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[Syllabus]

HBM514E Parallel Numerical Algorithms and Tools

Prof.Dr. M. Serdar ÇELEBİ
Computational Science and Engineering Program

Course Introduction

Science and engineering have undergone a major transformation at the research level as well as at the development and technology levels. The modern scientist and engineer spend more and more time in front of a laptop, a workstation, or a parallel supercomputer and less and less time in the physical laboratory or in the workshop.

In this course, we review and expand the role of parallelism in computing and introduce the parallel numerical programming models that serve as the basis for subsequent discussion of algorithm design, performance analysis, and implementation. We will learn parallel numerical computing techniques and algorithms, and have practical experiences writing parallel programs on a both shared memory and distributed memory computers. We will also focus on how numerical algorithms can be made efficient on these parallel computers. The goal of the course is to give the students sufficient skills in the area of parallel computing so that they will be able to (i) read and understand descriptions of parallel algorithms, (ii) understand, in general terms, the size of the potential gain in execution time for a given problem when ported to a parallel computer, (iii) choose a suitable parallel algorithm for a given problem, (iv) modify the standard algorithms, described in the course, so that they suit to a given non-standard problem, (v) write scalable parallel numerical algorithms for the scientific and engineering problems in general sense. We will concentrate upon the message-passing methods of parallel computing and use some standard parallel computing tools such as MPI (Message Passing Interface), OpenMP and Multilevel Parallel Programming (Hybrid programming) techniques for SMP and Distributed Computer Architectures. Algebraic equations, ODE's, PDE's, dense and sparse matrix operations, iterative and direct solution methods for large scale linear set of equations and FFT are re-revisited and their algorithms are reconstructed in terms of parallel programming concepts and tools learned in the course.

Pre-requisite: HBM 513E

Instructor: Prof. Dr. M. Serdar Çelebi
(Phone: 285 7012, E-Mail: mscelebi@itu.edu.tr)

Office: Informatics Institute Building, 2nd Floor, Room 214.

Office Hours: Wednesday 10:30 –12:00, Friday 10:30 – 12:00

Research Assistants:
Mehmet TUNÇEL (mehmet.tuncel@be.itu.edu.tr)
Derya BODUR (derya.bodur@be.itu.edu.tr)

Samet Demir (sametdemir@gmail.com)
Gözde İniş (gozdeinis90@gmail.com)

Lecture Hours: Monday 13:30 –16:30

Lab Hours: TBA

Textbooks:

1) ***Parallel Programming with MPI***, Peter S. Pacheco, Morgan Kaufmann, 1997.

2) ***Parallel Programming in C with MPI and OpenMP***, Michael J. Quinn, Mc Graw Hill, 2003.

3) ***Computational Mathematics: Models, Methods and Analysis***, Robert E. White, Chapman&Hall/CRC, 2004.

4) ***Using OpenMP***, Barbara Chapman et al., MIT press, 2008.

5) ***Introduction to Parallel Computing***, Petersen and Arbenz, Oxford University Press, 2004.

6) ***Introduction to Parallel Computing***, 2nd edition, Grama, Gupta, Karypis, Kumar, Pearson & Addision Wasley, 2003.

7) ***Using MPI-2: Advanced Features of the Message-Passing Interface,*** Gropp, Thakur, The MIT Press, 1999.

8) ***Fundamentals of Parallel Processing,*** H.F. Jordan and G. Alaghband, Prentice Hall, 2003.

9) ***Parallel Algorithms***, Casanova H., Legrand A. and Robert Y., CRC Press, 2009.

10) ***Parallel Scientific Computing in C++ and MPI,*** Karniadakis G. and Kirby R., Cambridge University Press, 2003.

11) ***Parallel Algorithms for Matrix Computations,*** K. A. Gallivan at al., SIAM, 1990.

12) ***Principles of Parallel Programming,*** Calvin Lin and Lawrence Snyder, Pearson International, 2009.

Course Web Page: http://hbmders.be.itu.edu.tr/

Lecture Location: Informatics Institute Building, 4th floor, Room 411.

Grading:

Homeworks (2)	16%
Term Project	18%
Mid-Term Exam	32%
Final Exam	34%

TENTATIVE CONTENT

Week 1: Message Passing Computing Review:
Communicators and Groups (Extended Review, self-study),
Derived Data Types.

