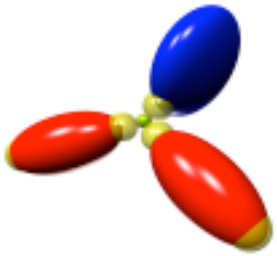
Simulations of hard bodies



Antonio Scala
SMC-ISC CNR-INFM Roma1 Italy

Cristiano De Michele
SOFT INFM-CNR and Dip. di Fisica - Univ. di Roma Italy

September 6, 2007

1 Workshop Details

1.1 Details

Timing
Number of days : 4
Start : 2007-04-16
end : 2007-04-19

Location of the activity
CECAM
46 allé e d'Italie
69007 Lyon
France

1.2 Description

No description provided

2 Requested Support

Simbioma

CECAM

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3 Participant List

Jeremy Schofield (jmschofi@chem.utoronto.ca)
Chemical Physics Theory Group, University of Toronto Canada

Wouter den Otter (w.k.denotter@utwente.nl)
University of Twente Netherlands

Thomas Voigtmann (tvoigtma@ph.ed.ac.uk)
Institute of Materials Physics in Space, German Aerospace Center (DLR) Germany

Chinmay Das (phycda@leeds.ac.uk)
Department of Physics and Astronomy,University of Leeds Great Britain

John H. Maddocks (John.Maddocks@epfl.ch)
EPFL, FSB-IMB Switzerland

Malvin H. Kalos (kalos1@llnl.gov)
Lawrence Livermore National Laboratory United States

Antonio Scala (antonio.scala@phys.uniroma1.it)
SMC-ISC CNR-INFM Roma1 Italy

Cristiano De Michele (cristiano.demichele@phys.uniroma1.it)
SOFT INFM-CNR and Dip. di Fisica - Univ. di Roma Italy

Galina Kalibaeva (Galina.Kalibaeva@roma1.infn.it)
Universita di Roma Italy

michele di pierro (michele.dipierro@roma1.infn.it)
Dip. Fisica La Sapienza Italy

4 Presentation List

Brownian dynamics simulations of liquid crystals under shear flow
Wouter den Otter
University of Twente, Netherlands
Abstract
An event-driven Brownian dynamics algorithm, in which hard particles diffuse freely from collision to collision, has been developed to simulate the dynamics of dense solutions of elongated rigid rods [1]. Using this code, we simulated the isotropic and nematic phases of rods with aspect ratios ranging from 10 to 60. The spinodal concentrations at the orientational ordering and disordering transitions were determined. The periodic collective orientational motions performed in a nematic phase under shear flow have been simulated for the first time [2,3]. We observed the director tracing out paths characterized as kayaking, wagging, flow-aligning or log-rolling, depending on the conditions of the simulation. The periods of these orbits follow a simple expression, independent of the type of the motion. Finally, the kayaking to wagging transition is shown to originate from a gradual loss of collectiveness.

References
[1] Y.G. Tao, W.K. den Otter, J.K.G. Dhont and W.J. Briels, J. Chem. Phys. 124 134906 (2006)

[2] Y.G. Tao, W.K. den Otter and W.J. Briels, Phys. Rev. Lett. 95, 237802 (2005)
[3] http://cbp.tnw.utwente.nl/Research/rods.html

