

## FINAL REPORT: CCP5 PROJECT ACTIVITIES 2002 - 2006

### The DL\_MESO Mesoscale Simulation Project.

The main focus of the Mesoscale project was to develop the simulation package DL\_MESO, which was entirely written by the appointed PDRA Dr R.S. Qin at Daresbury, with some assistance and advice from Dr. W. Smith (Daresbury). The package provides an integrated approach to mesoscale simulation. It offers the user the ability to set up a model system and select the preferred method for performing the simulation. The options are Lattice Boltzmann (LB) methods and Dissipative Particle Dynamics (DPD). A modern, object oriented, approach was adopted for writing DL\_MESO. The language used for the simulation code was C++ and the graphical user interface (GUI) was written in Java. By means of the GUI a system may be constructed, simulated, and then analysed. The package is now available, with documentation, to the academic community and has 70 registered users. 2 commercial companies have also obtained the software.

The DL\_MESO website is at [http://www.ccp5.ac.uk/dlmeso/DL\\_MESO.html](http://www.ccp5.ac.uk/dlmeso/DL_MESO.html)

Dr. Qin also undertook a number of scientific studies and collaborations. He collaborated with Prof. Coveney's group at UCL to adapt the DL\_MESO code for GRID use using WEDS software. A collaboration with Dr Emerson's group at Daresbury (CCP12) studied rare gas flow in microchannels. He collaborated with Prof. K.H. Luo at Southampton University, assisting PhD students to start work on simulating fuel cells. With Dr Shao at Brunel University he worked on semi solid processing and nucleation. In his own studies he investigated phase separation in binary fluid mixtures, the effect of flow on the kinetics of the solid-liquid interface, liquid-gas phase transitions in non-equilibrium fluids, the effect of flow on nucleation rate for binary fluids, the flow of particles and fibres and the effect of electropulsing on cell membranes. 5 publications have resulted from this work [1-5].

The Mesoscale project was managed by a steering committee under the chairmanship of Prof. D. Heyes (Surrey). Other members of the committee included J. Yeomans (Oxford), P.V. Coveney (London), C. Care (Sheffield Hallam), I Halliday (Sheffield Hallam), D. Emerson (Daresbury, for CCP12), A. Ferrante (Unilever), J. Harding (Sheffield), P.B. Warren (Unilever), W. Smith and R. Qin. Meetings of the steering group were held on 16/12/02, 27/6/03, 2/10/03, 23/1/04, 22/4/04, 18/2/05, 25/1/06.

The Mesoscale project also organised a series of workshops:

1. *Mesoscale modelling of Liquids. University of Oxford 20-21 March 2006.*
2. *Challenges in Mesoscale Models for Liquids: Simulation and Theory: University of Surrey 17 October 2005.*
3. *Particle Methods in Mesoscale Simulation: Daresbury Laboratory. 21 March 2005.*
4. *Developments and Applications of the Lattice Boltzmann Technique: Sheffield Hallam University 1 November 2004.*
5. *Mesoscale Modelling of Liquids: University of Surrey 19 April 2004.*
6. *CCP5 Lattice Boltzmann Workshop: Daresbury Laboratory 1 October 2003.*

The purpose of these workshops was to foster a mesoscale research community in the UK, to provide opportunity to review methodology and report progress in developing the DL\_MESO package. Dr Qin presented 6 talks at these workshops. In addition he presented an advanced course of four lectures on Mesoscale Simulation at the CCP5 Summer School in July 2005 and talks at the International Conference for Mesoscopic Methods in Engineering and Science, July 26 - 29, 2004, Brunswick, Germany and at Simulation and Modelling of Colloidal Systems, September 15 - 16, 2004, Sheffield, UK.

The continued development of DL\_MESO beyond the current grant period is the subject of a grant proposal submitted to EPSRC by W. Smith, R. Qin and D. Heyes in January 2006.

### The Work of the Daresbury Support Staff

**Dr W. Smith** has been associated with CCP5 since 1980 and **Dr M. Leslie** since 1983. Both are allocated 50% to the project and provide technical, scientific and administrative support.

