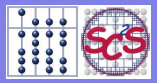
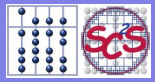


Algorithmen des Wissenschaftlichen Rechnens II

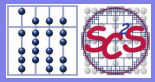
Algorithmen des Wissenschaftlichen Rechnens II

- Wahlfach Theoretische Informatik / Mathematik / . . .
- WS 2008/2009:
  - Termine Vorlesung: Mi 10:00-12:00 (MI HS 2)
  - Termine Übung: Di 14:00-16:00, 14-tägig (00.08.038)
  - exakter Zeitpunkt wird in der ersten Vorlesung festgelegt
- Menschen zum Anfassen:
  - Hans-Joachim Bungartz, Raum 02.05.054, Sprechstunde n.V.
  - Martin Buchholz, Raum 02.05.043
  - Stefan Zimmer, Raum 02.05.057



Motivation

- Algorithmen des Wissenschaftlichen Rechnens I:
  - Presentation of a selection of important modern methods in scientific computing
    - Fourier Transform
    - Space Filling Curves
    - Hierarchical Bases and Sparse Grids
- Algorithmen des Wissenschaftlichen Rechnens II:
  - Not a continuation of AWR I topics, but rather introducing further examples and giving deeper insight in
    - Molecular Dynamics Simulation
    - Sparse Grids
    - Algebraic Multigrid Methods
  - Note: AWR 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**

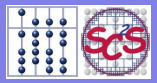
  1.1 Introduction
  1.2 Examples
  1.3 Essentials from Continuum Mechanics
  1.4 Molecular Dynamics – the Physical Model
  1.5 Molecular Dynamics – the Mathematical Model
  1.6 MD – Approximations and Discretization
  1.7 MD – Implementational Aspects
  1.8 MD – Parallelisation
  1.9 Molecular Dynamics – 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

- **Chapter 3: Algebraic Multigrid Methods**

  3.1 Multigrid Principle
  3.2 Algebraic Multigrids



Literature for Molecular Dynamics

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[2] M.P. Allen and D.J. Tildesley. Computer Simulation of Liquids. Oxford University Press (reprint), 2003.

[3] D. Frenkel and B. Smit. Understanding Molecular Simulation from Algorithms to Applications. Academic Press (2nd ed.), 2002.

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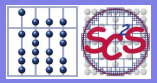

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[6] H.-J. Bungartz and M. Griebel. Sparse grids. Acta Numerica, 13:147–269, 2004.

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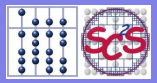

Literature for Algebraic Multigrid Methods

[8] 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.

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