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Student/Bachelor/Master Project: Incorporation of State-of-the-art Particle Interaction Potentials in the Molecular Dynamics Simulation Framework ls1 mardyn / AutoPas

Description: Molecular dynamics (MD) simulation is an important tool of process engineering used for detailed investigations of the behavior of liquids or gases. The appeal of the MD approach is the fact that thermodynamical properties of the substance at hand are automatically contained by the molecular interaction. Hence, the accurate description of the interaction by appropriate force potentials is essential. The scope of the present project is the extension of the available potentials of the MD framework ls1 mardyn / AutoPas [NIE14,SEC21]. The framework is able to efficiently simulate huge molecular ensembles relying on the Lennard–Jones force potential while utilizing auto-tuning schemes to improve the computational speed. The task will be to incorporate additional state-of-the-art interaction potentials like the Mie potential, the Morse potential, the Buckingham potential or the Tang-Tönnies potential with respect to the aforementioned auto-tuning capabilities. Afterwards, the performance of the code will be examined by applying the new force potentials to previously investigated test cases.

Prerequisites: Good command on C++; knowledge of MPI; experience in handling large software frameworks favorable

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References:

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[SEC21] S. Seckler, F. Gratl, M. Heinen, J. Vrabec, H.-J. Bungartz, P. Neumann. ls1 mardyn: AutoPas in ls1 mardyn: Massively parallel particle simulations with node-level auto-tuning. J. Comput. Sci. 50, 101296, 2021