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

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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.

[1] H. R. Larsson, B. Hartke, D. J. Tannor, *J. Chem. Phys.* **2016**, *145*, 204108.

[2] H. R. Larsson, D. J. Tannor, *J. Chem. Phys.* **2017**, *147*, 044103.