NERSC Requirements Workshop

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Lattice gauge theory

and some other HE theory

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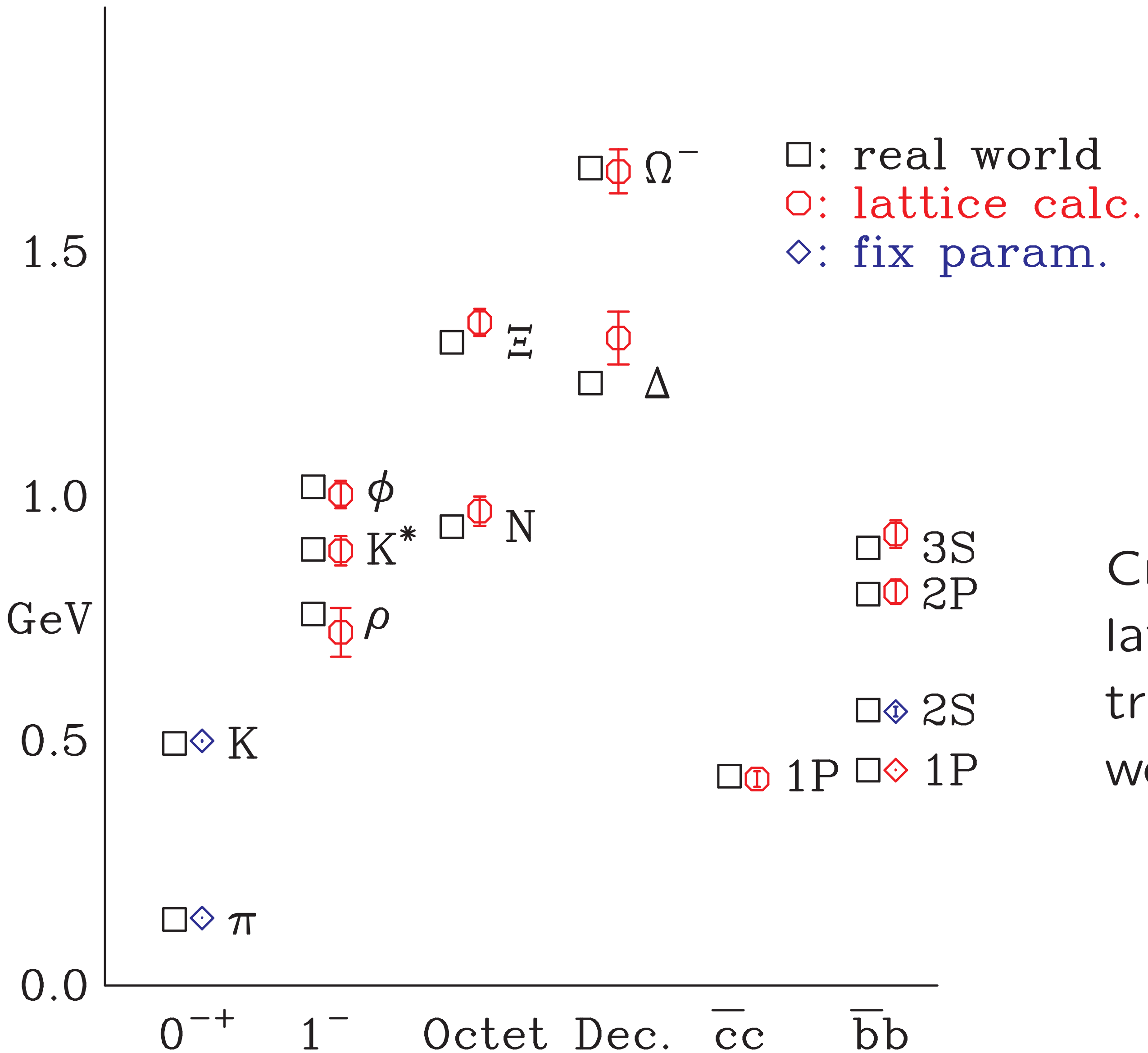
Help from: Paul Mackenzie (Fermilab)



Crude comparison of lattice hadron spectrum to the real world.

Lattice Gauge Theory

First-principles computations in QCD
Also, computations in other strongly coupled field theories

- Find hadronic factors to get fundamental physics from experiments
- Understand structure and interactions of hadrons, maybe even nuclei
- Understand QCD: confinement and chiral symmetry breaking
- Other strongly interacting theories (what if we don't find the Higgs?)
- Quark-gluon matter at high temeratures (RHIC, LHC, early universe) or high densities (neutron stars)

HEP theory projects at NERSC now:

- Production and analysis of QCD configurations with dynamical quarks, (Doug Toussaint) (MILC collaboration)
- Heavy quarks, using the MILC collaboration lattices (Junko Shigemitsu) (HPQCD collaboration)
- Computation of perturbative processes. (Zvi Bern)
- 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)
- Strongly coupled Higgs (what if LHC doesn't find a low mass Higgs?) (George Fleming) (start-up)
- Chiral gauge theory and mirror fermions. (Erich Poppitz) (startup)

The same list, organized by motivation:

- Calculate hadronic factors, relate theory to experiment: (Doug Toussaint) (MILC collaboration) (Junko Shigemitsu) (HPQCD collaboration)
- Understand QCD backgrounds to LHC data (Zvi Bern)
- LHC, RHIC, early universe, neutron stars (QCD at high T and pressure) (Bernd Berg)
- Understand seeming "fine tunings" in standard model, (Don Sinclair), (George Fleming))
- Explore possibilities for new (deeper?) theories. (Erich Poppitz)

The lattice QCD environment

- US funding: DOE HEP, DOE NP, DOE USQCD, NSF
- Note nuclear physics LGT projects are also at NERSC
- World resources (from USQCD proposal)
  - USA: 2007: est. 15 teraflops-sustained
  - Germany, 2007: est. 10-15 teraflops-sustained
  - Japan, 2007: est. 14-18 teraflops-sustained
  - Italy, 2007: est. 5 teraflops-sustained
  - UK, 2007: est. 4-5 teraflops-sustained

estimates by USQCD executive committee

1 LGT TF $\approx$ 5 linpack TF

How accurate a result do we need in five years?