## **Technical Support**

**Dr. Smith's** primary role in the current grant has been the development of the general- purpose simulation code known as DL\_POLY [6]. This has included: (i) conversion of the code to modular F90 form (ii) development of symplectic integration algorithms; (iii) incorporation of the relaxed shell model for polarisation; (iv) incorporation of many body Tersoff potential; (v) production of documentation; (vi) supervising development work on DL\_POLY\_3 (the domain decomposition version of DL\_POLY) (vii) adapting the code for HPCx; (viii) user support and advice; (ix) development of analysis tools; (x) maintenance of benchmarking suite; (xi) user registration and licensing. He has also supervised the development of the flagship code DL\_MESO by R. Qin, and assisted in a number of scientific projects.

**Dr Leslie's** role is to support users of the Static Simulation Programs and DMAREL (a static lattice, energy minimisation program for calculating the properties of crystalline materials and deriving model potentials) and to develop the DL\_MULTI (distributed multipole molecular dynamics) program and associated analysis software and support users exploiting this code in studies of molecular crystals.

## **Scientific support:**

**Dr Smith** has supported the following collaborations:

*Computer simulation of powders* with C. Yong (Daresbury) and K. Kendall (Birmingham) to determine the properties of granular materials from first principles. EPSRC project ended 2004.

1. *Passivation of Gold Nanoclusters in Supercritical Solvents* with M. Lal (Liverpool) and M Plummer (Daresbury).
2. *Ionic Diffusion in Grain Boundaries* with J. Harding (UCL/Sheffield), N. Allan (Bristol), J. Purton (Daresbury) and D. Harris (UCL).
3. *Radiation Damage Studies of Zirconia* with M. Dove, K. Trachenko (Cambridge) and I. Todorov (Daresbury).

**Dr Leslie** has supported the following collaborations:

1. *Studies of molecular crystal morphologies* with S. Price (UCL).
2. *Studies of molecular liquids* with P. Popelier (Manchester).

## **Administrative support.**

Both **Dr Smith** and **Dr Leslie** are members of the Executive Committee (Dr Leslie acting as Secretary). They support workshops and the Annual Meeting (Dr Leslie providing the delegate handbook) and help to organise visits by overseas speakers. **Dr Smith** supports the CCP5 Summer Schools, maintains the CCP5 program library and DL\_POLY website and manages the CCP5 funds held at Daresbury. **Dr Leslie** is the manager of the CCP5 infoweb, maintains the CCP5 website and administers the mailing list and email distribution list.

## **The Executive Committee**

The CCP5 Executive Committee consists of a chairman, six academic researchers and two Daresbury staff. The following people have served on the committee during the current grant: Prof. P.M. Rodger (current Chairman, Warwick), Prof. J.H Harding (past Chairman, Sheffield), Dr. D.W. Lewis (UCL), Dr. D. Sayle (Cranfield), Dr. N. Deleeuw (UCL/Birkbeck), Dr D. Duffy (UCL), Dr. M.S. Islam (Surrey), Dr. K. Travis (Bradford), Dr R.A. Jackson (Keele), Dr D. Willock (Cardiff), Dr M. Wilson (Durham), Dr. M. Leslie (Daresbury) and Dr. W. Smith (Daresbury). In the grant period 9 Executive Committee meetings took place: 9/1/03, 1/5/03, 11/9/03, 19/1/04, 30/3/04, 7/1/05, 18/5/05, 21/9/05, 11/1/06.

## **Meetings and Workshops**

The CCP5 Annual General Meeting attracts an international participation. The meeting is also the occasion of the CCP5 Forum where wider project issues (e.g. future directions) are discussed. The AGMs are always well attended particularly by research students and researchers new to the field.

**The AGMs organised in the 2002-2006 grant period are as follows.**

**Computational Techniques and Applications to Materials Modelling:** University of Keele 30 August – 2 September 2005. Speakers included D. Rapaport (Bar Ilan), M.J. Gillan (UCL), N. Quirke (Imperial), D.W.

Lewis (UCL), J. Harding (Sheffield), P.M. Rodger (Warwick). Topics included first principles methods, hydrodynamics and molecular dynamics, hydrated zeolites and nanoflows.

***New Perspectives in Modelling and Simulation: Theory and Applications:*** University of Sheffield 1 - 4 September 2004. Speakers included A. Fuchs (Paris), D. Cleaver (Sheffield), F. Bresme (Imperial), S. Owens (BNFL), C. Dettmann (Bristol), C. Care (SHU), D. Brown (Savoie), G. Jackson (Imperial). Topics included nanoporous materials, liquid crystals, molecular chaos, nanocomposites, vitrification, solvation processes and polymers.

