OSCER

State of the Center Address

Henry Neeman, OSCER Director

September 25, 2003

Oklahoma EPSCoR
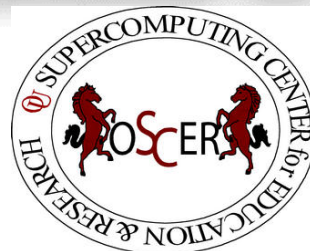
Oklahoma Supercomputing Symposium 2003

Outline

- Who, What, Where, When, Why, How
- What Does OSCER Do?
  - Education
  - Research
  - Dissemination
  - Resources
- OSCER's Future and How to Get Involved
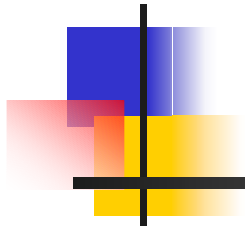- A few quick thanks

Who, What, Where, When, Why, How

What is OSCER?

- Multidisciplinary center within OU's Department of Information Technology
- OSCER provides:
  - Supercomputing **education**
  - Supercomputing **expertise**
  - Supercomputing **resources**: hardware, storage, software
- OSCER is for:
  - Undergrad students
  - Grad students
  - Staff
  - Faculty
  - Their collaborators

Who is OSCER? Academic Depts

- Aerospace & Mechanical Engineering
- Biochemistry & Molecular Biology
- Biological Survey
- Botany & Microbiology
- Chemical Engineering & Materials Science
- Chemistry & Biochemistry
- Civil Engineering & Environmental Science
- Computer Science
- Electrical & Computer Engineering
- **NEW! Finance**
- **NEW! History of Science**

- Industrial Engineering
- Geography
- Geology & Geophysics
- **NEW! Library & Information Studies**
- Management
- Mathematics
- Meteorology
- Biochemistry & Molecular Biology
- **NEW! Petroleum & Geological Engineering**
- Physics & Astronomy
- Surgery
- Zoology

Over 130 faculty & staff in 23 depts in Colleges of Arts & Sciences, Business, Engineering, Geosciences and Medicine – with more to come!

Who is OSCER? Organizations

- Advanced Center for Genome Technology
- Center for Analysis & Prediction of Storms
- Center for Aircraft & Systems/Support Infrastructure
- Cooperative Institute for Mesoscale Meteorological Studies
- Center for Engineering Optimization
- Department of Information Technology
- **NEW! Fears Structural Engineering Laboratory**
- Geosciences Computing Network
- Great Plains Network

- **NEW! Human Technology Interaction Center**
- Institute of Exploration & Development Geosciences
- **NEW! Instructional Development Program**
- **NEW! Laboratory for Robotic Intelligence and Machine Learning**
- Langston University Department of Mathematics
- Microarray Core Facility
- National Severe Storms Laboratory
- **NEW! NOAA Storm Prediction Center**
- Oklahoma EPSCoR

Expected Biggest Consumers

- Center for Analysis & Prediction of Storms: daily real time weather forecasting

- Advanced Center for Genome Technology: on-demand genomics

- High Energy Physics: Monte Carlo simulation and data analysis

Who Are the Users?

156 users so far:

- 35 OU faculty
- 34 OU staff
- 77 students
- 10 off campus users
- … more being added every month.

