OU NSF CI-TEAM Project: Creating a Multistate Grid

Henry Neeman, Director

OU Supercomputing Center for Education & Research

University of Oklahoma

Iowa State University DOSAR Workshop, Friday April 6 2007

People

Things

How to Build a Multistate Grid

To make a prairie

It takes a clover and one bee.

One clover, and a bee, and reverie.

The reverie alone will do,

If bees are few.

– Emily Dickinson, 1858

OU's NSF CI-TEAM Project

OU recently received a grant from the National Science Foundation's Cyberinfrastructure Training, Education, Advancement, and Mentoring for Our 21st Century Workforce (CI-TEAM) program.

Objectives:

- Teach general HPC concepts to a broad audience
- Provide Condor resources to the national community
- Teach users to use Condor and sysadmins to deploy and administer it
- Teach bioinformatics students to use BLAST over Condor

OU NSF CI-TEAM Project

Cyberinfrastructure Education for Bioinformatics and Beyond

Objectives:

- **teach** students and faculty to use **FREE** Condor middleware, stealing computing time on idle PCs;
- **teach** system administrators to deploy and maintain Condor on PCs;
- **teach** bioinformatics students to use BLAST on Condor;
- **provide** Condor Cyberinfrastructure to the national community (**FREE**).

OU will provide:

- **Condor pool** of 750 desktop PCs (already part of the **Open Science Grid**);
- **Supercomputing in Plain English** workshops via videoconferencing;
- Cyberinfrastructure **rounds** (consulting) via videoconferencing;
- **drop-in CDs** for installing full-featured Condor on a Windows PC (Cyberinfrastructure for **FREE**);
- **sysadmin consulting** for installing and maintaining Condor on desktop PCs.

OU's team includes: High School, Minority Serving, 2-year, 4-year, masters-granting; 11 of the 15 institutions are in 4 EPSCoR states (AR, KS, NE, OK).

OU NSF CI-TEAM Project

Participants at OU
(29 faculty/staff in 16 depts)

- Information Technology
  - OSCER: **Neeman (PI)**   ⴹ ⴺ ⴺ ⴺ
- College of Arts & Sciences
  - Botany & Microbiology: Conway, Wren
  - Chemistry & Biochemistry: **Roe (Co-PI)**, Wheeler
  - Mathematics: White
  - Physics & Astronomy: Kao, **Severini (Co-PI)**, Skubic, Strauss
  - Zoology: Ray
- College of Earth & Energy
  - Sarkeys Energy Center: Chesnokov
- College of Engineering
  - Aerospace & Mechanical Engr: Striz
  - Chemical, Biological & Materials Engr: Papavassiliou
  - Civil Engr & Environmental Science: Vieux
  - Computer Science: Dhall, Fagg, Hougen, Lakshmivarahan, McGovern, Radhakrishnan
  - Electrical & Computer Engr: Cruz, Todd, Yeary, Yu
  - Industrial Engr: Trafalis
- OU Health Sciences Center, Oklahoma City
  - Biochemistry & Molecular Biology: Zlotnick
  - Radiological Sciences: **Wu (Co-PI)**
  - Surgery: Gusev

Participants at other institutions
(19 faculty/staff at 14 institutions)

- California State U Pomona (**masters-granting, minority serving**): Lee
- Contra Costa College (**2-year, minority serving**): Murphy
- Earlham College (**4-year**): Peck
- Emporia State U (**masters-granting, EPSCoR**): Pheatt, Ballester
- Kansas State U (**EPSCoR**): Andresen, Monaco
- Langston U (**masters-granting, minority serving, EPSCoR**): Snow
- Oklahoma Baptist U (**4-year, EPSCoR**): Chen, Jett, Jordan
- Oklahoma School of Science & Mathematics (**high school, EPSCoR**): Samadzadeh
- St. Gregory's U (**4-year, EPSCoR**): Meyer
- U Arkansas (**EPSCoR**): Apon
- U Central Oklahoma (**masters-granting, EPSCoR**): Lemley, Wilson
- U Kansas (**EPSCoR**): Bishop
- U Nebraska-Lincoln (**EPSCoR**): Swanson
- U Northern Iowa (**masters-granting**): Gray

The Challenge of Teaching HPC

- Computational Science & Engineering (CSE) 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 Cyberinfrastructure (CI), which is seen as very hard to learn.

- **CI can be hard to learn**: few materials for novices; most documents written for experts as reference guides.

