A tale of GPUs and FPGAs: Prospects of modern computing architectures for MCTDH calculations

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The past decade has seen tremendous advances in available computing power as well the breakthrough of new computing architectures, e.g., graphics processing units (GPUs), field-programmable gate arrayfields (FPGAs) or Intel's Xeon Phi. However, MCTDH simulations have rarely taken advantage of these new architecture. An exception is the use of GPUs (along with some machine learning techniques) to speed up potential evaluations in multi-layer MCTDH/CDVR simulations [1]. The speedup achieved allowed for the first rigorous state-to-state simulation of a six atom reaction, i.e., $H+CH_4 \rightarrow H_2+CH_3$, [2] and the first calculation of initial-state selected reaction probabilities on accurate ab initio PES for the same reaction [3, 4].

GPUs are well suited for linear algebra operations and have a high memory bandwidth. Thus, performing MCTDH simulations could potentially benefit a lot from running on GPUs. The low memory requirement of MCTDH is particularly helpful as GPUs often have a rather limited amount of memory available. However, taking advantage of the power of GPUs comes at the cost of learning to think according to the GPU architecture as well as careful program design and implementation.

In this talk I will introduce the basic architecture of GPUs, discuss the implementation of Shepard interpolated and neural network PES on GPUs and give some perspective of how MCTDH simulations could benefit from modern computing architectures such as GPUs and FPGAs.

[1] R. Welsch and U. Manthe, J. Chem. Phys. **138**, 164118 (2013).

[2] R. Welsch and U. Manthe, J. Phys. Chem. Lett. **6**, 338 (2015).

[3] R. Welsch and U. Manthe, J. Chem. Phys. **141**, 051102 (2014).

[4] R. Welsch and U. Manthe, J. Chem. Phys. **141**, 174313 (2014).