Dissipative particle dynamics: Where do we stand on predictive application?

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1 State of the art

Dissipative particle dynamics (DPD) has seen widespread uptake since its inception as a relatively simple and inexpensive coarse-grained modelling tool ideally suited to the study of soft condensed matter systems. DPD is perhaps unusual in that its development has been driven as much by the needs of industry as by academic research. Despite the scientific advances and the early industrial applications, there remain several open questions both in the foundations of the method and in advanced applications, which prevent the method being used in a predictive fashion in an industrial setting. These questions include:

- Do robust parameterization methods exist that enable predictive simulations?
- Can such coarse-grained potentials be extended to different families of compounds or are they molecule/system-dependent?
- Is the application of electrostatics in DPD solved or not?
- How do we treat solvents of different nature?
- Do many-body method play an important role in predictive applications?
- What is the real computational gain in DPD? Time and length scales?
- Many industrial applications of DPD involve interactions with surfaces; can DPD provide realistic representation of these?
- Does the software exist to support predictive simulations?
- Do we have analytics to extract appropriate data from simulations, e.g., viscosity
- How could we describe specific ion interactions or ion interactions beyond simple ad-hoc parameters?

The workshop aimed to bring together leaders on the DPD community from academia and industry to address these open questions and to develop pathways to overcome challenges.

2 Major outcomes

This workshop brought together the leaders in the field to ask the question, where can DPD offer predictive insight currently, and what is required to improve the method and application to enable improved predictive capability in the future? The workshop was dominated by

discussion on four key areas; parameterization, applications, new methods and software. All of the talks were of high quality and covered topics such as the introduction of hydrogen-bonding into DPD, coupling DPD to higher length scale simulations and how to simulate surfaces effectively.

The workshop was able to answer most of the posed challenges.

- There are parameterization methods that enable predictive simulations although work is always ongoing
- Coarse-grained potentials should be considered system-dependent mot of the time
- The application of electrostatics is not solved, rather started.
- Progress is being made on solvents of different natures although there is plenty to do
- Many-body methods look like they should play an important role but are not yet fully exploited
- The computational gain is real but sacrifices must be made in accuracy
- Realistic representation of surfaces is important and some work has tackled this. However, more work is required
- In part, software does exist but more could be done (see community needs section)
- We have some good analytics but often not in an accessible repository and the tools can be extended (e.g., viscosity)
- Capturing specific ions effects are crucial to move the field on but no compelling strategy for parameterisation exists.

On this last point, the current best practice for charged ions is to assume they behave as charged water beads. Whilst the few groups who have simulated charge systems have used this approximation with good results, focussed work is required to be able to differentiate the behaviour of different ions. No consensus was reached at the workshop about how to tackle this challenge.

The workshop hosted a number of individuals from industrial organisations and the participants were impressed by the use of the DPD method in the research of BASF, Proctor & Gamble, Unilever and IBM. The first three of these organisations have produced workflows internal to their organisations to deploy the DPD method to key industrial challenges. The latter, IBM, are developing methodologies to parameterise the DPD method using experimental data in conjunction with the STFC Hartree Centre.

The need for clean, verified, experimental data was highlighted by a number of participants at the workshop. Currently, high-quality data is limited in the literature. The DPD community (and other communities) would benefit from good data (e.g., critical micelle concentrations, aggregation numbers, phase data) for pure surfactants. This data could be used to ratify simulation results and to train models.

A talk of particular note for the development of industrially useful predictive simulations was a GPU re-write of DL_MESO (sponsored by ECAM) with significant performance improvements. It is not unreasonable to assign an order of magnitude reduction in the cost of DPD simulations of DL_MESO calculations with this GPU dedicated version. With such a cost saving the application of DPD to industrial problems becomes more financially attractive.

The workshop assessed the community need for exascale. Most of the participants use very modest compute power, In the order of a couple of nodes. A smaller number of participants utilise 10-20 nodes at a time for simulations. The consensus was that exascale does not present a big step up for the community, rather that interesting scientific challenges need to be solved first. The main role exascale could play is in rapid screening of candidate systems for formulated product companies. This requires accurate models, efficient computation and appropriate workflows to be available.

3 Community needs

The DPD community needs discussed were separated into two related sections; software and support.

It was felt that identifying a European community code (e.g. DL_MESO or Espresso) to focus development upon would be highly desirable in two areas. Firstly, when lobbying the European commission for funding and secondly to ensure community developed functionality is available to all researchers in astable and well tested platform. The chosen community code would be the main European code of choice for DPD and could be validated with LAMMPS. Long-term funding would be required for this venture.

Whilst a number of analytics tools exist to extract data from simulation trajectories, these tools are often distributed across multiple research groups in different countries. Often poorly documented, these tools do not get utilised outside of the group from which they were developed. A positive outcome of the workshop would be if a repository could be developed and maintained where analytics codes could be deposited and used and further developed by other researchers. This should prevent many cases of the 're-invention of the wheel' in research projects. Note that there are a few general analytics tools available such as MD analysis and UMMAP.

In terms of usability of DPD methodologies, a significant amount of workshop time was dedicated to exploring the possibility of a dedicated user forum in which researchers around the globe could discuss challenges and successes as well as a portal for asking for help. This, coupled to a more informative set of tutorials was seen as a potential major boost to the community. A set of tutorial reviews were proposed to help with the latter point and the developers of DL_MESO and multiple workshop participants agreed to contribute.

4 Funding

Funding channels were not discussed with regards to scientific research as it was felt that the normal routes were appropriate.

However, long-term funding of community codes (see community needs section) was deemed to be a priority for the community. This funding would enable DPD codes chosen by the community to have well resourced development to ensure correctness and stability of the

codes. No specific funding rules were identified but it was felt that the traditional routes did not facilitate software development well.

5 Will these developments bring societal benefits?

The potential impacts of developing and applying more predictive DPD models and methods is significant. The method has proven already to be beneficial to developing improved formulated products as can attested to by multiple industrial participants examples at the workshop. Further scientific developments and those made to simulation and analytics codes will lead to models which better represent industry products and processes which in turn will lead to an increased understanding of the mode of action of these products.

Improved simulation codes combined with an efficient strategies for tackling key scientific challenges will allow the development of improved models allowing scientists to design new products in-silico which will reduce the number of time consuming experiments that need to be performed.

Ultimately the impact will be to enhance de novo formulation design, shorten time to market, provide an adaptive response to supply chain variability, and encourage the adoption of formulation for sustainability. The ability to formulate virtually allows for acceleration of R&D processes, smoother development of new products, especially for high value manufacturing markets where growth arise

from high R&D intensive efforts.

The next few years will be particularly exciting. New methodologies are currently being developed to tackle scientific challenges and improved simulation codes and analytics methodologies are becoming available. It is therefore planned to repeat this workshop in three years' time, to review our success and look further ahead.

6 Participant list

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