Comparison: National Center for Supercomputing Applications, with tens of millions in annual funding and 18 years of history, has about 2100 users.*
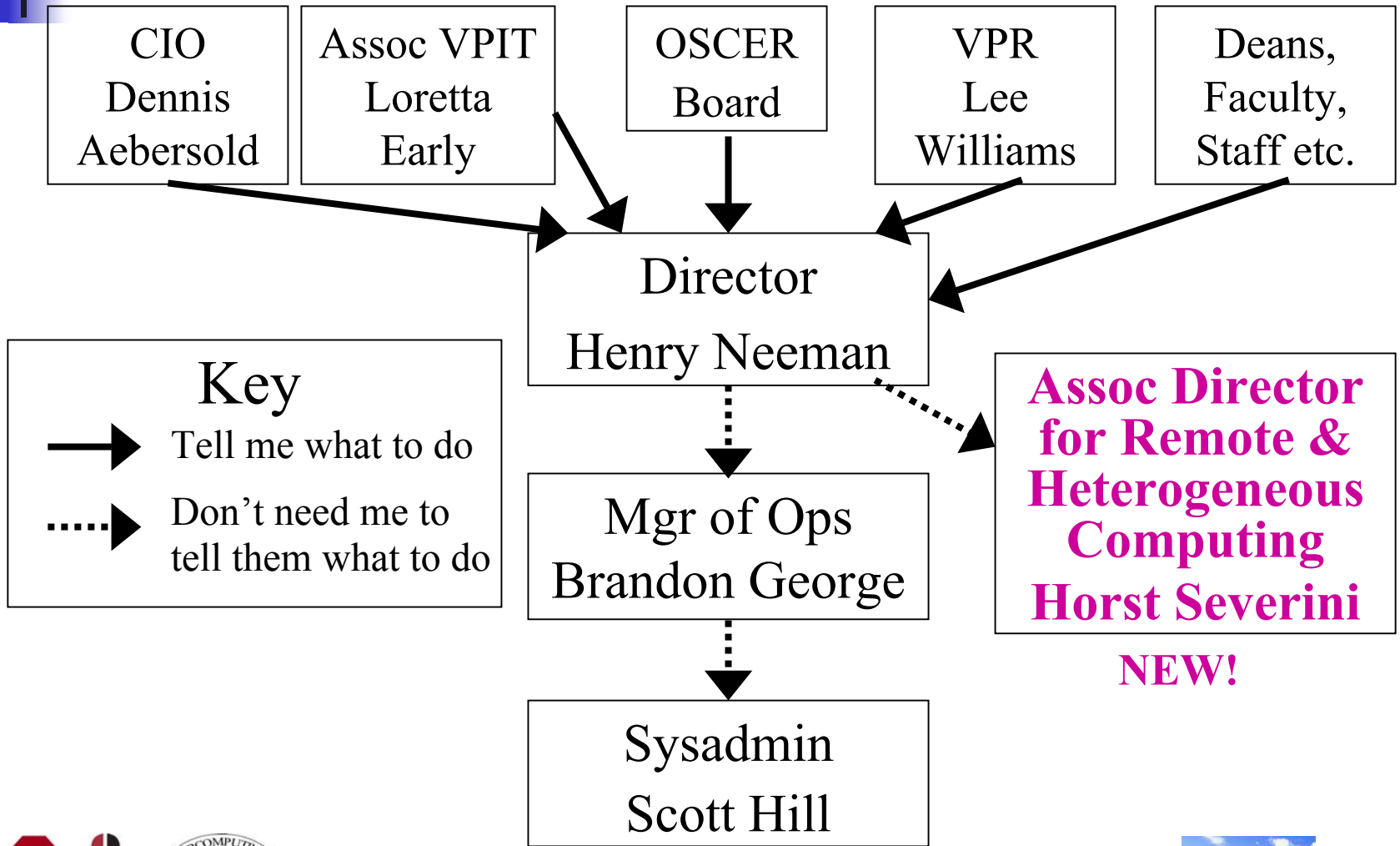
* Unique usernames on modi4, titan and cu

OSCER Structure

CIO Dennis Aebersold

Assoc VPIT Loretta Early

OSCER Board

VPR Lee Williams

Deans, Faculty, Staff etc.

Director Henry Neeman

Key
→ Tell me what to do
⋯▶ Don't need me to tell them what to do

Mgr of Ops Brandon George

Assoc Director for Remote & Heterogeneous Computing Horst Severini
NEW!

Sysadmin Scott Hill

Oklahoma EPSCoR

Vice President for Research
University of Oklahoma

Who Works for OSCER?

- Director: Henry Neeman
- Manager of Operations: Brandon George
- System Administrator: Scott Hill (funded by CAPS)
- **NEW! Associate Director for Remote & Heterogeneous Computing Horst Severini**

Left to right:
Henry Neeman,
Brandon George,
Scott Hill

Horst Severini

OSCER State of the Center Address
Oklahoma Supercomputing Symposium 2003

Oklahoma EPSCoR

Vice President for Research
University of Oklahoma

10

OSCER Board

- **Arts & Sciences**
  - Tyrrell Conway, Microbiology
  - Andy Feldt, Physics & Astro
  - Pat Skubic, Physics & Astro
- **Engineering**
  - S. Lakshmivarahan, Comp Sci
  - Dimitrios Papavassiliou, Chem Engr
  - Fred Striz, Aerospace & Mech Engr
- **Geosciences**
  - Kelvin Droegemeier, Meteorology/CAPS
  - Tim Kwiatkowski, G&G
  - Dan Weber, CAPS

L to R: Papavassiliou,
IBM VP for HPC Peter Ungaro,
Skubic, Striz, Neeman,
Droegemeier, Weber

Not pictured: Feldt,
Lakshmivarahan, Kwiatkowski

Where is OSCER?

For now:

- Machine Room: Sarkeys Energy Center 1030 (shared with Geosciences Computing Network; Schools of Meteorology, Geography, Geology & Geophysics; Oklahoma Climatological Survey, etc)

  Schedule a tour!

