Predictive Lattice QCD

Andreas S. Kronfeld

Fermilab
Preface
Predictive Lattice QCD

QCD is quantum chromodynamics, the modern theory of the strong (nuclear) force. Quarks & gluons $\Rightarrow$ hadrons.

Lattice QCD is a way to calculate long-distance properties with a lot of computing—$O(10)$ Tflop-years’ worth.

Any computational enterprise is more persuasive if it can predict something before it’s been measured.
PC Clusters at Fermilab
Introduction: the long and short of QCD.

Reflection: Why are we here?

Challenge: obstacles to lattice QCD.

Success: numerical simulation + effective field theory.

Predictions: calculations preceding measurements.

Outlook: influences on flavor physics and beyond.
The Long & Short of QCD
Quantum chromodynamics is part of the Standard Model.

SU(3) gauge symmetry.

Mathematically almost like QED, “just messier.”

QCD possesses asymptotic freedom, so at short distances perturbation theory is accurate and quantitative.

Chromodynamics is not like electrodynamics at all.
Lagrangian of QED, QCD

\[ \mathcal{L}_{\text{QED}} = -\frac{1}{4} F_{\mu \nu} F^{\mu \nu} - \bar{e} (\not\!D + m_e) e \]

\[ D^\mu = \partial^\mu + i e A^\mu \]

\[ F_{\mu \nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \]

\[ \mathcal{L}_{\text{QCD}} = -\frac{1}{4} F^{a}_{\mu \nu} F^{\mu \nu a} - \bar{q}_i (\not\!D_{ij} + m_q) q_j \]

\[ D_{i j} = \partial^\mu \delta_{i j} + g t^a_{i j} A^{\mu a} \]

\[ F^{a}_{\mu \nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^{a}_\mu A^{b}_\nu \]

\( U(1) \) photon \( A_\mu \)

\( SU(3) \) gluons \( A^a_\mu \)

electron \( e \)

electron \( q_i \)
QCD compared to QED

In QED, virtual electron-positron pairs screen the bare charge:

\[ F(r) = -\frac{\alpha(r)}{r^2}, \quad \alpha = \frac{e^2}{4\pi} \]

In QCD, gluons, as well as quarks, carry color. They anti-screen:

\[ F(r) = -\frac{4\alpha_s(r)}{3r^2}, \quad \alpha_s = \frac{g^2}{4\pi} \]
Asymptotic Freedom

\[ \alpha_{sF}(r) \equiv -\frac{3}{4} r^2 F(r) \]
Asymptotic Freedom Rocks

Because of asymptotic freedom, QCD is the “star” of the SM.

It is theoretically consistent at all length scales in contrast to the U(1) and Higgs sectors, where triviality says the theory must be replaced at some high scale.

QCD’s short-distance behavior can be calculated accurately.

Multi-GeV energies, multi-GeV temperatures, high densities.
Single-jet Cross Section

CDF Run II Preliminary

$K_T D = 0.7 - 0.1 < |y| < 0.7$

- Data
- Systematic Errors
- NLO (CTEQ61)
- NLO Uncertainties

$L = 145 \text{ pb}^{-1}$

NLO: JETRAD

$\mu_R = \mu_F = p_T^\text{MAX}/2$

No Had. / Und. Event Correction

DØ Run II preliminary

$\sqrt{s} = 1.96 \text{ TeV}$

$L = 378 \text{ pb}^{-1}$

- $|y| < 0.4$ (x10)
- $0.4 < |y| < 0.8$

NLO QCD
CTEQ6.1M

$\mu_R = \mu_F = p_T$

Agreement between data and NLO QCD PT over 8 orders of magnitude!
Running of $\alpha_s$

- **$\tau$ decay**
- **lattice QCD**
- **high-$E$ scattering**

![Running of $\alpha_s$](image)
Prize-worthy

The Nobel Prize in Physics 2004

"for the discovery of asymptotic freedom in the theory of the strong interaction"

David J. Gross

H. David Politzer

Frank Wilczek

1/3 of the prize
USA

1/3 of the prize
USA

1/3 of the prize
USA

Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, USA

California Institute of Technology, Pasadena, CA, USA

Massachusetts Institute of Technology (MIT), Cambridge, MA, USA

b. 1941

b. 1949

b. 1951
Long Distances

QCD is enormously successful at short distances, but ...

... at distances greater than $1 \text{ fm} = 10^{-15} \text{ m}$, QCD forces become strong.

Quantitatively, the perturbation series breaks down.

Qualitatively, quarks and gluons are confined into hadrons.
General-purpose tools—symmetry, unitarity, renormalization group, etc.—are not enough to calculate even the simplest properties of hadrons (masses, decay constants, ...).

What is needed is a definition of quantum field theory, including gauge theories like QCD, that is non-perturbative from the outset.

With such a tool, we could solve old problems—like the calculation of the hadron spectrum ...

... and new problems in particle, nuclear, & astro physics.
On Beyond QCD
Parts of the “Standard Model” are Laws of Nature

- gauge symmetry $SU_c(3) \times SU_L(2) \times U_Y(1)$
- gauge quantum numbers of quarks, leptons

Parts are known, but not understood

- EWSB: $SU_L(2) \times U_Y(1) \rightarrow U_{EM}(1)$
- Flavor: fermion masses and mixing
Standard Quark Fields

two-component fields, with weak isospin $\frac{1}{2}$

\[
\begin{align*}
(u_d)_L & \quad (c_s)_L & \quad (t_b)_L \\
\{u_R, d_R, c_R, s_R, t_R, b_R \}\text{ which do not} & \\
\text{one-component fields, with weak isospin 0}
\end{align*}
\]

which interact with $W$s
SU_L(2) symmetry is chiral and, thus, forbids quark masses

masses couple Left and Right

Standard Model introduces one scalar doublet \( \phi \)

\[
y^u_{11} \bar{u}_R (\phi^0 \phi^+) \left( \begin{array}{c} u \\ d \end{array} \right)_L + y^d_{11} \bar{d}_R (\phi^- \phi^{0*}) \left( \begin{array}{c} u \\ d \end{array} \right)_L + \text{h.c}
\]

Electroweak symmetry breaking: \( \langle \phi^0 \rangle \neq 0 \)
Also have

\[ y_{13}^u \bar{u}_R (\phi^0, \phi^+) \begin{pmatrix} t \\ b \end{pmatrix}_L + y_{13}^d \bar{d}_R (\phi^-, \phi^{0*}) \begin{pmatrix} t \\ b \end{pmatrix}_L + \text{h.c.} \]

(and all other combos)

So, as well as quark masses, these interactions lead to all sorts of generation-changing interactions.

Provides the Standard source of \( CP \) violation.

We know only that something like this happens; we do not know if the details are so simple.
Masses and CKM

Masses

- \( m_u < m_d; \) \( m_c > m_s; \) \( m_t > m_b. \)

Cabibbo-Kobayashi-Maskawa (CKM) matrix

\[
V = \begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
V_{cd} & V_{cs} & V_{cb} \\
V_{td} & V_{ts} & V_{tb}
\end{pmatrix}
\]

Complex elements violate \( CP \)
Why are we here?

Several mysteries in the microscopic world ...

- electroweak symmetry breaking
- (full) origin of $CP$ violation
- pattern of quark masses

... without which we cannot exist.

Hence, we want to study the microscopic couplings of quarks.
Where are the quarks?

Alas, the strong interactions are, well, too strong.

Experiments do not detect quarks, they detect hadrons.

To “measure” quark properties, theorists have to
- understand why (quark confinement)
- calculate effects of the strong interactions
Almost all the mass of ordinary matter comes from the chromodynamic energy of gluons and quarks whizzing around inside protons and neutrons.
Lattice QCD
Lattice Gauge Theory

Feynman functional-integral formulation of QFT:

- everything is a (infinite-dimensional) integral.

Field theory defined on a space-time lattice.

Wilson (1974) showed how to put non-Abelian gauge symmetries into lattice field theory.

A simple and compelling explanation of confinement.
Spacetime Lattice

Spacing $a$ gives UV cutoff

Box-size $L$ gives IR cutoff

Euclidean metric $t = ix_4$ yields positive weight

$L = N_s a$

space $\rightarrow$

time $\uparrow$

$\Box-size L$ gives IR cutoff
Lattice QCD

Lattice gauge theory provides a non-perturbative definition of the Lagrangian of lattice QCD. The Lagrangian has 1 + $n_f$ parameters.

Lattice gauge theory + numerical simulation allows one to compute the integrals numerically.

With $a \neq 0$ and $L, L_4 < \infty$, the problem is finite.

With positive weights, Monte Carlos methods work.
Many Scales in QCD

- Characteristic scale, $\Lambda_{\text{QCD}}$, around $m_\rho = 770$ MeV
- Coupling $\alpha_s(q) \sim 1$ for $q \sim 250$ MeV
- Chiral symmetry scale $m_K^2/m_s \approx 2500$ MeV

- Light quarks: $m_u, m_d \ll m_s \sim 80$ MeV $\ll \Lambda_{\text{QCD}}$
- Heavy quarks: $m_b \gg m_c \approx 1400$ MeV $> \Lambda_{\text{QCD}}$
- Top quark: $m_t \approx 175$ GeV, so decays before hadronizing.
Many Scales in Lattice QCD

QCD scales

MC scales
Mercedes: So, some dude at Cornell won the Nobel Prize in physics this year [1982]. Do you know him?

Andreas: Yes, I know Ken Wilson.

Mercedes: What did he do?

Andreas: He studied how to approach problems with more than one length scale. He said to study one scale at a time.

Mercedes: What’s so clever about that?
Effective Field Theories

A powerful framework for separating physics at different length scales.

Effective Lagrangian

- “short-distance” physics lumped into coefficients,
- “long-distance” physics described by operators.

Cascade of EFTs; matching calculations.
EFTs in Lattice QCD

- Chiral perturbation theory for the pion cloud to extrapolate in light quark mass.

- Symanzik theory of cutoff effects for gluons and light quarks.

- Heavy-quark theories (HQET and NRQCD) for cutoff effects of heavy quarks.
Lattice Fermions

Naïve: 16 species per field, lately called “tastes”.

Wilson: 1 taste (flavor), but hard chiral symmetry breaking
⇒ fine tuning ⇒ $m_q > 0.7m_s$ [JLQCD, QCDSF, ...].

Staggered: still 4 tastes per field, but remnant of chiral
symmetry ⇒ $m_q > 0.15m_s$ [MILC].

Ginsparg-Wilson (domain wall or overlap): flavor simple, full
chiral symmetry.
The Berlin Wall

$\text{cost} \propto \left( \frac{m^2_V}{m^2_{PS}} \right)^3 L^{4+1} a^{-(4+3)}$

- cost for Wilson
- 3 times faster
- cost for staggered

Plot from Jansen, Ukawa & Gottlieb
hep-lat/0311039

$a = 1/11 \text{ fm measured in simulation}$

$a = 1/22 \text{ fm extrapolated}$
Chiral Extrapolation

The slow-down at small quark mass has two important implications:

- extrapolations in light quark masses are needed;
- only staggered quarks are, so far, light enough to take chiral perturbation theory as a guide.

Other methods catching up: 3-5 years behind.
Quenched Approximation

Full QCD has (expensive) quark loops.

Replace $\det M$ with 1, and compensate by shifting bare gauge coupling and bare masses. “Dielectric”.

Arguably OK if all light quarks had mass $m_q \sim \Lambda$. 

A thing of the past!
Success (at last)
Staggered Quarks

Staggered fermions have always been fast.

Discretization effects $O(a^2)$, but “large”.

Traced to “taste-changing” interactions.

Systematically removed by Orginos, Sugar, & Toussaint:

Remaining $O(a^2)$ removed by Lepage

the “asqtad action”: $O(\alpha_s a^2)$, $O(a^4)$ and “small”.
Gold-plated Quantities

Some quantities are under much better control:

- 1 hadron in the initial state & 0 or 1 in the final state;
- stable, or narrow and not too close to threshold.

Chiral extrapolation must also be under control!

Narrow $D^*$, $\phi$, ... not gold-plated, but perhaps not bad.

