LAGOM: A Python/C++ package for quantum dynamics with and without MCTDH

Henrik R. Larsson

Institut für Physikalische Chemie, Christian-Albrechts-Universität, 24098 Kiel, Germany

A program package has been developed that is capable of performing quantum dynamics for distinguishable particles with time-dependent full CI and MCTDH, either using the conventional approach or using our newly developed dynamical pruning approach [1, 2]. The package is mostly written in Python3 and C++14. Advantages and disadvantages of these programming languages in the context of scientific computing are discussed. It is shown why C++ and similar languages are essential for an efficient implementation of dynamically pruned quantum dynamics. It is further shown how MCTDH can be implemented in Python without jeopardizing performance.