Lattice QCD and NERSC requirements

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Lattice Gauge Theory at NERSC

First-principles computations in QCD
Computations in other strongly coupled field theories

- Find hadronic factors to get fundamental physics from experiments
- Understand structure and interactions of hadrons
- Understand QCD: confinement and chiral symmetry breaking
- Other strongly interacting theories (could the Higgs be composite?)
- Quark-gluon matter at high temperatures (early universe) or high densities (neutron stars)

Current HEP LQCD projects at NERSC

- Production and analysis of QCD configurations with dynamical quarks, (Doug Toussaint) (MILC collaboration)
- Heavy quarks, using the MILC collaboration lattices (Junko Shigemitsu) (HPQCD collaboration)
- Parameters for Wilson-type quarks (Carleton DeTar)(USQCD collaboration)
- High temperature QCD in volumes about the size of a RHIC collision. (Bernd Berg)
- Field theories that might explain composite Higgs particles, and other approaches to the low quark mass limit. (Don Sinclair)

Example: signs for new physics

$$\begin{pmatrix} d_W \\ s_W \\ b_W \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d_m \\ s_m \\ b_m \end{pmatrix}$$

CKM matrix: "weak eigenstates" of quarks are mixtures of "mass eigenstates".
If the standard model is complete, that matrix must be unitary.
So look to see if rows are magnitude one and orthogonal.
If not, you are on the trail of physics beyond the standard model.

A current example:

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9999(6)$$
$$|V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2 = 1.067(47)$$

Biggest errors from V_{us} and V_{cs} respectively. V_{us} can be found from

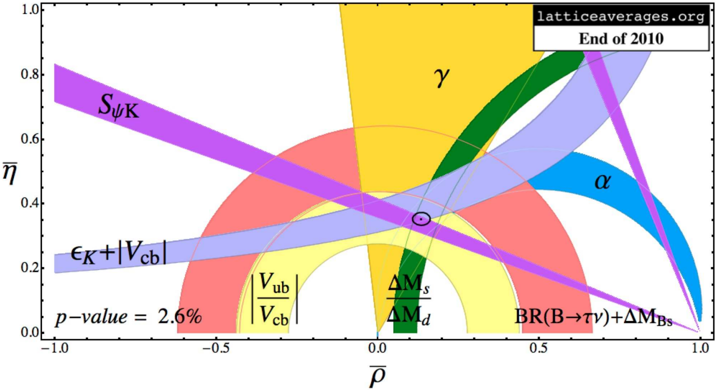
$$\Gamma(K \to l\nu) = (constants) \times |V_{us} f_K|^2 \quad .$$

This is an example of the generic form

$$\text{experiment} = (constants) \times \text{fundamental} \times \text{lattice} \quad .$$

Need to find f_K from lattice calculations. (Note: V_{ub} isn't known to good fractional accuracy, it doesn't matter much in the above equation because it is small.)
J. Beringer *et al.*, (PDG) Phys. Rev. D **86**, 010001 (2012)

A “unitarity triangle”:



Global fit of the CKM unitarity triangle [?]. The constraints labeled $\epsilon_K + |V_{cb}|$, $|V_{ub}/V_{cb}|$, $\Delta M_s/\Delta M_d$, and $\mathrm{BR}(B \to \tau\nu) + \Delta M_{B_s}$ all require LQCD input, while the others require minimal or non-lattice theoretical input. The solid ellipse encloses the 1σ region. (From 2011 USQCD proposal, thanks!)

Improvements in next few years?

From a USQCD proposal 2011 (thanks!)

Quantity	CKM element	Present exp. err.	Present lat. err.	2014 lat. err.	2020 lat. err.
f_K/f_π	$\|V_{us}\|$	0.2%	0.6%	0.3%	0.1%
$f_+^{K\pi}(0)$	$\|V_{us}\|$	0.2%	0.5%	0.2%	0.1%
$D \to \pi\ell\nu$	$\|V_{cd}\|$	2.6%	10.5%	4%	1%
$D \to K\ell\nu$	$\|V_{cs}\|$	1.1%	2.5%	2%	$< 1\%$
$B \to D^{(*)}\ell\nu$	$\|V_{cb}\|$	1.8%	1.8%	0.8%	$< 0.5\%$
$B \to \pi\ell\nu$	$\|V_{ub}\|$	4.1%	8.7%	4%	2%
$B \to \tau\nu$	$\|V_{ub}\|$	21%	6.4%	2%	$< 1\%$
ξ	$\|V_{ts}/V_{td}\|$	1.0%	2.5%	1.5%	$< 1\%$
ΔM_s	$\|V_{ts}V_{tb}\|^2$	0.7%	10.5%	5%	3%

