Computational Advances and Precision Kaon Physics

Lattice QCD simulations are now regularly being done with physical values for the light, strange and charm quarks. This allows many complicated phenomena to be investigated with direct impact on experiments. One example is the precision kaon physics being pursued by the RBC and UKQCD Collaborations, where the first calculation of direct CP violation in kaon decays has been done. In order to reduce the errors on this result, advances in algorithms and software are needed. Here we discuss the zMobius formulation of Domain Wall Fermions and the improvments it has led to date. The CPS code is currently being evolved to utilize the Grid software of Peter Boyle, to be ready to exploit Intel's Knights Landing architecture when it becomes available early next year. An early target for our research is the reduction of the errors on this direct CP violation calculation as soon as the Knight's Landing machines become available.

Knights Landing

- Kaon decays to two pions are well measured experimentally.
- The Standard Model predicts the details of these decays, but requires knowledge of quark properties inside kaons/pions.
- Knowledge of quark properties is determined from first principles through Lattice QCD.

SciDAC-3 HEP
Paul MacKenzie, PI

Robert Mawhinney
Columbia University

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Direct CP violation in kaons

- For kaons, the size of the violation of charge conjugation (particle ↔ antiparticle) and parity (physical process ↔ mirror image of process) symmetry (CP symmetry violation) is determined by the values for

$$\eta_{00} = \frac{A(K_L \to \pi^0 \; \pi^0)}{A(K_s \to \pi^0 \; \pi^0)} = \epsilon - 2\epsilon'$$

$$\eta_{+-} \equiv \frac{A(K_L \to \pi^+ \; \pi^-)}{A(K_s \to \pi^+ \; \pi^-)} = \epsilon + \epsilon'$$

- Non-zero values are found by experiments, so CP violation exists:

$$|\epsilon| = (2.228 \pm 0.011) \times 10^{-3}$$

$$\mathrm{Re}(\epsilon'/\epsilon) = (1.65 \pm 0.26) \times 10^{-3}$$

- To relate ε to the Standard Model, quark properties in mesons are needed. These are contained in a parameter, called B_K, while all other terms in this formula can be measured independently.

$$\varepsilon_K = \kappa_\varepsilon \, C_\varepsilon \, \hat{B}_K \, \mathrm{Im}(\lambda_t) \left\{ \mathrm{Re}(\lambda_c)[\eta_1 \, S_0(x_c) - \eta_3 \, S_0(x_c, x_t)] - \mathrm{Re}(\lambda_t) \, \eta_2 \, S_0(x_t) \right\} e^{i\pi/4}$$

- B_K is currently known to 1.3% accuracy, after many years of lattice QCD work (Eur. Phys. J. C74 (2014) 2890).

$$\hat{B}_K = 0.7661(99)$$

- Many other lattice calculations, particularly involving heavy quarks, are also used to relate different Standard Model parameters to experiment.
- A first complete calculation for ε' has recently been completed by the RBC and UKQCD Collaborations (arXiv:1505.07863) yielding

$$\mathrm{Re}(\epsilon'/\epsilon) = (0.138 \pm 0.515_{stat} \pm 0.443_{sys}) \times 10^{-3}$$

- This result is slightly over 2σ from the experimental value
- Many important theoretical physics techniques are required in this calculation and the value is sensitive to physics beyond the Standard Model
- The biggest numerical hurdle is the calculation of disconnected quark diagrams, which are only connected only by gluons and are statistically noisy
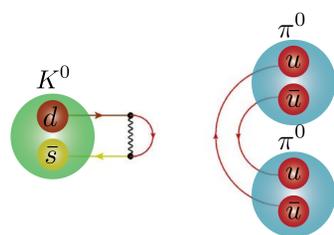

## Algorithmic and Software Improvements

- These direct calculations of K→ ππ amplitudes already incorporate a large number of sophisticated algorithmic and theoretical techniques:
  * G-parity boundary conditions to get two moving pions in a box with the correct kinematics
  * Lanczos algorithm to calculate low modes
  * All-to-all propagators with low mode deflation
  * Pion sources and sinks split in time
  * Subtraction of the vacuum intermediate state to reduce statistical errors
  * Non-perturbative renormalization to normalize the matrix elements correctly
- Faster computers will reduce statistical errors
- The systematic errors can also be markedly reduced with more computation.
- Current steps to improve the calculation:
  * Improve methodology: zMobius formulation for the quarks
  * Ready our software for the next generation of computers:

Improving Domain Wall Fermion Algorithms

- These complicated kaon properties can only be calculated if our discretized system has all of the symmetries of the continuum system.
- Domain wall fermions provide this, by adding a fifth dimension to our problem and localizing the left and right handed quarks on opposite boundaries of the fifth dimension
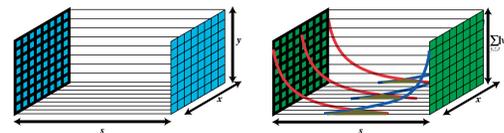
- This increases the computation cost by substantial factor
- Reducing L_s, the length of the fifth dimension, while preserving the symmetries, reduces the cost.
- Mobius Domain Wall Fermions are a variant formulation with reduced L_s (arXiv:1206.5214)
- Making the parameters in the Mobius formulation complex reduces L_s further. This is called zMobius and was developed by Blum, Izubuchi, Jung, Lehner and Syritsyn at BNL.
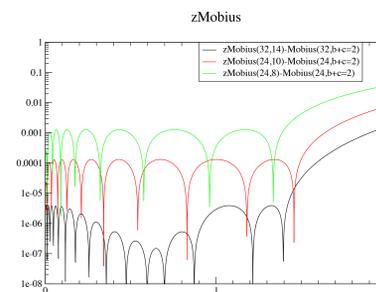
zMobius

