Fall 2008  
Georgia Tech, CSE 6140  
Tu/Th 8:05am - 9:25am  
Classroom: KACB Room 2447

Computational Science & Engineering (CSE) Algorithms  
http://www.cc.gatech.edu/~bader/COURSES/GATECH/CSE6140-Fall2008/

Instructor: Prof. David A. Bader, KACB 1332, 404-385-0004, bader@cc  
Office Hours: Tuesday/Thursday 9:30am-10:30am  
Teaching Assistant: Xin Sun, xinsun@cc.gatech.edu  
TA Office Hours: Friday 4PM-6PM, Klaus Room 1305  

Textbooks:

Course Description: This course will introduce students to designing high-performance and scalable algorithms for computational science & engineering applications. The course focuses on algorithm design, complexity analysis, experimentation, and optimization, for important science and engineering applications. Students will develop knowledge and skills concerning:
  - the design and analysis of real-world algorithms employed in computational science and engineering applications, and
  - performance optimization of applications using the best practices of algorithm engineering.

Pre-requisites: design and analysis of algorithms (CS 3510).  
Students (from the Sciences, Engineering, and Computing) interested in algorithmic applications in science and engineering are encouraged to take this course.

This course can be taken for satisfying the theory breadth requirement by computer science graduate students (M.S. and non-theory Ph.D. students). This course cannot be taken by ACO students to satisfy their core requirement and theory Ph.D. students in computer science to satisfy the theory breadth requirement.

Grading:

- (25 %) Midterm
- (25 %) Final
- (25 %) Project
- (20 %) Homework
- (5 %) Class participation
CLASS POLICIES

1. Class announcements will be sent to the Georgia Tech T-Square mailing list, see http://t-square.gatech.edu/.

2. Please let me know as soon as possible if you will need to re-schedule an exam, or have any special needs during the semester.

3. Each student must read and abide by the Georgia Tech Academic Honor Code, see www.honor.gatech.edu.

4. Plagiarizing is defined by Websters as “to steal and pass off (the ideas or words of another) as one’s own: use (another’s production) without crediting the source.” If caught plagiarizing, you will be dealt with according to the GT Academic Honor Code.

5. When working on homework, you may work with other students in the class. However; you must turn in separate copies of the homework with the following written on it: your name and the names of everyone with whom you collaborated.

6. Homework is due by the end of lecture on the given due date. Late homeworks will not be accepted without a legitimate excuse and approval from the instructor.

7. No collaboration is permitted on exams. The midterm and final exams will be in-class, closed-book exams. You will be allowed to take a “cheat sheet” (double-sided 8.5 x 11 sheet of paper) into each exam.

8. Unauthorized use of any previous semester course materials, such as tests, quizzes, homework, projects, and any other coursework, is prohibited in this course. Using these materials will be considered a direct violation of academic policy and will be dealt with according to the GT Academic Honor Code.

9. For any questions involving these or any other Academic Honor Code issues, please consult me, my teaching assistants, or www.honor.gatech.edu.
Coverage of Topics

The course balances the use of theory and practice in algorithm design by presenting the student with case studies from application domains. After an introduction to computational science and engineering applications, algorithm theory, and realistic models of computation, the course consists of two modules. The first focuses on the design and analysis of real-world algorithms, with an application walk-through from algorithmic techniques to construction of the algorithm and finally application-level performance. The second module focuses on attaining high-performance implementations through algorithm engineering. These modules develop the theoretic framework and complements the study with examples from real-world problems using implementations on modern computing systems.

Computational Science & Engineering Introduction

1. Overview of Computational Sci. and Engr. Applications; characteristics and requirements
2. Computability and Complexity
3. Ideal and Realistic Models of Computation
4. Design of Parallel Algorithms
5. Performance Analysis
6. Multi-scale, multi-discipline applications

Real-World Algorithms: Techniques to Applications

1. Algorithms for Genomics: Divide and Conquer, cache-aware data structures, string algorithms
2. Sequence similarity searching: dynamic programming, string algorithms, local alignments, BLAST
3. Parallel Sorting by Regular Sampling: Randomized algorithms, load balancing, partitioning, merging, and sorting
4. Scientific visualization: greedy algorithms, 3d surface construction, marching cubes
5. Graph partitioning: NP-completeness, approximation algorithms, adaptive mesh refinement
6. Graph analysis: search algorithms, semantic networks, betweenness centrality

