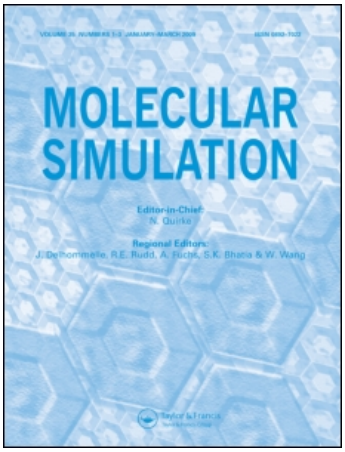


Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

CECAM Workshop: 'Dissipative particle dynamics: addressing deficiencies and establishing new frontiers' (16-18 July 2008, Lausanne, Switzerland)

John K. Brennan[a]; Martin Lísal[b]
[a] US Army Research Laboratory, Weapons and Materials Research Directorate, Aberdeen Proving Ground, MD, USA [b] E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals of the ASCR, Ústí nad Labem, Czech Republic

To cite this Article Brennan, John K. and Lísal, Martin(2009) 'CECAM Workshop: 'Dissipative particle dynamics: addressing deficiencies and establishing new frontiers' (16-18 July 2008, Lausanne, Switzerland)', Molecular Simulation, 35: 9, 766 — 769
To link to this Article: DOI: 10.1080/08927020902902783
URL: http://dx.doi.org/10.1080/08927020902902783

Molecular Simulation
Vol. 35, No. 9, August 2009, 766–769

Taylor & Francis
Taylor & Francis Group

REPORT

CECAM Workshop: 'Dissipative particle dynamics: addressing deficiencies and establishing new frontiers' (16–18 July 2008, Lausanne, Switzerland)

John K. Brennan[a]* and Martin Lísal[b]

[a]*US Army Research Laboratory, Weapons and Materials Research Directorate, Aberdeen Proving Ground, MD 21005-5066, USA;* [b]*E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals of the ASCR, v. v. i., 165 02 Prague 6-Suchdol, Czech Republic and Department of Physics, Faculty of Science, J.E. Purkinje University, 400 96 Ústí nad Labem, Czech Republic*

(*Received 4 March 2009; final version received 17 March 2009*)

In this report, we summarise highlights of a workshop sponsored by the Centre Européen de Calcul Atomique et Moléculaire on the dissipative particle dynamics method (DPD) held during 16–18 July 2008, at the Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland. We present our motivation for organising the workshop, followed by a description of the technical program, and finally a summary of a group discussion on future directions for the DPD method is given.

Keywords: mesoscale; simulation; dissipative particle dynamics

1. Introduction

The Centre Européen de Calcul Atomique et Moléculaire (CECAM) has more than a decade's tradition of sponsoring short-duration, intimate workshops on modelling and simulation. Workshops can be focused on a specific methodology of wide interest, or a particular field of science that has benefited from simulation and modelling. An aim of CECAM workshops is to provide an effective forum for establishing personal contacts and for ample exchange of ideas, often with an emphasis on discussion rather than on formal presentations. The world's leading researchers in the field are often active participants in CECAM workshops and tutorials.

A workshop sponsored by CECAM on the dissipative particle dynamics method (DPD) was held during 16–18 July 2008, at CECAM's new headquarters located in the campus of the Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland. The location, on the shores of Lake Léman (Lake Geneva), provided a picturesque backdrop to three days of excellent presentations and posters on the DPD method. The workshop was attended by 47 scientists from 19 different countries in Europe, Asia, North and South America. A majority of the attendees formally participated in the workshop, with 35 of the 47 participants presenting either a talk or a poster. The workshop was co-organised by John K. Brennan of the US Army Research Laboratory (APG, MD, USA) and Martin Lísal of the Academy of Sciences of the Czech Republic (Prague) and J.E. Purkinje University (Ústí nad Labem).

In this report, we briefly summarise some of the highlights of the meeting. We begin by presenting our motivation for organising the workshop, followed by a description of the technical program, and finally a summary of the group discussion on future directions for the DPD method is given.

2. Motivation

Since its development a little over 15 years ago, DPD [1,2] has become a robust tool for the study of soft condensed matter including polymer melts, blends and composites, surfactants and colloids. DPD allows for simulation studies at length and time scales that are inaccessible using molecular-level methods, the reasons for which are twofold. First, larger length scales can be simulated since the internal degrees-of-freedom of the molecules that a DPD particle is intended to represent are included in an averaged way or effectively ignored. Secondly, the weakly-repulsive particle interactions lend themselves to stable integrations of the equations of motion at longer time steps.