- Henry's office: SEC 1252

- Brandon & Scott's office: SEC 1014

OSCER is Moving in 2004

OU recently broke ground on a new weather center complex, consisting of the National Weather Center building and the Peggy and Charles Stephenson Research and Technology Center, which will house genomics, robotics, the US Geological Survey and OSCER.

OSCER will be housed on the ground floor, in a glassed-in machine room and offices, directly across from the front door – a showcase!

Scheduled opening: 2004

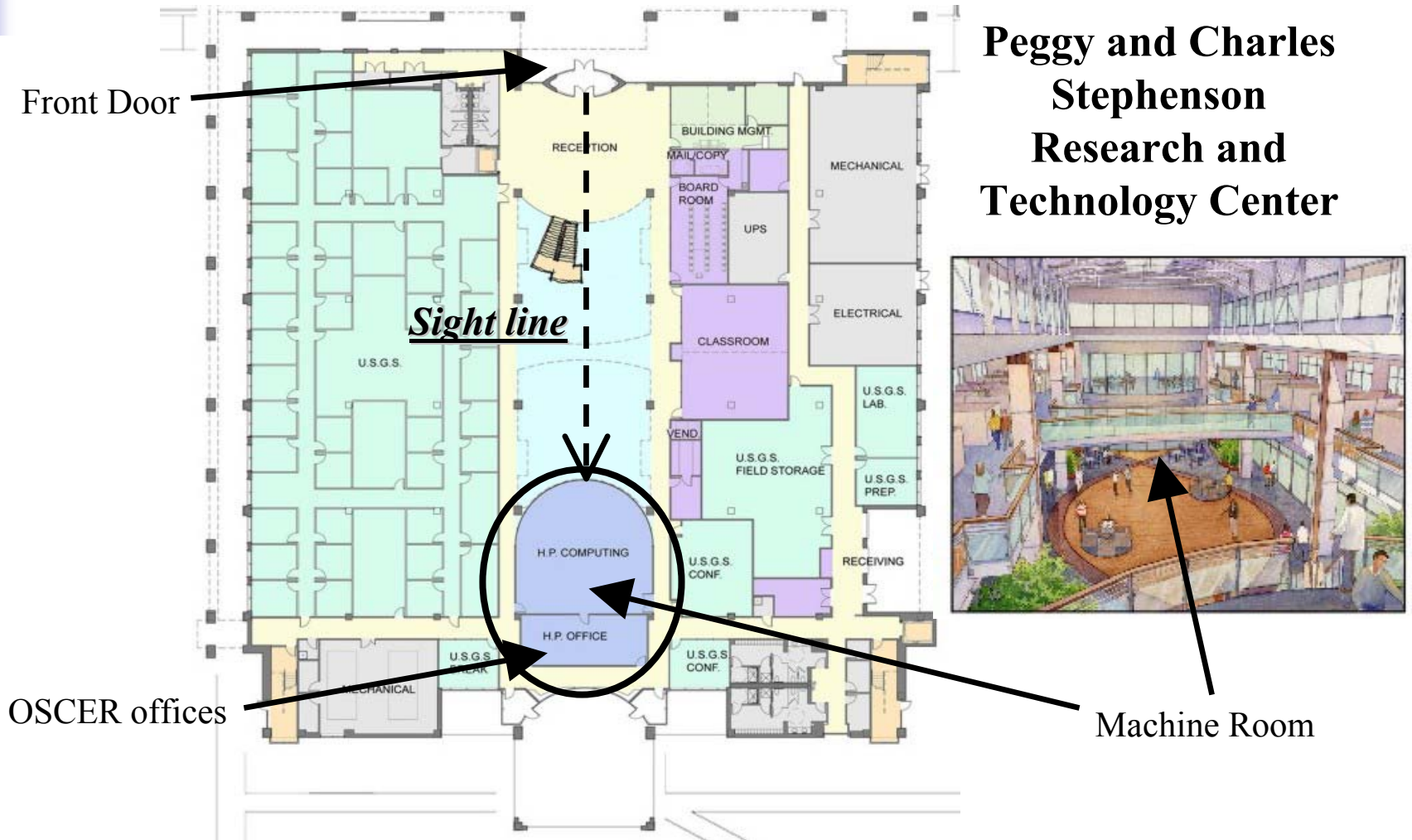# Where Will OSCER Move to?

Front Door

Sight line

OSCER offices

Peggy and Charles Stephenson Research and Technology Center

Machine Room

Why OSCER?

- Computational Science & Engineering has become sophisticated enough to take its place alongside experimentation and theory.

- Most students – and most faculty and staff – don't learn much CSE, because it's seen as needing too much computing background, and needs HPC, which is seen as very hard to learn.

- HPC can be hard to learn: few materials for novices; most docs written for experts as reference guides.

