CL^{2}QCD - Part 2

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Unit Tests, Maintainability and Portability

- It is desirable to be able to test every single part of code on its own and to have as little code duplication as possible (*Test Driven Development* [Beck, 2002] and *Clean Code* [Martin, 2008] concepts). These concepts are followed during CL^{2}QCD development, visible in code structure (see Figure 2).
- Unit tests implemented utilizing the BOOST[7] and CMAKE unit test frameworks.
- Regression tests for the OpenCL parts are absolutely mandatory due to runtime compilation.
  ⇒ Both the architecture and the used compiler can lead to miscompilations of the kernels.
- Reliable tests allow to recognize such situations quickly and simplify error location drastically. Most important, this can prevent the user from wasting computing time.
- LQCD functions are local ⇒ analytic results to test against can be calculated.
- Dependence on the lattice size often easily predictable. Varying the lattice size in the tests, or in general the parameters of the considered function, is important as errors may occur in certain parameter ranges only.
- Crucial aspect to guarantee maintainability and portability of code is to avoid dependence of the tests on specific environments. For example, if random numbers are used (e.g. for trial field configuration), then the test result depends not only on the used PRNG but also on the hardware in a multi-core architecture.

[7] See http://www.boost.org .

Performance of $\not{D}$

Wilson $\not{D}$ implementation:

- Very good performance on various lattice sizes (Figure 3);
- Outperforms literature values (see [Bach et al., 2013]);
- Utilizes ∼ 80% of peak memory bandwidth on AMD Radeon HD 5870, Radeon HD 7970 and FirePro S10000;
- Code runs also on NVIDIA devices ⇒ lower performance since AMD was primary development platform and no optimization were carried out.

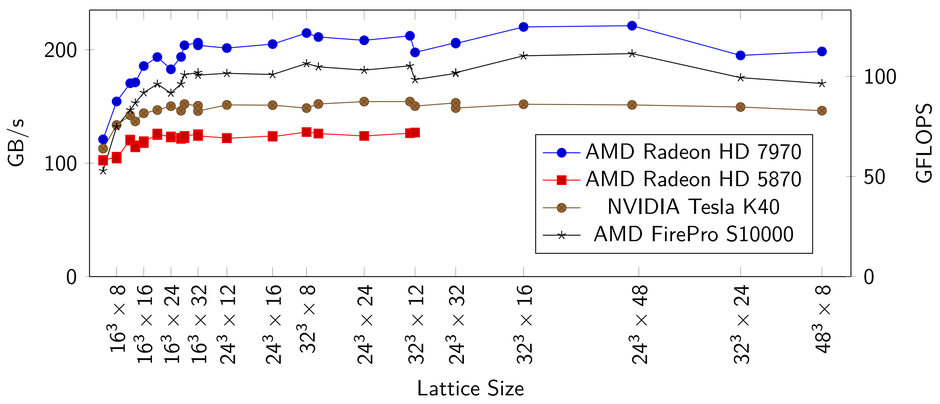

Figure 3: *Performace of Wilson $\not{D}$ kernel for various lattice sizes on different devices in double precision.*

Staggered D_{KS} implementation:

- Good performance on various lattice sizes (Figure 4);
- Utilizes ∼ 70% of the peak memory bandwidth on the AMD Radeon HD 5870 and AMD Radeon HD 7970;
- Recent development ⇒ implementation can be further optimized;
- So far no other benchmark for a possible comparison is present in the literature;
- Code runs also on NVIDIA, showing good performance.

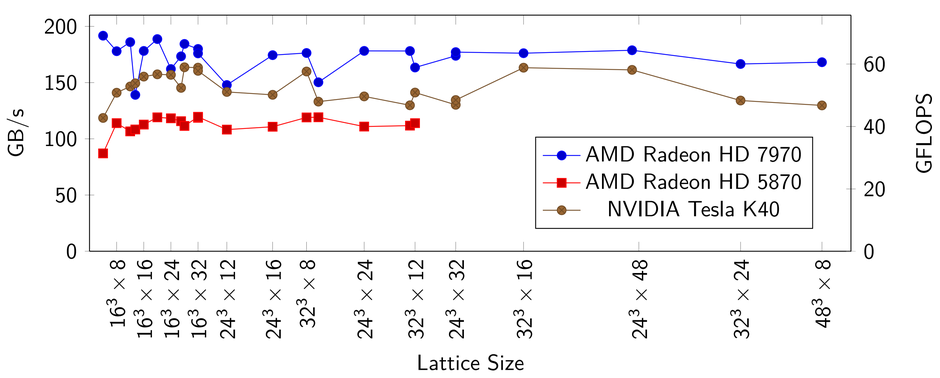

Figure 4: *Performace of D_{KS} kernel for various lattice sizes on different devices in double precision.*

Algorithmic Performance

Full HMC application:

- It performs very well compared to the reference CPU-based code `tmLQCD` [Jansen and Urbach, 2009] (see Figure 5) whose performance was taken on one LOEWE -CSC node.
- The older AMD Radeon HD 5870 is twice as fast as `tmLQCD`. The newer AMD FirePro S10000 again doubles this performance.
  ⇒ Gain a factor of 4 in speed, comparing a single GPU to a whole LOEWE -CSC node.
- Price-per-flop ratio: Much lower for the GPUs used then for the used CPUs.