The fundamentals of the DPD method are now fairly well established [3–7], as are the technical subtleties [8,9] and some coarse-grain parameterisation techniques, with improvements consistently being introduced, e.g. [10]. Moreover, the similarities between the molecular dynamics and the DPD methods make it a rather simple method to implement since the methods share a common

*Corresponding author. Email: jbrennan@arl.army.mil

ISSN 0892-7022 print/ISSN 1029-0435 online

DOI: 10.1080/08927020902902783
http://www.informaworld.com

Picture of Lake Léman from the shores of Ouchy.

framework and many of the same computational *tricks-of-the-trade* can be utilised. Extensions of the DPD method which impose energy conservation have also been introduced allowing for heat as well as momentum exchange between particles [11,12]. All of these factors have led to a plethora of DPD simulation studies that have provided insight into a variety of phenomena that occurs at the mesoscale, though typically for polymer systems. However, DPD is beginning to be applied in other areas such as biophysics, e.g. the simulation of biomembranes and lipid bilayers. Furthermore, it is expected that DPD will play an ever-increasing role in multiscale modelling approaches through bridging of the atomistic and continuum scales. In such approaches, atomistic simulations are performed to build the DPD models, followed by DPD simulations that provide the necessary input to the continuum codes. Implementations of such approaches can circumvent assumptions in the continuum codes since the mesoscale simulations can provide more accurate estimates of the thermodynamic state within the localised regions compared to a constitutive equation.

However, further work is required to continue to establish a viable foundation for appropriately interpreting the results of such approaches. The overall goal of this workshop was to begin a dialogue on 'what still needs to be done', in particular: (a) to determine if the methodology and parameterisation can be improved; (b) to identify areas where the method is under-utilised; and (c) to identify new applications and the issues that may be slowing these applications. During this workshop, we hoped to address the following questions:

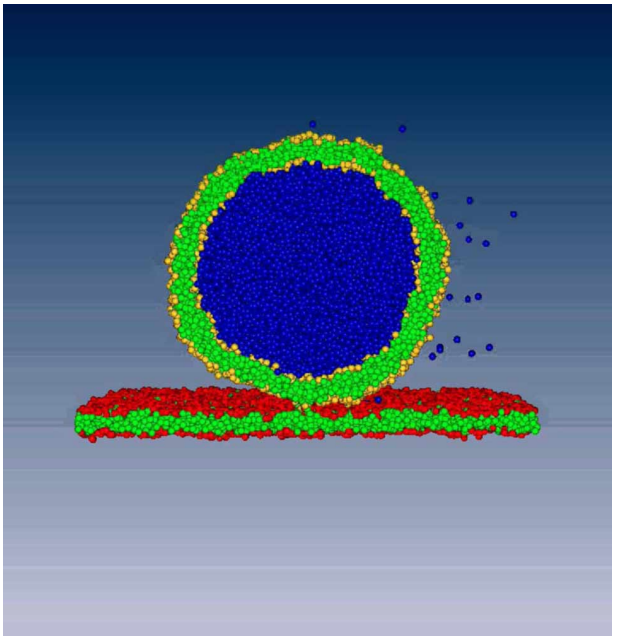
i) What are the challenges limiting the use of DPD in other areas of study?
ii) What are the solutions to overcome these challenges?
iii) Can a standard protocol be developed to generate DPD model parameters?
iv) Can a better link between atomistic modelling and continuum modelling be made via DPD, thus creating a multiscale modelling protocol?
v) Would it be useful to generate a freeware DPD web site (analogous to the MCCCS Towhee code [towhee.sourceforge.net]), which would include various versions of DPD algorithms and computational tools, along with parameter and model potential databases?

3. Technical program

A total of 19 talks were presented during the workshop, where the workshop was comprised of four technical sessions: (i) Technical aspects of the DPD method; (ii) Parameterisation and model development; (iii) Various applications; and (iv) Approaches beyond conventional DPD. To kick-off the workshop on day 1, Rob Groot (Unilever Research, Vlaardingen, The Netherlands) gave a review of the DPD method along with a brief history of its development. Next, Josep Bonet Avalos (Universitat Rovira i Virgili, Tarragona, Spain) described the constant-energy version of the DPD approach, including a discussion on its drawbacks, future directions and possible generalisations of the method. This was followed by a talk from Ignacio Pagonabarraga (University of Barcelona, Spain) on using non-pairwise additive potentials for DPD simulation of high-density contrast systems, such as coexisting phase interfaces or surface wetting. The final talk of the morning session was given by Tomoyuki Kinjo (Toyota Central R&D Labs, Nagakute, Japan) who presented a microscopic basis for developing coarse-grain models for the DPD method.

The afternoon session of day 1 was dedicated to examining some of the various approaches to parameterising DPD model parameters. Maurizio Fermeglia (University of Trieste, Italy) presented the state-of-the-art in mapping atomistic models onto mesoscale models, while Karl Travis (University of Sheffield, UK), Reinier Akkermans (Accelyrs, Cambridge, UK), and Martin Nilsson Jacobi (Chalmers U. of Tech., Göteborg, Sweden) presented novel approaches for determining DPD model parameters.