- We need a new approach: HPC and CSE for computing novices – OSCER's mandate!

Why Bother Teaching Novices?

- Application scientists & engineers typically know their applications very well, much better than a collaborating computer scientist ever would.

- Commercial software lags far behind the research community.

- Many potential CSE users don't need full time CSE and HPC staff, just some help.

- One HPC expert can help dozens of research groups.

- Today's novices are tomorrow's top researchers, especially because today's top researchers will eventually retire.

How Did OSCER Happen?

Cooperation between:

- OU High Performance Computing group: currently over 130 faculty and staff in 23 departments within 5 Colleges
- OU CIO Dennis Aebersold
- OU VP for Research Lee Williams
- Williams Energy Marketing & Trading Co.
- OU Center for Analysis & Prediction of Storms
- OU School of Computer Science
- Oklahoma EPSCoR Director Frank Waxman
- Encouragement from OU President David Boren, OU Provost Nancy Mergler, Oklahoma Congressman J.C. Watts Jr. (now retired), OU Assoc VPIT Loretta Early, various Deans

OSCER History

- Aug 2000: founding of OU High Performance Computing group
- Nov 2000: first meeting of OUHPC and OU Chief Information Officer Dennis Aebersold
- Jan 2001: Henry's "listening tour:" learning about what researchers needed – education!!!
- Feb 2001: meeting between OUHPC, CIO and VPR; draft white paper about HPC at OU
- Apr 2001: Henry appointed IT's Director of HPC
- July 2001: draft OSCER charter released
- Aug 31 2001: OSCER founded; 1st Supercomputing in Plain English workshop presented

OSCER History (continued)

- Sep 2001: OSCER Board elected
- Nov 2001: hardware bids solicited and received
- Dec 2001: OU Board of Regents approval
- March – May 2002: machine room retrofit
- Apr & May 2002: supercomputers delivered
- Sep 2002: 1st annual OU Supercomputing Symposium
- **Oct 2002: first paper about OSCER's education strategy published**
- **Dec 2002: CAPS real time weather forecasts go live**
- **Sep 2003: NSF MRI grant for Itanium2 cluster**

What Does OSCER Do?

What Does OSCER Do?

- Teaching
- Research
- Dissemination
- Resources

OSCER Teaching

OSCER Teaching

- Workshops
  - Supercomputing in Plain English
  - Parallel Programming
- Rounds and ride-alongs
- Academic coursework
- Web-based materials

Supercomputing in Plain English

An Introduction to High Performance Computing

Henry Neeman, Director
OU Supercomputing Center for Education & Research
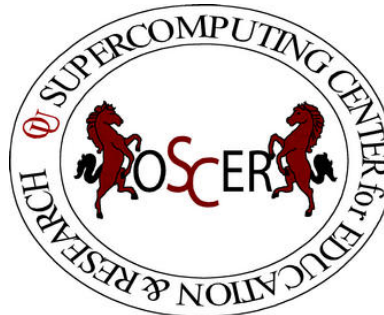
Supercomputing in Plain English

Supercomputing in Plain English workshops target not only people who are sophisticated about computing, but especially students and researchers with strong science or engineering backgrounds but modest computing experience.

Prerequisite: 1 semester of Fortran, C, C++ or Java

Taught by analogy, with minimal use of jargon, and assuming very little computing background.

Materials:

http://www.oscer.ou.edu/education.html

Workshop Topics

- Overview

- The Storage Hierarchy

- Instruction Level Parallelism

- High Performance Compilers

- Shared Memory Parallelism

- Distributed Parallelism

- Grab Bag: Scientific Libraries, Visualization, Grid Computing

Teaching: Workshops

- Supercomputing in Plain English
  - Fall 2001: 87 registered, 40 – 60 attended each time
  - Fall 2002: 66 registered, c. 30 – 60 attended each time
  - Spring 2004: to be announced
- **S. Lakshmivarahan parallel programming workshops (over 40 registered for each)**
  - **Performance evaluation (Nov 2002)**
  - **MPI (Nov 2002)**
- **NEW! Parallel programming workshop (Sep 2003)**
… and more to come.

Parallel Programming Workshop 2003

NEW! MPI programming workshop presented as part of Oklahoma Supercomputing Symposium 2003

- working with:
  - Dr. David Joiner of the Shodor Education Foundation, National Computational Science Institute
  - Dr. Paul Gray of the University of Northern Iowa
- Demand is so high that we're holding a second workshop later in Fall 2003.
  - > 100 registrations for 58 seats (OU overflow bumped)
  - includes over 30 visitors from 15 institutions in 7 states (AR, KS, LA, MO, OK, SD, TX)

Teaching: Rounds

Rounds: interacting regularly with several research groups one-on-one (or one-on-few)

- Brainstorm ideas for applying supercomputing to the group's research
- Coding: design, develop, debug, test, benchmark
- Learn new computing environments
- Write papers and posters

Fall 2003: meeting with about 20 research groups weekly, biweekly or monthly

Teaching: Rounds Ride-Alongs

Ride-alongs: students in CS 1313 (Programming for Non-majors) get extra credit for taking the supercomputing tour and "riding along" on a round: a "living lab" of scientists & engineers in their native habitat.

