“Chemical Engineering Education and the role of Cyberinfrastructure”

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Cyberinfrastructure Elements in ChE Education

- Integrated computing in ChE core courses
- New computing applications – CFD, molecular modeling
- New curricular themes (NSF workshops)
- Web-based experiments
- Increased usage of audio/video/multimedia
- Internet 2
- Distance Education
- Grid computing

computing

simulation

learning communities

e-books

collaboration

wireless

multimedia

visualization

digital libraries

distance education

portals

collaboration

teaching and learning

data acquisition

Internet 2

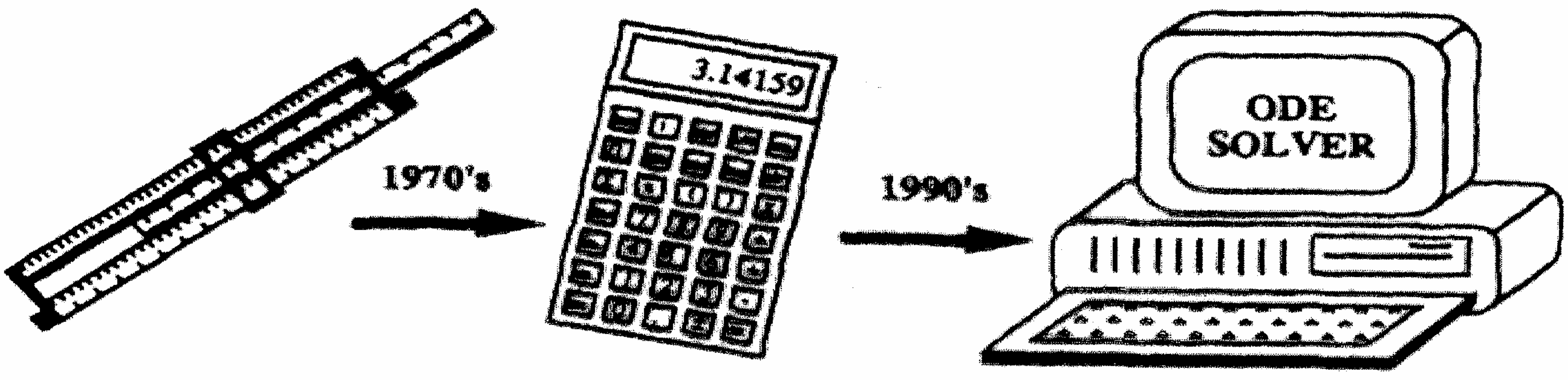
4

Technology Drivers

- wireless, handheld devices
- household LANs (audio, video, appliances – toasternet)
- disintermediation (e.g., shopping)
- integrated voice, data, video networks
- voice communication with computers

New Digital Generation

- Lives with pervasive microprocessors and telecommunications (e.g., cell phones)
- Napster, Playstation, Pokemon
- Demands computer interaction, plug and play
- Learns through experimentation, group interaction



Paradigm shifts in chemical engineering education.

Integrated Computing in the ChE Curriculum

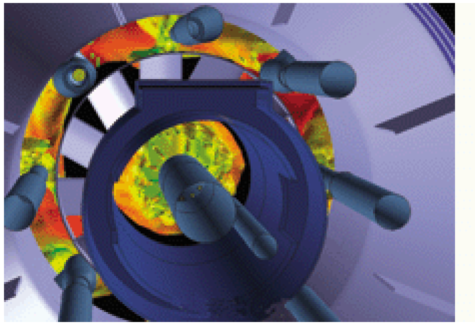
- White paper by CACHE Corporation (www.cache.org)
- Teaching computer programming
- Teaching information technology
- Use of process simulators (sophomore-senior)
- Course software packages ($1 \leq n \leq 11$) - how many ?
- Prototypical approaches at six universities

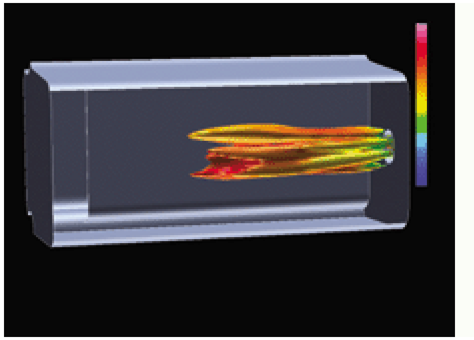
Numerical vs. Analytical Approaches in Modeling Physical Behavior

- Need to learn both approaches (advantages and disadvantages)
- Need to re-examine role of detailed analytical solutions (training for industry vs. graduate school)
- Use fewer simplifying assumptions in numerical solutions
- Public can run simulators in science museums, so ChE education can find a way
- Observations can come from physical experiments and numerical experiments
- CFD software is important new element for cyberinfrastructure (Fluent, FEMLAB)

Reasons for modeling and simulation

- Fundamental understanding of the process is possible under correct assumptions
- Sensitivity analysis
- Aid in scaling systems to either larger or smaller throughputs
- Aid in optimization and control strategies





Flare Modeling

- Challenging project that requires coupled physical processes be modeled
- These processes include
  . complex chemical reactions

  . soot formation

  . radiation

  . turbulent fluid flow

Approaching the Problem…

STARTING POINT

Governing Transport Equations

- .Mass
- .Species
- .Momentum
- .Energy

Reaction Models

Infinitely Fast Chemistry
vs
Finite Rate Chemistry

Non-premixed combustion
vs
Premixed combustion

Pollutant Models

Radiative Heat Transfer Models

Species conservation equation is too simple:

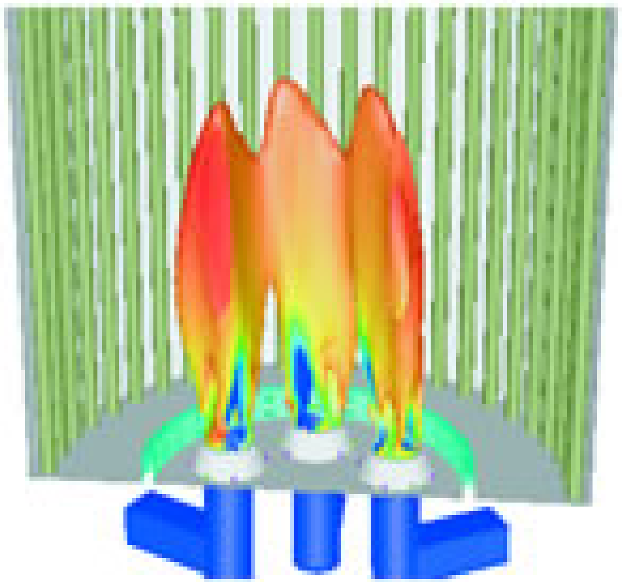
$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_j}(\rho\, u_j Y_i) = \frac{\partial}{\partial x_j}\left(\rho D_i \frac{\partial Y_i}{\partial x_j}\right) + R_i$$

CFD

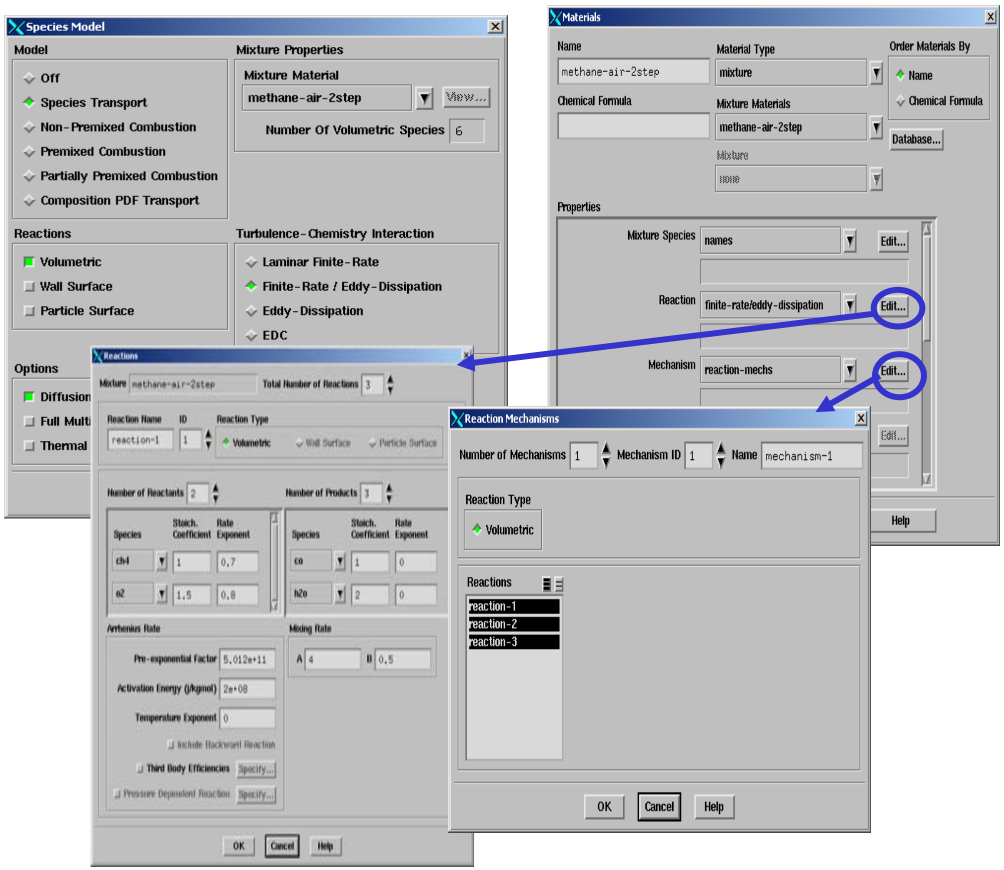
- CFD is a powerful numerical tool for simulating the complicated fluid flow, heat transfer, and chemical reactions in a combustion system
- CFD has gained in popularity in recent years due the dramatic increase in computer power
- CFD is based on fundamental physics and not on empirical functions
- In dealing with combustion simulations, the complexity of the problem requires the CFD engineer to have specialized knowledge to set up complex 3-D CFD simulations and interpret the results
- FLUENT 6.1, C-SAFE and FEMLAB3.0 are options