- **We need a new approach**: CI and CSE for computing novices!

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 to Create a Multistate Grid?

- Grids **aren't** primarily about technology!
- You need to recruit **people**, by offering them more than you ask them to provide.
1. Go to their institution.
2. Give a really fun and interesting talk about your stuff.
3. Tell them that they can use your stuff for free.
4. Make them commit to using your stuff.
5. Help them use your stuff.
6. If possible, get them to visit you and see your stuff.

OU NSF CI-TEAM Project

Participants at OU
(29 faculty/staff in 16 depts)

- <u>Information Technology</u>
  - <u>OSCER</u>: **Neeman (PI)** E M Ǝ Ш
- College of Arts & Sciences
  - <u>Botany & Microbiology</u>: Conway, Wren
  - <u>Chemistry & Biochemistry</u>: **Roe (Co-PI)**, Wheeler
  - <u>Mathematics</u>: White
  - <u>Physics & Astronomy</u>: Kao, **Severini (Co-PI)**, Skubic, Strauss
  - <u>Zoology</u>: Ray
- College of Earth & Energy
  - <u>Sarkeys Energy Center</u>: Chesnokov
- College of Engineering
  - <u>Aerospace & Mechanical Engr</u>: Striz
  - <u>Chemical, Biological & Materials Engr</u>: Papavassiliou
  - <u>Civil Engr & Environmental Science</u>: Vieux
  - <u>Computer Science</u>: Dhall, Fagg, Hougen, Lakshmivarahan, McGovern, Radhakrishnan
  - <u>Electrical & Computer Engr</u>: Cruz, Todd, Yeary, Yu
  - <u>Industrial Engr</u>: Trafalis
- OU Health Sciences Center, Oklahoma City
  - <u>Biochemistry & Molecular Biology</u>: Zlotnick
  - <u>Radiological Sciences</u>: **Wu (Co-PI)**
  - <u>Surgery</u>: Gusev

Participants at other institutions
(19 faculty/staff at 14 institutions)

- <u>California State U Pomona</u> (**masters-granting, minority serving**): Lee
- <u>Contra Costa College</u> (**2-year**, **minority serving**): Murphy
- <u>Earlham College</u> (**4-year**): Peck
- <u>Emporia State U</u> (**masters-granting**, **EPSCoR**): Pheatt, Ballester
- <u>Kansas State U</u> (**EPSCoR**): Andresen, Monaco
- <u>Langston U</u> (**masters-granting**, **minority serving, EPSCoR**): Snow
- <u>Oklahoma Baptist U</u> (**4-year**, **EPSCoR**): Chen, Jett, Jordan
- <u>Oklahoma School of Science & Mathematics</u> (**high school, EPSCoR**): Samadzadeh
- <u>St. Gregory's U</u> (**4-year**, **EPSCoR**): Meyer
- <u>U Arkansas</u> (**EPSCoR**): Apon
- <u>U Central Oklahoma</u> (**masters-granting**, **EPSCoR**): Lemley, Wilson
- <u>U Kansas</u> (**EPSCoR**): Bishop
- <u>U Nebraska-Lincoln</u> (**EPSCoR**): Swanson
- <u>U Northern Iowa</u> (**masters-granting**): Gray

NSF EPSCoR RII Proposal

- The National Science Foundation sponsors a program in Oklahoma that every 3 years gives the state approximately $9M for a few research themes.

- In 2007, OSCER in collaboration with several other Oklahoma institutions is proposing Cyberinfrastructure (supercomputing) as one of the themes – statewide supercomputing available for **<u>free</u>**.

16 institutions, 134 people

Cameron U (3)
- **Mathematics:** Argyros, Zhao
- **Physical Science**: Nalley

East Central U (2)
- **Chemistry:** Myers
- **Mathematics**: Ferdinand

Langston U (2)
- **Mathematics & Physics:** Snow
- **Computer Information Sciences**: Tiako

Oklahoma Baptist U (4)
- **Biology:** Jett
- **Chemistry:** Jordan
- **Mathematics:** Hobbs
- **Physics:** Chen

