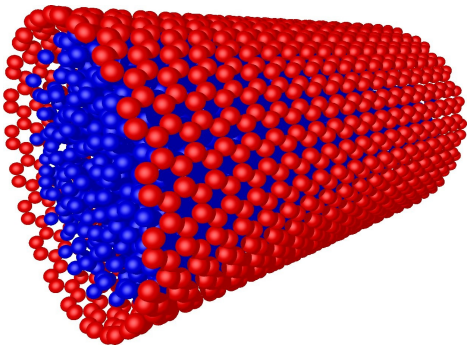
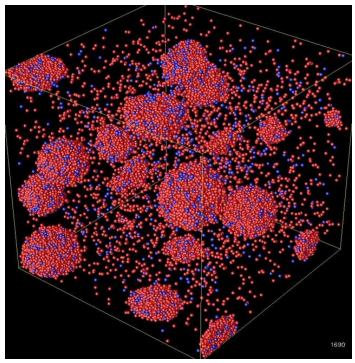
IDP Mathematik: Analysis of numerical precision requirements of Molecular Dynamcis Simulations

In order to predict or analyse thermodynamic material properties like pressure or potential energy of a material, molecular dynamic simulations are getting more and more important. A typical example is the simulation of a mixture of two different gases with millions of molecules by studying the interaction of the single particles.





At the beginning of a timestep the positions and velocities of the molecules are given. From the positions, forces between the molecules can be determined, and the molecules are moved according to those forces.

Such a simulation programme called ls1/Mardyn has been realized over the last few years in a cooperation of the HLRS (Höchstleistungsrechenzentrum Stuttgart), University Paderborn, TU Kaiserslautern and our chair, facing the challenges of large amounts of data and high computational intensity neccessitating the efficient use of supercomputers and clusters.

An important aspect is the precision of the floating point representation, with which molecular dynamics simulations are carried out, as algorithms become numerically instable and the results are worthless, if the precision is too low.
However, from a programming point of few, low precision would be preferable. Vector extensions to modern CPUs such as Intel SSE and Intel AVX offer twice the performance for single precision floating point (SP) numbers compared to double precision (DP). Even worse, the performance of SP calculations may be an order faster on accelerator hardware like GPUs. Moreover, compilers and / or hardware may offer fast low-precision approximations to expensive operations like inverse square-root, which are then not IEEE-compliant any more.
Also algorithmical tweaks are possible, depending on the precision required. E.g. could expensive calculations of the interatomic forces be replaced by table lookups followed by interpolation, the payoff however may depend of the hardware used [2].

Commonly, single precision is considered to be sufficient, however, there exist also applications where double precision is required. From literature no clear statement can be made, when which precision is appropriate [1,3]. To some extend, SP floating point numbers have been found insufficient in a preceeding student research work [10] for the simulation of fluids modelled by rigid-body multi-centered molecules, however no in-depth analysis has been performed, which parts of the simulation are sensitive to a reduction of precision.
The objective of this work is twofold: first close this gap in theory, determining the precision requirements of the various parts of a rigid-body multi-centered molecular dynamics simulation, well-funded on numerical experiments. In the second part, known optimisation techniques like table-

lookups or fast-math algorithms can be exploited where suitable and their effect on performance can be examined.

If favoured, also the GPU version of ls1/Mardyn can be included in the evaluation, as the efficiency of optimisations like the table lookup may be different (as table-lookup and interpolation fit perfectly to the gpu texture cache, however the resulting precision may be low).

Summary of the project steps:

- Literature search about existing approaches to the problem, resulting in a summary of the state-of-the-art
- Definition or extension of existing measures for the precision of the steps of a molecular dynamics simulation (e.g. energy conservation, force relative mean-square error) explicitly taking the rotational degrees of freedom into account.
- Realisation of numerical experiments, including mixed-precision representations(e.g. single precision for the position calculation of the molecules, double precision of the force calculation).
- Implementation of performance optimisations like inverse-square-root or table-based force lookup. Analysis of these optimizations with respect to the required precision and the performance benefit.

Requirements for the candidate:

- good programming skills, experience in c++-development in linux of advantage
- basic knowledge in numerical programming
- interest in hardware-aware programming
- interest in a challenging topic

This topic can also be offered as a bachelor or master thesis. If the outcome is good, a publication of the results in an internationally recognized journal is possible.

Contact:
Please send an informal application stating your previous experiences as well as your knowledge or skills to Wolfgang Eckhardt (eckhardw@in.tum.de).

References:

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[2] Nilsson, L.: Efficient table lookup without inverse square roots for calculation of pair wise atomic interactions in classical simulations In: *Journal of Computational Chemistry,* **2009***, 30*, 1490-1498

[3] Bowers, K. J.; Chow, E.; Xu, H.; Dror, R. O.; Eastwood, M. P.; Gregersen, B. A.; Klepeis, J. L.; Kolossvary, I.; Moraes, M. A.; Sacerdoti, F. D.; Salmon, J. K.; Shan, Y. & Shaw, D. E.
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