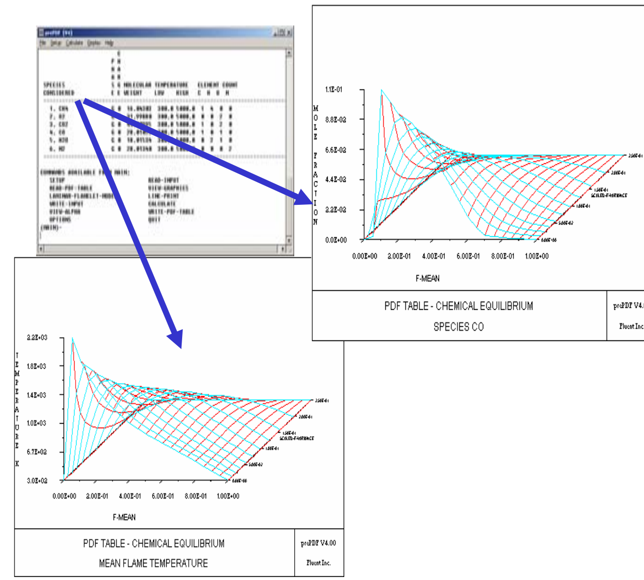
CFD Solution Methodology

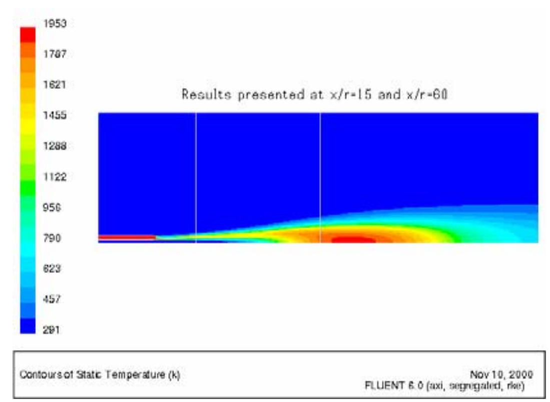
- Mesh generation
- Flow specification
- Calculation (numerical solution)
- Analysis of Results



Fluent Capabilities...







Summary of the NSF Workshops (2003)
(see http://web.mit.edu/che-curriculum)

- Changes in science and the marketplace call for extensive changes to the chemical engineering curriculum
- The enabling sciences are: biology, chemistry, physics, mathematics
- There is a core set of organizing chemical engineering principles, emphasizing molecular level design
  - Molecular Transformations, Multi-scale Analysis, Systems
- Chemical engineering contains both product and process design
- There is agreement on the general attributes of a chemical engineer

Molecular Transformations

- Molecular transformations: the molecular basis of chemical engineering
  - goals: students recognize that properties can be changed by changing structure via qualitative and quantitative computation
- Molecular Basis of Thermodynamics (Sophomore)
  - intro quantum and stat mech, equilibria, 1st Law, 2nd Law, equations of state, phase transitions
- Classification of Molecules (Sophomore)
  - qualitative concepts (“hydrophilic”, “hydrophobic”), quantitative structure-property correlations, macromolecules, biological interactions
- Molecular Basis of Reaction Rates (Sophomore or Junior)
- Molecular Basis of Other Properties and Constitutive Equations (Junior)
  - transport properties, effects of polymer/biomolecular conformations, mixture properties, some elements of molecular biology
- Special Topics (Junior/Senior electives)
  - interfacial phenomena, nucleation/growth, material props, directed evolution

Multi-Scale Analysis

- Multi-scale analysis: Application of chemical engineering principles over many scales of length and time
- Interfaces and Assemblies (Sophomore)
  - adsorption, extraction, interfaces, Brownian motion, molecular forces, nucleation, colloidal interactions, molecular assemblies
- Homogeneous Reactor Engineering (Sophomore)
  - PFR and CSTR
- Multi-scale descriptions of reactive systems (Junior)
  - Integrated approach to continuum momentum, heat and mass transfer with reactivity, stochastic processes, heterogeneous systems and interfacial phenomena
- Beaker-to-Plant: Implementation of Multi-scale Principles for Product and Process Design (Senior)
  - design of a product and process to make the product: polymer, drug delivery system (includes lab component for making of prototype)

Systems

- Systems: tools for synthesis, analysis and design of processes, units and collections thereof
- Introduction to Systems (Sophomore)
  - conservation laws for simple dynamic and steady state systems
  - build model for experimental dynamic system
  - collect and analyze lab data
  - build numerical simulation for simple models
  - parameter estimation (exposure to complexity and uncertainty)
  - construct equipment/sensor
- Introduction to Molecular Systems (Junior)
  - stochastic systems and molecular level reactions as systems
  - simulation as an enabling technology
  - use of models in predicting system behavior (analysis) and in shaping system behavior (synthesis)
  - energy and mass integration, design for the environment
  - optimization principles for design, parameter estimation and decision-making
  - examples from microelectronics, catalysis, systems biology, stochastic kinetics

- Systems and the Marketplace (Senior)
  - multi-scale systems: separation and resolution of time and length scales
  - design and analysis of feedback
  - monitoring, fault detection and sensitivity analysis
  - design experience: economics/business skills, safety, marketing, environmental impact, life cycle analysis, ethics, globalization, IP
  - process operations
  - planning, scheduling, and supply chains
  - Tie-in with Beaker to Plant (Process and Product Design)

Possible Case Studies

- Desalination of sea water
- Hydrogen from biomass
- Synthesis of specialty polymers
- Global climate change
- Regional air quality analysis
- Production, separation, and purification of natural products and recombinant proteins
- Reconstruction of cellular networks. Design of cells and biomolecules
- Insulin regulation
- Pharmacokinetic and pharmacodynamic models
- Biomedical control systems
- Drug patch design
- The human body as a chemical process
- Environmental cycles (water, carbon, nitrogen, etc.)
- Chemical plant design and operation
- Cell design (human, animal, plant) and regulation of metabolic pathways
- Product design