NEW! Library & Information Studies has started participating.

Talks are underway now with the Departments of History of Science, Philosophy and English to extend the ride-along program to students studying scientists and engineers from a humanities perspective.

CS also has a proposal for their Data Networks course to extend ride-alongs to the IT networking group.

Teaching: Academic Coursework

- Scientific Computing (S. Lakshmivarahan)
- **NEW! Computer Networks & Distributed Processing (S. Lakshmivarahan) teaches MPI on OSCER's Linux cluster**
- **NEW! Nanotechnology & HPC (L. Lee, G.K. Newman, H. Neeman)**
- Supercomputing presentations in other courses
    - Industrial & Environmental Transport Processes (D. Papavassiliou)
    - undergrad numerical methods (U. Nollert)
    - Advanced Numerical Methods (R. Landes)
    - **NEW! Human Technology Interaction Center REU (R. Shehab)**

OU Nano/HPC Teaching Team
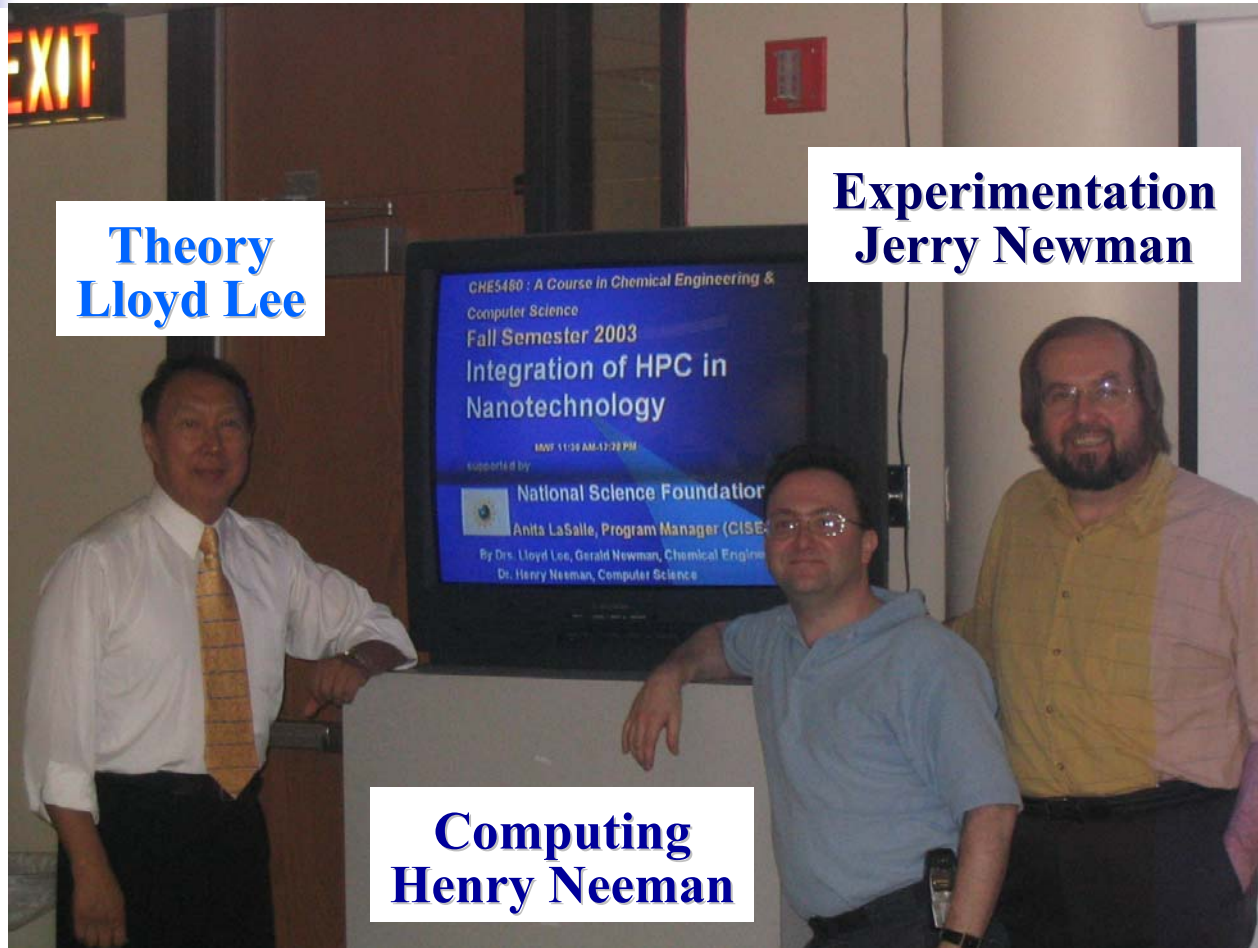
Theory
Lloyd Lee

Experimentation
Jerry Newman

Computing
Henry Neeman

NEW!

