Bringing the Grid to Chemical Engineering

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Bringing the Grid to Chemical Engineering

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National Center for Supercomputing Applications
National Computational Science Alliance
University of Illinois at Urbana-Champaign
A Chemical Engineer
Started Modern Digital Computing!

John von Neumann
B.S. Chemical Engineering
ETH Zurich
Outline of Presentation

• Introducing the Grid
• New Directions in Computing
• Challenges to the Chemical Industry
• The Chemical Engineer’s Workbench
• The Killer App for the Grid: Tele-Immersion
• Conclusions
The Grid Links People with Distributed Resources on a National Scale

Computers
- Supercomputers
- Experimental Facilities

Collaborative Environments

High-Speed Networks
- Databases
- Mass Storage

http://science.nas.nasa.gov/Groups/Tools/IPG
Imagine a national computing and information infrastructure that allowed everyone to access the information resources of the nation in much the same way that one accesses electrical power today; an "Information Power Grid"
The Grid Can Unify Enterprise Business Processes

Before

Business Team  Design and Engineering Teams  Manufacturing Team  Operations Team

After

Virtual Integrated Team  Product Design Data & Resources

http://science.nas.nasa.gov/Groups/Tools/IPG
FY98 Assembling the Links in the Grid with NSF’s vBNS Connections Program

NCSA Distributed Applications Support Team for vBNS

27 Alliance sites running...

...16 more in progress.

1999: Expansion via Abilene
vBNS & Abilene at 2.4 Gbit/s

Source: Charlie Catlett, Randy Butler, NCSA
How Applications Teams Drive the Alliance

- Cosmology
  - Metacomputing
- Environmental Hydrology
  - Immersive Collaboration
- Chemical Engineering
  - Virtual Prototyping
- Bioinformatics
  - Distributed Data
- Nanomaterials
  - Remote Microengineering
- Scientific Instruments
  - Virtual Observatories

- Multidiscipline Domains
- Multiscale Interactions
- Complex Geometries
- Full-up Virtual Prototyping
- Large Scale Optimization
NCSA Industrial Partners
Drive Innovation

- Allstate Insurance Co.
- Boeing Company
- Caterpillar Inc.
- Eastman Kodak Co.
- FMC Corporation
- Ford Motor Company
- J. P. Morgan
- Motorola, Inc.
- Phillips Petroleum Co.
- SABRE Group, Inc.
- Schlumberger
- Sears, Roebuck & Co.
- Shell Oil Company
Enterprise Management- Convergence of Commercial and Technical Computing

• The Web Browser as a Universal Interface
  – To Data, Video, Instruments, Computing

• Virtual Teams In Business and Research
  – Intranets and Collaborative Environments

• Emergence of Distributed Object Architecture
  – Java, ActiveX, CORBA, Integrated Thru the Web

• From Scientific Visualization to Info. Viz.
  – Data Mining Petabyte Archives

• Microprocessor Market Convergence
  – NT/Intel Challenging UNIX/RISC
The Continuing Exponential Agent of Change

1985
Cray X-MP
Cost: $8,000,000
60,000 watts of power
No Built in Graphics
56 kbps NSFnet Backbone

1997
Nintendo 64
Cost: $149
5 watts of power
Interactive 3D Graphics
64 kbps ISDN to Home
TOP500 Systems by Vendor - A Market Revolution

TOP500 Reports: http://www.netlib.org/benchmark/top500.html
Shared Memory Microprocessors
Replacing Vector Systems in Top 500

PVP Systems

SMP + DSM Systems

Number of Systems

Europe
Japan
USA

Vector Processors

Microprocessors

TOP500 Reports: http://www.netlib.org/benchmark/top500.html
NCSA is Combining Shared Memory Programming with Massive Parallelism

Doubling Every Nine Months!

- SN1
- Origin
- Power Challenge
- Challenge

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<th>SGI Processors</th>
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High-End Architecture 2000-
Scalable Clusters of Shared Memory Modules

Each is 4 Teraflops Peak

- NEC SX-5
  - 32 x 16 vector processor SMP
  - 512 Processors
  - 8 Gigaflop Peak Vector Processor

- IBM SP
  - 256 x 16 RISC Processor SMP
  - 4096 Processors
  - 1 Gigaflop Peak RISC Processor

- SGI Origin Follow-on - SN1
  - 8 x 256 RISC Processor DSM
  - 2048 Processors
  - 2 Gigaflop Peak EPIC Processor
NASA Computational Aerosciences

- First-of-a-kind aerodynamic sim. of adv. ASTOVL in near-hover ground effect with strong fountain

- 8X speedup on compressor analysis code, 5X for combustion flow solver
- Design time reduced from 18 to 14 months by 9/97
- $3.33 million saved per design

http://science.nas.nasa.gov/Groups/Tools/IPG
Simulation of Convective Mixing

- 512x512x512 Grid
- 285,000 CPU-Hours on PSC T3D
- Bottom Half Stable, Top Half Unstable (Thermal Diffusivity Varies with Height)
- Color Shows Temperature Fluctuations (Red Hot, Blue Cool)

Constant Temperature on Top

Constant Heat Flux on Bottom

Cooler Descending Plume

LCSE, University of Minnesota
High-End Computing Enables
High Resolution of Flow Details

1024x1024x1024-
A Billion Zone
Computation of
Compressible Turbulence

This Simulation Run
on Los Alamos SGI
Origin Array

U. Minn.SGI Visual
Supercomputer
Renders Images

Vorticity
Harnessing Distributed UNIX Workstations - University of Wisconsin Condor Pool