Event-driven simulations of hard bodies
Cristiano De Michele
SOFT INFM-CNR and Dip. di Fisica - Univ. di Roma , Italy
Abstract
The technical details of a novel event-driven algorithm for simulating hard bodies (HB) will be illustrated. This new algorithm differently from previous ones relies on evaluation of distance between objects of arbitrary shape and - in order to optimize collision detection between elongated objects - on a new nearest-neighbour list based on oriented bounding boxes. The possibility of decorating hard bodies on their surface with spherical sites (sticky spots), that interact through an attractive step potential, will be also explained. Noticeably addition of sticky spots to HB offers many new interesting applications of this new code, and they will be discussed also shortly.
A first application of this new code was the study of the statics [1] and the dynamics [2] of hard ellipsoids (HE). Another application was the simulation of hard spheres decorated with sticky spots. Using such objects, two recently studied primitive models of network forming liquids - a primitive model for water [3] and for silica [4] - have been simulated and some results about their dynamics will be shown. Furthermore a mixture of hard ellipsoids of different size and elongation, decorated with sticky spots has proved to be a good model for a chemical gel, already investigated experimentally. Finally some work on biophysical systems is in progress, more specifically antibody-antigene interaction is being investigated, using a system of HE decorated with sticky spots, polydisperse in size and shape and some possible applications to proteins will be also discussed.

References
[1] C. De Michele and A. Scala and R. Schilling and F. Sciortino *Molecular correlation functions for uniaxial ellipsoids in the isotropic state*, J. Chem. Phys. **124** 104509 (2006)

[2] C. De Michele and R. Schilling and F. Sciortino *Dynamics of uniaxial hard ellipsoids*, In preparation (2007)

[3] C. De Michele and S. Gabrielli and P. Tartaglia and F. Sciortino *Dynamics in the Presence of Attractive Patchy Interactions*, J. Phys. Chem. **110** 8064-8079 (2006)

[4] C. De Michele and P. Tartaglia and F. Sciortino *Slow dynamics in a primitive tetrahedral network model*, J. Chem. Phys **125** 204710 (2006)

Event-Driven Simulations using Energy Discontinuities
Jeremy Schofield
Chemical Physics Theory Group, University of Toronto, Canada
Abstract
A scheme for performing event-driven, asynchronous simulations of hard bodies will be outlined that makes use of discretizations of a continuous potential and the exact solution of free motion of asymmetic bodies. The method is illustrated for rigid systems interacting via orientationally-dependent point potentials. Event-driven simulations will be contrasted with simulations based on elegant new symplectic integration schemes for rigid systems interacting by more conventional continuous potentials.

Event-Driven Stochastic Dynamics
Thomas Voigtmann
Institute of Materials Physics in Space, German Aerospace Center (DLR), Germany
Abstract
The simulation of interacting Brownian particles is an important tool in condensed matter and biophysics. To study the interplay of excluded-volume effects and stochastic motion, the hard-sphere system with Brownian dynamics (BD) is one of the most important reference systems for condensed-matter theories, especially at high densities. Yet, the simulation of stochastic differential equations (e.g., the Langevin equation) including the singular hard-sphere potential is not straightforward. In this talk, we will discuss how the event-driven (ED) approach for the simulation of hard-core potentials, and conventional stochastic dynamics algorithms can be merged to form an ED-BD approach to the simulation of Brownian hard spheres. This approach can be extended to include other singular interactions (e.g., the square-well system), and inertial effects.

First-Passage Algorithms for Brownian Motion
Malvin H. Kalos
Lawrence Livermore National Laboratory, United States

Abstract
We will review the mathematical basis for generating Green's functions for the diffusion equation based on first-passage decomposition, and some technical details of how these are used in efficient event-driven simulations of hard bodies. Possible generalizations will be discussed, along with issues for effective parallel algorithms.

References
Oppelstrup et al., Phys. Rev. Letts, 97, 230602 (2006)

Kalos, Lesesque, and Verlet, Phys. Rev., A9, 2178(1974)

Bortz, Kalos, and Lebowitz, J. Comput. Phys. 17, 10 (1975)

Martinez, Marian, Kalos, and Perlado, "Synchronous Parallel Kinetic Monte Carlo," in preparation, J. Comput. Phys.