Algorithm Engineering

1. Modeling of the Memory Hierarchy
2. Cache-friendly, cache-aware, and cache-oblivious algorithms
3. Ideal and realistic models of parallel computation
4. Parallel and distributed algorithms and applications
5. Parallel disk models
6. Problem solving frameworks
7. Tools for Performance analysis
8. Experimental methods and validation
## Fall 2008, Tentative Course Schedule

<table>
<thead>
<tr>
<th>Week</th>
<th>Date</th>
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<th>Topic</th>
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<tbody>
<tr>
<td>1</td>
<td>19 Aug</td>
<td>1</td>
<td>Intro. to Computational Science &amp; Engineering</td>
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<td>21 Aug</td>
<td>2</td>
<td>Modern Computer Architecture, Models of Computation, Multicore</td>
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<td>2</td>
<td>26 Aug</td>
<td>3</td>
<td>Projects</td>
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<td>28 Aug</td>
<td>4</td>
<td>Real-world algorithm analysis</td>
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<td>3</td>
<td>2 Sep</td>
<td>5</td>
<td>Performance Analysis, High-Performance Computing</td>
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<td>4 Sep</td>
<td>6</td>
<td>Realistic models of computation, Disk models, cache-oblivious algorithms</td>
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<td>4</td>
<td>9 Sep</td>
<td>7</td>
<td>Practical Graph Algorithms (Guest Lecturer)</td>
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<td>11 Sep</td>
<td>8</td>
<td>Multi-scale, Multi-physics applications (Guest Lecturer)</td>
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<td>5</td>
<td>16 Sep</td>
<td>9</td>
<td>Review of Computability and Complexity</td>
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<td>18 Sep</td>
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<td>Petascale CSE Applications</td>
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<td>23 Sep</td>
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<td>IBM Cell processor and algorithms</td>
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<td>25 Sep</td>
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<td>Graph Partitioning (with Nodal Coordinates)</td>
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<td>Graph Partitioning (Spectral Methods)</td>
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<td>2 Oct</td>
<td>14</td>
<td>Multi-Grid Methods</td>
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<td>8</td>
<td>7 Oct</td>
<td>15</td>
<td>Midterm</td>
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<td>9 Oct</td>
<td>16</td>
<td>Parallel Sorting by Regular Sampling</td>
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<td>14 Oct</td>
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<td><strong>Fall Break</strong></td>
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<td>16 Oct</td>
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<td>Large-scale Graph and Multithreaded Algorithms</td>
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<td>21 Oct</td>
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<td>Real-world Connectivity Algorithms (Routing, Distance)</td>
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<td>23 Oct</td>
<td>19</td>
<td>Real-world Centrality Algorithms (Informatics and Interactions)</td>
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<td>28 Oct</td>
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<td>Biological Sequence Alignment and Searching</td>
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<td>Computational Biology/Phylogeny</td>
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<td>12</td>
<td>4 Nov</td>
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<td>Realistic models of parallel computation</td>
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<td>6 Nov</td>
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<td>Vectorized Algorithms and Techniques</td>
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<td>Productivity Metrics and Frameworks</td>
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<td>13 Nov</td>
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<td>Algorithm Engineering and Performance</td>
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<td>14</td>
<td>18 Nov</td>
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<td>Project Presentations</td>
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<td>20 Nov</td>
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<td>Experimental Methods and Validation</td>
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<td>27 Nov</td>
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<td><strong>Thanksgiving Break</strong></td>
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<td>16</td>
<td>2 Dec</td>
<td>29</td>
<td>Problem Solving Environments for Discrete Algorithms</td>
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<td>4 Dec</td>
<td>30</td>
<td>Special Topics: Open Problems in CSE Algorithms</td>
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<td>17</td>
<td>8 Dec</td>
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<td><strong>Final Exam</strong> (2:50pm-5:40pm)</td>
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Additional Readings:


