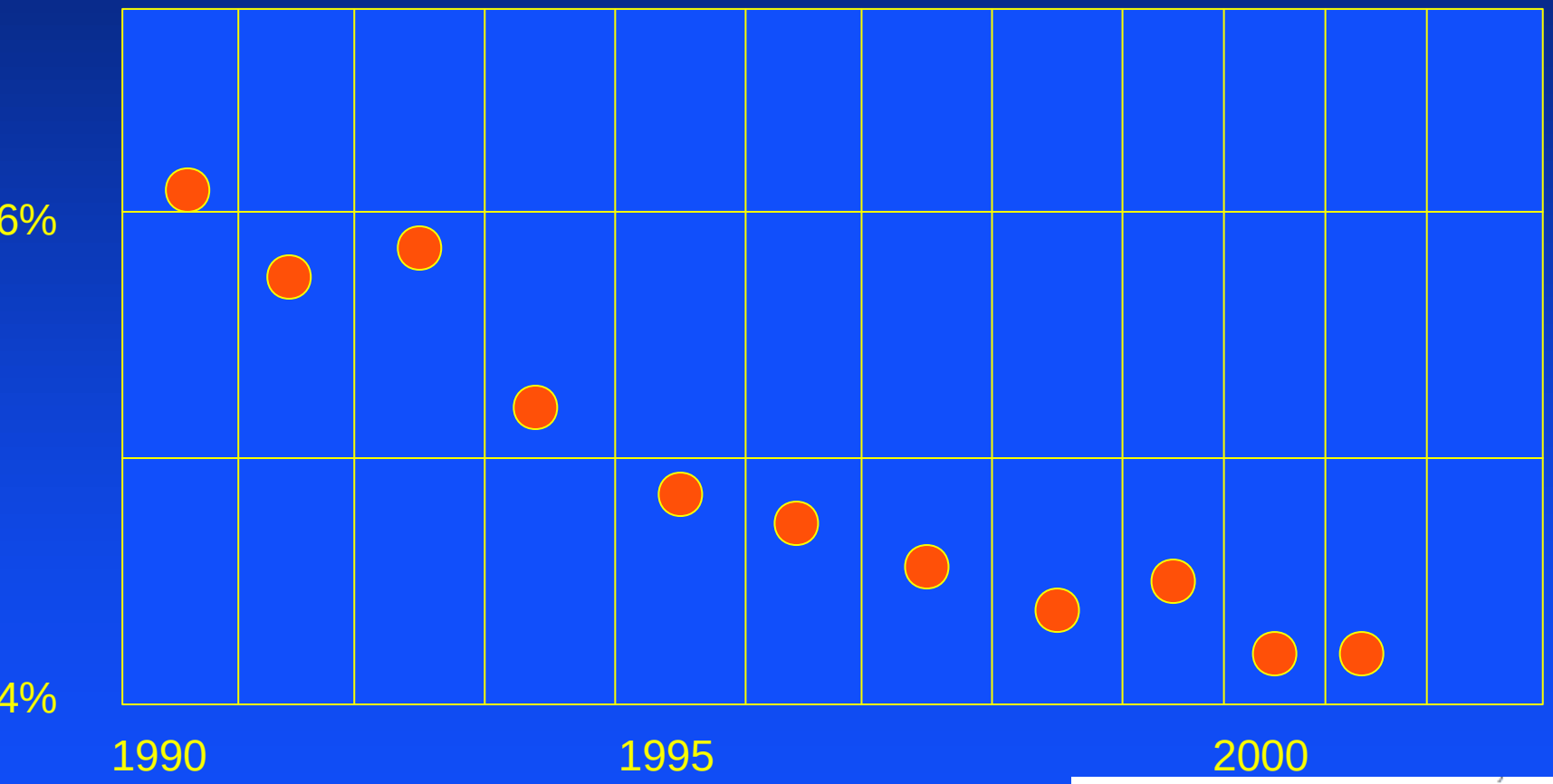
R&D Intensity For the Chemical Industry



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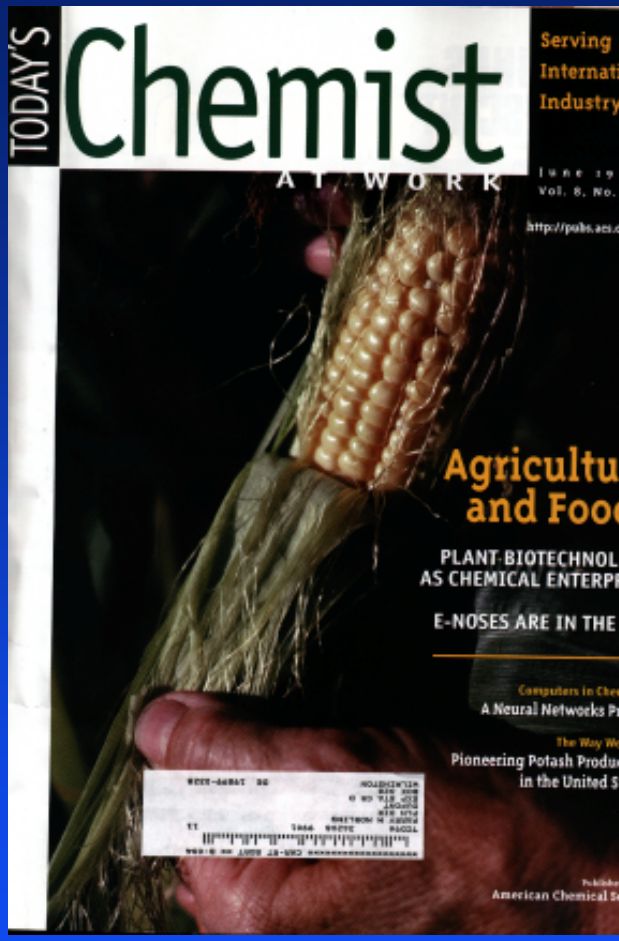
Concern Today

- Are we walking away from discovery research and breakthrough technologies?
- Will Innovation be a means of not only remaining competitive but also of growing?
- Are there new directions in R&D for the chemical industry?

What's Ahead for the Chemical Industry?

- Economic and Scientific Forces at work