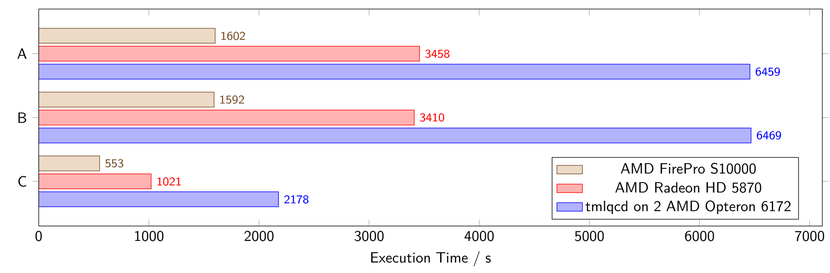

Figure 5: *HMC performance for different Setups A, B and C (setup A having the smallest fermion mass) for $N_\tau = 8, N_\sigma = 24$. The HMC is compared on different GPUs and compared to a reference code [Jansen and Urbach, 2009] running on one LOEWE -CSC node.*

Multi-GPU:

- On-board memory is the biggest limiting factor on GPUs ⇒ using multiple GPUs is of interest, see e.g. [Babich et al., 2011].
- In CL^{2}QCD it is possible to split the lattice in time direction.
- Figure 6 shows the weak (constant lattice size per GPU) and strong (constant total lattice size) scaling of the CG solver on one SANAM node (up to 4 GPUs) [Bach et al., 2014].
- The overlapped computation and transfer utilize direct GPU-to-GPU communication for best performance. To handle a variety of hardware configurations, the best possible data transfer method is choosen via benchmarking at application startup.

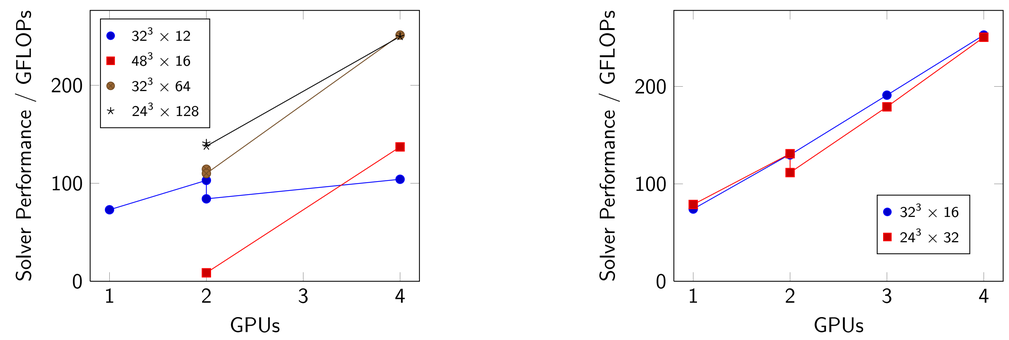

Figure 6: *Strong (left) and weak (right) scaling of the CG solver on the AMD FirePro S10000 GPU in SANAM for multiple lattice sizes.*

Conclusions and Perspectives

- We presented the OpenCL-based LQCD application CL^{2}QCD. It has been successfully applied in finite temperature studies on LOEWE -CSC and SANAM supercomputers (see Table 2), providing a well-suited basis for future applications.[8] CL^{2}QCD is available at

  `http://code.compeng.uni-frankfurt.de/projects/clhmc`

- In $N_f = 2$ Lattice QCD studies we explore the phase diagram of QCD, in particular aiming at the chiral limit, where the order of the chiral transition is not resolved yet. This is done in two independent investigations:
  - Studies employing **Twisted Mass Wilson fermions** [Burger et al., 2011; Ilgenfritz et al., 2009; Philipsen and Zeidlewicz, 2010], aiming directly at the chiral limit at zero chemical potential.
  - Studies of the phase structure of QCD at purely **imaginary chemical potential** μ with Wilson and staggered fermions [Bonati et al., 2013; Philipsen and Pinke, 2014]. Results obtained here can be used to constrain the physical phase diagram of QCD.
- Additional features will be added to CL^{2}QCD according to the needs of the physical studies. In the near future, these will cover:
  - Extension of Wilson fermions to $N_f = 2 + 1$ flavours and implementation of the clover discretization.
  - Optimizations of performances of staggered fermions and inclusion of improved staggered actions.

[8] In particular, there will be an upgrade of LOEWE -CSC, which will be equipped with AMD FirePro S10000 GPUs with 6 GB memory each.

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