# COSC 594 – 004
# **Scientific Computing for Engineers**

**Web page for the course:**
http://bit.ly/cs594-2012

## CS 594 – 004
## Wednesday's 1:30 – 4:30

- **Scientific Computing for Engineers**
- **Spring 2012 - 3 credits**
  - Jack Dongarra
  - with help from:
    - George Bosilca
    - Jakub Kurzak
    - Shirley Moore
    - Stan Tomov
    - Vince Weaver
- **Class will meet in Room C-233, Claxton Building**

2

# To Get Hold of Us

- **Email: dongarra@cs.utk.edu**
  - Room: 413, Claxton
  - Phone: 974-8295
- **Office hours:**
  - Wednesday 11:00 - 1:00, or by appointment
- **TA: Blake Haugen, bhaugen@utk.edu**
  - Rm 352, Claxton Complex, 974-
  - OH: Wednesday's 10am-12am or by request

3

# Four Major Aspects Of The Course:

1. Start with current trends in high-end computing systems and environments, and continue with a practical short description on parallel programming with MPI, OpenMP, and pthreads. Put together a cluster and experiment.
2. Deal with numerical linear algebra solvers: both direct dense methods and direct and iterative methods for the solution of sparse problems. Algorithmic and practical implementation aspects will be covered.
3. Illustrate the modeling of problems from physics and engineering in terms of partial differential equations (PDEs), and their numerical discretization using finite difference, finite element, and spectral approximation.
4. Various software tools will be surveyed and used. This will include PETSc, Sca/LAPACK, MATLAB, and some tools and techniques for scientific debugging and performance analysis.

4

## Grades Based on:

- 30% on weekly homework
  (the lowest homework grade will be dropped)
- 30% on a written report and presentation
  (20 pages circa.)
- 30% on a final exam (2 hours)
- 10% on class participation.



## Homework

- Usually weekly
- Lowest grade will be dropped
- Must be turned in on time (no late homework)
- Don't copy someone else's homework.
- Sometimes problems, sometimes programming assignment, sometimes requiring running a program to find the solution.

## Homework (continued)

- We expect an analysis and detailed discussion of the results of your efforts.
  - The program itself is not very interesting.
- Programming in C or Fortran.
- Will go over the assignments the week they are due.
- See class web page weekly for details.

7

## Using the SInRG Clusters

Grig:

- 128x Intel Xeon 3.2 GHz
  - 64 Nodes
  - 4G RAM
  - Myrinet 2000

Mordor:

- AMD Opteron 8358 2.4Ghz
  - 8 nodes (128 cores)4x (16 cores total)
  - 32G RAM
  - GigE
  - 2x Myricom 10G PCI-E Cards

Battlecat:

- 8x Intel Core 2 Duo 2.13 GHz
  - 8 Nodes
  - 2 GB RAM
  - Gig-E

8

## Build a Cluster

- Form subgroups
- Each subgroup will get a cluster to put together and experiment with.
  - Intel dual core based with a GPU from Nvidia and AMD
- Put software on and run experiments

9

## Project

- Topic of general interest to the course.
- The idea is to read three or four papers from the literature (references will be provided)
- Implement the application on the cluster you build
- Synthesize them in terms of a report (~10-15 pages)
- Present your report to class (~30 mins)
- New ideas and extensions are welcome, as well as implementation prototype if needed.

10

## Remarks

- Hope for very interactive course
- Willing to accept suggestions for changes in content and/or form

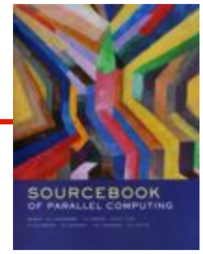
11

## Final Exam

- In class
- Will cover the material presented in the course
- ~2 hours

12

# Material




- **Book:**
  - The Sourcebook of Parallel Computing, Edited by Jack Dongarra, Ian Foster, Geoffrey Fox, William Gropp, Ken Kennedy, Linda Torczon, Andy White, 2002, 760 pages, ISBN 1-55860-871-0, Morgan Kaufmann Publishers.
- **For each lecture a set of slides will be made available in pdf or html.**
- **Other reading material will be made available electronically if possible.**
- **The web site for the course is:**
  - http://bit.ly/cs594-2012