Molecular dynamics of hard constrained systems
Galina Kalibaeva
Universita di Roma, Italy
Abstract
As soon as the study of macromolecules became available to numerical investigations, an always increasing requirement for faster algorithms to investigate the whole spectrum of the time scales involved in their dynamics developed. Polymer dynamics is one of the best known phenomena showing this wide range of time scales and for which there is a need for ever faster molecular dynamics methods. We want to represent a polymer by hard spheres linked by bond constraints (a free joint chain). The dynamics can be separated into collisions and a (free) propagation of the polymers in between them. It has been thought until recently that models involving hard spheres are incompatible with constraints, so that not many attempts to bridge the two approaches have been made so far. We demonstrate the possibility of including constraints in hard systems and apply it to a simple case of a dimer, where analytical solution is on hand and Lagrange multipliers remain constant during the propagation in between collisions. Then we extend the solution to more complex structures and observe that, starting from a trimer, the solution for the free propagation is no more analytical, because the Lagrange multipliers become time-dependent functions. Therefore, instead of an analytical solution, we developed two algorithms for polymer dynamics: finite time step algorithm based on Velocity Verlet, and a finite time predictor, which is a generalization of discontinuous molecular dynamics (DMD) for constrained hard spheres. The collision solution is solved taking into account the impulsive contribution from the constraints.

Molecular dynamics simulation of three dimensional crosses
Chinmay Das

Department of Physics and Astronomy,University of Leeds , Great Britain

Abstract

We consider a system of three dimensional “crosses”, particles that consist of three mutually perpendicular line segments of length L rigidly joined at the mid-points. The model has the structural properties of an ideal gas, yet the dynamic properties of a strong glass former. Because of zero volume of the line segments, they never overlap and a Monte Carlo or a traditional molecular dynamics with discrete time steps are not applicable for the present system and an event driven algorithm becomes necessary. A binary event tree structure, along with neighborlist based on overlap of spherocylinders around the line segments, leads to a fast algorithm which allows us to follow the dynamics of the model for a large number of collision events.

References

Ketel, Das, and Frenkel, PRL, 94, 135703 (2005).
Das, Ketel, and Frenkel, (to be communicated, 2007)

The Impetus-Striction formulation of Holonomically Constrained Lagrangian Dynamics

John H. Maddocks
EPFL, FSB-IMB, Switzerland

Abstract

In the presence of holonomic constraints there is considerable freedom in the choice of conjugate variable adopted to construct a Hamiltonian form of the dynamics. The impetus-striction formulation exploits this freedom to construct a Hamiltonian form of the dynamics in which the constraint appears as either one level set of an integral of the system, or as an exponentially attracting level set of the dynamics.

5 Program

Day 1: April 16 2007

Session : 1 Introduction
15:30 to 16:00 : Welcome

16:45 to 17:30 : Presentation
The Impetus-Striction formulation of Holonomically Constrained Lagrangian Dynamics
John H. Maddocks

17:30 to 17:45 : Coffee Break

17:45 to 18:30 : Discussion

Day 2: April 17 2007

Session : 2 Event Driven Molecular Dynamics
09:00 to 09:45 : Presentation
Molecular dynamics of hard constrained systems
Galina Kalibaeva

09:45 to 10:30 : Presentation
Molecular dynamics simulation of three dimensional crosses
Chinmay Das

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation
Event-Driven Simulations using Energy Discontinuities
Jeremy Schofield

11:45 to 12:30 : Presentation
Event-driven simulations of hard bodies
Cristiano De Michele

15:30 to 18:30 : Discussion

Day 3: April 18 2007

Session : 3 Event Driven Brownian Dynamics
09:00 to 09:45 : Presentation
First-Passage Algorithms for Brownian Motion

Malvin H. Kalos

09:45 to 10:30 : Presentation
Brownian dynamics simulations of liquid crystals under shear flow
Wouter den Otter

10:30 to 11:00 : Coffee Break

11:00 to 11:45 : Presentation
Event-Driven Stochastic Dynamics
Thomas Voigtmann

15:30 to 18:30 : Discussion

Day 4: April 19 2007

Session : 4 Closing
09:15 to 09:30 : Closing word

09:30 to 12:30 : Discussion

6 Organizer's report

6.1 Conclusions.

The workshop has brought together a small but focused group of scientists from different fields and countries, who have highly appreciated and exploited the possibility, after the talks in the mornings, of having long and clarifying exchanges of ideas during the afternoons.

