Accelerating Lattice QCD Calculations on GPU-Enabled Systems

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in collaboration with

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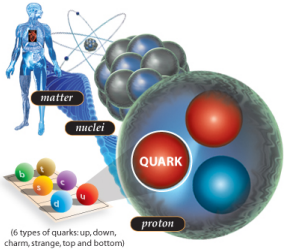
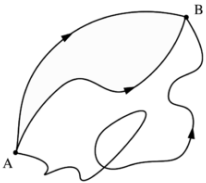
Outline

- QCD is the dynamical theory of quarks and gluons

$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{2}\mathrm{Tr}(F_{\mu\nu}F_{\mu\nu}) + \sum_{i=1}^{N_f} \overline{\psi}^{(i)} \left(\not{D} + m^{(i)} \right) \psi^{(i)} + i\theta \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \mathrm{Tr}(F_{\mu\nu}F_{\rho\sigma})$$

- Quantum Field Theory, Non-Abelian gauge group
- Elementary degrees of freedom are quarks and gluons transforming in the fundamental representation of SU(3)





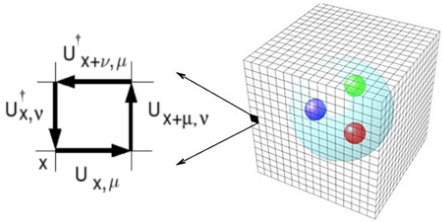
- Feynman's path integral approach

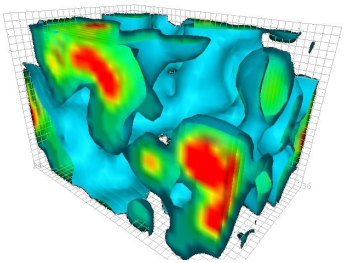
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\Phi] \mathcal{O} e^{-S(\Phi)}$$

- QCD must be regularized both in the UV and IR
- The formulation on the lattice which provides regularization for $a > 0$ and $V = L^4 < \infty$

- Discretization of space-time on a 4-dimensional hypercubic lattice
- Ascribe fermionic degrees of freedom to lattice sites, Gauge bosons to links
- Controlled discretization errors, typically $\mathcal{O}(a^2)$
- Continuum limit approached as

$$a \to 0 \qquad L \to \infty$$





- Infinite dimensional path integral $\to$ high dimensional sum
- Analytically integrate fermionic degrees, importance sampling (fermion determinant)
- Hybrid Monte Carlo (HMC) and variants update the quark and gluon fields

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{\text{all links}} dU_i \mathcal{O} e^{-S(U)} \to \overline{\mathcal{O}} = \frac{1}{Z} \prod_{\text{configurations}} \mathcal{O}(U)\, P(U)$$

- Gauge field generation (Hybrid Monte Carlo methods)
- Evaluating the Path Integral:
  There are $4V$ links. $V = 40^3 \times 256 \rightarrow 4V = 65M$ links
- Typically requires “capability machine”
  (can solve one large problem in the shortest possible time)

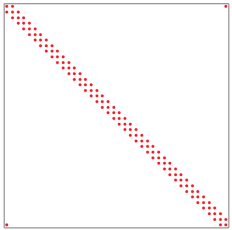
12k GPU cluster at JLab

- Analysis of gauge field configurations
- Propagator calculations, Contractions
- Parallelization on independent gauge field configurations
- Typically a “capacity machine” suffices
  (can solve many smaller problems simultaneously)

- Main consumer of computational power in Lattice QCD calculations:
- Solution to a large linear system of equations (dimension 10^9 and larger)

$$Dx = b$$

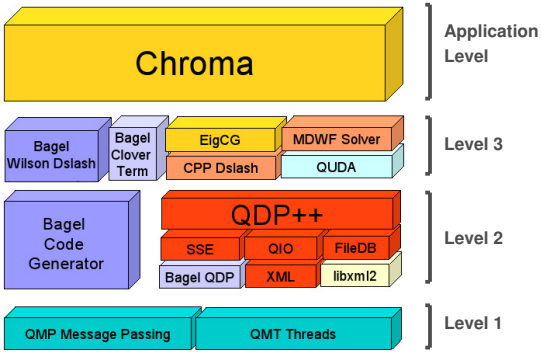
  where D is the discretized Dirac operator, a large sparse matrix
- Typically done by conjugate gradient algorithm (or similar)
- Requires efficient: Dx multiplication
  $y = ax + b$ linear algebra and $r = x \cdot y$ scalar product, global sums



