Parallel Programming Techniques

Intro to PSC

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PITTSBURGH SUPERCOMPUTING CENTER

What is the PSC?

PSC is a joint effort between:

- Carnegie Mellon University
- University of Pittsburgh
- Westinghouse Electric Company

PSC's Mission

- Enable solutions to important problems in Science and Engineering by providing leading-edge computational resources to the national community.
- Advance computational science, computational techniques and the National Information Infrastructure.
- Educate researchers in high performance techniques and their applications to science and engineering.
- Assist the private sector in exploiting high performance computing for their competitive advantage.
  - Alcoa
  - Pfizer
  - Chevron
  - USX

PSC's Mission (continued)

In meeting our mission, we've developed valuable programs and resources, including:

- Computational resources
- Partnerships with other research centers and universities
- Biomedical Supercomputing Initiative
- Scientific Visualization research and support
- The Corporate Program
- Networking Research and Operations

There are numerous research and development efforts currently underway at PSC.

Disciplines

Grants of time on our supercomputers are awarded to researchers from many disciplines, including:

- Chemistry
- Physics
- Atmospheric Science
- Materials Science
- Engineering
- Geological Science
- Astronomy
- Biophysics
- Biochemistry
- Neuroscience
- Economics and Social Science

John Pople, a pioneer researchers at PSC, was awarded the 1998 Nobel Prize in chemistry.

Peter Kollman, of the University of California at San Francisco, used PSC's T3D and T3E extensively for his Microsecond Villin Headpiece Folding Simulation.

Machine Environment: Supercomputers

ginger.psc.edu

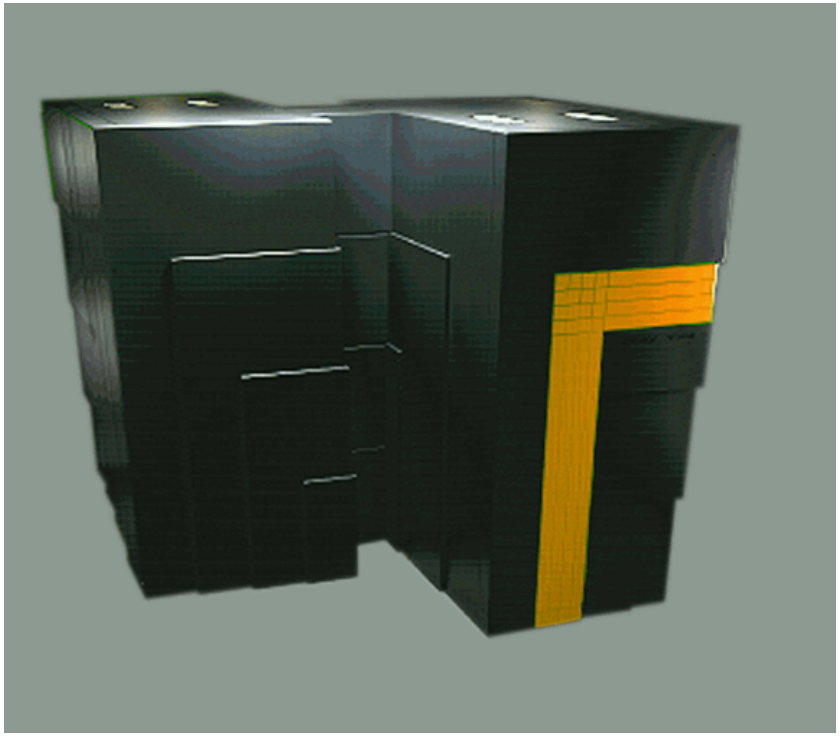
J90 ginger	
Number of Processors	**8**
Processor Peak Speed **Peak Aggregate Speed**	**200 MFLOPs** **1.6 GFLOPs**
Clock Cycle	**10 nsec**
Memory	**128 MW**
Operating System	**Unicos 9.0.2.5 with AFS**

Machine Environment: Supercomputers

intel2.psc.edu

Intel Cluster	
Number of Compute Nodes	**20**
Processor Speed	**10 – 400Mhz** **10 – 550Mhz**
Numbers of Compute Processors	**80**
Memory	**1 Gbyte per Node**
Operating System	**Linux**

Machine Environment: Supercomputers



jaromir.psc.edu

MPP (Massively Parallel Processing Platform) CRAY T3E

- **PSC's T3E supercomputer is currently rated number 85 as of November 2001.**
- **512 application processors running at 450 Mhz.**
- **Machine's theoretical peak speed : about 460 GFlops.**
- **128 MB/processor**

Machine Environment: Supercomputers

lemieux.psc.edu

Compaq Terascale Computing System Alphaserver SC LeMieux

- PSC's Alphaserver SC is currently the fastest academically available machine in the world
- 3024 processors (760 nodes) running at 1 GHz
- Theoretical peak 6048 GFlops
- Each node is 4 processor SMP with 4 Gbytes of memory

Machine Environment: Supercomputers

golem.psc.edu

Cray J90 Golem

- 2 Storage Tek robotic silos
  - 6000 internally stored tapes per silo

Login Procedures

- Users can access the PSC Computing Platforms by using SSH

Changing Passwords

- VMS front ends – set password
- AFS – kpasswd
- T3E(jaromir) – passwd
- FAR(golem) – ssh to golem then choose the password reset selecton

Disk Quota

- VMS – 10,000 blocks
- AFS – 50 Mbytes
- T3E – 20 Mbytes in $HOME
- T3E – 32 Gbytes in $TMP
- Far – No quota

Online Information

- http://www.psc.edu
- VMS – bulletin
- T3E – news

Using the T3E

- ssh jaromir.psc.edu
- Use scp, kftp or far to retrieve files
- Keep only scripts and source code in your home dir
- Run executables from $TMP
- Store output to far
- Remove files when you are finished

Using FAR

- ssh golem.psc.edu
- Change your password by selecting passwd
- Exit

Storing and Retrieving Files

- far get file1 file1
- far get file1 file2 file3 $TMP
- far store file1 file1
- far store file1 file2 file3 output
- far rget dir – copies an entire subtree
- far rstore dir dir – stores entire subtree

Moving around in far

- Enter far simply by typing far
- cp – copies files
- mkdir – create a directory
- mv – renames a file
- pwd – prints the current directory name
- rm – deletes a file
- rmdir – deletes an empty directory

Recommended Storage

- Use tar to combine multiple small files

tar cvf file.tar *

far store file.tar file.tar

far get file.tar .

tar xvf file.tar

Accounting

- Usage tracked in Service Units
- 1 SU is approx. 1 computing hour on 1 PE

Allocations

- Participants interested in obtaining production time on PSC systems should apply for a grant.
- http://www.psc.edu/grants/grants.html
- Who can apply?

Post-Docs, Professors and Research Staff

Workshops

- Networking
- Biomedical
- Application Specific
- Parallel Programming

Consultation

- Hotline

  1-412-268-6350

  1-800-221-1641

Staffed six days a week:

  Mon-Fri 9AM-8PM

  Sat 9AM-4PM

Remarks Email

- Mail to remarks@psc.edu
- Response on or before the next business day
- Include pertinent information in the email to save time

Exercises

- Login to jaromir

  ssh jaromir.psc.edu
- Reset your password

  passwd
- Create a file

  emacs test.txt

Exercises Cont.

- Store the file to far

  far store test.txt test.txt
- List the files in far

  far ls
- Rename the file

  far mv test.txt test2.txt

Exercises Cont.

- Retrieve the new file to your temporary directory

  far get test2.txt $TMP

- Move to the temporary directory and then list the file

  cd $TMP

  ls