We have shown how to perform event-driven Langevin-dynamics simulations for hard bodies. This is extremely relevant for the blossoming field of condensed soft-matter, where many-body systems have typically length scales beyond the atomic and the molecular so that pair interactions can be well described by hard interactions.

We have shown and analysed some successful approaches to the simulation of non-spherical hard-bodies. Following such new techniques, it should be now possible to study many-bodies system taking account of the detailed shape of its constituents.

We have explored some possibilities for taking into account holonomic constraints in hard-body systems. A new possibility for simulating in an event-driven fashion polymeric chains has emerged and open an exciting field to explore, whose success could contribute in having faster simulations of proteins and polymers.

It is even more clear now that event-driven dynamics, apart their interest for simplified model systems with discontinuous potentials, represent an opportunity of performing faster simulations for colloidal, liquid crystals and granular systems and of performing faster equilibration for atomic, molecular and polymeric systems.

6.2 Recommendations.

The methods for simulating hard-bodies taking into account shape, constraints and for implementing stochastic dynamics require techniques and methods that go beyond the classical standard Molecular or Brownian Dynamics codes for continuous potentials. The first step to allow the wide and interdisciplinary scientific community interested in exploring hard-systems is to develop libraries for building easily simulation codes for hard systems. In fact, while for continuous systems there are excellent books, reviews and even efficient all-purpose codes, in the

case of hard-body systems there is a strong initial ”coding barrier” to be overcomed before being able to address scientific questions. A final goal would be to have also for hard systems an efficient all-purpose code. We hope that the developing of such libraries and of a general code will be supported by ESF; we observe that such aims are in line with the 2007 ESF Forward Look European Computational Science: the Lincei Initiative ”from computer to scientific excellence”.

In order to have realistic simulations for a wider range of soft-condensed matter systems, it is necessary to include the effects of hydrodynamics in event-driven simulations of hard-bodies systems. The very preliminary discussions initiated in the workshop should be pursued until the development of an effective code.

Algorithms developed in the fields of robotics, virtual reality, game design and computational geometry share a naturally strong overlap with what is used and what is necessary for the simulation of hard-bodies systems. It is necessary to investigate the literature of such fields and develop relations with scientists of such communities to avoid re-discoveries and speeding up the process of developing an uniform paradigm for simulating hard objects with complex shapes and constraints.

The workshop has suffered from a lack of participation from the granular community; this issue must be corrected developing stronger contacts with such community from the participants of the workshop. It is hopeful that a new, wider workshop will subsume the results and the improvements reached at the end of a two-three years period. It is necessary a wider interdisciplinary participation, especially form the fields of granular simulations and computer science.

The new simulations of the dynamics of hard-bodies systems are still in their infancy and require the newborn community to continue existing and grow; we hope to reach such objective in the next two-three years ESF will support periodic visits among the people who have contributed to the workshop and also to all the other people that have expressed their interest being unable to participate.

7 Key references

[1] De∼Michele, C. and Scala, A. and Schilling, R. and Sciortino, F. *Molecular correlation functions for uniaxial ellipsoids in the isotropicstate*, J. Chem. Phys. **124** 104509 (2006)

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[3] van∼Zon, R. and Schofield, J. *Numerical implementation of the exact dynamics of free rigid bodies*, cond-mat/0607529 ()

[4] Scala, A. and De∼Michele, C. and Voigtmann, Th. *Event-Driven Brownian Dynamics for Hard Spheres*, cond-mat/0607040 , submitted to J. Chem. Phys. ()

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