A sampling of applications of the DPD method was given on day 2, with the morning session focused on polymer systems. Bernard Rousseau (CNRS/Université Paris-Sud, Orsay, France) presented work on chain entanglement, which was followed by Patrice Malfreyt's talk (CNRS/University of Blaise Pascal, Clermont-Ferrand, France) on friction and compression of polymer brushes. Sudip Roy (Technical University of Darmstadt, Germany) presented work on DPD simulations of polymer miscibility with application to fuel cell membrane morphology, which was followed by a talk by Venkat Ganesan (University of Texas, Austin, TX, USA) on simulating the structures and dynamics of polymer nanocomposites.

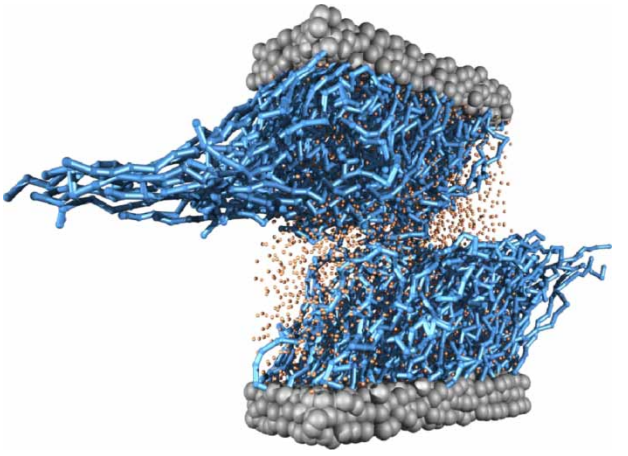


DPD simulation of vesicle (reproduced by permission of J. Shillcock).

The afternoon session of day 2 comprised of DPD simulations outside the realm of the typical application to polymer systems. Julian Shillcock (University of Southern Denmark, Odense, Denmark) presented work on the simulation of biomembranes and vesicles, while Rob Groot demonstrated an application of the method to surfactant systems. Samy Merabia (LPMCN University of Lyon 1, France) presented a DPD study on the dynamics of the de-wetting of thin films, which was followed by Henry Bock's (Heriot-Watt University, Edinburgh, UK) talk on surfactant self-assembly in carbon nanotube-based materials.

Day 3 of the workshop comprised talks that incorporated the DPD method into other simulation methodologies. Martin Lísal (Academy of Sciences of the Czech Republic) started the morning by giving a talk on the reaction ensemble DPD method for simulating polymer reaction equilibria. Hans Fraaije (Leiden University, The Netherlands) then presented a sampling of projects which utilised the DPD approach as part of the Chemistry Unified Language Interface (Culgi) and finally, Rafael Delgado Buscalioni (Universidad Autonoma de Madrid Cantoblanco, Spain) demonstrated the use of the DPD approach as a multiscale link between atomistic simulations and continuum hydrodynamics modelling via an adaptive coarse-graining technique.

A total of 16 posters were also presented during the workshop. The topics of the posters covered a wide range of study, including various novel applications and extensions of the DPD approach. Electronic copies of all talks and posters are available on the CECAM website (http://www.cecam.org/workshop-5-188.html).



DPD simulation of polymer brushes under shear (reproduced by permission of P. Malfreyt).

Following the formal presentations, a group discussion was initiated that resulted in a scintillating exchange of ideas. Several issues were raised by participants regarding the current shortcomings of the DPD method. For example, a suggestion was made that improved thermostatting mechanisms are still required, especially for non-equilibrium applications. Also, a general consensus was that one still needs to spend considerable effort in developing parameters predicated upon the phenomena one wishes to simulate. Moreover, more reliable parameterisation methods, in particular for conversion from DPD units to real units for comparison with experimental data are needed. Another critical deficiency is in our understanding and interpretation of the underlying physics of the dynamics of DPD systems.

Regarding the specific questions posed at the start of the workshop, the group discussion offered several key thoughts worth noting.

What are the challenges limiting the use of DPD in other areas of study?

In addition to developing reliable parameterisation methods and gaining an understanding of the underlying physics of the dynamics, several specific issues were raised, including: (a) modelling solid walls with typical DPD soft potentials is troublesome; (b) time scales are still limited in polymer-particle systems (even after coarse-graining); (c) the treatment of polymer entanglement requires further work; (d) for rheological applications, more work is required to establish the link between dissipative forces and viscosity.

What are the solutions to overcome these challenges?

While more limitations than actual solutions were raised, the open dialogue and exchange of ideas were encouraging. Numerous possible routes to pursue in overcoming these challenges were suggested,

conveying a general feeling that solutions are indeed on the horizon.