***Simulation of Materials -Techniques and Applications:*** University of Cardiff 8 – 11 September 2003. Speakers included T Darden (NIH), F. Mueller-Plathe (Bremen), A Cormack (NYSU), G Pacchioni (Milano-Bicocca), S. Price (London), P.M. Rodger (Warwick), P. Sherwood (DL), G Kneller (CNRS), R.W. Grimes (Imperial), G. Watson (Dublin). Topics included methods of calculating electrostatics, polymer coarse-graining models, silicate glasses, electronic properties of point defects, crystal polymorphism, crystal nucleation and inhibition, QM/MM methods, multiscale relaxational phenomena in liquids, compositional optimisation and density functional theory of surfaces.

***Advances in Simulations of Molecules and Materials:*** University of Durham 9 – 12 September 2002. Speakers included G. Seder (MIT), S Clark (Durham), J Clarke (UMIST), C Zannoni (Bologna), F. Schmid (Bielefeld), A. Mulholland (Bristol), J. Essex (Southampton), N. Allen (Bristol). Topics included first principles structure prediction, non local exchange functions, polymers, liquid crystals, enzyme catalysed reactions, drug design and solid solutions.

**The workshops organised were:**

***CCP5 organised 6 Mesoscale Simulation workshops (see section A1)***

***Proton Conduction in Diverse Media:*** Cambridge 11 – 12 April 2005. (Part sponsored with EPSRC). The purpose of this meeting was to bring together researchers working on a wide range of materials where conduction of protons is an important phenomenon, for example fuel cell membranes, biological membranes and inorganic zeolites.

***Symposium in honour of Professor Julian Clarke to mark his retirement.*** (UMIST) October 2004. The invited speakers were: Austen Angell (Arizona), Les Woodcock (UMIST), David Heyes (Surrey), Chin Yong (Daresbury), Doros Theodorou (Athens), Karl Travis (Sheffield) and Wouter den Otter (Twente, the Netherlands).

***Hydrogen in Oxides:*** 21 April 2004 The Royal Institution. Organised by the Materials and Characterisation Group of the Institute of Physics in association with the ISIS Muon Group, Rutherford Appleton Laboratory, the Materials Research Centre, University College London, the EPSRC Nanotechnology Network "Theory and Experiment in Extreme Nanotechnology" and CCP5. This was a one-day meeting which aimed to bring together theorists and experimentalists concerned with all aspects of hydrogen in oxides, including the newly discovered possibility of electronic conduction and other issues of practical concern to oxide electronic materials and gate dielectrics, as well as protonic conduction, hydrogen mobility, fuel cells, nano-porous materials and mineralogy.

***Complex Inorganic Materials: Crystal Growth, Inhibition and Dissolution - Linking Experiment and Theory:*** 23rd - 24th October 2003, University of Reading. The workshop covered the field of dissolution, growth and inhibition of inorganic solids, often containing complex molecular ionic species such as carbonates, sulphates, phosphates or nitrates.

***Modelling of Materials: Atomistic and Ab Initio Approaches:*** Oxford 9 – 10 April 2003. The Theoretical Chemistry Group of the Royal Society of Chemistry and CCP5 co-organised this meeting. The meeting, was concerned with developments in methodology and algorithms for atomistic and ab initio simulations, as well as their applications. The following invited speakers attended the meeting: Neil Allan (Bristol), Emilio Artacho (Cambridge), Christian Elsaesser (Freiburg), Steve Parker (Bath), David Pettifor (Oxford), Joost VandeVondele (Zurich) and Mark Wilson (UCL)

***Joint CCP3/CCP5 Workshop on Nanoscale Modelling:*** Cambridge 6 – 7 January 2003. CCP3 and CCP5 (with support from the IRC in Nanotechnology, the EPSRC Network on Theory and Experiment in Extreme Nanotechnology, and the Thin Films and Surfaces Group of the Institute of Physics) organized a joint workshop on the modelling and simulation of nanostructures. Invited speakers included: Malcom Green (Oxford), Mike Payne (Cambridge), Alan Windle (Cambridge), Mads Brandbyge (Lyngby), Paulette Clancy (Cornell), Merfyn Miles (Bristol), Richard Palmer (Birmingham), Tchavdar Todorov (QUB), Richard Friend (Cambridge)

**Accelerating dynamical simulations March 2004.** A meeting held jointly with SIMU organised by M.P. Allen and G. Kneller.