Putting together theory, computing and experimentation in a single engineering course (nanotechnology)

Teaching: Web-based Materials

Web-based materials:

- "Supercomputing in Plain English" (SiPE) slides
- Links to documentation about OSCER systems
- Locally written documentation about using local systems
- Introductory programming materials (developed for CS1313 Programming for Non-Majors): Fortran 90, C

OSCER Research

OSCER Research

- OSCER's Approach
- New Collaborations
- Rounds
- Grant Proposals

Research: OSCER's Approach

- Typically, supercomputing centers provide resources and have in-house application groups, but most users are more or less on their own.

- OSCER's approach is unique: we partner directly with research teams, providing supercomputing expertise to help their research move forward faster (rounds).

- This way, OSCER has a stake in each team's success, and each team has a stake in OSCER's success.

Research: New Collaborations

- OU Data Mining group
- OU Computational Biology group – Norman campus and Health Sciences (OKC) campus working together
- **NEW! Grid Computing group: OSCER, CAPS, Civil Engineering, Chemical Engineering, High Energy Physics, Aerospace Engineering, Computer Science**
- **NEW! Real Time Learning from Data group**
- **NOW FORMING! Scientific Visualization group**
- **NOW FORMING! Real Time & On Demand HPC group**
- … and more to come

Research: Rounds

<u>Rounds</u>: interact regularly with several research groups one-on-one (or one-on-few)

- Brainstorm ideas for applying supercomputing to the group's research
- Coding: design, develop, debug, test, benchmark
- Learn new computing environments
- Write papers and posters

Fall 2003: meeting with almost 20 research groups weekly, biweekly or monthly

Research: Grant Proposals

- OSCER provides text not only about resources but especially about education and research efforts (workshops, rounds, etc).

- Faculty write in small amount of money for:
  - funding of small pieces of OSCER personnel;
  - storage (disk, tape);
  - special purpose software.

- In many cases, OSCER works with faculty on developing and preparing proposals.

- OSCER now has a line item in the OU proposal info sheet that all new proposals have to fill out.

Proposals: Funded

- R. Kolar, J. Antonio, S. Dhall, S. Lakshmivarahan, "A Parallel, Baroclinic 3D Shallow Water Model," DoD - DEPSCoR (via ONR), $312K

- L. Lee, J. Mullen (Worcester Polytechnic), H. Neeman, G.K. Newman, "Integration of High Performance Computing in Nanotechnology," NSF, $400K

- J. Levit, D. Ebert (Purdue), C. Hansen (U Utah), "Advanced Weather Data Visualization," NSF, $300K

- D. Papavassiliou, "Turbulent Transport in Wall Turbulence," NSF, $165K

- D. Weber, H. Neeman, "Adaptation of the Advanced Regional Prediction System to the Modeling Environment for Atmospheric Discovery," NCSA, $210K

- M. Richman, A. White, V. Lakshmanan, V. De Brunner, P. Skubic, "Real Time Mining of Integrated Weather Data," NSF, $950K

Proposals: Funded (cont'd)

- D. Weber, K. Droegemeier, "MEAD: Portal Interfaces, Data Ingest and Analysis, Surface Hydrology Coupling," NCSA, $150K

- **NEW! D. Papavassiliou, "Scalar Transport in Porous Media," ACS-PRF, $80K**

- **NEW! H. Neeman, K. Droegemeier, K. Mish, D. Papavassiliou, P. Skubic, "Acquisition of an Itanium Cluster for Grid Computing," NSF, $340K**

- **NEW! K. Droegemeier et al., "Engineering Research Center for Collaborative Adaptive Sensing of the Atmosphere," NSF, $17M (total), $5.6M (OU)**

- **NEW! K. Droegemeier et al., "Linked Environments for Atmospheric Discovery (LEAD)," NSF, $11.25M (total), $2.5M (OU)**

OSCER-RELATED FUNDING TO DATE: $31M total, $11M to OU

Proposals: Pending

- **NSF Science of Learning Center:** T. Trafalis, M. Richman, V. Lakshmanan, D. Hougen, G. Kosmopolou, "Multidisciplinary Center for Learning from Data in Real Time", $23.5M

