ACMS60212/40212 Advanced Scientific Computing, Spring 2012

Instructor: Zhiliang Xu

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Class time and place: MWF 9:35am – 10:25am, E.J. Debartolo Hall 311

Office hours: M, 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:	10%
4 projects:	60%
Final project including project presentation:	30%

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
3. G. Hager, G. Wellein, Introduction to High Performance Computing for Scientists and Engineers, ISBN-978-1-4398-1192-4

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