**CCP5 sponsored 8 regional meetings** providing postgraduate students with an opportunity to present talks to their peers and discuss scientific issues in a friendly atmosphere.

- *Northern Atomistic Simulation Group (NASG) Meeting #1.* Daresbury Laboratory 5 January 2005.
- *Northern Atomistic Simulation Group (NASG) Meeting #2.* Sheffield University 5 December 2005.
- *South West Computational Chemists (SWCC) Meeting #1.* Bristol University September 2002.
- *South West Computational Chemists (SWCC) Meeting #2.* Cardiff University September 2003.
- *South West Computational Chemists (SWCC) Meeting #3.* University of Bath October 2004.
- *South West Computational Chemists (SWCC) Meeting #4.* Southampton University October 2005.
- *London Atomistic Simulation Group (LASG) Meeting. #2* Imperial College London, July 2003.
- *London Atomistic Simulation Group (LASG) Meeting#1* University College London June 2002.

**CCP5 sponsored 3 RSC Industrial Molecular Modelling Group "Young Materials Modellers" Forums.** These events gave young Ph.D. students an opportunity to present their work to an audience including industrialists and academics.

- *RSC MMG "Young Materials Modellers" Forum* May 2003 (Daresbury).
- *RSC-MMG "Young Materials Modellers" Forum* September 2005 (Oxford)
- *RSC-MMG "Young Materials Modellers" Forum* May 2004 (Daresbury)

## Education in Simulation Methods

**The Methods in Molecular Simulation Summer Schools** are run annually by CCP5 under sponsorship from the European Commission, under the Marie Curie Actions programme (from 2004), for a target audience of 60 or more postgraduate students. EPSRC funding was used to sponsor the 2002 and 2003 schools and also to sponsor extra UK students to attend the School beyond the quotas permitted by EU rules. The School lasts nine days and introduces the fundamentals of molecular simulation through an intensive series of lectures and practical sessions involving real problem solving exercises in applied computational science. The first week is devoted to basic material every student needs to know, followed by two days of specialised, advanced courses on scientific areas of high current interest. Research plenary lectures are provided by internationally leading speakers. The attendance is international. The Schools are strongly supported by the simulation community, both in the United Kingdom and overseas, and receive enthusiastic assistance from speakers from all countries. For the period 2002-2006 the Summer CCP5 sponsored and organised two Summer Schools at King's College London in 2002 and 2003 and two at Cardiff University in 2004 and 2005. The accumulated attendance at these workshops was 280 students. The 2006 School was also held at Cardiff and 70 students were registered.

The CCP5 Summer School is managed by a working group consisting of: Prof. J. Harding (Sheffield), Dr. J. Anwar (Bradford), Dr. K. Travis (Sheffield), Dr K. Refson (RAL), Dr W. Smith (DL), Dr. P. Camp (Edinburgh) and Dr P. Lindan (Canterbury). The working group met on 14 occasions: 29/10/02, 28/2/03, 15/5/03, 14/11/03, 4/2/04, 29/4/04, 22/9/04, 12/11/04, 7/1/05, 18/5/05, 14/9/05, 24/11/05, 27/1/06, 26/5/06.

**Other Training Events:** Training events have been organised for the use of the DL\_POLY simulation code, often in collaboration with EPCC and other computer centres. In these sessions, a small number of students (10~20) were given hands-on training in the use of the DL\_POLY code: 3/4/03 (DL), 10/2/03 (EPCC), 18/6/04 (RI), 16-20/8/04 (Oak Ridge), 25/10/04 (EPCC), 27/4/95 (DL), 15/9/05 (RAL).

## Visitor's Programme

CCP5 seeks to strengthen links between UK simulation scientists and colleagues overseas. An important aspect of this is the frequent invitation of overseas experts to the UK to visit and lecture at several UK Universities. As well as providing grounds for future collaborations, the programme helps to promulgate new and important methods. The invited speakers in the grant period were:

**Prof. Francesc Illas** (University of Barcelona) April 2006. Professor Illas is an expert in the application of a range of quantum chemistry methods to elucidate properties of magnetic materials and to investigate surface structures/properties and catalytic processes.

