Lattice QCD based on OpenCL

[arXiv:1209.5942, accepted for Computational Physics Communications]

Christopher Pinke

–

with M. Bach, V. Lindenstruth and O. Philipsen

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Institute for Theoretical Physics
Goethe-University Frankfurt

HIC for FAIR
Helmholtz International Center

HGS-HIRe for FAIR
Helmholtz Graduate School for Hadron and Ion Research

New Horizons in Lattice Field Theory
Natal, March 22, 2013

Life on the lattice…

State of the art LQCD …

- …is (persistently) one of the most computing intensive problems in science
- …uses big computing clusters ($\rightarrow$ parallelization)

LQCD simulations fall roughly in 2 categories:

- Ensemble creation: Hybrid Monte Carlo (HMC)
- Observable evaluation: m_π, $\overline{\psi}\psi$, …

Consequently, lots of improvements in numerics have been achieved…

"(Wall)Time is Money (CPU hrs)"

Meanwhile in the continuum. . .

1994

⇒
⇒
⇒
⇒

2003

NEED FOR SPEED MOST WANTED: GPUs

	Chip	Peak SP [GFLOPS]	Peak DP [GFLOPS]	Peak BW [GB/s]
AMD Radeon HD 5870	Cypress	2720	544	154
AMD Radeon HD 6970	Cayman	2703	683	176
AMD Radeon HD 7970	Tahiti	3789	947	264
NVIDIA Tesla M2090	Fermi	1331	665	177
NVIDIA GeForce GTX 680	Kepler	3090	258	192
AMD Opteron 6172	Magny-Cours	202	101	42.7
AMD Opteron 6278	Interlagos	307	154	51.2
Intel Xeon E5-2690	Sandy Bridge EP	371	186	51.2

- LQCD can greatly benefit from GPUs
- Today‘s computing clusters incorporate GPUs (eg AMD based **LOEWE-CSC** in Frankfurt)
- Existing LQCD applications based on `CUDA` (eg **QUDA**):

  $\rightarrow$ vendor specific

What is expensive?

Dominant part of typical LQCD simulation (for small m_f):

$$D\,\psi = \phi \Leftrightarrow \psi = D^{-1}\,\phi$$

- D: sparse matrix
- Krylov-space solvers (CG, BiCGStab, ...)
- Most expensive ingredient: Hopping Matrix $\not{D}$:
  read/write: 2880 Bytes $\leftrightarrow$ perform 1632 FLOPS

(for Wilson, per site)

$\rightarrow$ Low numerical density

$\Rightarrow$ LQCD always memory bandwidth limited

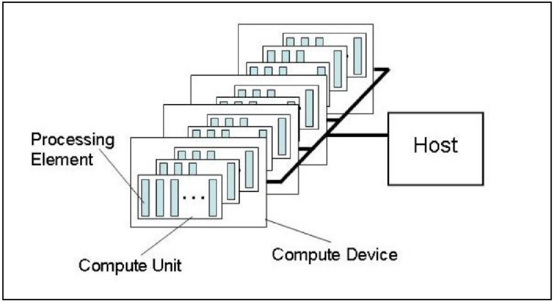
"Flops don't count"

M. Clark

OpenCL

Concept

- Development platform for heterogeneous/hybrid systems
- OpenCL-programming is device and hardware independent (contrary to `CUDA`)

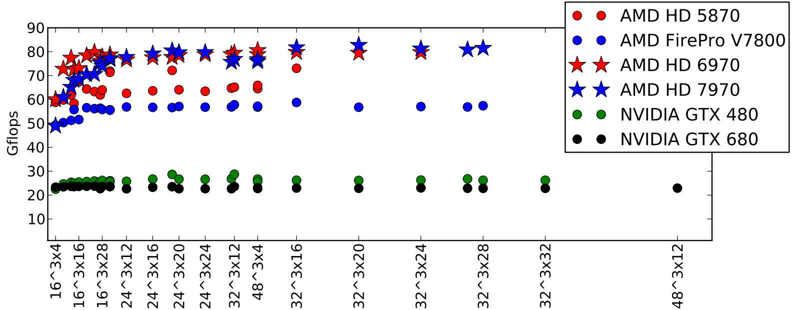


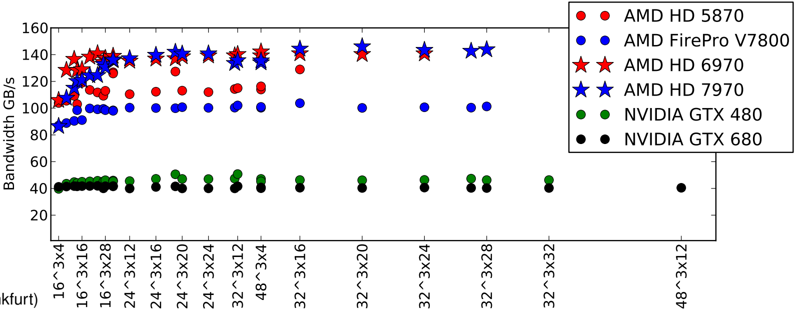
OpenCL Specification 1.1

Lattice QCD based on OpenCL [arXiv:1209.5942]

- New LQCD code developed in Frankfurt
  - Host program implemented using `C++`
- based on OpenCL $\rightarrow$ applicable to CPUs and GPUs
- Applications:
  - SU(3) Heatbath
  - HMC / Inverter for Twisted Mass Fermions
- All calculations carried out on OpenCL devices
- Future plans:
  - multiple devices
  - more fermion discretizations
  - hybrid algorithms
  - ...

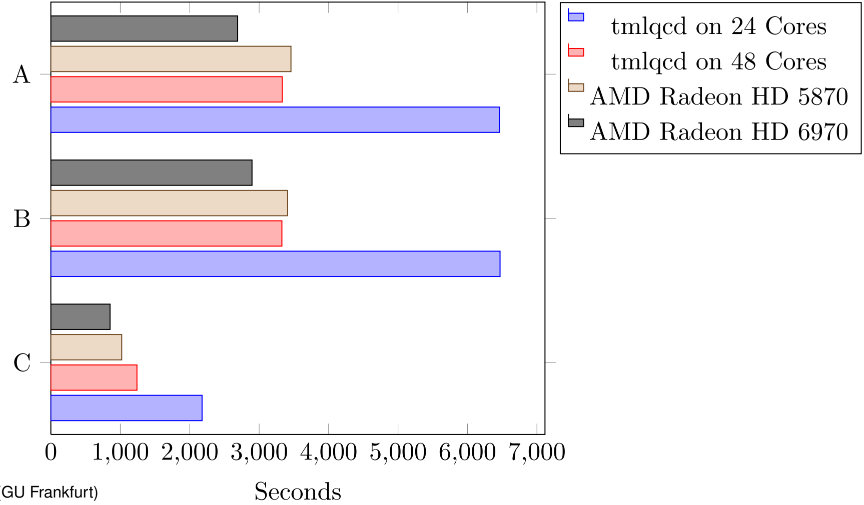
$\not{D}$ performance





HMC performance

Reference: `tmlqcd` (Jansen, Urbach) on 2 and 4 LOEWE-CSC 12-core CPUs (`MPI` parallel)



Conclusions & Perspectives

- LQCD can be accelerated by GPUs
- New LQCD application based on OpenCL developed in Frankfurt, showing good performance
- Currently investigating Multi-GPU usage

Physics applications

- Finite T studies with $N_f = 2$ twisted mass Wilson fermions
- Exploratory studies at imaginary chemical potential with $N_f = 2$ Wilson fermions