ACMS60212/40212 Advanced Scientific Computing, Spring 2013

Instructor: Zhiliang Xu

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Class time and place: MWF 9:35am - 10:25am, Jordan Hall of Science 310

Office hours: W 3:00pm – 4:00pm, HH226

Prerequisite: ACMS60690/ACMS40390 or equivalent. Significant experience in C/C++ programming and applications to science or engineering.

This course covers fundamental materials necessary to use high performance computing to support research in science and engineering. There is a special emphasis on algorithm development, computer implementation, and the application of these methods to specific problems in science, engineering.

Topics to be covered:

- 1. Review of C/C++ programming for scientific computing, data management for developing code for scientific computation. Computer implementation of data structure (doubly linked list, tree etc), algorithms (Hash table, Stack, fast searching algorithm etc).
- 2. Parallel Computing, MPI basics
- 3. Parallel algorithms for implementing direct and iterative methods for solving system of linear equations
- 4. Sub-domain decomposition method for solving time-dependent partial differential equations on large domains.
- 5. Mesh Generation, Adaptive Mesh Refinement and Scientific Visualization
- 6. Computing on GPUs
- 7. Monte Carlo and stochastic simulations
- 8. If time permits, parallel implementation of finite element method for solving elliptic equations

Grades: Course grades will be based on homework and projects. Homework and projects should be done individually or in small groups. Undergraduate and graduate students will have different assignments.

Homework: 4 projects: Final project including project presentation:	10% 60% 30%
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The Notre Dame Academic Code of Honor Pledge is observed in this course. "As a member of the Notre Dame community, I will not participate in or tolerate academic dishonesty." **Textbooks:**

- 1. A. Grama, A. Gupta, G. Karypis, V. Kumar, Introduction to Parallel Computing, ISBN-0-201-64865-2
- 2. G.E. Karniadakis, R.M. Kirby II, Parallel Scientific Computing in C++ and MPI, A Seamless Approach to Parallel Algorithms and Their Implementation, ISBN-9780521520805

References:

- 1. V. Eijkhout, E. Chow, R. van de Geijn, Introduction to High-Performance Scientific Computing by (Public draft)
- 2. Numerical Recipes in C: The Art of Scientific Computing. Cambridge University Press, second edition, 2002.
- 3. Iterative Methods for Linear and Nonlinear Equations by C.T. Kelley, SIAM 1995
- 4. J. Sanders, E. Kandrot, CUDA by Example: An Introduction to General-Purpose GPU Programming, ISBN-10: 0131387685