- Mature businesses may need to be replaced
- Will chemical companies embrace the life sciences, advanced materials, nanotechnology or????



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Council for Chemical Research Study

Each dollar invested in chemical R&D produces 2 dollars in income over a seven year period

17% rate of return

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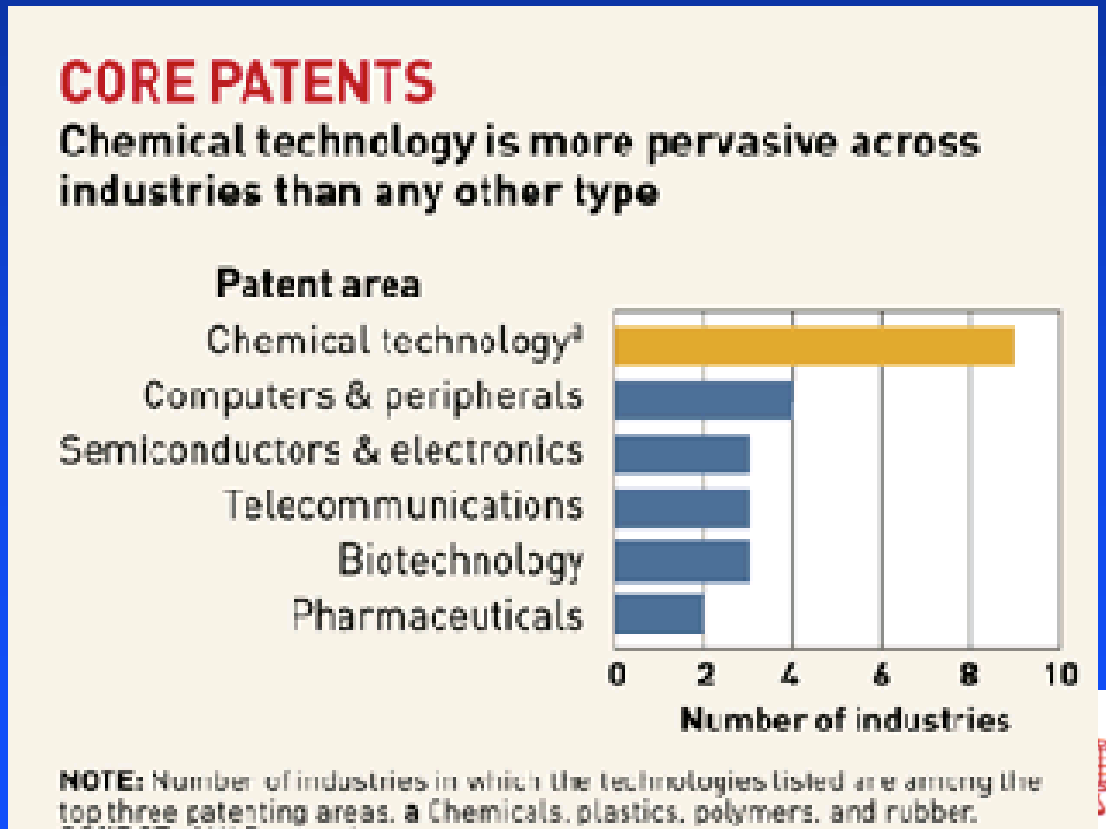
Council for Chemical Research Study