Can a standard protocol be developed to generate DPD model parameters?

Agreement among participants was that this is not currently possible since parameterisation is still highly system dependent. Moreover, one needs to spend the appropriate effort in developing parameters based upon the phenomenological features that one wants to preserve in the simulation. Interestingly, it was mentioned that while a true physical basis of the DPD parameters may be lacking, one can utilise this aspect since it allows greater flexibility in tuning the model parameters. Suggestions were made on several occasions to consider moving away from the Groot–Warren δ- and χ-parameter approach altogether [6,7], and on to the more general form of the Pagonabarraga–Frenkel non-pairwise additive potential approach [13].

Can a better link between atomistic modelling and continuum modelling be made via DPD, thus creating a multiscale modelling protocol?

The final two presentations of the workshop by Fraaije and Delgado-Buscalioni clearly showed this to be possible with quite satisfactory results. The DPD approach within this context is quite promising.

Would it be useful to generate a freeware DPD web site (analogous to the MCCCS Towhee code (towhee.sourceforge.net)), which would include various versions of DPD algorithms and computational tools, along with parameter and model potential databases?

Consensus was that this was reasonable with some participants agreeing to contribute parameters and parameterisation protocols to such a database. Indeed, the LAMMPS suite of simulation software appears to be heading in this direction, where open-source parallel versions of DPD code are available (http://lammps.sandia.gov/).

4. Conclusion

The CECAM workshop forum once again provided an atmosphere conducive for extensive discussion and exchange of ideas amongst participants. We greatly appreciate the opportunity that the director Mauro Ferrario and the CECAM Scientific Council provided us to organise this workshop. We would like to thank the EPFL for providing more than adequate facilities. Finally, we would like to acknowledge the help of the administrative staff whose efforts made the workshop possible, Emilie Bernard, Suzy Eichenberger, Jordi Brusa, and Emmanuelle Foltzer.

It is our hope that from the beginnings of a formal dialogue to address the deficiencies of the DPD approach that in the end it will further our ability to simulate behaviour at the mesoscale. We hope that the workshop will stimulate new developments in a number of areas, including parameterisation, establishing a theoretical foundation of the dynamics, as well as continued novel applications of the method. We anticipate another workshop within the next several years, where an assessment of the progress in these areas along with others can be made.

References

[1] P.J. Hoogerbrugge and J.M.V.A. Koelman, *Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics*, Europhys. Lett. 19 (1992), pp. 155–160.

[2] J.M.V.A. Koelman and P.J. Hoogerbrugge, *Dynamic simulations of hard-sphere suspensions under steady shear*, Europhys. Lett. 21 (1993), pp. 363–368.

[3] Y. Kong, C.W. Manke, W.G. Madden, and A.G. Schlijper, *Simulation of a confined polymer in solution using the dissipative particle dynamics method*, Int. J. Thermophys. 15 (1994), pp. 1093–1101.

[4] A.G. Schlijper, P.J. Hoogerbrugge, and C.W. Manke, *Computer simulation of dilute polymer solutions with the dissipative particle dynamics method*, J. Rheol. 39 (1995), pp. 567–579.

[5] P. Español and P.B. Warren, *Statistical mechanics of dissipative particle dynamics*, Europhys. Lett. 30 (1995), pp. 191–196.

[6] R.D. Groot and P.B. Warren, *Dissipative particle dynamics: bridging the gap between atomistic and mesoscopic simulation*, J. Chem. Phys. 107 (1997), pp. 4423–4435.

[7] R.D. Groot and T.J. Madden, *Dynamic simulation of diblock copolymer microphase separation*, J. Chem. Phys. 108 (1998), pp. 8713–8724.

[8] A.F. Jakobsen, *Constant-pressure and constant-surface tension simulations in dissipative particle dynamics*, J. Chem. Phys. 122 (2005), 124901.

[9] R.D. Groot, *Electrostatic interactions in dissipative particle dynamics-simulation of polyelectrolytes and anionic surfactants*, J. Chem. Phys. 118 (2003), pp. 11265–11277.

[10] K.P. Travis, M. Bankhead, K. Good, and S.L. Owens, *New parameterization method for dissipative particle dynamics*, J. Chem. Phys. 127 (2007), 014109.

[11] J. Bonet Avalos and A.D. Mackie, *Dissipative particle dynamics with energy conservation*, Europhys. Lett. 40 (1997), pp. 141–146.

[12] P. Español, *Dissipative particle dynamics with energy conservation*, Europhys. Lett. 40 (1997), pp. 631–636.

[13] I. Pagonabarraga and D. Frenkel, *Dissipative particle dynamics for interacting systems*, J. Chem. Phys. 115 (2001), pp. 5015–5026.