Laboratory Experience

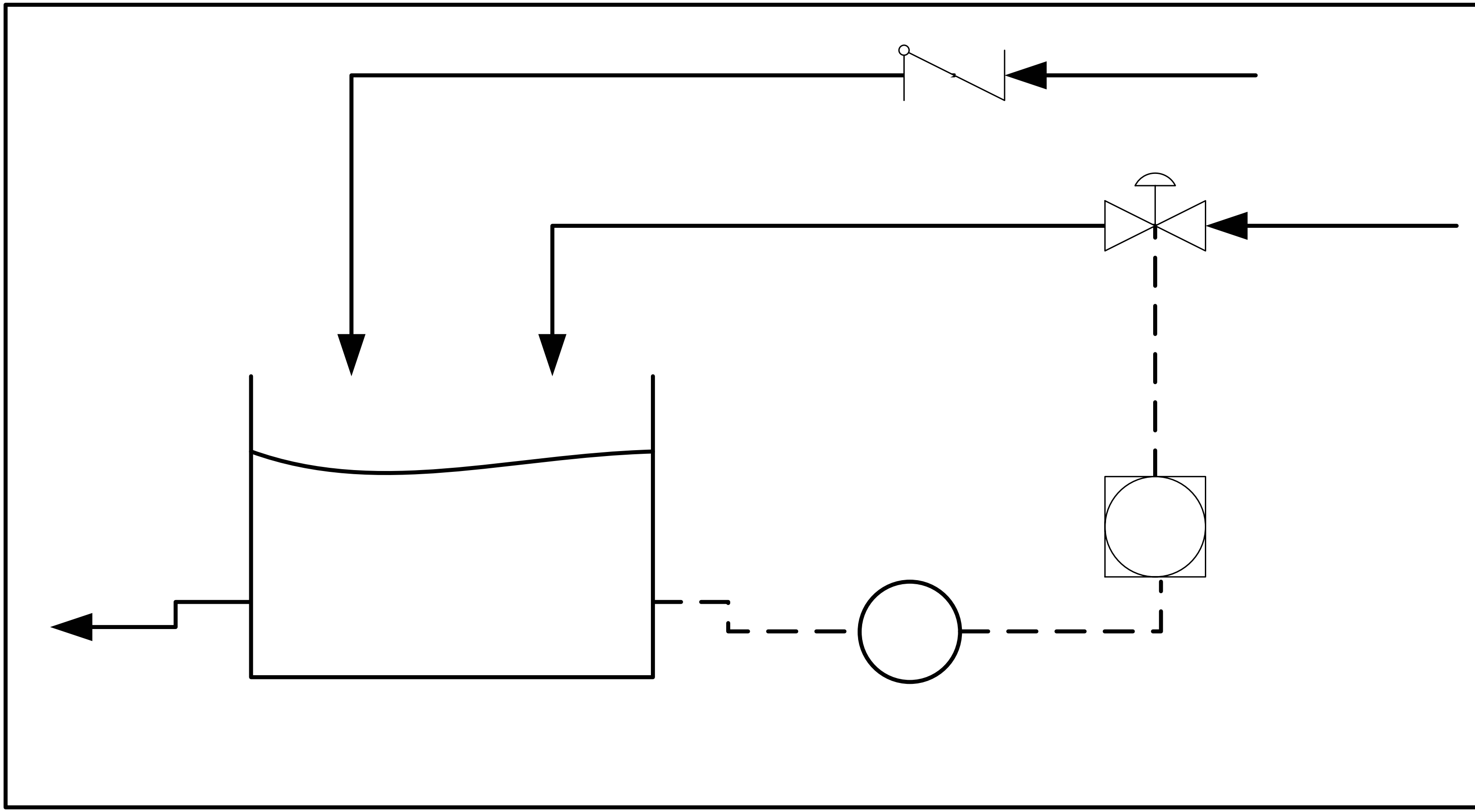
- Includes VLAB, ILAB and hands-on
- Will teach:
  - teamwork and communication skills
  - ability to handle real (i.e., messy) problems and data
  - open-ended problem-solving
  - safety
  - environmental and regulatory issues
  - reinforcement and visualization of concepts from courses
- Can also teach
  - experimental design
  - basic lab techniques and instrumentation