- **DOE EPSCoR:** S. Nandy, M. Strauss, J. Snow, "Oklahoma Center for High Energy Physics Research," $4.5M

- **NSF Course, Curriculum & Laboratory Improvement:** M. Atiquzzaman, H. Neeman, L. Fink, "Development of a Data Networks Course with On-site Mentoring by Practitioners," $75K

Proposals: to be Submitted

- **NSF CISE Research Infrastructure**: "Acquisition of a Scientific Visualization Platform" (Oct 2003)

- **NSF Major Research Infrastructure**: "Acquisition of a Real Time and On Demand High Performance Computing Platform" (Jan 2004)

- **NSF IGERT**: "Educating the Next Generation of Cross-Disciplinary High Performance Computing Mentors," $2.95M (preproposal Jan 2004)

OSCER Dissemination

OSCER Dissemination

- Local symposia
- Parallel programming workshop
- Talks, papers, posters
- Publicity

Supercomputing Symposium 2002

- Participating Universities: OU, Oklahoma State, Cameron, Langston, U Arkansas Little Rock

- Participating companies: Aspen Systems, IBM

- Other organizations: OK EPSCoR, COEITT

- 69 participants, including 22 students

- Roughly 20 posters

Supercomputing Symposium 2003

- Participating Universities: over 100 visitors from 35 schools in 13 states & Puerto Rico

- Participating organizations: NSF, 9 companies, 11 other groups

- Academic Sponsors: OK EPSCoR, OU VPR, Great Plains Network, OU IT, OSCER

- Industry sponsors: Aspen Systems, Atipa Technologies, Dell Computer Corp, Infinicon Systems, Perfect Order

- Over 250 participants, including almost 100 students

- Roughly 50 posters, many by students

- Keynote speaker: Peter Freeman, head of NSF CISE

- Symposium 2004 already being planned

Parallel Programming Workshop

NEW! MPI programming workshop presented as part of the Oklahoma Supercomputing Symposium 2003

- working with:
  - Dr. David Joiner of the Shodor Education Foundation, National Computational Science Institute
  - Dr. Paul Gray of the University of Northern Iowa
- Demand is so high that we are holding a second workshop later in Fall 2003.
  - > 100 registrations for 58 seats (OU overflow will be bumped)
  - includes over 30 visitors from 15 institutions in 7 states (AR, KS, LA, MO, OK, SD, TX)

Disseminating OSCER

- Talk, Poster: OU Supercomputing Symposium 2002
- Paper, Talk: 3rd LCI International Conference on Linux Clusters, October 2002 ("Supercomputing in Plain English: Teaching High Performance Computing to Inexperienced Programmers")
- Talk: EDUCAUSE Southwest Regional Conf 2003
- Poster: NCSA/Alliance All Hands Meeting 2003
- Talk: OU Information Technology Symposium 2003
- Talk: OU VPR Brown Bag Series, Sep 2003
- Talk, Poster: Oklahoma Supercomputing Symposium 2003
- Papers (various) acknowledging OSCER

OSCER Resources

OSCER Resources

- IBM Regatta p690 Symmetric Multiprocessor
- Aspen Systems Pentium4 Xeon Linux Cluster
- IBM FAStT500 FiberChannel-1 Disk Server
- Qualstar TLS-412300 Tape Library
- **Itanium2 cluster coming soon!**

OSCER Hardware: IBM Regatta

32 POWER4 CPUs (1.1 GHz)

32 GB RAM

218 GB internal disk

OS: AIX 5.1

Peak speed: 140.8 GFLOP/s*

Programming model:
shared memory
multithreading (OpenMP)
(also supports MPI)

*GFLOP/s: billion floating
point operations per second

`sooner.oscer.ou.edu`

Oklahoma EPSCoR

G P N

Vice President for Research
University of Oklahoma

OSCER Hardware: Linux Cluster

270 Pentium4 XeonDP CPUs

270 GB RAM

8.7 TB disk

OS: Red Hat Linux 7.3

Peak speed: > 1 TFLOP/s*

Programming model:
distributed multiprocessing
(MPI)

Aspen Systems

*TFLOP/s: trillion floating
point operations per second

boomer.oscer.ou.edu

IBM FAStT500 FC-1 Disk Server

- 2.2 TB hard disk: 30×73 GB FiberChannel-1

- IBM 2109 16 Port FiberChannel-1 Switch

- 2 Controller Drawers (1 for AIX, 1 for Linux)

- Room for 60 more drives: researchers buy drives, OSCER maintains them

- Expandable to 13 TB at current drive sizes

Tape Library

- Qualstar TLS-412300
- Reseller: Western Scientific
- Initial configuration
  - 100 tape cartridges (10 TB)
  - 2 drives
  - 300 slots (can fit 600)
- Room for 500 more tapes, 10 more drives: researchers buy tapes, OSCER maintains – expandable to 120 TB
- Software: Veritas NetBackup DataCenter, Storage Migrator
- Driving issue for purchasing decision: weight!