Week 2: Virtual Topologies

LAB 1: MPI Review

Week 3: Parallel I/O, Remote Memory Access and Dynamic Memory Management

LAB 2: MPI : Derived Data Types

Week 4: Graph Theory

LAB 3: MPI : Virtual Topology

Week 5: Domain Decomposition and Graph Partitioning Algorithms

LAB 4: MPI : Graph Based Virtual Topology

Week 6: Numerical Algorithms: Matrix Multiplications
Canon, Fox, DNS Algorithms

LAB 5: MPI : Advanced MPI-2 Features (Parallel I/O, RMA, DMM)

Week 7: Dense Matrix Operations: Direct Methods
Gauss Elimination, LU Decomposition, Factorizations

LAB 6: OpenMP: Review

Week 8: Iterative Methods and Sparse Matrices:
Jacobi, Gauss-Seidel, SOR, Red-Black Ordering, Thomas Algorithm

LAB 7:	Applications:1) Matrix Multiplication: Fox and Canon Algorithms, 2) N dimensional integral using Monte Carlo Method
Week 9:	Algorithms for ODE's and PDE's based on Finite Difference: Multi-coloring Algorithms
LAB 8:	Application1: Solution of PDE's based on MPI
Week 10:	Algorithms for ODE's and PDE's based on Finite Difference: Multi-coloring Algorithms
LAB 9:	Application2: Solution of PDE's based on MPI
Week 11:	Multi-level Programming: OpenMP+MPI and OpenMPI
LAB 10:	Application1: Solution Methods for Linear Set of Equations
Week 12:	Non-Stationary Matrix Methods: CG and GMRES
LAB 11:	Application2: Solution Methods for Linear Set of Equations
Week 13:	Performance İssues and Parallel Profiling
LAB 12:	Multilevel Programming: OpenMP+MPI and OpenMPI
Week 14:	FFT
LAB 13:	Performance Analysis Tools: Thread Checker, TAU, Intel Trace Analyzer, Vtune

LAB & SUPPLEMENTARY NOTES

1. Performance Analysis Tool I: Thread Checker
2. MPI Lab Notes (Three Labs)
3. OpenMP Lab Notes (Two Labs)
4. PDE Lab Notes
5. Monte Carlo Lab Notes
6. Matrix Multiplication Lab Notes

7. OpenMPI Lab Notes
8. Performance Analysis Tool II: TAU lab Notes, Vtune

TERM PROJECT

A Term Project will be assigned for writing a parallel algorithm using MPI, OpenMP or Hybrid programming. In your project, either an initial and boundary value problem or your pre-approved problem will be programmed by using parallel algorithms which will be teach in class. Profiling, Analysis, Performance and Scalability tests are going to be implemented for variety of test cases.

ADDITIONAL REFERENCES

1) William Gropp, E. Lusk and R. Thakur, ***Using MPI-2: Advanced Features of the Message-Passing Interface***, The MIT Press, 1999.
2) S. Goedecker and A. Hoisie, ***Performance Optimization of Numerically Intensive Codes***, SIAM, 2001.
3) Rajat P. Garg and I. Sharapov, ***Sun BluePrints: Techniques for Optimizing Applications***, Sun Microsystem Press, 2002.
4) Seyed H. Roosta, ***Parallel Processing and Parallel Algorithms***, Springer Verlag, 2000.
5) Peter Pacheco, ***Parallel Programming with MPI***, Morgan Kaufmann Pub., 1997.
6) Xavier C., Iyengar S.S. and Lyengar S.S., ***Introduction to Parallel Algorithms,*** Wiley Series, 1998.
7) Dongarra, Foster, Fox, Gropp, Kennedy, Torczon, White, ***Sourcebook of Parallel Computing***, Morgan Kauffman, 2003.
8) Koniges, ***Industrial Strength Parallel Computing***, Morgan Kauffman, 2000.
9) David E.K., Ahmed S. and Venkatakrishnan, ***Parallel Numerical Algorithms,*** Icase/Larc Interdisciplinary Series in Science and Engineering, Vol 4, 1997.
10) Kumar V., ***Introduction to Parallel Computing: Design and Analysis of Parallel Algorithms***, Addison-Wesley, 1994.
11) Van Der Welde, ***Concurrent Scientific Computing,*** Springer, 1994.
12) Almasi G.S. and Gottlieb A., ***Highly Parallel Computing***, 2nd ed., Benjamin/Cummins, CA, 1994.
13) Akl S.G., ***The Design and Analysis of Parallel Algorithms***, Prentice Hall, Englewood Cliffs, NJ, 1989.
14) Akl S.G., ***Parallel Computation: Models and Methods***, Prentice Hall, Upper Saddle River, NJ, 1997.

15) Berman K.A. and Paul J.L., ***Fundamentals of Sequential and Parallel Algorithms***, PWS Publishing, Boston, 1997.
16) Chaudhuri P., ***Parallel Algorithms: Design and Analysis***, Prentice Hall, Englewood Cliffs, NJ, 1992.
17) Gibbons A. and Rytter W., ***Efficient Parallel Algorithms***, Cambridge University Press, New York, 1988.
18) Jaja J., ***An Introduction to Parallel Algorithms***, Addison-Wesley, Reading, MA, 1992.
19) Smith J.R., ***The Design and Analysis of Parallel Algorithms***, Oxford University Press, New York, 1993.
20) Quinn M.J., ***Designing Efficient Algorithms for Parallel Computers***, McGraw-Hill, New York, 1987.
21) Freeman T.L. and Phillips C., ***Parallel Numerical Algorithms***, Prentice Hall, Englewood Cliffs, NJ, 1992.

Additional Extended Bibliography on Parallel Computing will be provided.