Progress report for 12272: Hydronamic Theory of Wet Particle Systems

MercuryDPM: Accomplished and future

Chris de Jong

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1 About MercuryDPM

MercuryDPM is an open source discrete particle simulation code developed at the University of Twente. The code serves as an important toolkit to perform research of new contact laws and as an alternative method to discover new phenomena. The code is constantly validated by researchers in universities, including the University of Twente and the University of Birmingham. Because of close relations between researchers doing experiments and the developers of this code, MercuryDPM will stay one of the world leading codes for discrete particle simulations.

2 STW Project 12272

For STW project 12272: "Hydronamic Theory of Wet Particle Systems" new contact laws for adhesion and specialised geometries have been implemented in the code. This allows researchers to investigate and test the validity of different contact laws and see the effect of such changes without performing expensive and time-intensive experiments.

The MercuryDPM team is on the verge of the first official of the package. This version will be released after some minor changes as version 1.0. So far major improvements to the code include support for multiple platforms, and better documentation and tutorials. To prevent coding errors going unnoticed the MercuryDPM team has implemented both unit-tests and self-tests for the code to make sure that any change made to the code will not compromise scientific results.

3 Future work

Development of the next version of MercuryDPM has also started; using experience gained over the last few years with both our academic users and industry, a new direction has been chosen. This new code, informally called Mercury 2.0, has a new layer of tools available on top of the code. These tools include easy to use interfaces for researcher so less effort is required to set up new simulations. The MercuryDPM team feels that these tools have to be added to further strengthen our position as one of the world's leading simulation packages for these kind of simulations.

Focus for this new version especially lays on a single, easy to use interface with extensive support for data analysis. Expectations are that this unified interface means that less training is required to gain familiarity with the code and training time for both new personnel, as well as requiring less time for existing users to stay up to date with the latest methods and developments available.

Because of tight integration with infrastructure required for performing these kind of simulations, researchers no longer require training in these systems. Because of a total transparent layer between the definition of the simulation parameters and the actual execution of the simulation, people will be no longer required to have extensive knowledge of the systems used internally such as Linux, which are not directly relevant for research.

4 Summary

Work done includes:

- Implement new contact laws required for this project
- Add support for special geometries, including periodic boundaries within cylindrical coordinate systems
- Implement short-range non-contact forces into the contact detection
- Add support for particles with prescribed trajectories to implement rough moving walls
- Refine documentation
- Create step-by-step tutorials for wet particle simulations
- Automatic optimisation of parameters for contact detection
- Implement thorough testing infrastructure
- Improve cross-platform support

Future work includes:

- Release version 1.0
- Integrate our simulation software with our infrastructure
- Create a more easy-to-use interface for researchers
- Rewrite tools to allow quick and efficient data analysis

5 Information

More information about MercuryDPM can be found on our website:
`http://mercurydpm.org`