13

# Other Sources

- Will use material from the internet (manuals, papers)
- Will use a variety of book sources; including
  - Ian Foster
    - » Designing and Building Parallel Programs
  - Alices E Koniges
    - » Industrial Strength Parallel Computing
  - Jack Dongarra, Iain Duff, Danny Sorensen, Henk van der Vorst
    - » Numerical Linear Algebra for High Performance Computers
  - Ananth Gramma et al.
    - » Introduction to Parallel Computing
  - Michael Quinn
    - » Parallel Programming
  - David E. Culler & Jaswinder Pal Singh
    - » Parallel Computer Architecture
  - George Almasi and Allan Gottlieb
    - » Highly Parallel Computing

14

## Important Place for Software

- Netlib - software repository
  - Go to http://www.netlib.org/

15

## What will we be doing?

- Learning about:
  - High-Performance Computing.
  - Parallel Computing
  - Performance Analysis
  - Computational techniques
  - Tools to aid parallel computing.
  - Developing programs in C or Fortran using MPI and perhaps OpenMP.

16

## Outline of the Course

1. January 11: Introduction to Class & High Performance Computing
2. January 18: Dense Linear Algebra
3. January 25: Parallel programming paradigms and their performances
4. February 1: Data Parallel Languages
5. February 8: Message Passing Interface (MPI)
6. February 15: Performance Evaluation and Tuning
7. February 22: MPI I/O
8. February 29: OpenMP and Hybrid MPI/OpenMP programming
9. March 7: Partitioned Global Address Space (PGAS) languages
10. March 14: Accelerators/GPUs

March 23 – Spring Break

11. March 28: Projection and its importance in scientific computing
12. April 4: Discretization of PDEs and Tools for the Parallel Solution
13. April 11: Sparse Matrices and Optimized Parallel Implementations
14. April 18: Iterative Methods in Linear Algebra
15. April 25: A look at PageRank
16. May 2: Class Final



## What you should get out of the course

In depth understanding of:

- Why parallel computing is useful.
- Understanding of parallel computing hardware options.
- Overview of programming models (software) and tools.
- Some important parallel applications and the algorithms
- Performance analysis and tuning techniques.

## Background

- C and/or Fortran programming
- Knowledge of parallel programming
- Some background in numerical computing.



## Computer Accounts

- For much of the class computing you can use one of our set of computer clusters. More on this later
- If you have an account in the Department you have access to the clusters.
- Cluster of PC's:
  - http://icl.cs.utk.edu/iclhelp/ look under clusters

CS 594 - **Scientific Computing for Engineers**

http://bit.ly/cs594-2012

Homework #1
January 11, 2012
Due: January 25, 2012

I would like you to implement a version of the following mathematical operations:

- the 2-norm of a vector,

$$\| x \|_2 = \sqrt{x^T x} = \sqrt{\sum_{i=1}^{n} x_i * x_i}$$

- matrix - vector multiplication,

$$y = y + A * x$$

$$y_i = y_i + \sum_{j=1}^{n} A_{i,j} * x_j, \text{for } i = 1, \ldots, n$$

- matrix multiplication

$$C = C + A * B$$

$$C_{i,j} = C_{i,j} + \sum_{k=1}^{n} A_{i,k} * B_{k,j}, \text{for } i, j = 1, \ldots, n$$

The point of this assignment is not to write software, but to look at the performance for each of your implementations and try to explain why you are getting the performance you see and what you could do to increase the performance. You should produce a software implementation for each and run some experiments on various systems, in particular use processors from battlecat, grig, and mordor clusters. I would like to see a report and analysis of your results, perhaps some plots of your performance data for n between say 10 and 1000. Please verify and convince me that you are computing the correct results in each case. Let me know what computers you used and how you are getting the performance results as well.

Our TA will have a set of timer you can use to measure the execution time of your programs. See the course webpage for details.

You can find out information on various processors at:
http://www.cpu-world.com/CPUs/index.html
http://www.cpu-world.com/sspec/index.html

21