Lattice QCD based on OpenCL

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Introduction

Quantum Chromodynamics (QCD) is the theory of the strong interactions between elementary particles. Since an analytical treatment is not possible, it is well established to study QCD in numerical simulations via a discretized version, Lattice QCD (LQCD). State-of-the-art lattice simulations require high-performance computing and constitute one of the most compute intensive problems in science. Graphics Processing Units (GPUs) have become an interesting alternative to classical CPUs as they offer fast computing facilities at a very attractive price-per-flop ratio. So far, however, most applications in this field have been based on NVIDIA CUDA, locking the software to run on hardware by the single vendor NVIDIA. As a rather new alternative, OpenCL offers a vendor independent developement platform, and, in addition, allows for executing the code also on classical CPUs. We have developed the first LQCD application based on OpenCL for Wilson fermions, in particular concentrating on so-called twisted Mass Wilson fermions [1].

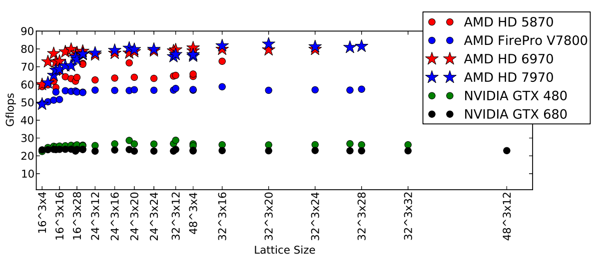

Figure 1: $\not{D}$ performance in Gflops for different lattice sizes on a variety of GPUs.

Performance results

LQCD simulations are always memory bound, meaning they have a low numerical density. Hence, the most compute intensive part, the application of the $\not{D}$ operator, benefits most strongly from an optimal usage of memory bandwidth. We were able to utilize more than 70 % of the available memory bandwidth for all lattice sizes on a variety of AMD GPUs, outperforming published performances of CUDA based codes (Figure 1). The code also works on NVIDIA GPUs, although with reduced performance, as no optimization has been performed for that hardware.

A full LQCD application is the so-called Hybrid Monte-Carlo (HMC) algorithm, which is used to generate ensembles of gauge configurations. Our HMC implementation for twisted-mass Wilson fermions shows a speedup factor of four running on an AMD FirePro V7800 compared to a CPU based reference code running on a single AMD Opteron 6172 socket with 12 cores (Figure 2). In addtion we could show an additional performance increase on the newer generations of AMD GPUs, AMD RADEON HD 6970, substituting the overall good picture of performance and applicability of our code.

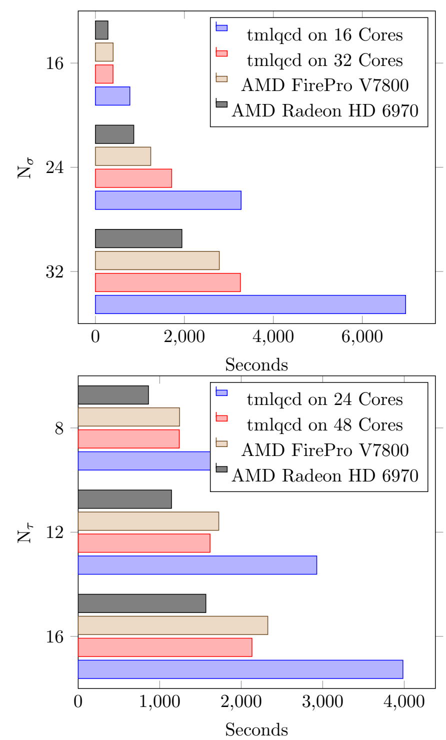

Figure 2: HMC runtimes in seconds using $\mu = 0.1$, $m_\pi = 520$, $\beta = 3.9$ and $\kappa = \kappa_c = 0.160856$ for fixed $N_\sigma = 8$ and $N_\sigma = 24$, respectively, compared to reference code "tmlqcd".

Acknowledgements

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References

[1] M. Bach, V. Lindenstruth, O. Philipsen, C. Pinke, "Lattice QCD based on OpenCL", arXiv:1209.5942 [hep-lat]

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