Wilson $\not{D}$ is $12V \times 12V$ complex sparse matrix

- The QUDA library provides CUDA-accelerated linear solvers
- Highly-optimized operations, mixed precision, domain-decomposition methods
- QUDA has been successfully applied to the post-Monte Carlo analysis phase

- Software architecture for Lattice Field Theory
- Layered software architecture:
- Domain science (application) level, implements algorithms in terms of high-level domain-specific interfaces
- Level 3 (optimization): Plug-in functionality, e.g. linear solvers
- Data-parallel level, provides data types and operations for Lattice Field Theory
- Threading and Message Passing level: Provides abstractions for multi-core/node



Data types

- C++ template library with data-parallel expressions for lattice field theory
- QDP++ captures the tensor index structure of lattice QCD types

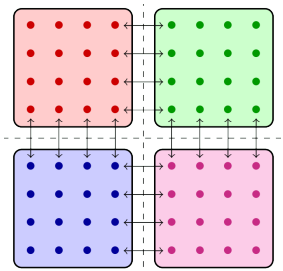
	Lattice	Spin	Color	Reality	built-in
`Real`	Scalar	Scalar	Scalar	Scalar	REAL
`LatticeColorMatrix`	Lattice	Scalar	Matrix	Complex	REAL
`LatticePropagator`	Lattice	Matrix	Matrix	Complex	REAL
`LatticeFermion`	Lattice	Vector	Vector	Complex	REAL

- These data types are implemented with C++ templates

```
typedef
OLattice< PSpinVector< PColorVector< RComplex<REAL>,Nc>,Ns»
LatticeFermion;
```

Parallelization

- `OLattice` ascribes its elements to an N_d-dimensional grid
- The grid is parallelized across multiple MPI ranks



MPI parallelization of the data-parallel container

Operations

- QDP++ provides an "embedded domain-specific, data-parallel language", like HPF
- Whole-array elemental operations, e.g. `z = a * x + y` where a, b and c are arrays.
- Array selection, the ability to refer to subsets of an array, e.g. `z[rb[0]] = a * x + y`
- `Shift` operations as building blocks for stencil operations, e.g. `shift( U[mu] * psi , FORWARD , mu )`
- Configure time parameters: Number of space-time N_d, spin N_s and color N_c indices.
- I/O routines, RNG, etc.

QDP++ (summary)

- It's a virtual machine for Lattice QCD calculations which abstracts architectural details with a high-level interface

- Just adding Level-3 libraries opens a serious Amdahl's law issue:

  On Blue Waters, adding QUDA to Chroma, for our HMC production we see a factor ~ 2 improvement

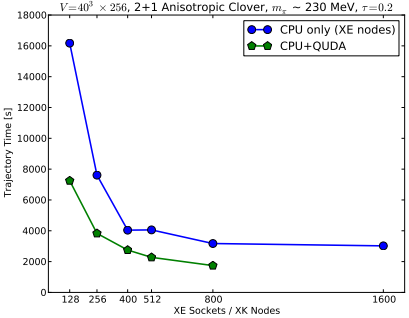
  Many calculations are not accelerated, we are constantly moving data between CPU and GPU memories

- this motivates to move *all* of Chroma to the GPUs
- QDP++ is a framework worth targeting because

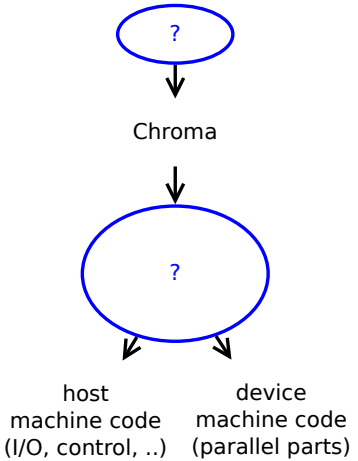
  It implements virtually all functionality of Chroma,

  it is relatively compact,

  and getting it onto GPUs can have an immediate, large impact.