Oklahoma EPSCoR G P N

Vice President for Research
University of Oklahoma

The Newest Addition

- **In Sep 2003, OSCER received an NSF Major Research Instrumentation grant: "Acquisition of an Itanium Cluster for Grid Computing."**

- **We'll be buying a new cluster, using Intel's new 64-bit CPU, the Itanium2 (16 to 64 CPUs).**
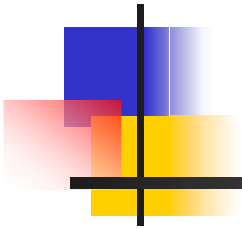

`schooner.oscer.ou.edu`

OSCER's Future and How to Get Involved

What Next?

More, MORE, **MORE!**

- More users

- More rounds

- More workshops

- More collaborations (intra- and inter-university)

- **MORE PROPOSALS!**

How Can You Get Involved?

To get involved with OSCER:

- Send e-mail to **`hneeman@ou.edu`**.

- By OSCER Board policy, to be eligible to use OSCER resources, you must be either:
  - an OU faculty or staff member, or
  - a student working on a research or education project directed/co-directed by an OU faculty or staff member, or
  - a non-OU researcher working on a project that has, as one of its PI/Co-PIs, an OU faculty or staff member.

A Bright Future

- OSCER's approach is unique, but it's the right way to go.

- People are taking notice nationally – e.g., you!

- We'd like there to be more and more OSCERs around the country:

  - local centers can react better to local needs;

  - inexperienced users need one-on-one interaction to learn how to use supercomputing in their research.

A Few Quick Thanks

Thank You: Sponsors

- Academic sponsors
  - Oklahoma EPSCoR (Frank Waxman)
  - OU Office of the VP for Research (Lee Williams)
  - Great Plains Network (Jerry Niebaum, Greg Monaco)
  - OU Department of Information Technology (Dennis Aebersold, Loretta Early)
  - OSCER
- Industry sponsors
  - Aspen Systems Inc.
  - Atipa Technologies
  - Dell Computer Corp
  - Infinicon Systems
  - Perfect Order

Thank You: Speakers

- **KEYNOTE:** Peter Freeman, National Science Foundation
- T. H. Lee Williams, University of Oklahoma
- Jason Levit, Cooperative Institute for Mesoscale Meteorological Studies/NOAA Storm Prediction Center
- David Joiner, Shodor Education Foundation Inc.
- Paul Gray, University of Northern Iowa
- Joel Snow, Langston University Mathematics/Physics
- Stephen Wheat, Intel Corp.
- Greg Monaco, Great Plains Network
- S. Lakshmivarhan, University of Oklahoma
- Jose Castanos, IBM

Thank You: Panelists

- Jay Boisseau, Texas Advanced Computing Center/ University of Texas at Austin: cancelled because of family loss – our condolences
- Geoffrey Dorn, BP Center for Visualization/ University of Colorado at Boulder
- Maria Marta Ferreyra, Carnegie Mellon University
- Steven Jennings, University of Arkansas Little Rock
- John Matrow, Wichita State University
- Richard Sincovec, University of Nebraska Lincoln

Thank You: Organizers

- OSCER
  - Brandon George
  - Scott Hill
- School of Meteorology
  - Alicia Zahrai
- OU Department of Information Technology
  - Ashlie Cornelius
  - Kim Haddad
  - Lisa Hendrix
  - Erin Hughes
  - Pam Jordening
  - Matt Runion
  - Matt Singleton
  - Michelle Wiginton
  - Alan Wong
  - Matt Younkins
- College of Continuing Education
  - Debbie Corley
  - Melvyn Kong
  - Amy Patterson

- University of Kansas Access Grid team
  - Ken Bishop
  - John Eslich
- Volunteer drivers of presenters
  - Mohammed Atiquzzaman
  - Kelvin Droegemeier
  - Dean Hougen
  - Horst Severini
  - Jim Summers

Thank You: Participants

- Over 250 participants registered including:
    - Over 125 OU faculty, staff and students
    - Over 100 visitors
    - 35 universities
    - 13 states and Puerto Rico
    - Over 50 posters
- Thank you for making the Oklahoma Supercomputing Symposium 2003 such a success!

To Get Involved with OSCER

- E-mail **hneeman@ou.edu**!

- Let's collaborate!

Have a safe trip home!