What will this mean for computing requirements?

Example of possible smoking gun

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

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:

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9977(5_{ud})(12_{us})(0_{ub})$$

Biggest error from V_{us}, which 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.)

Improvements in five years?

From a USQCD proposal 2008 (thanks!)

CKM elem.	Quantity	2008 exp. err.	2008 latt. err.	2014 latt. err.	error from non-lattice theory
V_{us}	f_K/f_π	0.3%	0.9%	0.3%	-
V_{us}	$f_{K\pi}(\vec{p}=0)$	0.4%	0.5%	0.2%	1%(ChPT)
V_{cd}	$D \to \pi l \nu$	3%	11%	4%	-
V_{cs}	$D \to K l \nu$	1%	11%	2%	5%(ν scatt.)
V_{cb}	$B \to D^* l \nu$	1.8%	2.4%	0.8%	<2%(Incl. $b \to c$)
V_{ub}	$B \to \pi l \nu$	3.2%	14%	4%	10%(Incl. $b \to u$)

Note at least one case where experimental error is 1/10 theory error

- need to keep up

A “unitarity triangle”.

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, $a \to a/\sqrt{2}, N_{points} \to 4 \times N_{points}$.

Worse condition number, $CG \to \sqrt{2}CG$.

Chiral extrap – from current $m_l \approx 0.1 m_s$ to $m_l \approx 0.8 m_s$, CG iterations up by $1/.8 = 1.25$.

Finite volume effects $\propto e^{-m_\pi L}$, $L \to L + 1$ fm, $4^3 -> 5^3 fm = 2$X.

SUMMARY:

$4_{stat.} \times 4_{disc.} \times \sqrt{2}_{cond.} \times 1.25_{chiral} \times (5^3/4^3)_{volume} \approx$ 55

Algorithm improvements might make this better

New developments

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

- The area that I think is likely to show major growth is studies of Higgs particle physics. A burst of computational activity about 15 years ago died out, but anything other than a standard model Higgs at the LHC will start a gold rush.

Some guesses on growth in 3-5 years:
My guess -DT or provided by PI

- MILC(Toussaint) factor of 20 = 400 M XT4
- HPQCD(Shigemitsu) personel limited, 0 to 18M XT4
- QCD Perturbation Theory (Bern) 1.5 M XT4 next year relatively small
- Hot QCD in small volume (Berg) 100M doubtful
- Chiral QCD, (Sinclair) possibly just small increases
- Strongly coupled QCD, (Fleming) Possible explosive growth
- New theories. (Poppitz) probably remain relatively small
- New projects coming in — There are other US groups doing computational high energy theory — a real wildcard

QCD with 3(or 4) dynamical quarks

Case Study

MILC collaboration

Claude Bernard (Washington University)(PI)
Carleton DeTar (University of Utah)(PI)
Steve Gottlieb (Indiana University)(PI)
Urs Heller (American Physical Society)(PI)
Jim Hetrick (Pacific University)(PI)
Bob Sugar (Univ. of Calif. Santa Barbara)(PI)
Doug Toussaint (University of Arizona)(PI)
Postdocs and grad students
Combine with Fermilab lattice collaboration for “heavy-light” physics

- Study the fundamental strong interaction (QCD)
- Especially, calculations needed to get fundamental parameters
- Precise calculations could expose new physics
- Quark masses, quark mixing angles, dark matter cross section

- 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
- Two-stage process: First generate and store "lattices", then re-process them to calculate hadron properties. Same basic codes, but second stage can also be embarrassingly parallel.

Current usage

- NERSC: 13 M Franklin 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
- Generating configurations with "HISQ" (next generation) action while analyzing current "Asqtad" (used for last ten years) action.
- Current generation: $64^3 \times 144$ lattice, using 6144 cores, two simulation time units takes 5.5 hours (think $\approx 10^{-23}$ seconds) Uses about 70 GB memory (not much by current standards) Limited mostly by memory and IPC bandwidth

What role does NERSC play in this?

- Only a few machines can do the largest lattices with lightest quarks.
- Currently that would be Franklin, Kraken (ORNL CRAY) and Intrepid (ANL BGP).
- presumably NERSC's incoming system
- Also, convenient debug/development environment

2-3 years ahead

Goals: reduce errors on masses and mixings to one percent

(Lattice spacing 0.06 fm at the physical quark mass!)

$96^3 \times 144$ lattice

Approximately a factor of 20 increase in flops.

Only a factor of 4 increase in memory and IO

Why more flops per byte?

Mostly because we are resolving more length scales:

UV cutoff	0.06×10^{-13} cm.
Hadronic size	1×10^{-13} cm
Simulation box size	6×10^{-13} cm
$\frac{1}{m_{quark}}$	70×10^{-13} cm

Computational challenges and possibilities

Need to understand 100-core chips or GPU's
(Hopefully we will be supported by compilers/ software libraries)
Need to implement any new algorithm developments
(Of course, predicting a good idea is impossible)
Need to keep human resources available and **focussed**
(no joke — this may be the largest challenge)