Second phase: Is chemical technology significant to other industries?



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Some Techniques and Approaches: Enabling Innovation in the Chemical Industry

- Green Chemistry
- Modeling and simulation
- High Throughput Experimentation- Combichem

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What is Green Chemistry?

Involved in the invention, design, and application of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.

Selection of feedstocks, reagents, alternative reactions, solvents, lower use of energy for environmentally benign and safer products and processes.

Ultimately replaces end-of-pipe controls for pollution prevention

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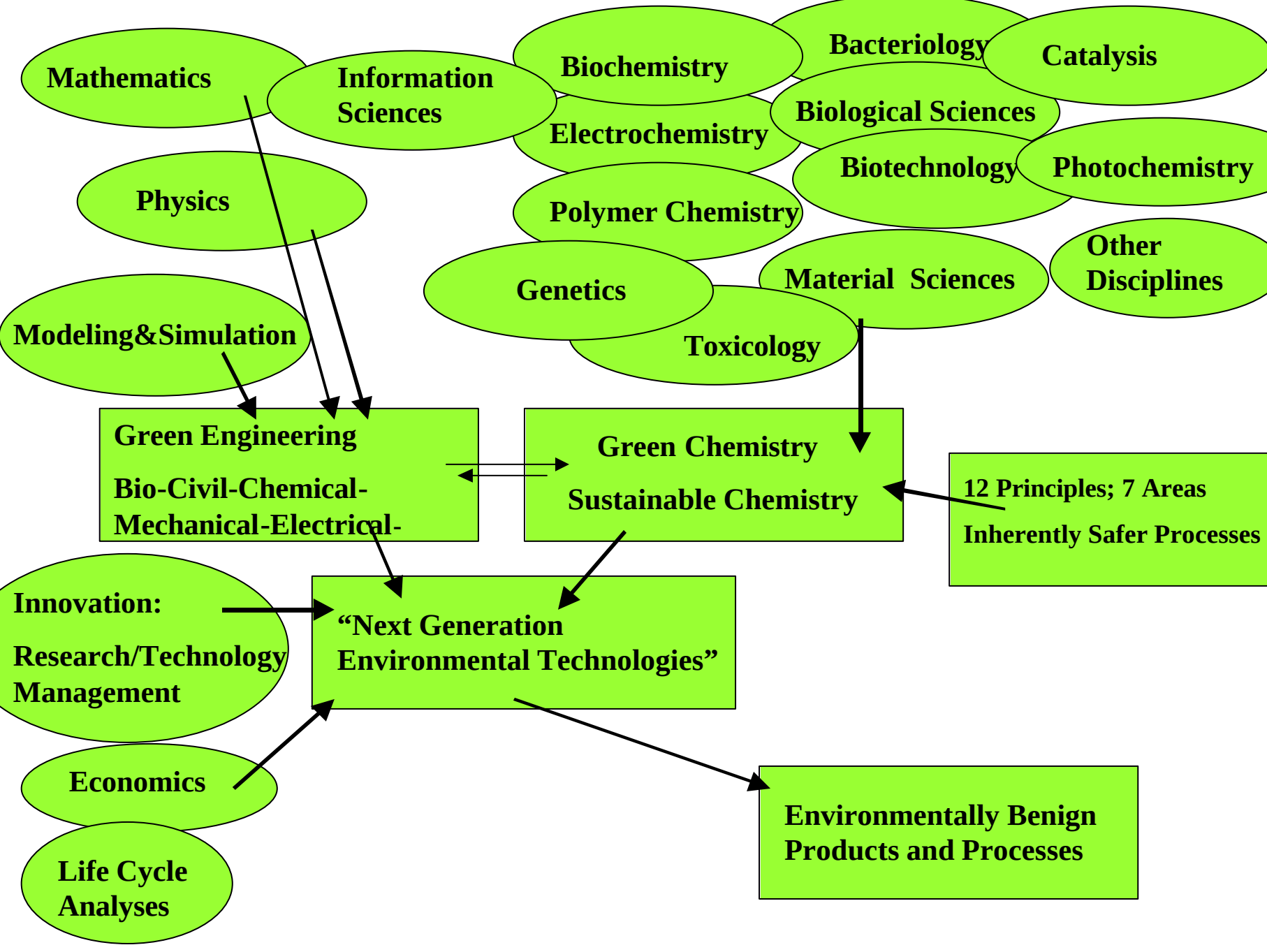

