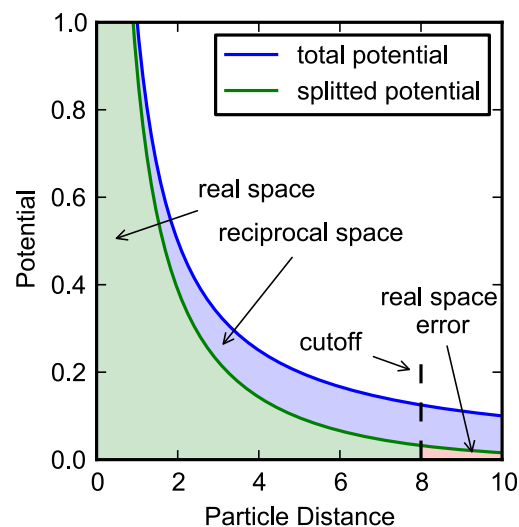


## Master's thesis: Advanced methods for long-range PPPM dispersion solvers

**Topic:** Until recently, development of long-range dispersion solvers for Molecular Dynamics codes has been discouraged by the belief that their computational overhead would make their application unaffordable. We were recently able to show that this belief is flawed and that a clever use of our developed PPPM dispersion solver can provide simulations that are more accurate and more efficient.



In this project you will work on methods to either increase the efficiency or range of applicability of these solvers. This can include:

- development of advanced error estimates for inhomogeneous systems
- development of parameter selection routines that render possible simulations at minimum cost while ensuring accurate simulation results
- implementation of advanced techniques for further increasing the efficiency and range of applicability of the solver
- optimization of the method to work efficiently on GPU-supported systems

**Requirements:** You should have a background in engineering, material science, simulation sciences, natural sciences, computer sciences, applied mathematics, or a related area, and a general interest in numerical simulations and code development. Advanced programming skills in C++ and Python are highly encouraged.