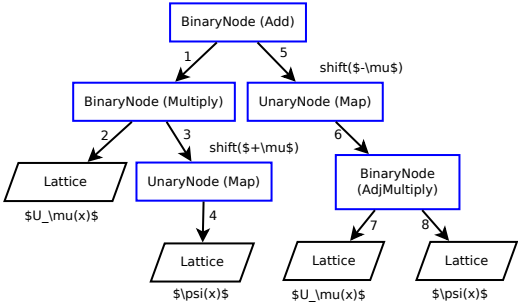
- To date no GPU programming framework can off-load “expressions” to accelerators
  - QDP++ uses *expression templates* to implement operations on the data-parallel container
  - Although CUDA supports C++ templates, refactoring of the Chroma code into “kernels” would be needed
- GPU programming frameworks expose “explicitly managed memory domains”
  - Program control flow determines the order of data accesses, i.e. host or device
  - It’s impractical to add memory copy instructions to the Chroma source code (over 400K C++ code lines)
- Data layout optimization, CUDA kernel tuning, etc.



- QDP-JIT implements QDP++ API with support for NVIDIA GPUs
- Automatic off-loading of expressions to the accelerators
- Multi-GPU support
- Dynamic PTX code generation
- Additional Just-In-Time (JIT) compilation step
- Data layout is optimized for coalesced memory accesses
- Automatic memory transfers via a 'software cache'
- Automatic tuning of CUDA kernels
- Only a general-purpose C++ compiler is required to build the application
  On the compute nodes: No additional compiler is needed, only the CUDA kernel driver

- We use the "structural information" in expression templates to build code generators
- In analogy to static compilers, unparsing the program AST interfaces to a code generator
- However, our approach implements unparsing the AST with the C++ visitor pattern
- While traversing the AST we issue calls to a code generator (PTX)
- NVIDIA JIT compiler generates GPU code

$$U_\mu(x)\psi(x+\hat{\mu}) + U^\dagger_\mu(x-\hat{\mu})\psi(x-\hat{\mu})$$

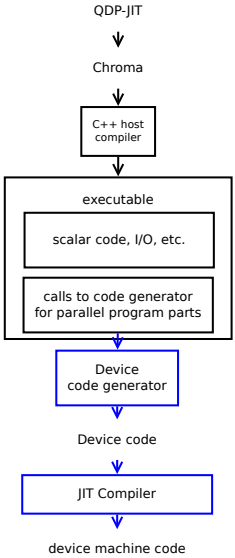


Syntax tree for a simple 1-dimensional nearest-neighbor derivative operator

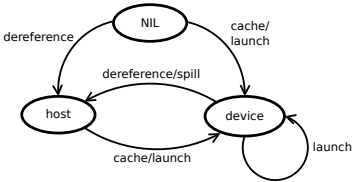
- Standard CUDA code generation toolchain:

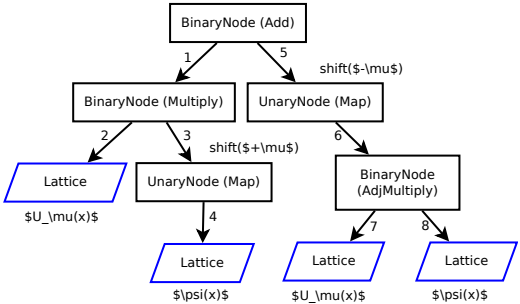
$$\text{CUDA C/C++} \xrightarrow{\text{NVCC}} \text{PTX} \xrightarrow{\text{Linux driver}} \text{GPU code}$$

- PTX (Parallel Thread eXectution), virtual, low-level, machine and instruction set architecture
- The Linux driver JIT-compiles PTX to machine code
- We skip the compilation with NVCC by directly generating our kernels in the PTX language



- We use the “dynamic information” in expression templates to identify data fields
- Prior to a kernel launch we make all data fields available in GPU memory
- The dynamic nature of memory accesses → Use a “cache” for GPU memory
- The cache dynamically spills “least recently used” data fields to CPU memory