Mathematics
Information Sciences
Biochemistry
Bacteriology
Catalysis
Biological Sciences
Electrochemistry
Biotechnology
Photochemistry
Physics
Polymer Chemistry
Other Disciplines
Genetics
Material Sciences
Modeling&Simulation
Toxicology
Green Engineering
Bio-Civil-Chemical-
Mechanical-Electrical-
Green Chemistry
Sustainable Chemistry
12 Principles; 7 Areas
Inherently Safer Processes
Innovation:
Research/Technology
Management
"Next Generation
Environmental Technologies"
Economics
Life Cycle
Analyses
Environmentally Benign
Products and Processes

Case studies : 24 plus 47 examples of bio-based processes

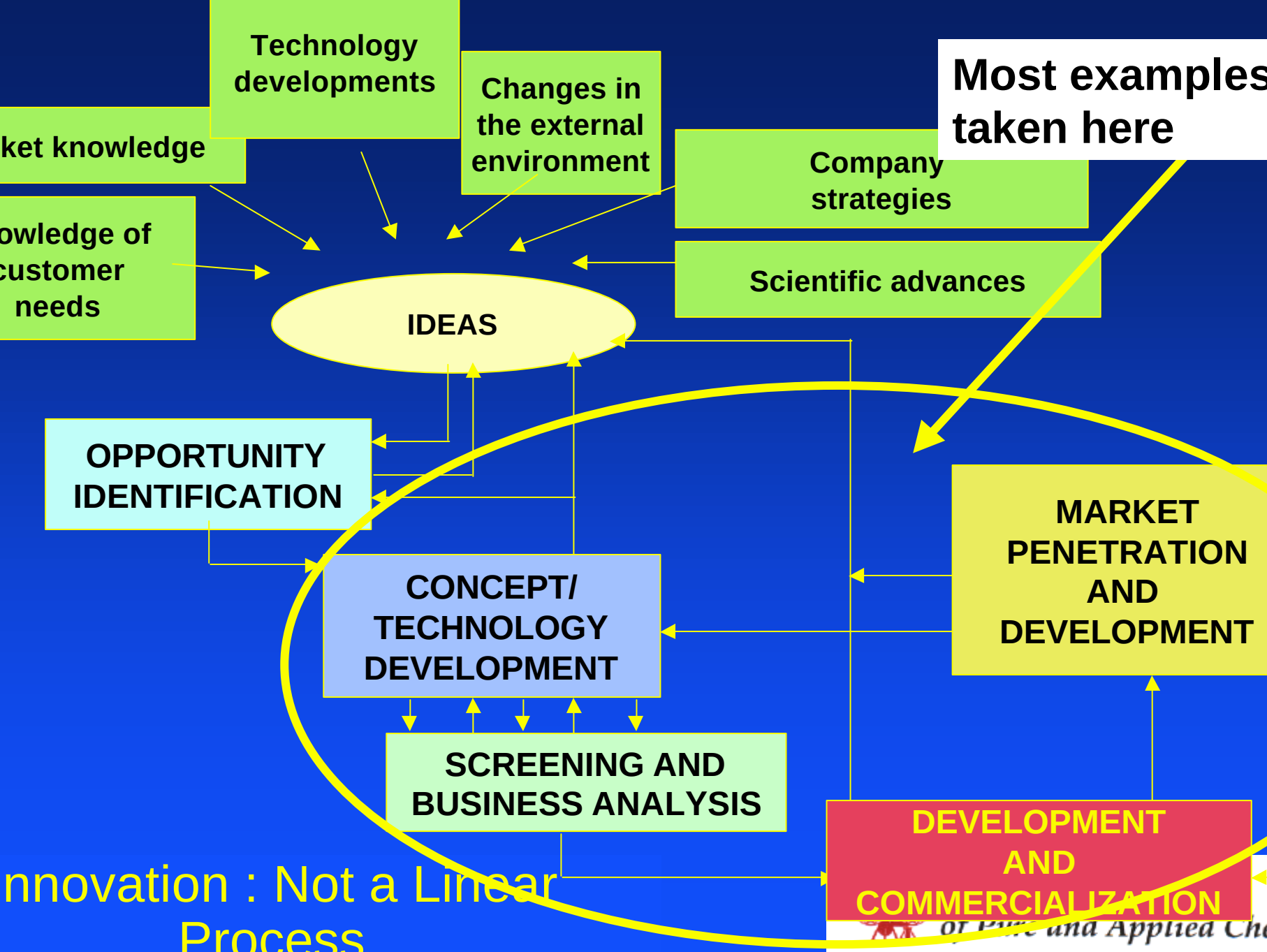
Study: “Next Generation Environmental Technologies: Benefits and Barriers” RAND 2003

Description of the chemistry and/or science and technology involved. Sectors affected now and in the future

Immediate and longer term benefits

Barriers to commercialization