Cyberinfrastructure and Laboratory Experiments

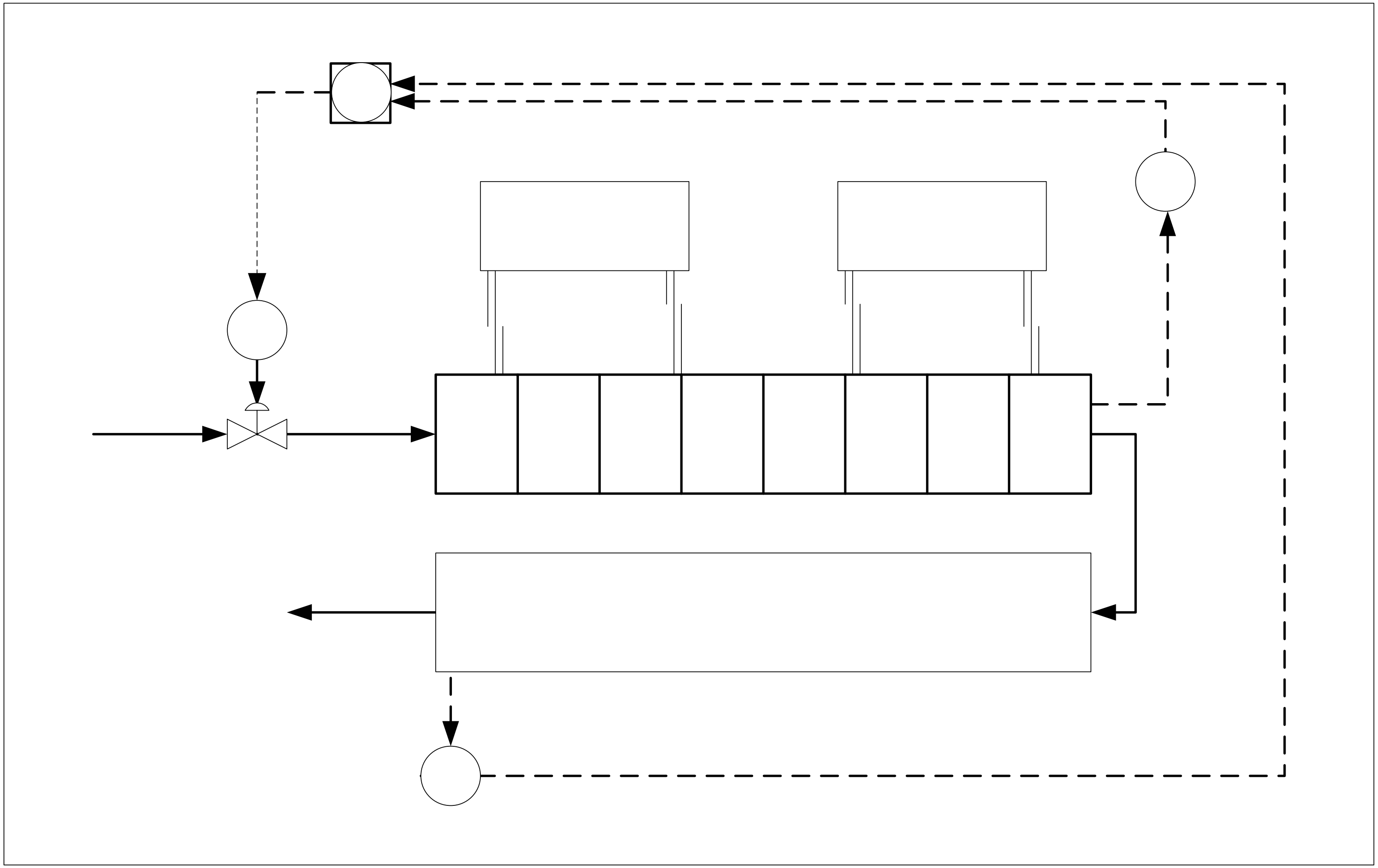
- Lab equipment can be connected to Internet for remote operation
- Permits sharing of experimental systems among universities
- Offers a way to reinforce lecture concepts with live demonstrations (web-connected classrooms classrooms)
- Should not be viewed as a way to decrease the undergraduate laboratory experience
- Experiments developed by U. Tennessee (Chattanooga), MIT, U. Texas, U. Florida

Dynamics and Control Experiments (UT-Austin)

