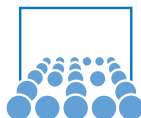


Algorithms of Scientific Computing II

0. Introduction

Hans-Joachim Bungartz



Algorithmen des Wissenschaftlichen Rechnens II

- Elective topic in Theoretische Informatik / Mathematik / ...
- WS 2010/2011:
 - Lecture: Mi 10:15-11:45 (MI 02.07.023)
 - Tutorial: Mo 16:00-18:00, every second week (MI 02.07.023)
 - Exam date will be discussed on the lecture
- People:
 - Hans-Joachim Bungartz, Room 02.05.054
 - Daniel Butnaru, Room 02.05.036
 - Wolfgang Eckhardt, Room 02.05.055

Motivation

- Algorithms of Scientific Computing I:
 - Presentation of a selection of important modern methods in scientific computing
 - Fourier Transform
 - Space Filling Curves
 - Hierarchical Bases and Sparse Grids
- Algorithms of Scientific Computing II:
 - Not a continuation of ASC I topics, but rather introducing further examples and giving deeper insight in
 - Molecular Dynamics Simulation
 - Sparse Grids
 - Algebraic Multigrid Methods
 - Note: ASC II exists in two variants
 1. Sparse Matrices (Prof. Th. Huckle)
 2. Scientific Computing (Prof. Th. Huckle)
 3. This semester's program (see above)

Outline of the Lecture

- **Chapter 1: Molecular Dynamics Simulation**

- 1.1 Introduction
- 1.2 Examples
- 1.3 Essentials from Continuum Mechanics
- 1.4 Molecular Dynamics – the Physical Model
- 1.5 Molecular Dynamics – the Mathematical Model
- 1.6 MD – Approximations and Discretization
- 1.7 MD – Implementational Aspects
- 1.8 MD – Parallelisation
- 1.9 Molecular Dynamics – Examples of Nanofluidic Simulations
- 1.10 Numerical Methods for Long-Range Potentials







- **Chapter 2: Sparse Grids**

- 2.1 Hierarchical Basis and Sparse Grids
- 2.2 Optimization via Discretization
- 2.3 Recurrences and Complexity
- 2.4 Numerical Quadrature on Sparse Grids








Outline of the Lecture (2)

- **Chapter 3: Algebraic Multigrid Methods**
 - 3.1 Multigrid Principle
 - 3.2 Algebraic Multigrids

Bibliography I

-  M.P. Allen and D.J. Tildesley, *Computer simulation of liquids*, Oxford University Press (reprint), 2003.
-  G. A. Bird, *Molecular gas dynamics and the direct simulation of gas flows*, Oxford Science Publications, Oxford Engineering Science Series 42, 1994.
-  William L. Briggs, Van Emden Henson, and Steve F. McCormick, *A multigrid tutorial (2nd ed.)*, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2000.
-  H.-J. Bungartz, *Rekursive Verfahren und hierarchische Datenstrukturen in der numerischen Analysis*, Skript zur Vorlesung.
-  H.-J. Bungartz and M. Griebel, *Sparse grids*, *Acta Numerica* **13** (2004), 147–269.
-  Robert D. Falgout, *An introduction to algebraic multigrid computing*, *Computing in Science and Engg.* **8** (2006), no. 6, 24–33.

Bibliography II

-  D. Frenkel and B. Smit, *Understanding molecular simulation from algorithms to applications*, Academic Press (2nd ed.), 2002.
-  M. Griebel, S. Knapek, G. Zumbusch, and A. Caglar, *Numerische simulation in der molekulardynamik*, Springer Verlag, 2004.
-  J. M. Haile, *Molecular dynamics simulation*, Wiley Professional Paperback Edition, 1997.
-  Wm. G. Hoover, *Molecular dynamics*, Lecture Notes in Physics 258, Springer, 1986.
-  J. Israelachvili, *Intermolecular & surface forces*, Academic Press (2nd ed.), 2001.
-  D. Rapaport, *The art of molecular dynamics simulation*, Cambridge University Press, 1995.
-  R.J. Sadus, *Molecular simulation of fluids theory, algorithms and object-orientation*, Elsevier, 1999.

Bibliography III



Irak Yavneh, *Why multigrid methods are so efficient*, Computing in Science and Engg. **8** (2006), no. 6, 12–22.