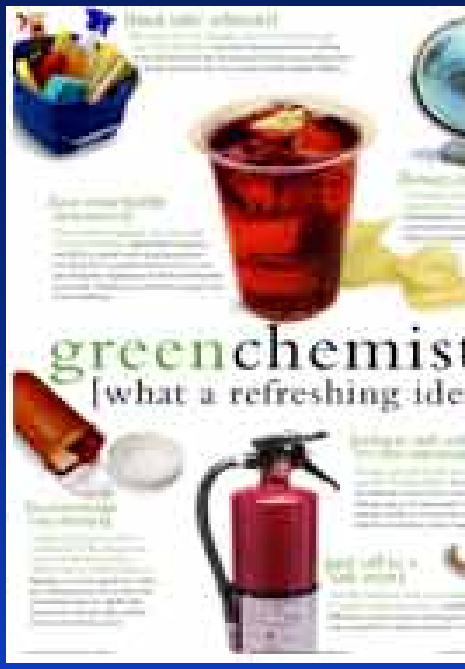
Government role


Technology developments
Changes in the external environment
ket knowledge
owledge of customer needs
Company strategies
Scientific advances
IDEAS
Most examples taken here
OPPORTUNITY IDENTIFICATION
CONCEPT/ TECHNOLOGY DEVELOPMENT
MARKET PENETRATION AND DEVELOPMENT
SCREENING AND BUSINESS ANALYSIS
DEVELOPMENT AND COMMERCIALIZATION
nnovation : Not a Linear Process

Use of supercritical or liquid CO2 as solvent

- **Surfactants enabling use of supercritical CO2 as solven in dry cleaning**
- **Production of fluoropolymers**
- **Use in computer chip manufacture**

A three step process replaced a six step process for manufacture of ibuprofen



o-based processes – 47 including:

Use of genetically altered *Echerichia coli* to produce adipic acid, Catechol, and substitute for BHT

1,3 propanediol from glucose

biopulping

Biocatalytic Production of 5-Cyanovaleramide.