(almost) elastic $\rho$, $\Delta$, $K \rightarrow \pi\pi$ much, much harder.
The MILC Ensembles

- MILC Collaboration = dozen or so physicists at Arizona, UCSB, APS, Indiana, Pacific, Utah, Washington U. (St. Louis)
- Improved staggered quarks (asqtad action)
- 2 + 1 flavors of light quarks in sea
- Lattice spacings $a = 1/8, 1/11$ fm.
Many (valence and sea) $m_q$ down to $0.15 m_s$.

Several hundred lattice gauge fields per ensemble

- sub-% statistical errors (importance sampling).

Freely available over the internet.
Several groups started looking at light hadrons (MILC), hadrons with bottom quarks (HPQCD), & hadrons with charmed quarks (Fermilab).

All of the QCD scale was being probed.

A consistent picture emerged: after tuning $1 + n_f$ parameters, we checked 9 other mass splittings and decay constants.
Update: $\Omega^-$ works too!
Because staggered quarks come in four tastes, we have used $[\text{det}_4 M]^{1/4}$ for $\text{det}_1(D + m)$.

But $\text{det}_4 M^{1/4}$ looks non-local and, hence, terrifying.

Several theoretical and numerical studies are suggestive that the "$1/4$-root trick" is acceptable.

Nevertheless, "not proven:" not proven right; not proven wrong either.
Summary So Far

Lattice QCD with improved staggered quarks agrees with Nature for 5+9 gold-plated quantities.

Only improved staggered fermions have achieved the following:

- 2+1 flavors of sea quark
- Quarks light enough for chiral perturbation theory
- Very promising for flavor physics and all QCD.
Marciano suggests taking $f_\pi/f_K = 1.210(4)(13)(1)$ [MILC] to get the Cabibbo angle $\tan \theta_{12} = |V_{us}|/|V_{ud}|$

Quark masses [MILC/HPQCD]

- strange $m_s(2 \text{ GeV}) = 76(0)(3)(0)(7) \text{ MeV}$
- $2m_s/(m_u + m_d) = 27.4(4)$; $m_u/m_d = 0.43(8)$

Strong coupling [HPQCD] $\alpha^{(5)}_{\text{MS}}(M_Z) = 0.1177(13)$
Predictions
Predictive Lattice QCD

Any numerical simulation is a messy enterprise.

An end-to-end test is a fair demand.

Compute something before it’s been measured.

Success (?)! in a strongly-coupled field theory.

Use calculations of unmeasurable quantities to learn more about deep questions about quarks.
Fortunately, we are in a position to make some:

- semi-leptonic form factor of the $D$ meson, $f_+(q^2)$
- normalization,
- shape;

- leptonic decay of the $D$ meson, $f_D$;
- mass of the $B_c$ meson, $m_{B_c}$.

All being measured on the same time scale, or a little later!
Test several ingredients

<table>
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<th>Calculation</th>
<th>Light Sea</th>
<th>Light Valence</th>
<th>Heavy</th>
</tr>
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<tr>
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<td>★★★</td>
<td>★★★</td>
<td>★★★</td>
</tr>
<tr>
<td>leptonic $f_D$</td>
<td>★★★</td>
<td>★★★★</td>
<td>★★</td>
</tr>
<tr>
<td>$B_c$ mass</td>
<td>★★★</td>
<td>—</td>
<td>★★★★</td>
</tr>
</tbody>
</table>

Let’s see how we are doing!
$f_+^{D \to \pi(q^2)} \& f_+^{D \to K(q^2)}$
Semileptonic Decay

One example: $V_{cs}$ from semileptonic decay $D \to Kl!$, $E$.

Experiment $D \to Kl!$, $E$.