**Professor Dennis Rapaport** (Bar-Ilan University, Israel. August-September 2005) Prof. Rapaport visited Daresbury, Keele, Warwick, The Royal Institution and Imperial College and gave 5 seminars on subjects ranging from folding polymer chains, hydrodynamic instability, emergent behaviour and self assembly of virus capsules.

**Professor Peter Cummings** (Vanderbilt University and Oak Ridge. May-June 2005) Prof Cummings visited Imperial College, Guildford, Warwick, Daresbury and Sheffield. He gave 5 seminars on computational science, theoretical nanoscience and water and aqueous solutions at interfaces.

**Dr. J Shelley** (Schroedinger Inc., Portland. October – November 2004). Dr Shelley visited Oxford, King's College London, Cambridge and Daresbury. He gave 4 seminars on coarse graining methods, membranes and structured fluids.

**Professor P. Kusalik (Dalhousie, May 2003)**. Prof Kusalik visited Warwick, Belfast, London and Rutherford Laboratory and gave 4 seminars on crystallization and crystal growth.

**Professor S. Glotzer (Michigan, November 2002)**. Prof. Glotzer visited Oxford, Cambridge and Warwick and gave 3 seminars on the nanostructure of supercooled liquids.

**Professor John Kieffer (Michigan, November 2002)**. Prof. Kieffer visited Oxford, Cambridge and Warwick and gave 3 seminars on nanostructure assembly in hybrid polymer/inorganic systems and structural transformations in crystalline and amorphous inorganic materials.

**Professor Charusita Chakravarty** (Indian Institute of Technology-Delhi) May 2004. Her research interests include developing efficient path integral simulation methods for atomic and molecular systems and energy landscape approaches to understand phase transitions and dynamics of classical liquids and clusters. She gave seminars at Imperial College London, University of Cambridge and Daresbury Laboratory as well as attending the Symposium on Atomistic Simulation at Queen's University Belfast to mark the retirement of Professor Ruth Lynden-Bell.

**Dr Blas. Pedro. Uberuaga** ((Los Alamos National Laboratory) July 2004. Dr Uberuaga has research interests in defect diffusion in Plutonium, long-time annealing of radiation damage in ceramics, mechanics of carbon nanotubes, first-principles hyperdynamics and bulk silicon defect diffusion mechanisms. He gave talks at Loughborough University and Reading University and also visited Imperial College.

## Sponsored Collaborations

The purpose of this sponsorship is to provide a little travel money to help initiate new collaborations between research groups, with the objective of encouraging grant applications in the molecular simulation area. The following collaborations were sponsored in the grant period.

Jamshed Anwar, (King's College London), Ruslan Davidchack (University of Leicester), "*Calculation of the solid-liquid interfacial free energy of a water model*".

Dr Saiful Islam, (University of Surrey), Dr M Grazia Francesconi, (University of Hull), "*Computational studies of oxyfluoride superconductors*".

Dean C. Sayle, (Cranfield University), Stephen C. Parker, (University of Bath), "*Modelling the Structure and Ionic Conductivity of Nanoparticles and Thin Films*".

Robin Westacott, (Heriot-Watt University), Dr Mark Rodger, (University of Warwick), "*Phase transitions and thermodynamic stability of phases of solid water, including ices and gas hydrates*".

C Dettmann, (University of Bristol,) A. Samoletov, (University of Dundee), "*Ideas in thermostatted dynamics*".

David J Cooke (University of Cambridge), Stephen C Parker (University of Bath), "*To extend our previous work to consider the effect of salt solutions over a far greater range of concentrations and also to use the same methodology to consider other minerals (principally ZnO and TiO<sub>2</sub>) and the effect the salt solution has on mineral growth and dissolution*".

D.C. Sayle (RMCS, Cranfield Uni.), G.W. Watson, (Trinity College, Dublin), "*To develop a simulated amorphisation and recrystallisation methodology to explore structural features that evolve within a supported material*".

## PERFORMANCE STATISTICS

**Membership List:** CCP5 currently has 992 members. 294 are in the UK, 289 in other European countries and 409 elsewhere. Registration is by electronic submission of a WWW form completed by the new member. In 2004 there were 102 new members, 95 members were deleted from the list and 29 changed email address. The membership list is used to advertise CCP5 activities by Email to CCP5 members. We also publicise third party meetings in the area of computer simulation of condensed matter. We advertise job vacancies for CCP5 members in our field of activity. These are usually post-doctoral positions in the UK and Europe, and UK studentships.