Removal of metals from mine water by biotreatment

Pulp and paper processes

- **Delignification and bleaching of pulp in paper manufacture without the use of chlorine or chlorine dioxide;**
- **Activation of hydrogen peroxide with materials that mimic enzymes**

Production of polylactides

oduction of Hydrogen Peroxide directly from Hydrogen a Oxygen in CO2

ood Preservation – replacing chromated copper arsenate

nthesis of key intermediate for Monsanto's Roundup®

ntricon ® Termite Colony Elimination System

Benefits from NGETs

Environmental – Reduction in:

- Toxics (TRI) – (toxicity weighted index)
- Carcinogens- (specific chemicals removed from environment)
- Endocrine Disrupters- (Specific chemicals removed)
- Persistent materials- (quantity of specific chemicals)
- Greenhouse gases- (CO_2, Nitrous oxide, methane,…)
- Total waste generated- (total pounds), reduction of resources
- Damage to the eco-system- (specific materials)

Benefits from NGETs

Security

- **Critical materials**
- **Quantities of stored hazardous materials; terrorist targets**
- **Less energy; energy efficiency**
- **Worker safety**
- **Overall inherently safer processes**

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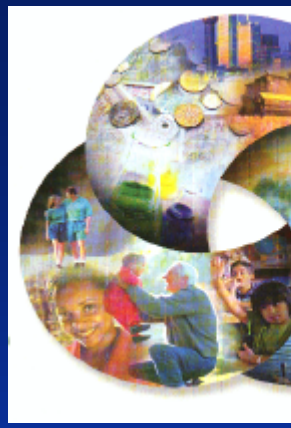
Benefits from NGETs



Performance/economics

- Quality, improved product performance
- New “green” markets
- Reduced manufacturing costs
- Reduced regulatory compliance costs

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Combinatorial Chemistry

- High throughput experimentation incorporates a variety of different technologies of which combinatorial chemistry is sometimes one.
- Combinatorial chemistry : the production of libraries of new materials representing permutations of variables

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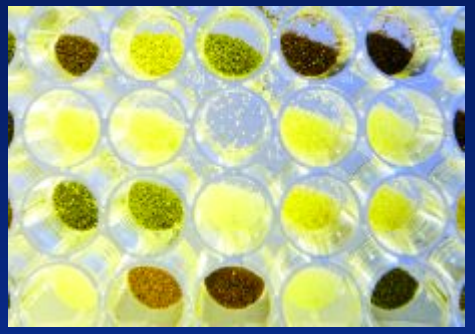
Combinatorial Chemistry

- Established drug discovery technology is refined with advances in synthesis, purification and analysis
- New government center helps industry develop high-throughput methods to measure material properties of polymers

Combinatorial Chemistry



- The field of catalysis where performance is often variable has much appeal for combinatorial chemistry
- Typically, spots representing a matrix of catalyst compositions are prepared by a robot on a plate or in microreactors. The array is then put into a reaction chamber from which measurements are taken and sent directly to a computer that manipulates the data and creates a graph visualizing the results.

Combinatorial Chemistry

- Symyx Technologies and Dow in a four year collaboration discover a new class of single-site catalysis for olefin polymerization; also with ExxonMobil
- Considerable activity outside US – Avantium Technologies (Netherlands) with Degussa, Pfizer and Millennium; HTE in Germany with BASF
- Challenge: software
- Challenge: study of catalyst deactivation
- "tools used today didn't exist 18 months ago"

Modeling and Simulation: Steps

- Understand a system
- Represent the system as a model (mathematical)
- Execute the model
- Operate the model in a discrete or continuous manner to determine the interactions between systems and components
- Analyze the results

Modeling and simulation techniques have taken over many aspects of the R&D environment – from modeling the labs we work in to simulating the the multiphysica world we live in.