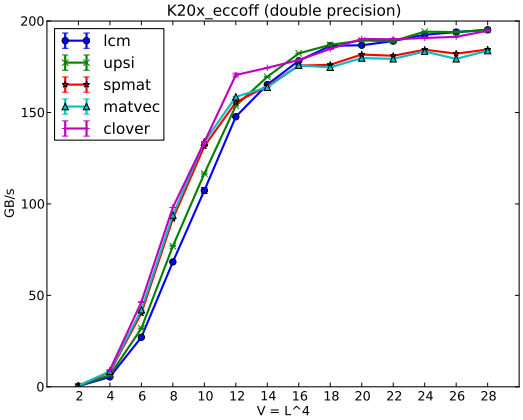
The leaf nodes include references to data fields

- We identified a set of relevant kernels

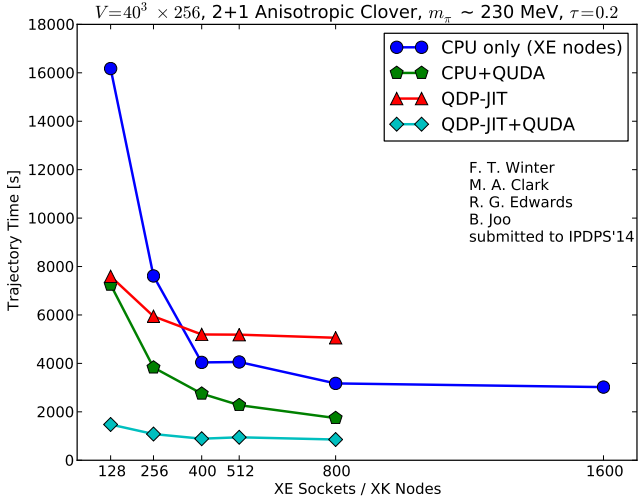
Test	Expression	flop/byte (DP)
`lcm`	$U_1 = U_2 * U_3$	0.458
`upsi`	$\psi_1 = U_1 * \psi_2$	0.5
`spmat`	$\Gamma_1 = \Gamma_2 * \Gamma_3$	0.62
`matvec`	$\psi_0 = U_1 * \psi_1 + U_1 * \psi_2$	0.64
`clover`	$\psi_0 = A * \psi_1$	0.525

- NVIDIA K20x GPU (GK110)
- Peak performance: 1.3 TFlops (DP)
- Peak memory bandwidth: 250 GB/sec (ECC disabled)

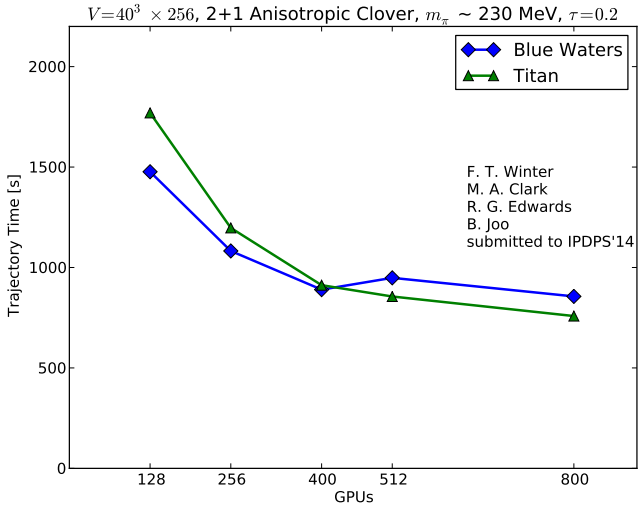
- "Performance shoulder" at around $V = 12^4$ due to SM occupancy
- Our generated kernel sustain up to 79% of peak memory bandwidth



- QDP-JIT allows us to deploy the full Chroma gauge-generation program in production on large-scale GPU-based machines such as Titan (OLCF)
- QUDA device interface understands QDP-JIT's datalayout
- Speedup factor of $\sim$ 11.0 on 128 GPUs/CPU sockets
- Speedup factor of $\sim$ 3.7 on 800 GPUs/CPU sockets



- The Blue Waters and Titan results are hardly distinguishable
- Our benchmark timings on these systems typically show some amount of fluctuation



Conclusions

- QDP-JIT provides a QDP++ API with support for the CUDA architecture
- QDP++ implements an embedded data-parallel language
- The expression templates are of enabling character for this work
- A JIT compiler from a low-level assembler to accelerator code is required
- This work reduced the computational cost for our production simulations on Titan by a factor of ~ 5

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