Oklahoma City U (2)
- **Computer Science:** Kazmierczak, Sells

Oklahoma Medical Research Foundation (1)
- Wren

Oklahoma School of Science & Math (1)
- **Computer Science:** Zimmer

St. Gregory's U (1)
- **Physical Sciences:** Meyer

National Severe Storms Lab (1)
- Wicker

U Central Oklahoma (2)
- **Physics & Engineering:** Lemley, Sanchez

Oklahoma State U (14)
- **Biochem & Molecular Bio:** Hoyt
- **Biosystems & Agriculture**: Storm
- **Botany**: Palmer
- **Chemistry:** Eastman, Lavine
- **Computer Science:** Dai, Li, Sarangan
- **Electrical Engineering:** Stine
- **Geology**: Atekwana
- **Management Science and Information Systems**: Sharda
- **Marketing**: Mowen
- **Mathematics**: Biinegar
- **Physics**: Mintmire

Rogers State University (1)
- **Mathematics and Sciences**: Soe

Southeastern Oklahoma State U (1)
- **Computer Science:** Morris

Southwestern Oklahoma State U (2)
- **Chemistry:** Linder
- **Computer Science:** Moseley

U Tulsa (9)
- **Biology:** Buchheim
- **Electrical Engineering:** LoPresti, Manikas
- **Mathematics & Computer Science:** Gamble
- **Mechanical Engineering**: Mohan, Shirazi
- **Petroleum Engineering:** Reynolds, Saricka, Shoham

EMEM

88 Participants @ OU

- **Aerospace & Mechanical Engr (6):** Altan, Attar, Lai, Siddique, Striz, Vedula
- **Biochemistry & Molecular Biology (2):** Mooers, Zlotnick
- **Botany & Microbiology (3):** Conway, Wallace, Zhou
- **Center for Analysis & Prediction of Storms (5):** Brewster, Brotzge, Gao, Kong, Weber (+ Carr, Droegemeier, Shapiro, Xue of Meteorology)
- **Chemical, Biological &Materials Engr (7):** Bagajewicz, Grady, Nollert, O'Rear Papavassiliou, Schmidtke, Striolo
- **Chemistry & Biochemistry (3):** Roe, Soloshonok, Wheeler
- **Cooperative Institute for Mesoscale Meteorological Studies (3):** Kogan, Mansell, Mechem
- **Civil Engr & Environmental Sci (7):** Hatami, Kolar, Mish, Muraleetharan, Nanny, Vieux, Zaman
- **Communication (1):** O'Hair
- **Computer Science (11):** Antonio, Atiquzzaman, Cheng, Dhall, Dong, Fagg, Gruenwald, Hougen, Lakshmivarahan, McGovern, Thulasiraman
- **Economics (1):** LaMarche

- **Electrical & Computer Engr (6):** Cruz, Ibrahim, Sluss, Tull, Yeary, Yu
- **Finance (1):** Linn
- **Geography (1):** Yuan
- **Industrial Engr (1):** Trafalis
- **K20 Center for Educational & Community Renewal (2):** Arana, O'Hair
- **Mathematics (2):** Gutman, White
- **Meteorology (7):** Carr, Droegemeier, Fedorovich, Richman, Shapiro, Straka, Xue
- **Oklahoma Biological Survey (1):** Broughton
- **OU Supercomputing Center for Education & Research (1):** Neeman
- **Radiological Sciences (1):** Wu
- **Petroleum & Geological Engineering (2):** Oliver, Zhang
- **Physics & Astronomy (10):** Abbott, Baron, Gutierrez, Kao, Milton, Parker, Severini, Skubic, Strauss, Wang
- **Sarkeys Energy Center (1):** Chesnokov
- **Surgery (1):** Gusev
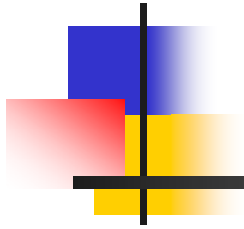- **Zoology (2):** Ray, Wang

OUHSC

OU's Supercomputing Education Strategy

OU's HPC Education Strategy

1. "Supercomputing in Plain English" workshops
2. Question-and-Answer
3. Cyberinfrastructure Tours
4. Rounds

Supercomputing in Plain English

Science and engineering faculty from all over America learn supercomputing at OU by playing with a jigsaw puzzle (NCSI @ OU 2004).

Supercomputing in Plain English

Supercomputing in Plain English (SiPE) workshops target 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, storytelling and play, with minimal use of jargon, and assuming very little computing background.

