The Development of Accelerated Quantum Molecular Dynamics for Complex Gas-Phase Reactive Systems

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A suite of programs called **A**ccelerated **Mol**ecular **D**ynamics with **C**hemistry (*AMolDC*) has been written, tested, and employed in order to perform time-dependent, multilevel QM/MM simulations.

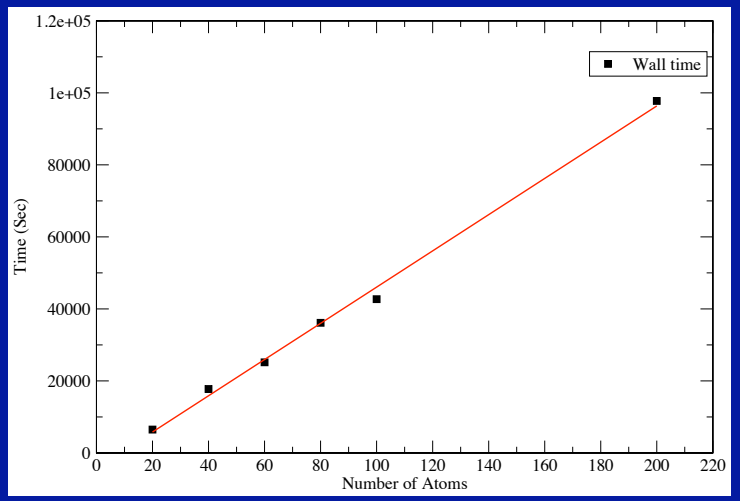
Demonstrated results:

-NVT simulations with extremely discontinuous potential[1]

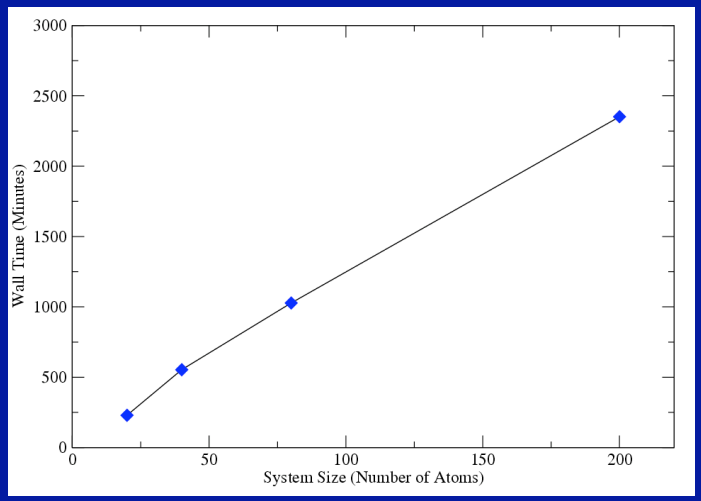
-capability of linear scaling with system size for nQM methodology[1]

-QM/MM linear scaling within serial and parallel implementation of ***AMolDC***

1. *J. Chem. Theory Comput.*, **2010**, *6*, 18.



H_2 NVT QM/MM simulation
400 atm, 1000K



Serial HF/6-31g**/ReaxFF

Parallel HF/cc-pVTZ/ReaxFF