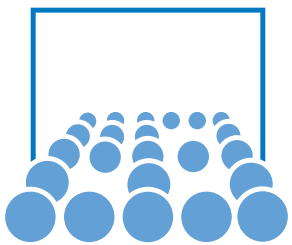
Algorithms of Scientific Computing II

0. Introduction

Hans-Joachim Bungartz



Algorithms of Scientific Computing II

- Elective topic in *Algorithms and Scientific Computing*-track (Master Computer Science)
- WS 2012/2013:
  - Lecture: Thu 10:00-12:00 (MI 02.07.023)
  - Tutorial: Tue 13:00-14:30, basically bi-weekly (MI 02.07.023)
    - 30.10.2012
    - 06.11.2012
    - 27.11.2012
    - 11.12.2012
    - 15.01.2013
    - 29.01.2013
    - 05.02.2013 (additional tutorial, for questions,...)
  - Exam date will be discussed on the lecture
- People:
  - Hans-Joachim Bungartz, Room 02.05.054
  - Alexander Heinecke, Room 02.05.036

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 three 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 The Multigrid Principle
  3.2 The Algebraic Multigrid Idea

Bibliography I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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.


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Bibliography III

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