#### MATERIALS AND ENVIRONMENT

Richard Braatz
John A. Burns
Pramod Khargonekar
PS Krishnaprasad
Tariq Samad
Ben Shapiro
Jerry Marsden
Brian Farrell
Igor Mezic
Navin Khaneja
Greg McRae

## **Big Problem Areas**

- control of clusters
- process and manufacturing control
- nano-technology
- thin films
- economic control
- supply chain management
- flow control
- geophysics (weather, environment, etc)

## **Overarching Themes**

# FOR MATERIALS / PROCESSING ENVIRONMENT / SOCIAL-ECONOMICS

#### **CONTROL = EVERYTHING**

- Modeling
- Computation
- Paradigm shifts
- Experiment/Verification

## Modeling

- multi-scale, time and space
- model reduction
- model identification
- heterogeneous model integration
- hierarchical
- uncertainty
- role of data/statistics/noise
- complex systems
- exploiting problem structure

## Computation

- algorithmic and software interfacing
- structured algorithms
- distributed computing
- dynamic resource allocation
- algorithmic development
  - » ADIFOR
  - » optimization
  - » sensitivity
- hierarchical/multiscale
- uncertainty/verification

## **Paradigm Shifts**

- data centric
- coordinated control
- complex systems
- spatially distributed (control, sensors...)
- multidisciplinary teaming
- control configured design (and other things, up front)

## **Experiment/Verification**

- physical
- computational
- interface (with modeling, computation)
- new technology (sensor, etc)

# **Possible Vignettes**

- up front design of chemical plants
- process control
- space applications
- sensitivity tools
- combustion modeling
- meteorology

## **TECH AREAS**

## **PAYOFFS**

- Nano Technology
  - » Nano Electronics
  - » Designer Chemistry
  - » Biological Materials
- Flow Control
  - » Chemically Reacting
  - » Aerodymanic
- Thin Films
  - » RCVD
  - » MBE
  - » IBD

- The "Future"
  - » "Smart Dust"
  - » The Next "Transistor"
  - » Embedded Intelligence
  - » Combustion
  - » GMR Devices
  - » Thin Film is \$300 Billion Industry

### **TECH AREAS**

- DESIGN OF MEMS
- Process Control
  - » Web
  - » Chemical
  - » Power Generation
  - » Pharmaceutical
  - » Injection Molding
- Supply Chain Management

### **PAYOFFS**

- Enabling New Products
  - » Component Integration
- Economic & Others
  - » \$ Billions Per Year
  - » Trees
  - » \$ Competitiveness
  - » Health

#### **AREAS**

- Nano Technology
  - » Nano Electronics
  - » Designer Chemistry
  - » Biological Materials
- Flow Control
  - » Chemically Reacting
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#### **ISSUES**

- Modeling for Control
  - » Quantum, MD, FE?
  - » Reduced Order Models?
  - » Interaction of Devices
- Modeling
  - » Computational Methods
- Process Sensor Based Control of Product Parameters
  - » Associated Modeling
  - » Model Reduction

#### **AREAS**

- DESIGN OF MEMS
- Process Control
  - » Web
  - » Chemical
  - » Power Generation
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#### **ISSUES**

- Model Reduction & ID
  - » Component Integration
- Large Scale Systems
  - » Modeling of Big Systems
  - » Integrated Health Management & Control
  - » Distributed PS
- Optimization

## **EDUCATION**

#### **EXPOSURE TO COMPUTING**

#### **!!! INTERDISCIPLINARY !!!**

#### MANUFACTURING PROCESS KNOWLEDGE

#### **RESEARCH NEEDS**

- BETTER SOLUTION METHODS FOR MULTIDISCIPLINARY SYSTEMS (FASTER, CHEAPER, MORE ACCURATE)
  - » CHEMICALLY REACTING FLOWS
  - » AEROELASTIC SYSTEMS
  - » COMPUTATIONAL CHEMISTRY
  - » TIME DEPENDENT PROBLEMS
  - » MOLECULAR DYNAMICS (MD CODES, ETC.)
- NUMERICAL METHODS THAT TRAVERSE DISPARATE TIME AND LENGTH SCALES
  - » CONTINUUM MODELS (FINITE ELEMENTS, ETC.)
  - » MOLECULAR DYNAMICS (MD and QM CODES, ETC.)
- LARGE-SCALE COMPUTATIONAL METHODS FOR DESIGNING, CONTROLLING AND OPTIMIZING UNDER UNCERTAINTY

# RESEARCH NEEDS - SIMULATION FOR DESIGN -

- NEW COMPUTATIONAL METHODS THAT ARE "DESIGN SPECIFIC"
  - » A NUMERICAL METHOD "GOOD FOR SIMULATION" ... MAY <u>NOT</u> BE GOOD FOR OPTIMIZATION OR CONTROL
- GEOMETRIC MODELING AND MESH GENERATION TOOLS
- MESH INDEPENDENT COMPUTATIONAL TOOLS FOR
  - » SENSITIVITY ANALYSIS
  - » OPTIMIZATION BASED DESIGN
- INTEGRATED PROBLEM SOLVING ENVIRONMENTS
  - » ARCHITECTURE SPECIFIC ALGORITHMS
  - » HIERARCHICAL ADAPTIVE MODELING FOR DESIGN & CONTROL
  - » VISUALIZATION