**Website and ftp server** The website publicizes CCP5 activities. It also contains links to the archive of the program library and electronic newsletters. There are 1200 visits per month to the main entry page and 5000 visits per month summed over all pages. The summary page for the program library attracts 500 visits per month, with the meetings, links, newsletter and DL\_POLY pages between 100-200. There are 500 downloads per month from the ftp server. 300 of these are program library files and 200 are from the newsletter archive. There are 400 downloads per month of the files from the textbook *Computer simulation of liquids* (Allen and Tildesley) Between 80 and 120 people per month download the DL\_POLY manuals and licences. The website now has an infoweb area which has replaced the newsletter.

**DL\_POLY:** There are 673 existing DL\_POLY licences, as follows: UK (126), Continental Europe (185) and the rest of the world (362). There are 910 users on the DL\_POLY news mailing list, through which they are kept up-to-date about software developments. Since its creation in April 2005 445 entries have been posted on the DL\_POLY online forum.

## Publications

- [1] R.S. Qin, “*Mesosopic interparticle potentials in the lattice Boltzmann equation for multiphase fluids*”, Phys. Rev. E. Vol 73 066703 (2006).
- [2] R.S. Qin and Y.H. Zhang, “*Lattice Boltzmann study of the effect of stirring on the migration rate of curved interface in binary slurries*”, Computers & Fluids, Vol 35/8-9 pp929-933 (2006).
- [3] Y.H. Zhang, R.S. Qin and D.R. Emerson, “*Lattice Boltzmann simulation of rarefied gas flows in microchannels*”, Physical Review E Vol. 71, 047702, (2005).
- [4] Y.H. Zhang, R.S. Qin Y.H. Zhang, R.W. Barber and D.R. Emerson, “*Lattice Boltzmann simulation of continuum and rarefied gas flows through microchannels*”, J Statistical Physics, Vol 121, pp257-267, (2005).
- [5] D.M. Heyes, J.B. Baxter, U. Tuzun and R.S. Qin, “*Discrete-element method simulation: from micro to macro scales*”, Philosophical Transactions of the Royal Society London A , Vol. 362, pp1853-1865, (2004).
- [6] W. Smith, C.W. Yong and P.M. Rodger, “*DL\_POLY: Application to Molecular Simulation*”, Molecular Simulation, **28** (2002) 385.
- [7] E.Mocaco, K.H. Luo and R.S.Qin, “*A study of micromixing enhancement by optimization of the obstacles layout in a T-shaped micromixer using the lattice Boltzmann method*”, submitted to the conference of micro and nanoscale flows: Advancing the engineering science and design. The proceeding will be published in IMechE.
- [8] R. Machado, K.H. Luo and R.S. Qin, “*Three-dimensional lattice Boltzmann simulation of microreaction in porous media*”, submitted to the conference of micro and nanoscale flows: Advancing the engineering science and design. The proceeding will be published in IMechE.
- [9] I. Bush, W. Smith and I.T. Todorov, “*A DAFT DL\_POLY Implementation of the Smoothed Particle Mesh Ewald Sum*”, Comput. Phys. Commun. Accepted 2006.
- [10] W. Smith, I. T. Todorov and M.Leslie, “*The DL\_POLY molecular dynamics package*”, Zeitschrift fur Kristallographie (Computational Crystallography), **220** (5-6), (2005)
- [11] I. T. Todorov, W. Smith, K. Trachenko and M.T. Dove, “*DL\_POLY\_3: Science on a Grand Scale via Massively Parallelised Molecular Dynamics Simulations*”, HPCx News, **6**, 12, (2005).
- [12] Ilian T. Todorov, William Smith, Kostya Trachenko and Martin T. Dove, “*DL\_POLY\_3: New Dimensions in Molecular Dynamics Simulations via Massive Parallelism*”, J. Mater. Chem. (2006) DOI: 10.1039/b517931a
- [13] I.T. Todorov and W. Smith, “*DL\_POLY\_3: the CCP5 national UK code for molecular dynamics simulations*”, Phil Trans. R. Soc. London A **362** (2004) 1.