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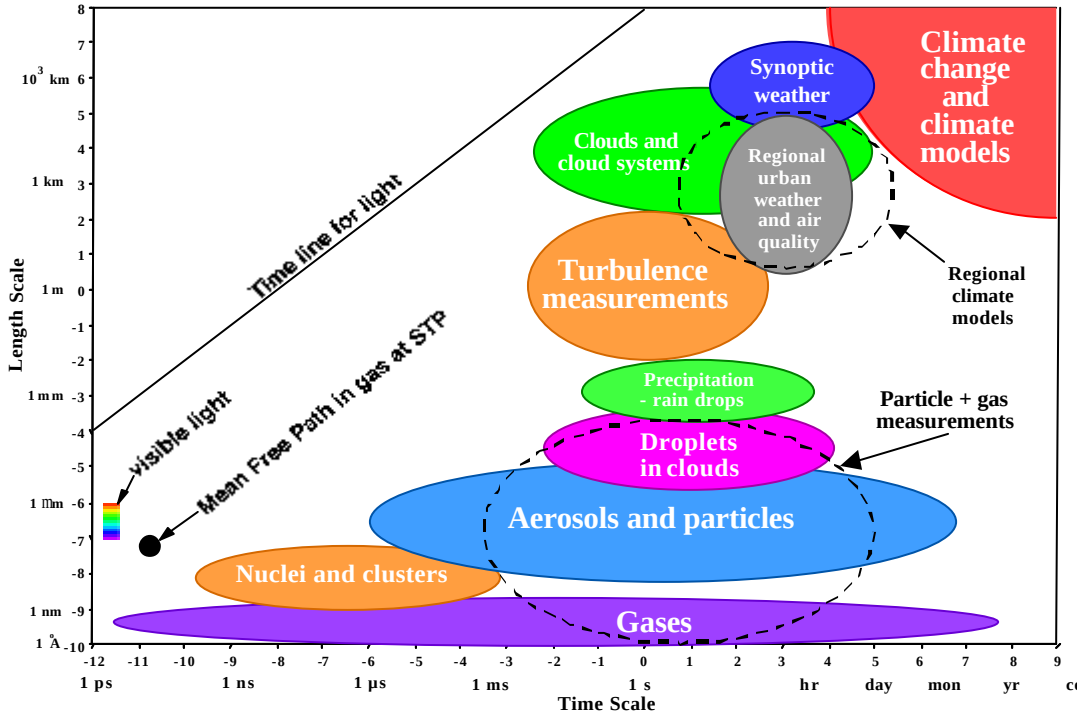
Modeling and Simulation

- Available to researchers for several decades
- More powerful each year
- Larger more intricate, iterative models
- Japan's Earth simulator; Los Alamos, Pacific Northwest National laboratory
- Climate modeling, material sciences, fluids and solid mechanics, biological systems; interactions of new drugs with cells and diseases.

Modeling and Simulation: Problems of scale

Pacific Northwest National Laboratory

Dimensions of Integration - Scale



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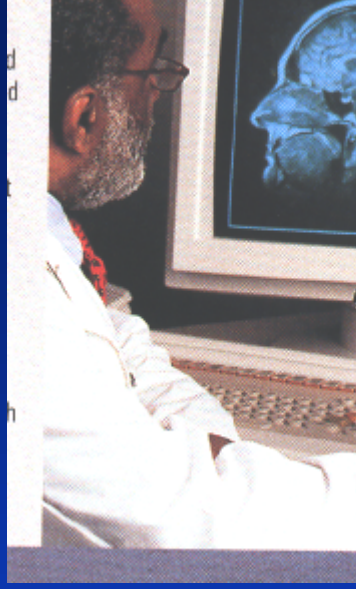
The U.S. Government Promoting Innovation



- Increasing Investment in R&D $123 billion up 7% from the 2003 request
- Networking and Information Technology R&D
- Nanotechnology
- Increasing the Federal Investment in IT

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Conclusions

- Chemical industry moving into new domains
- A number of tools and approaches are enabling chemical companies to be more effective in their R&D efforts
- The environment in the United States is favorable for innovation.