Seminar Particle Methods

Philipp Neumann

Arbeitsbereich Wissenschaftliches Rechnen
Fachbereich Informatik
Fakultät für Mathematik, Informatik und Naturwissenschaften
Universität Hamburg

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Organisational Aspects

- Please sign up to the mailing list PM-18, see seminar website!
- Timeline: 14.05., 28.05., 11.06., 18.06., 09.07. (Mondays, 14-16)
- Participation in sessions is mandatory (missing 1 session is OK)
- Deliverables: 35-min presentation + 10-page seminar paper
- Per seminar session:
  - Repetition round
  - 2 talks
  - After each talk: questions and discussion on topic *and* feedback on presentation style
- Today:
  - Introduction to the provided topics
  - Distribution of topics to people

List of Topics

1. Introduction to Particle Dynamics
2. Molecular Dynamics
3. Parallelization and High-Performance Computing for Particle Systems
4. Adaptive Resolution Scheme
5. Long-range Particle Interactions
6. Smoothed Particle Hydrodynamics
7. Software Frameworks for Particle Dynamics
8. Unidirectional Coupling Particles and Fluid Flow

Introduction to Particle Dynamics

- Newton's equations of motion
- Discretization of the underlying ordinary differential equations using Euler and Verlet methods
- Discussion of the accuracy of Euler and Verlet
- Implementation of simple toy problem

Getting started:

- D.C. Rapaport. The Art of Molecular Dynamics Simulation
- M. Griebel, S Knapek, G Zumbusch. Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications

Molecular Dynamics

- Description of the problem
- Molecule representations: rigid molecules vs. internal degrees of freedom (and respective extension of equations of motion by rotations)
- Implementation for short-range systems: complexity considerations, Verlet lists and linked-cell method
- Example applications from process engineering, chemistry and polymer dynamics
- Restrictions and limitations of the method

Getting started:

- D.C. Rapaport. The Art of Molecular Dynamics Simulation
- M. Griebel, S Knapek, G Zumbusch. Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications

Parallelization and High-Performance Computing for Particle Systems

- Domain and force decomposition
- Parallelization for linked-cells and Verlet lists
- Load balancing approaches for heterogeneous particle systems/hardware
- Performance evaluation based on literature review
- SIMD, shared- and distributed-memory parallelism

Getting started:

- D.C. Rapaport. The Art of Molecular Dynamics Simulation
- M. Griebel, S Knapek, G Zumbusch. Numerical Simulation in Molecular Dynamics: Numerics, Algorithms, Parallelization, Applications
- B. Hess et al. GROMACS4: Algorithms for Highly Efficient, Load-Balanced, and Scalable Molecular Simulation
- W.M. Brown, et al. Implementing molecular dynamics on hybrid high performance computers – short range forces
- S. Seckler et al. Load Balancing for Molecular Dynamics Simulations on Heterogeneous Architectures

Adaptive Resolution Scheme

- From fine-grained molecular dynamics to coarse-grained particle represenations
- Changing degrees of freedom on the fly
- Features and drawbacks of AdResS
- Hamiltonian AdResS

Getting started:

- M. Praprotnik, L. Delle Site, K. Kremer. Adaptive resolution molecular-dynamics simulation: Changing the degrees of freedom on the fly
- R. Potestio, S. Fritsch, P. Espanol, R. Delgado-Buscalioni, K. Kremer, R. Everaers, D. Donadio. Hamiltonian Adaptive Resolution Simulation for Molecular Liquids
- K. Kreis, R. Potestio, K. Kremer, A.C. Fogarty. Adaptive Resolution Simulations with Self-Adjusting High-Resolution Regions

Long-Range Particle Interactions

- Discussion of short-range and long-range effects
- Approaches to long-range particle interactions: barnes-hut and fast multipole methods
- Application examples

Getting started:

- W. Eckhardt. Efficient HPC Implementations for Large-Scale Molecular Simulation in Process Engineering (Sections 2.5, 9 and references therein)
- R. Beatson, L. Greengard. A short course on fast multipole methods

Smoothed Particle Hydrodynamics

- Description of the method
- Application in astrophysics and fluid dynamics
- Restrictions and limitations of the method

Getting started:

- V. Springel. Smoothed Particle Hydrodynamics in Astrophysics
- P. Gonnet. Efficient and Scalable Algorithms for Smoothed Particle Hydrodynamics on Hybrid Shared/Distributed-Memory Architectures

Software Frameworks for Particle Dynamics

- Discussion and presentation of software packages, including (self-made) toy simulation setups
- ESPResSo, LAMMPS, GROMACS, NAMD, ls1 mardyn, GADGET, ...

Getting started: see websites of the respective software frameworks, user manuals/documentation, and related papers

Unidirectional Coupling of Particles and Fluid Flow

- Examples (respiration in human lungs, etc.)
- Mapping mesh-based quantities to particle descriptions
- Visualization: path line visualization, using, e.g., ParaView with own flow data

Getting started:

- M. Griebel, T. Dornseifer, T. Neunhoeffer. Numerical Simulation in Fluid Dynamics, Section Visualization Techniques
- T. Henn, G. Thäter, W. Dörfler, H. Nirschl, M.J. Krause. Parallel dilute particulate flow simulations in the human nasal cavity
- Paraview documentation and user manual

Algorithm for Topic Distribution

1. Every participant chooses favorite topic. If there is no overbooking: END
2. If two or more participants want the same topic: second round of choice for these participants
3. If there is still an issue: coin flip :-)
4. Until 11 April: e-mail to philipp.neumann@uni-hamburg.de, confirming your participation and topic choice

Important Dates

- First draft of presentation: due two weeks before presentation
- Final draft of presentation: due one week before presentation (minor adaptions are still OK)
- 10-page seminar paper: due end of the lecture period (16 July)
  $\rightarrow$ 2-3 iterations with supervisor are recommended, starting at least on 15 June
- Submissions via e-mail to philipp.neumann@uni-hamburg.de