CEE 618 (Spring 2013):
Parallel Computing for Engineers

January 11, 2013

Course Description:

This course will introduce students to the state-of-the-art high performance parallel computing to solve engineering and science problems using fundamental physics including fluid dynamics. Computational tasks are focused on increasing speed of finding solutions and enlarging sizes of targeted problems (possibly) with higher accuracy. Students will develop knowledge and skills primarily concerning:

1. Basic serial/parallel programming languages and numerical algorithms (f90 and f03);
2. Parallelizing existing serial codes; and
3. Solving real-world problems (computational fluid dynamics and statistical physics).

Coverage of Topics:

Two main topics will be taught in parallel, which will be inter-correlated: (1) basic physics and fluid mechanics with examples and applications, and (2) computation with specific algorithms. Materials and concepts to be covered are:

- Topic I: Basic UNIX/Linux commands; FORTRAN 77/90 for serial computation; Basic parallel programming using MPI (Message Passing Interface) and OpenMP (Multiple Processing) with FORTRAN binding; distributed memory systems; queuing protocols (Portable Batch Systems (PBS)); parallel Monte Carlo techniques; parallel algorithms for matrix operation and linear algebra
- Topic II-A: Basic statistical physics (selectively); ensemble averages and fluctuations; partition functions for ideal gases; Markov chain and biased Monte Carlo; random walk theory and diffusion for environmental/chemical engineering applications; (Bayesian approaches)
- Topic II-B: Parallel Computational Fluid Mechanics (CFD) using OpenFOAM - basics and simple applications; Parallel Dissipative Hydrodynamics (DHD) including nano and colloidal particle motion in an aqueous phase; Scientific visualizations and parallel movie generation.

Course Schedule:

Lecture (2 hours) and Lab. (1 hour)
Friday, **9:30 a.m. – 12:30 p.m., POST 214 (Don Kim Lab)**

Instructor:

PROF. ALBERT S. KIM

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Course URL:	TBA & Links (`http://albertsk.org/courses/cee618s13/`)
Office Hours:	open, online, or by email appointment

Texts:

- Main Text: Instructor's selected handouts will be posted to the course web site. Students should download, print, and bring them to class (except the first class).
- Supplementary Textbooks and Reading Materials:

1. **Scientific Software Design: The Object-Oriented Way**, Damian Rouson, Jim Xia, and Xiaofeng Xu, Cambridge University Press, 2011
2. **Computer Simulation of Liquids**, by M. P. Allen and D. J. Tilldesley, Oxford Science Publications
3. **Understanding Molecular Simulation**, by Daan Frenkel and B. Smit, Academic Press
4. **Introduction to FORTRAN 90 for Engineers and Scientists** by Larry R. Nyhoff and Sanford Leestma
5. **FORTRAN 90 for Scientists and Engineers** by Brian Hahn
6. **Numerical Recipes in Fortran 90** by William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, and Michael Metcalf
7. **USING MPI: Portable Parallel Programming** with the Message-Passing Interface, by W. Gropp, E. Lusk, A. Skjellum, The MIT Press
8. **A Survey of Computational Physics: Introductory Computational Science** by Rubin H. Landau, Manuel Jose Paes, & Cristian C. Bordeianu, Princeton University Press, 2008.
9. `http://www.netlib.org/`

Grading scheme and policy:

Class Participation:	15 %	A or A+:	85 – 100 %
Quizzes:	15 %	B:	75 – 85 %
Homework ($\backsim$10):	20 %	C:	65 – 75 %
Midterm :	20 %	D:	below 65 %
Final Project:	30 %		

Lecture schedule:

- Refer to the course web site: `http://albertsk.org/courses/cee618s13/`