Condor Cycles

CondorView, Courtesy of Miron Livny, Todd Tannenbaum(UWisc)
NT Workstation Shipments Rapidly Surpassing UNIX

Solving 2D Navier-Stokes Kernel - Performance of Scalable Systems

Preconditioned Conjugate Gradient Method With Multi-level Additive Schwarz Richardson Pre-conditioner

(2D 1024x1024)

Source: Danesh Tafti, NCSA
The Grid Links Remote Sensors With Supercomputers, Controls, & Digital Archives

- Alliance Scientific Instrument Team
  - Radio Astronomy and Biomedicine
  - Collaborative Web Interface
  - Real Time Control and Steering

Starburst Galaxy M82
Sears Pioneers Massive Data Mining and Information Visualization at NCSA

- 1998 VLDB Survey Program Grand Prize Winner
  - Largest Database
    - 4.7 Terabytes of Data
  - 10 Terabyte Total Disk Space Capacity
    - Storage Provided by EMC

Image Courtesy of Michael Welge, NCSA and Sears
Challenges Facing the Chemical Industry

- Globalization, Competition
- Shorter Product Life Cycles
- Environmental Issues
- Emerging Technologies
- Capacity Expansions
- New Materials
- Etc.

All Involve Chemical Reactions

How Can The Grid Help Meet the Challenges?
Challenges - Complex Application Domains

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]

\[ \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u^2) = -2\Omega \times \rho u - \nabla p + \nabla \cdot (\mu \nabla \cdot u) \]

\[ \frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E u) = \nabla \cdot (k \nabla T) + Q_H - \nabla \cdot F^{\text{rad}} - p \nabla \cdot u \]
Challenges - The Problem of Scale

O(km)  O(cm)  O(nm)
Challenges-A Hierarchy of Modeling Systems With Uncertainty Everywhere

But: What Are the Effects of Uncertainties on Performance?
Alliance Chemical Engineering AT Team

- Gregory McRae, Chairman, MIT
- Jay Alameda, NCSA
- Paul Barton, MIT
- Ken Bishop, University of Kansas
- Richard Braatz, UIUC
- Klavs Jensen, MIT
- and you!!
The Chemical Engineer’s Workbench

A Computational System that:

• Provides an Integrated Environment for Process Modeling, Control, and Optimization

• Links Multiple Scales and Software Tools From Different Vendors

• Utilizes the “Best” Computing and Software Tools to Help Solve Practical Applications
Alliance Chemical Engineering Team
Developing the Chemical Engineer’s Workbench

• Web Interface for:
  – *Ab Initio* Chemistry Calculations
  – Dynamic Chemical Process Simulations
  – Implementation of Automated Parameter Estimation and Experimental Design Algorithms
  – Link Process Simulation Packages to *Ab Initio* Codes for Physical Properties
  – Data Mining, Analysis, & Visualization

• Testing of Prototype Workbench Using a Detailed Chemical Reactor Model
Algorithmic Developments

• Automatic Differentiation (ADIFOR Tool)
  – Numerical Optimization
  – Solving Stiff ODEs/PDEs

• Solution of Large Linear Algebra Problems
  – Process Flowsheet Simulation
  – Parameter Estimation and Optimization

• Solution of Integro-Partial-Differential Equations

• Parallel Methods for Uncertainty Analysis
Goal-Closing the Loop to Optimize Chemical Plant Operations

Measurements and Experimental Design

Grid Coupling:
Sensors
Networks
Data
HPC Models
Controls

Process Model

Parameter Estimation

Process Data

Control Signals

Plant-wide Control

Process
Goal: Create Collaborative Interface to Link Multiple Investigators With the Grid

- Interactive Discussion
- Detailed Visualization
- Reactor Simulation
- Current parameters in solution
- Status of Simulation

Ken Bishop, U Kansas Using NCSA Habanero
Goal-Integrating Digital Video Throughout the Enterprise

Interactive Virtual Environments

Create Digital Video Animation Concurrently with Supercomputing

Internet, vBNS

Application Teams

Desktop Video Conferencing

Digital Video Server

Individual Desktops

NCSA™

National Computational Science Alliance
The Killer Application for the Grid - Collaborative Tele-Immersion

CAVE

ImmersaDesk

Different Physical Implementations of the Alliance CAVE Software Libraries

Image courtesy: Electronic Visualization Laboratory, UIUC
Cave5d Enables Interactive Visualizations of Time-Varying, 3-Dimensional Vis5d Data Sets in CAVE Environments

Donna Cox, Robert Patterson, Stuart Levy, NCSAVirtual Director Team
Glenn Wheless, Cathy Lascara, Old Dominion Univ.
Goal - Create Shared Virtual Environment
CVD -- Collaborative Virtual Director

Donna Cox, Robert Patterson, Stuart Levy, NCSA Virtual Director Team
Glenn Wheless, Old Dominion Univ.
Goal-Linking the CAVE to the Desktop: Collaborative Java3D

Java 3D API HPC Application: VisAD
Environ. Hydrology Team, (Bill Hibbard, Wisconsin)
Steve Pietrowicz, NCSA Java Team
Standalone or CAVE-to-Laptop-Collaborative

NASA IPG is Adding Funding To Collaborative Java3D
Real Time Linked VR and Audio-Video Between NCSA and Germany Using SGI Indy/Onyx and HP Workstations

Data courtesy of Valerie Lehner, NCSA
Goal-Global Enterprise Management

Designer

ATM/IP Network

Supplier

Customer

Manufacturing Facility
How to Find Out More About the Alliance

See also http://alliance.ncsa.uiuc.edu