Scaling to better accuracy

How does the computing time scale with accuracy of result?
Suppose you want to reduce errors by factor of two.
You are already "balanced", so all errors are same order of magnitude.
So you must reduce them all by factor of two
Statistical errors $\propto N^{-1/2}$, so need factor of 4.
Discretization errors, go as a^2, $a \rightarrow a/\sqrt{2}$, $N_{points} \rightarrow 4 \times N_{points}$.
Worse condition number, $CG \rightarrow \sqrt{2}CG$.
Finite volume effects $\propto e^{-m_\pi L}$, $L \rightarrow L + 1$ fm,
$5.5^3 -> 6.5^3 fm = 1.7$X.
SUMMARY:
$4_{stat.} \times 4_{disc.} \times \sqrt{2}_{cond.} \times (6.5^3/5.5^3)_{volume} \approx$ 37
Algorithm improvements might make this better

New developments

- Five years is a long horizon for theorists' planning; entirely new directions might appear.

A “Case Study”

QCD with four dynamical quarks
MILC collaboration
Claude Bernard (Washington University)
Carleton DeTar (University of Utah)
Steve Gottlieb (Indiana University)
Urs Heller (American Physical Society)
Jim Hetrick (Pacific University)
Jack Laiho (Edinburgh)
Bob Sugar (Univ. of Calif. Santa Barbara)
Doug Toussaint (University of Arizona)
Ruth Van de Water (Fermilab)
Postdocs and grad students
Combine with Fermilab lattice collaboration for “heavy-light” physics

Case Study

- Use Monte Carlo simulation
- Generate properly weighted samples of QCD field configurations
- Basically doing the Feynman path integral numerically
- Molecular dynamics evolution of four (space+time) dimensional lattices with non-local forces coming from the quarks
- In common with many other large computational projects: Integration of hyperbolic PDE's, and iterative solution of sparse matrix problems.
- An extra kicker that boosts the flops needed: do everything a few thousand times to average over

Current simulations

- NERSC: 60 M Hopper hours this year
- Other resources from NSF centers, USQCD program (DOE)
- NERSC this year is about 20% of the total computing for this simulation program
- Starting a simulation with four dynamical quark flavors, at the physical quark masses, with lattice spacing 0.06 fm and spatial size 5.5 fm.
- Using 18432 Hopper cores, a simulation time unit takes 2.15 hours (physically, $\approx 10^{-23}$ seconds) Uses about 500 GB memory (not much by current standards) Limited mostly by memory and IPC bandwidths

4-5 years ahead

- Lattice spacing 0.03 fm at the physical quark mass!
  A lattice spacing small enough to resolve B physics
- Box size 7.5 fm
  A box large enough for a nucleon's "pion cloud", or a couple of nucleons
- $\rightarrow 256^3 \times 512$ lattice
- Four flavors of dynamical quarks, at their physical masses
- Approximately a factor of 150 increase in flops.
- Approximately a factor of 50 increase in memory and IO
- Why more flops per byte?
- Mostly because we are resolving more length scales:

Length scales in problem

UV cutoff	0.03×10^{-13} cm.
B quark Compton Wavelength	0.07×10^{-13} cm.
Hadronic size	1×10^{-13} cm
Simulation box size	7.5×10^{-13} cm
$\frac{1}{m_{quark}}$	70×10^{-13} cm

($1/m_{quark}$ affects flop count, but not lattice size.)
Generic discretization errors $\propto a^2$.

What does it take?

- HECH = "Hopper-equivalent core-hour"
- Generate lattices: 3.6×10^{10} HECH
- Hadron spectrum: 4.2×10^{10} HECH
- Three point functions: 10×10^{10}?? HECH
- Memory $\approx$ 25 TB ???

Disclaimer

This hypothetical case study is a scaling up of a project that we are now running at NERSC and other centers. Thus estimating time in hopper-equivalent core-hours is fairly straightforward. In making the time estimates we have not assumed any algorithmic breakthroughs, although it is possible that advances such as application of multigrid techniques for sparse matrix solution will bring significant improvement. Although the time estimate is made with a particular choice of discretization of the underlying differential equations, and a particular algorithm for the Monte Carlo sampling, we expect that the physical parameters of this sample problem will be what is needed in the 2017 time frame. Your mileage may vary.

Computational challenges

Need to efficiently use 100-core chips or GPU's
(Hopefully we will be supported by compilers/ software libraries)
Need to implement new algorithm developments
(Of course, predicting a good idea is impossible)
Need to manage and focus power of next-generation computers.