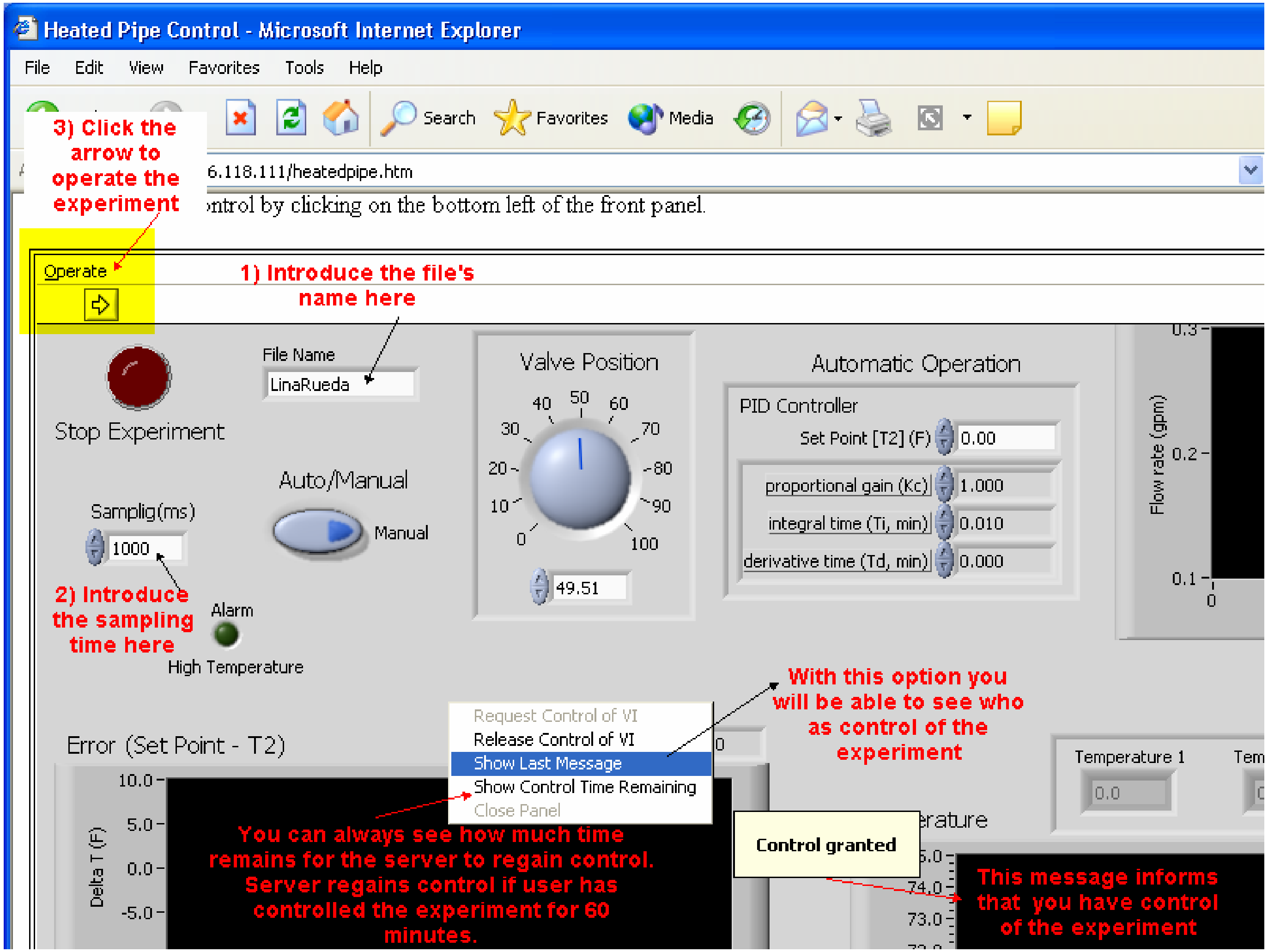
Liquid Level Control



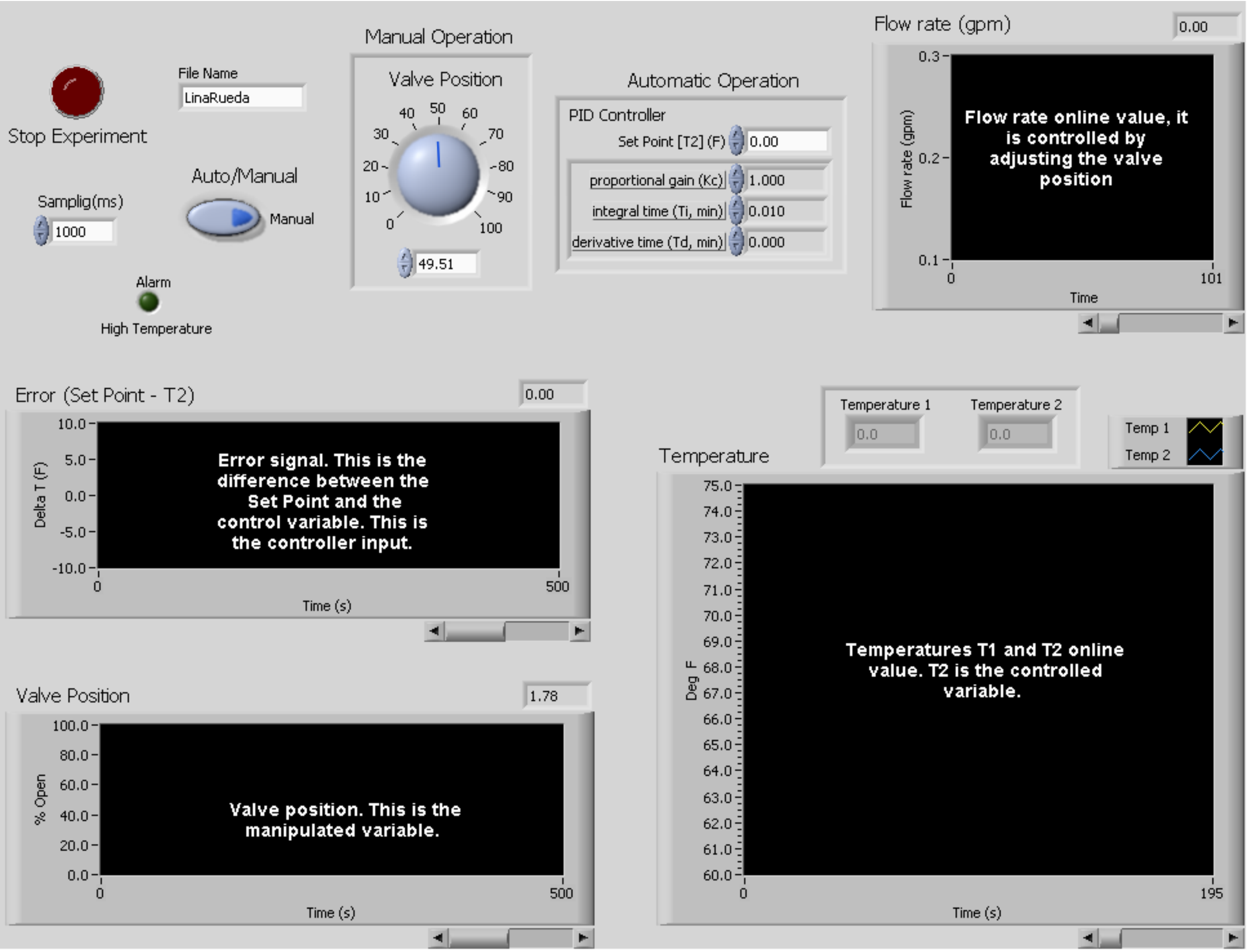
Heated Pipe Control



Computer Interface - 1



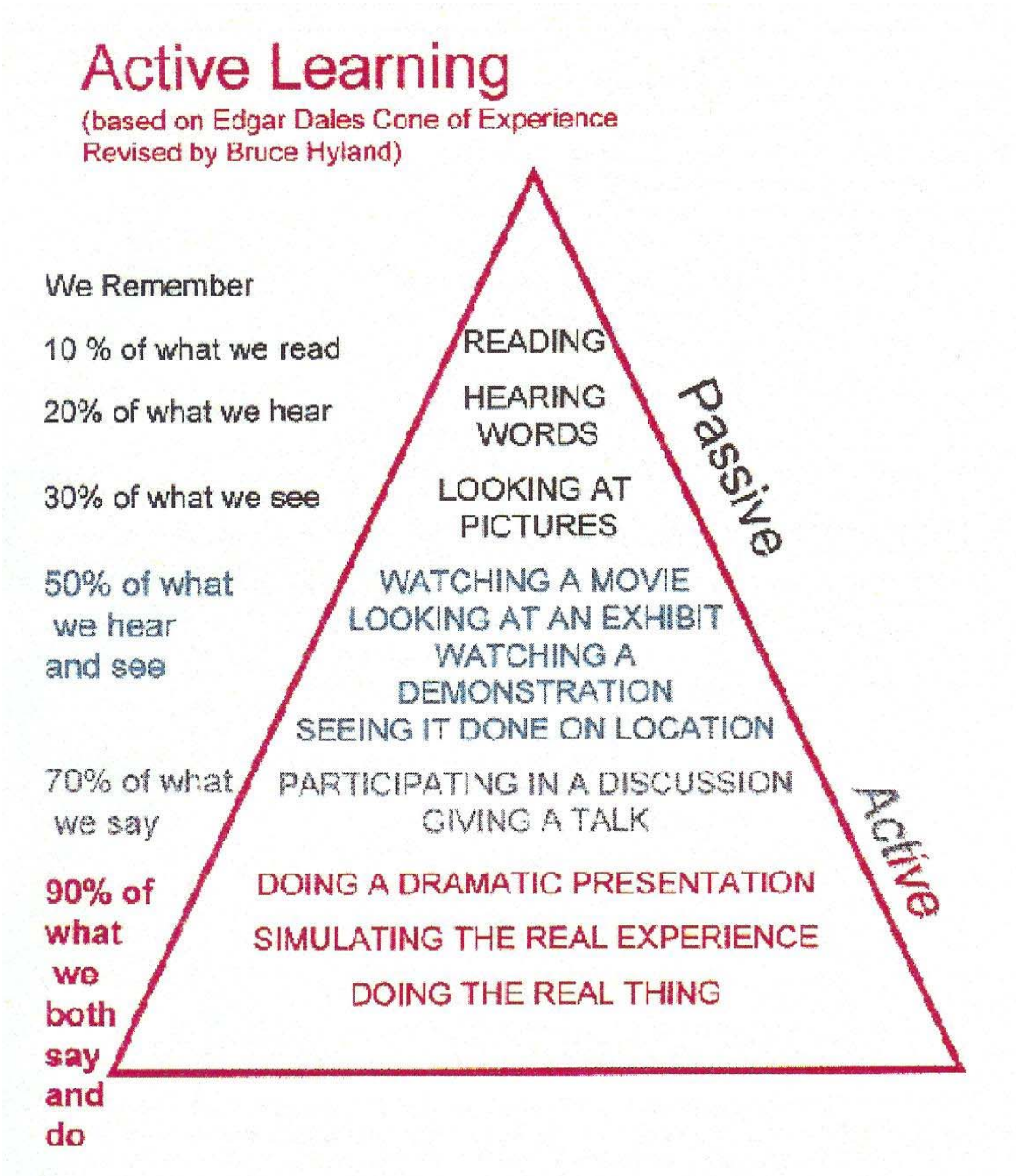
Computer Interface -2

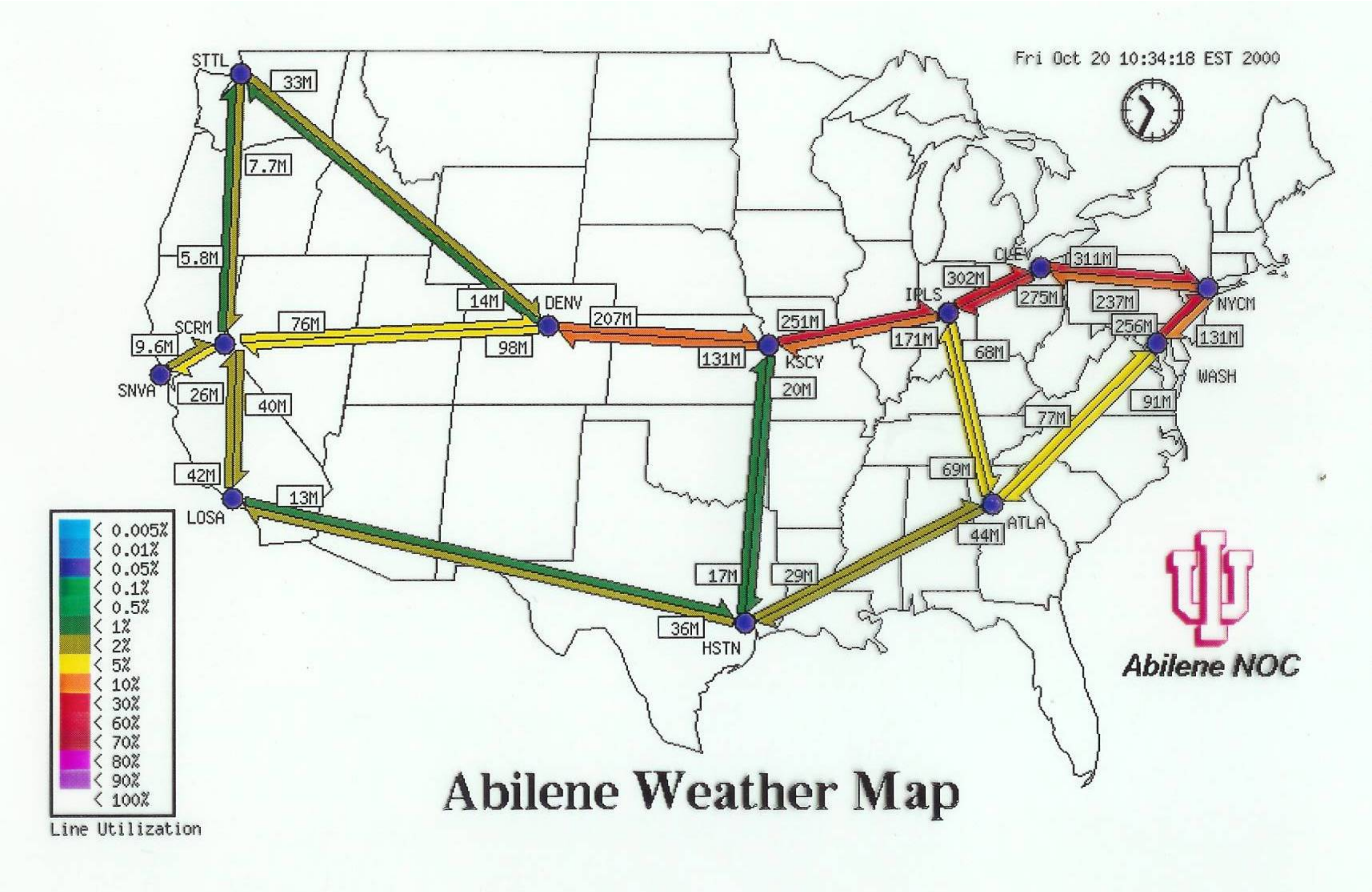


- Experiments can be run by students without extensive preparation or supervision (faculty or TA).
- Typical time to complete step testing and PI controller design is 1 to 2 hours per group (can be treated like a homework assignment)
- Most groups run the experiment from the department computer labs
- Experiments are also suitable for lecture demos.
- National Instruments software provides a good interface.

Multimedia and Computer-Based Learning

- Self-paced methods (checkpoints on learning or mastery of concepts)
- Interactive learning
- Increased use of audio/video, animation, simulation
- Making class materials readily available (web)
- Requires high bandwidth for effective use


Active Learning
(based on Edgar Dales Cone of Experience
Revised by Bruce Hyland)
We Remember
10 % of what we read
20% of what we hear
30% of what we see
50% of what we hear and see