- Can reduce L_s from 32 to 14 with very little change in the Dirac operator
- The number of iterations for a conjugate gradient solution increases markedly when moving from the original Domain Wall Fermion formulation to Mobius to zMobius.
- Improved preconditioners ameliorate this somewhat, but further improvements in preconditioners would be useful and would immediately lead to faster solves.
- Coding effort required to implement complex parameters and variant preconditioners in our high-performance codes (Jung).

zMobius in Generation of QCD Ensembles

- For precision measurements of the $K_L - K_S$ mass difference, we need QCD ensembles that include a physical charm quark and have small lattice spacing (1/a ≈ 3 GeV).
- The RBC and UKQCD Collaborations are generating 2+1+1 flavor Mobius DWF ensembles on Mira at the ALCF.
- Greg McGlynn (Columbia) and Chulwoo Jung (BNL) have implemented zMobius into our evolution code.
- We are running in production now on 12 racks of Mira, using zMobius with L_s = 14 in the molecular dynamics part of our L_s= 32 evolution.
- We see a factor of about 1.5 speedup from the use of zMobius.

zMobius in Measurements

- The all mode averaging technique of Blum, Izubuchi and Shintani (PRD 88 (2013) 9, 094503) allows many measurements to be done with reduced precision, or some other approximation. A correction term calculates the deviation between the approximation and the precise value, but is calculated less often, resulting in substantial reduction in cost.
- zMobius can easily play the role of the approximation, pushing to very small values for L_s.
- Currently in use for nucleon and heavy quark measurements. Being extended to other measurements, such as kaon physics.
- Speed-ups by a factor of a few are expected, in addition to O(10-100) speed-up already achieved with all mode averaging and deflation techniques.

Software Preparation for Next Generation Architectures

- The RBC and UKQCD Collaborations have used highly optimized BGQ code written by Peter Boyle of the University of Edinburgh for the conjugate gradient solvers in our ensemble generation and precision kaon calculations
- Peter Boyle has developed a new data parallel QCD library, called Grid, to exploit the next generation of architectures, particularly the Knights Landing from Intel.
- Grid is under active development by Boyle and Yamaguchi at the University of Edinburgh and Cossu at KEK in Japan, with more contributions from BNL and RBC members beginning.
- Evolving the CPS QCD codes to work with Grid is underway at BNL, lead by Chulwoo Jung.
- Our immediate task is to rewrite our K→πππ measurement code in Grid, to be ready to run on Cori, or other KNL hardware, by early 2016.
- Some information about Grid is presented here, based on Boyle's poster at Lattice 2015

  https://indico2.riken.jp/indico/getFile.py/access?contribId=24&sessionId=15&resId=0&materialId=poster&confId=1805

- Because Grid's underlying data layout allows parallelizatoin at the SIMD, OpenMP and MPI level, very high efficiency is achieved for code that is written in C++.

We present progress on a new C++ data parallel QCD library. It enables the description of cartesian fields of arbitrary tensor mathematical types.

Ddata parallel interface, conformable array syntax with Cshift and masked operation (c.f. QDP++, cmfortran or HPF).

Three distinct forms of parallelism are transparently used underneath the single simple interface:
- MPI task parallelism
- OpenMP thread parallelism
- SIMD vector parallelism.

The SIMD vector parallelism achieves nearly 100% SIMD efficiency due to the adoption of a virtual node layout transformation, similar to those in the Connection Machine.

This ensures identical and independent work lies in adjacent SIMD lanes. SSE, AVX, AVX2, AVX512 and Arm Neon SIMD targets are implemented.

The library is under development. Solvers for Wilson, Domain, and multiple 5d chiral fermions (Cayley, Continued fraction, partial fraction) are implemented.

GRID parallel library

- Geometrically decompose cartesian arrays across nodes (MPI)
- Subdivide node volume into smaller virtual nodes
- Spread virtual nodes across SIMD lanes
- Use OpenMP+MPI+SIMD to process conformable array operations
- Same instructions executed on many nodes, each node operates on four virtual nodes
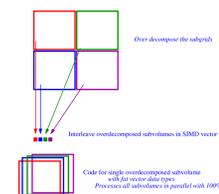
- Conclusion: Modify data layout to align data parallel operations to SIMD hardware
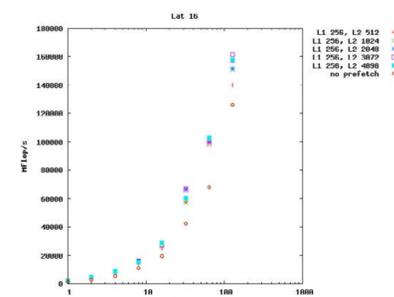- Conformable array operations simple and vectorise perfectly

```
std:vector<int> grid ({ 8,8,8,8 });
std:vector<int> simd_layout ({ 1,1,2,2 });
std::vector<int> mpi_layout  ({ 1,1,1,1 });

CartesianGrid Grid(grid,simd_layout,mpi_layout);

LatticeColourMatrix A(Grid);
LatticeColourMatrix B(Grid);
LatticeColourMatrix C(Grid);

A = B * C;
```


- New algorithms and evolution of our code base will allow us to exploit the new resources as soon as they become available.
- Precision calculations continue to improve constraints on the Standard Model

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