Microfluidics & Nanofluidics

Band 5

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Dissipative Particle Dynamics

Simulation of Microfluidic Systems With Fluid Particle Methods on High Performance Computers

Shaker Verlag
Aachen 2009

Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at http://dnb.d-nb.de.

Zugl.: Freiburg, Univ., Diss., 2009

Printed in Germany.

ISBN 978-3-8322-8305-6
ISSN 1866-5411

Shaker Verlag GmbH • P.O. BOX 101818 • D-52018 Aachen
Phone: 0049/2407/9596-0 • Telefax: 0049/2407/9596-9
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This thesis proves that realistic problems in microfluidics can be solved with *Dissipative Particle Dynamics* (*DPD*) and in fact that this method can be used as a supplementary tool in an engineering design process of constructing microfluidic devices. This work is presented in two parts. *Part I* deals with the simulation approach of fluid particle methods, the setting of appropriate pressure boundary conditions and their application to a microfluidic problem with aggregating microspheres. In *Part II* the parallelization approach and its performance is presented, including new algorithms to handle large numbers of different species efficiently, or to optimize the load balancing in heterogeneous simulation problems. As *DPD* and its extensions leave room for interpretations, and many authors have adapted it in different contexts, first a literature review is given in the introduction Chapter 1.

Part I presents in Chapter 2 the theory behind *DPD* and introduces the basic equations that describe the dynamics of the *fluid particles*. Extensions to the original approach are explained that implement additional degrees of freedom to further improve the hydrodynamic description of fluids and colloidal suspensions. As a central part of this work, the *Quaternion* approach is introduced to describe the dynamics of arbitrarily shaped objects in an elegant and numerically efficient manner. Finally, the applied *Velocity-Verlet* based integration schemes for fluid particles and rigid objects are presented.

In Chapter 3, fluid properties and hydrodynamic behavior is discussed together with the application of appropriate pressure boundary conditions that are typically used in *Molecular Dynamics* (*MD*). The viscosity of the fluids is measured with *Lees-Edwards boundary conditions* for different model parameter such as repulsion, density or the random force. For pressure boundary conditions the *Reflecting Boundary* and the *Gravitational* methods are validated in detail.

In Chapter 4 it is shown that *DPD* can represent adequately the aggregation of 335 suspended polystyrene beads of diameter $d = 150\mu$m at a measured maximum *Reynolds number* of $\mathsf{Re} = 5.4$. Experiment and simulation are matched by a set of dimensionless numbers such as *Reynolds number*, *Peclet number*, *Mach number* as well as the drag coefficient for spherical objects. The *Peclet number* could be determined to $\mathsf{Pe} \approx 2300$, which is sufficiently large to neglect thermal motion of the spherical objects. The hydrodynamic flow field and hydrodynamic drag is validated against *CFD* simulation as well as analytical solutions and corresponds well within the relevant Re range of 0 to 10.

Part II presents in Chapter 5 the applied *Distributed Memory* parallelization strategy with *Domain Decomposition*, new simulation concepts and the structure of the parallelized program. The two new concepts of a *Multi-Species Identification* and *Master Object scheme* allow simplification of a general code design, especially if rigid objects are used. The *Multi-Species Identification scheme* encodes material definition parameters and indices of different moving objects into one single value and allows for an efficient realization of managing material properties in multiprocessor environments, independent of the complexity of the simulated system. The *Master Object* concept for *Quaternions* can handle any number of differently shaped objects just by defining so-called *Master Objects* and calculating only changes in orientation with respect to the initial configuration.

Finally, Chapter 6 shows the versatility of the developed code with tests on different platforms ranging from a low cost Opteron cluster with 12 CPUs up to a NEC Xeon cluster with 400 CPUs in comparison to a shared memory system. The developed code reaches a linear *Scale-up* of almost 70% on 64 CPUs, with approximately 100 million particles and of 74% with 1.5 million particles on 16 CPUs. The performance has been kept at an optimum level with a new *Time Dependent Load Balancing* suitable for fluid particle and rigid object simulations. As it is independent of a local density distribution it increases the performance in the considered test case by a factor of 15.