Materials: **http://www.oscer.ou.edu/education.php**

Registrations: almost 200 since 2001, plus many downloads of streaming video

SiPE Workshop Topics

- Overview

- The Storage Hierarchy

- Instruction Level Parallelism

- High Performance Compilers (mostly a discussion of parallelism issues)

- Shared Memory Parallelism

- Distributed Parallelism

- Grab Bag: Scientific Libraries, I/O libraries, Visualization

SiPE Overview Talk is for Everyone

The "Supercomputing in Plain English" Overview talk, which contains very little overtly technical material, has been presented to dozens of groups ranging from schoolchildren to top researchers.

Anyone who's used a computer for e-mail or websurfing understands enough about computing to understand the fundamental issues of supercomputing – if these issues are presented carefully.

SiPE Overview Talk Recipients

- Courses at OU
    - Chem Engr: Industrial & Environmental Transport Processes (D. Papavassiliou)
    - CS: Research Methods (A. Fagg)
    - Engineering Numerical Methods (U. Nollert)
    - Math: Advanced Numerical Methods (R. Landes)
    - Electrical Engr: Computational Bioengineering (T. Ibrahim)
- Research Experience for Undergraduates at OU
    - Ind Engr: Metrology REU (T. Reed Rhoads)
    - Ind Engr: Human Technology Interaction Center REU (R. Shehab)
    - Meteorology REU (D. Zaras)
- External
    - American Society of Mechanical Engineers, OKC Chapter
    - Oklahoma State Chamber of Commerce
    - National Educational Computing Conference 2006
    - Sooner Lions Club

- Other Universities
    1. SUNY Binghamton (NY)
    2. Bradley University (IL)
    3. Cameron University (OK)
    4. El Bosque University (Colombia)
    5. Louisiana State University
    6. Midwestern State University (TX)
    7. Northwestern Oklahoma State University
    8. Oklahoma Baptist University
    9. Oklahoma City University
    10. Oklahoma State University – OKC
    11. Oral Roberts University (OK)
    12. St. Gregory's University (OK)
    13. Southeastern Oklahoma State University
    14. Southwestern Oklahoma State University
    15. Texas A&M University - Commerce
    16. University of Arkansas Little Rock
- High Schools and High School Programs
    - Oklahoma School of Science & Mathematics
    - Oklahoma Christian University's Opportunity Bytes Summer Academy
    - Dept of Energy National Scholarship Finalists
    - Ardmore High School (OK)

Question & Answer

After either participating in a SiPE workshop or watching the associated SiPE video, each person:

1. answers a set of review questions available on the OSCER website;

2. formulates 3 questions about the material in the workshop.

Usually people do these in groups, so the number of question answered together can be substantial.

Many of these questions lead to detailed discussions of a CI issue.

CI Tours

Empirically, we've discovered that taking students on a tour of Cyberinfrastructure (e.g., a big cluster) is an unforgettably visceral experience.

Basically, anyone who hasn't taken the tour has great difficulty understanding the ideas – and anyone who has gets it pretty quickly.

Rounds

OU undergrads, grad students, staff and faculty learn
how to use supercomputing in their specific research.

Why Rounds?

- **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.

What are Rounds?

Rounds: interacting regularly with several research groups

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

Has now evolved into **supercomputing help sessions**, where many different groups work at the same time.

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.

- Library & Information Studies: on-campus internships
- History of Science: like CS students

Okla. Supercomputing Symposium

Wed Oct 3 2007 @ OU

Over 170 registrations already!

2003 Keynote:
Peter Freeman
NSF
Computer &
Information
Science &
Engineering
Assistant Director

2004 Keynote:
Sangtae Kim
NSF Shared
Cyberinfrastructure
Division Director

2005 Keynote:
Walt Brooks
NASA Advanced
Supercomputing
Division Director

2006 Keynote:
Dan Atkins
Head of NSF's
Office of
Cyberinfrastructure

**2007 Keynote:
Jay Boisseau
Director
Texas Advanced
Computing Center
Univ Texas Austin**

FREE!

`http://symposium2007.oscer.ou.edu/`

OU NSF CI-TEAM Project: Creating a Multistate Grid
Iowa State DOSAR Workshop, Friday April 6 2007

To Learn More OSCER

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

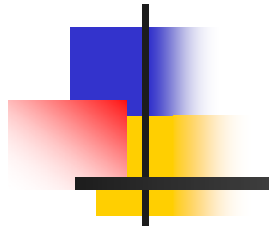http://symposium2007.oscer.ou.edu/

OU NSF CI-TEAM Project: Creating a Multistate Grid
Iowa State DOSAR Workshop, Friday April 6 2007

29

Thanks for your attention!

Questions?