\[ q^2 = m_D^2 + m_K^2 - 2m_D E \]

\[ \frac{d\Gamma}{dE} = \frac{G_\mu^2 m_D}{12\pi^3} |V_{cs}|^2 p^3 |f_+(E)|^2 \]

\[ \langle K(p_K) | V^\mu | D(p_D) \rangle = f_+(E) \left[ p_D + p_K - m_D^2 - m_K^2 \frac{q^2}{q^2} \right]^\mu \]

\[ + f_0(E) m_D^2 - m_K^2 \frac{q^2}{q^2} q^\mu \]
and DK results (hep-ph/0408306, accepted for PRL)

\[ V_\mu D f q_2 p D p > m_2 D m_2 q_2 q_\mu f_0 q_2 m_2 D m_2 q_2 q_\mu f_0 f^+ \text{experiment} \]
$D \rightarrow Kl\nu$:

$$f_{+}^{D \rightarrow K}(0) = 0.73(3)(7)$$

$$f_{+}^{D \rightarrow K}(0) = 0.78(5) \quad [\text{BES, hep-ex/0406028}]$$

$D \rightarrow \pi l\nu$:

$$f_{+}^{D \rightarrow \pi}(0) = 0.64(3)(6)$$

$$f_{+}^{D \rightarrow \pi}(0) = 0.87(3)(9) f_{+}^{D \rightarrow K}$$

$$f_{+}^{D \rightarrow \pi}(0) = 0.86(9) f_{+}^{D \rightarrow K} \quad [\text{CLEO, hep-ex/0407035}]$$

dominant error: heavy quark discretization
$D \rightarrow Kl\nu$ vs. $q^2$

$D \rightarrow Kl\nu$

$f_+ (q^2)/f_+ (0)$

$q^2/m^2_{D_s^*}$

- lattice QCD [Fermilab/MILC, hep-ph/0408306]
- $1\sigma$ (statistical)
- $2\sigma$ (statistical)
$D \rightarrow Kl\nu$ vs. $q^2$

![Graph](image)

- **Experiment** [FOCUS, hep-ex/0410037]
- **Lattice QCD** [Fermilab/MILC, hep-ph/0408306]

1σ (statistical)
2σ (statistical)
Summary of Form Factors

BES and CLEO-III have confirmed the normalization, on the same time scale as our calculations.

FOCUS confirmed the shape, after we were finished.

CLEO-c will improve the measurements.

Lattice can systematically improve: few % foreseeable.

Prototype for $B \rightarrow \pi l \nu$, which yields $|V_{ub}|$. 
**$f_{Ds} \& f_D$**

- Meson decay constants parametrize $D \rightarrow l\nu$, etc.
- Experiments measure $|V_{cd}|f_D$ and $|V_{cs}|f_{Ds}$ ...
- ... so take $|V_{cd}|$ and $|V_{cs}|$ from CKM unitarity.
- CLEO-c is measuring them.
- A test of chiral perturbation theory for staggered quarks.
- Prototype for $f_B$: no experiment will measure $|V_{ub}|f_B$. 
Chiral Extrapolation

Dots are PDG.
Error bars are latQCD.
Linear extrap (demo).
Fancier versions of χPT get closer & improve CL.
Consider two quantities with different dominant uncertainties:

- \( \phi_s = f_{Ds} \sqrt{m_{Ds}} \) not sensitive to light quarks
- \( R_{d/s} = \frac{\phi_d}{\phi_s} \) most uncertainties cancel, (not most of the uncertainty cancels).
Chiral Extrapolation $f_{DS}$

Interpolate in valence $m_q$ to get down to real $m_s$.

Extrapolate in sea $m_u$ to get down to real $m_l$. 

MILC coarse
sea $am_s = 0.05$
A separate linear fit, shown for illustration.
\[ \phi_s = f_{D_s} m_{D_s}^{1/2} (\text{GeV}^{3/2}) \]

- only log taste violations removed
- almost all taste violations removed
- \(0.3493 \pm 0.0049\)
- 3.9%
Chiral Extrapolation $f_D$

$m_q = m_l$

$$R_{qs} = f_D m_D^{1/2} f_D m_D^{1/2}$$

- $a = 0.121$ fm
- staggered $\chi$PT fit (to 60 points)
- taste violations removed
C. Aubin et al., hep-lat/0506030 (PRL)

\[ R_{d/s} = 0.786(04)(05)(04)(42) \]
\[ \phi_s = 0.349(05)(10)(15)(14) \text{ GeV}^{3/2} \]

\[ f_{D_s} = 249 \pm 3 \pm 7 \pm 11 \pm 10 \text{ MeV} \]

\[ f_{D^+} = 201 \pm 3 \pm 6 \pm 9 \pm 13 \text{ MeV} \]

\[ f_{D^+} = 223 \pm 17 \pm 3 \text{ MeV} \]

CLEO-c, hep-ex/0508057
Comparison

![Graph showing comparison of $f_{D^+}$ and $f_{D_s}$ with $n_f$ as the x-axis and $f$ in MeV as the y-axis. The graph includes data points from hep-ph/9711426 [Fermilab], hep-lat/0206016 [MILC], hep-lat/0506030 [Fermilab + MILC], hep-ex/0508057 [CLEO-c], and the PDG average.](image-url)
$B_c$
Meson composed of a beautiful anti-quark and a charmed quark.