70% of what we say
90% of what we both say and do
READING
HEARING WORDS
LOOKING AT PICTURES
WATCHING A MOVIE
LOOKING AT AN EXHIBIT
WATCHING A DEMONSTRATION
SEEING IT DONE ON LOCATION
PARTICIPATING IN A DISCUSSION
GIVING A TALK
DOING A DRAMATIC PRESENTATION
SIMULATING THE REAL EXPERIENCE
DOING THE REAL THING
Passive
Active



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< 100%
Line Utilization
Abilene NOC
Abilene Weather Map

Internet2 Applications

- Interactive collaboration and instruction
- Real-time, sensor-based modeling and simulation
- Multi-site computation and database processing
- Shared virtual reality – “tele-immersion”

Distance Learning – Delivery Technologies

- Internet – “web-based courses”
- Interactive video
- CD ROMs
- Broadcast and cable video
- Satellite
- Audioconferencing
- Print/media based

Drivers for Web-based Learning

- Constituency driven
  - Workforce development
- Industry practices in CBT
  (e.g., 90% of all training at Dell)
- Increased interaction outside of class via asynchronous learning
- Not necessarily lower cost but private DE providers are profitable

Internet-Based Delivery

- Technology used to enhance learning experience
- Technology used to deliver course
- Telepresence achieved via high bandwidth (> 1 MB/s)
- Students can be in class or at a distance (or both)

Course Management Tool Features (Blackboard, WebCT)

- Conferencing, on-line chat, and email (privacy question)
- Student progress tracking and self-evaluation
- Student/group project organization, work areas, homepages
- Grade maintenance/distribution
- Access control
- Auto-marked quizzes
- Automatic index generation
- Course calendar
- Course content searches

Grid Computing

- Alternative to PC clusters (or Big Iron)
- Building momentum on many campuses and in industry
- Utilizes slack processing resources in individual PCs
- Modeled after SETI@home (5M desktops)
- Attractive for big computational projects (weather prediction, oil reservoirs, gene research)

New Technology Will Change Research and Instruction and Also Cyberinfrastructure

- Groupware
- Virtual experiments
- Desktop computing (Moore’s law)
- Mobile computing
- Query of image content
- Use of intelligent agents
- Speech synthesis and text to speech conversion