Project PN-III-P1-1.1-TE-2016-1279

Scientific report for the period 01.05.2018 – 29.11.2018

During the first stage of the project (01.05.2018-31.12.2018), the following activities have been carried out:

1. Recruitment of a PhD student and a postdoctoral researcher

The PhD student selected for the project is Janos Szoverfi, with whom I also worked during my previous young research teams grant. He has acquired experience in molecular dynamics simulations on graphical processing units, using biomolecular force fields.

Recruitment for the postdoctoral researcher took more time than originally planned, because of the chronic lack of suitably qualified applicants for research projects in Romania. Finally, we managed to hire Dr Lorand Czipa, he obtained his PhD in physics at the Babes-Bolyai University earlier this year. Dr Czipa has experience in Fortran programming of various physics models.

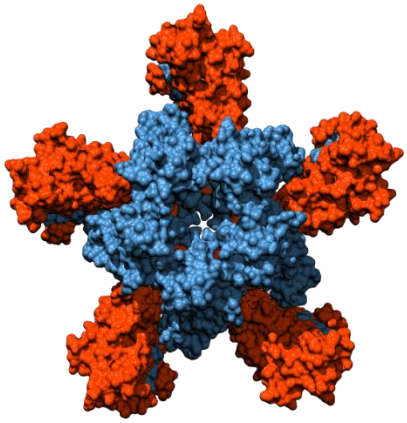
2. Improving Monte-Carlo exploration for basin-hopping global optimization of colloidal particles

During this activity we explored various strategies for efficient step taking on quite complex potential energy hypersurfaces, due to the fact that colloidal building blocks usually have quite small-range interactions, complicating the whole landscape. Their shape and interaction anisotropy also complicates MC steps, one should avoid high-energy starting structures in order for the moves to be efficient. Taking too small steps is not efficient for the exploration of the landscape either. After trying several step taking methods, we found that the best scheme that works for our systems is a hybrid approach, in which Cartesian steps are taken after each minimization step, while rotational steps are taken only intermittently, depending on the system (on average, every second or third step). The step taking moves have to be combined with the basin-hopping parallel tempering (BHPT) method, in order to efficiently explore the rough landscapes of colloidal particles. We found that BHPT works best if it can manage an acceptance ratio of 0.5 both in the low and high temperature regions. For this, the temperature is the main parameter that had to be adjusted.

3. Optimizing the evaluation of rigid-body potentials on GPUs

For this activity, we evaluated in depth the GPU code for the AMBER molecular mechanics force field (version 12), as it is interfaced with the GMIN and OPTIM programs of the Wales group. The local rigidification scheme of the Amber force field, already implemented in GMIN and OPTIM, works by evaluating the intramolecular forces as well, and setting them to zero after each energy/gradient evaluation. The implemented scheme is quite flexible, as it allows for relaxation of the rigidified

molecules as well. However, the GPU implementation of the Amber force field makes it impossible to use custom Lennard-Jones interactions, for example we cannot use only the repulsive part of the Lennard-Jones equation to model excluded volume interactions. The code calculates sigma and epsilon values for the original LJ equation from the supplied LJ coefficients in the parameter topology file, and uses those values for subsequent potential evaluation in the GPU code. We are currently exploring whether using the coefficients directly affects the performance of the GPU energy and force evaluations. Also, the lack of a vacuum model programmed for GPUs means that Generalized Born solvation terms are evaluated even when the external dielectric is set to 1, which obviously slows down the computation, compared to the vacuum case. We are therefore in the process of implementing the rigid-body Coulomb and LJ interactions as a separate model, using as a template the existing addressable LJ model implemented for CUDA.



We also did some benchmarking of system sizes accessible through CUDA MD simulations, using Amber 14. We managed to simulate a pentamer of CCMV dimers for almost 2 microseconds, reaching about 14 ns/day on two nVidia Tesla K40m GPUs (200523 atoms).

4. Implementing the developed potentials into OPTIM

Since during my last project we successfully modified the SANDBOX routine of GMIN and OPTIM to include a variety of site-site interactions for binary systems, we built on this experience to create an easy-to-use implementation of our coarse-grained models in this framework. We will finish implementing an addressable version of the Lennard-Jones interaction, combined with Coulombic interactions by the end of the reporting period. Addressable systems are of great interest, and it is expected that such colloidal building blocks can be used for very efficient data storage in the future. Therefore, studying the dynamics of addressable particles is one of the goals of the project, as their directional interaction is directly relevant to the topic.

5. Creating an algorithm for seeded global optimization

We modified the MODULAR keyword implemented in GMIN to allow for global optimization with a certain seed structure, during which the seed is not affected by MC moves. To do this, the algorithm resets the forces acting on each particle of the seed at each energy evaluation step, and relaxes the structure during the final quenches. There is a possibility to grow the seeded structure, starting from one of the lowest saved structures, adding a specified number of particles into the system. We could run benchmarks on known systems, and for example seeding systems of Janus particles with a cluster in

a Bernal spiral configuration indeed drives the system towards Bernal spiral structures, as if they would grow out of that seed. However, with the seeded global optimization it is possible to miss the real global minimum, if it is of a completely different configuration. Therefore, the best use of seeded global optimization is to study the effect of structural growth in one or two dimensions of a certain motif. We plan to use the algorithm further, to study structural growth in three dimensions in case of asymmetric triblock Janus particles, but the expected complexity of the potential energy landscape will make even seeded global optimization very difficult.

6. Other relevant activities

Visits

I visited the group of Prof. David Wales FRS at the University of Cambridge between 11-18 November 2018. During this time I presented my current research topics to them, and we discussed several new ideas for collaboration. I also had the opportunity to do some joint debugging of the GMIN CUDA code.

Conferences

Members of my group attended two conferences this year:

a. MolMod 2018, organized by UBB Cluj-Napoca – oral presentation by Janos Szoverfi and myself
b. International Conference on Chemistry, organized by the Hungarian Technical Scientific Society of Transylvania – oral presentation by Janos Szoverfi

Refereeing

During this stage of the current project, I refereed papers submitted to Nature Communications.

Sfantu Gheorghe, on 29.11.2018

Dr Szilard Fejer