Unusual beast

- contrast with $B_s$ & $D_s$, $\psi$ & $\Upsilon$: $\nu_c = 0.7$.
- no annihilation to gluons
4:00 p.m. One West
Joint Experimental Theoretical Physics Seminar
Saverio D'Auria, University of Glasgow
$B_c^+$ : Fully Reconstructed Decays and
Mass Measurement at CDF
QCD Theory & $B_c$

- Three main tools
  - potential models
  - potential NRQCD
  - lattice QCD

All treat both quarks as non-relativistic
- charmed quark is pushing it, $v_c^2 = 0.5$. 
Prediction: $\alpha_s, m_b, m_c$ taken from bottomonium and charmonium spectrum

Use latNRQCD for $b$ and Fermilab method for $c$.

We calculate two mass splittings

\[ \Delta_{\psi \Upsilon} = m_{B_c} - \frac{1}{2}(\bar{m}_\psi + m_\Upsilon) \]  \hspace{1cm} \text{quarkonium baseline} \\
\[ \Delta_{D_s B_s} = m_{B_c} - \frac{1}{2}(\bar{m}_{D_s} + \bar{m}_{B_s}) \]  \hspace{1cm} \text{heavy-light baseline}
Error Analysis

Everything is gold-plated, in the sense that the mesons are all stable, and far from threshold.

Statistical error is straightforward & small.

Uncertainty from $a^{-1}$, $m_b$, $m_c$ easy to propagate: latter two are ±10, ±5 MeV.

Main problem is to estimate the discretization effect for the heavy quarks.
Discretization Effects

(short distance mismatch) • (matrix element)

- Use calculations of tree-level mismatches
- Wave hands for one-loop mismatches
- Estimate matrix elements in potential models
- Check framework with other calculations
Results

Splittings:

\[ \Delta_{\psi \Upsilon} = 39.8 \pm 3.8 \pm 11.2^{+18}_{-10} \text{ MeV}, \]
\[ \Delta_{D_s B_s} = -\left[1238 \pm 30 \pm 11^{+37}_{-37}\right] \text{ MeV}, \]

Meson mass:

\[ m_{B_c} = 6304 \pm 4 \pm 11^{+18}_{-10} \text{ MeV}, \]
\[ m_{B_c} = 6243 \pm 30 \pm 11^{+37}_{-37} \text{ MeV}, \]

More checks on quarkonium baseline, so it is our main result.
Comparisons

$m_{B_c}^{n_f=0} = 6386 \pm 9 \pm 15 \pm 98 \text{ MeV} \quad \text{[Phys. Lett. B 453, 289 (1999)]}$

$m_{B_c}^{2+1} = 6304 \pm 4 \pm 11^{+18}_{-0} \text{ MeV} \quad \text{[hep-lat/0411027 → PRL]}$

$m_{B_c}^{\text{expt}} = 6287 \pm 5 \text{ MeV} \quad \text{[CDF, W&C seminar, 12/3/2004]}$

hep-ex/0505076
Outlook
The “end of the beginning” of non-perturbative QCD even if staggered quarks prove not to be the last word, other methods are only 3-5 years behind.

This advance opens the way to applications in flavor physics, RHIC and, of course, the LHC

QCD calculations of moments of parton densities;

new strong dynamics breaking $SU_L(2) \times U_Y(1)$. 
Mind the gap!
It’s new physics!
Thanks

MILC Collaboration

Junior collaborators Masataka Okamoto, Ian Allison, Matthew Nobes, Christopher Aubin, ...

Don Holmgren and Amitoj Singh