Physics & Computing Challenges in Lattice QCD

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Original Invitation

• Talk about “Machine Learning Challenges in Complex Multiscale Systems”

• Title of a TUM Institute for Advanced Study "Focal Period"
  • (I helped organized)

• Alas, you will hear about lattice QCD instead.
Outline

- Nonperturbative QCD & some lattice QCD results
- Basics of lattice gauge theory
- Software
- QCD random number generators
- Solvers for quarks
- Bayesian curve fitting
- Upcoming physics challenges

some ML speculation
Emergent Phenomena in QCD & Some Lattice QCD Highlights
nuclear physics

nuclear forces

hadron-hadron interactions

hadrons

confinement & $\chi$SB

neutron stars

excited states

phase shifts

weak decays

phase transitions in early universe

hadron structure: pdfs, $\chi^N \rightarrow \chi^N$
neutron stars
excited states

phaseshifts

hadron-hadron interactions

weak decays

hadrons

confinement & χSB

hadron structure: pdfs, χN → χN

jets

nuclear physics

nuclear forces
Non-Abelian gauge fields have nontrivial topology (in $d = 4$).

Suppose, as $x \to \infty$, $A_\mu(x) \to g^{-1}(x) \partial_\mu g(x)$. Then

$$Q = \frac{1}{24\pi^2} \int_{S^3} d^3 \sigma \varepsilon^{\mu \nu \rho \sigma} \text{tr}[(g^{-1} \partial_\nu g)(g^{-1} \partial_\rho g)(g^{-1} \partial_\sigma g)] \in \mathbb{Z}$$

$$= \frac{1}{32\pi^2} \int_{\mathbb{R}^4} d^4 x \varepsilon^{\mu \nu \rho \sigma} \text{tr}[F_{\mu \nu} F_{\rho \sigma}], \quad F_{\mu \nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu]$$

Leads to the possibility of strong CP violation, if $\theta \neq 0$ and $m_u \neq 0^*$;

- lattice QCD: $m_u = 2.16(11)$ MeV, so $m_u = 0$ is disfavored;
- neutron EDM: $\theta \equiv \theta_{\text{QCD}} + \arg M_{\text{quark}} < 10^{-11}$, which is mind boggling.

* Yes, Mike, I know.
QCD Hadron Spectrum

π...Ω: BMW, MILC, PACS-CS, QCDSF; ETM (2+1+1);
η-η': RBC, UKQCD, Hadron Spectrum (ω);
D, B: Fermilab, HPQCD, Mohler&Woloshyn

compilation updated from arXiv:1203.1204

B mesons offset by –4000 MeV

numerous quarkonium omitted
Excited States

e.g., Hadron Spectrum Collaboration, *PRD 83* (2011) 111502

- Future applications to glueball spectra, hybrids, excited baryons, & mixing.
CKM Unitarity:

\[ |V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 \stackrel{?}{=} 1 \]
\[ |V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2 \stackrel{?}{=} 1 \]
Kinematic Distributions

- Experimental data from LHCb [arXiv:1403.8044, arXiv:1509.00414] and earlier experiments; right plot’s theory preceded measurement:

- arXiv:1510.02349 also contains predictions for the ratio, the flat terms, etc.
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Synopsis

- Nonperturbative QCD is rich: return to some current challenges at end.
- Low-lying hadron spectrum agrees with experiment at 2% level & better.
- Excited states are more challenging, but progress recently is rapid.
- Quark flavor physics, with sub- to few-percent uncertainties:
  - includes several validated predictions—$D_{(s)}$ decay constants & form factors, $B_c$ mass ➔ over 12 years ago!
  - and $B_c^*$ mass, yet to be seen in experiments.
- Lattice QCD is now a reliable tool for precision physics.
Lattice Gauge Theory
Lattice Gauge Theory

• Infinite continuum: uncountably many d.o.f. (⇒ UV divergences);

• Infinite lattice: countably many; used to define QFT;

• Finite lattice: finite dimension \( \sim 10^9 \), so compute integrals numerically.

\[
\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} \exp(-S)[\bullet]
\]

\[
= \frac{1}{Z} \int \mathcal{D}U \text{Det}(\mathcal{D} + m) \exp(-S_{\text{gauge}})[\bullet']
\]
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\[
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\]

\[
L = N_s a
\]

\[
L = N_s a
\]
Algorithmic Issues

e.g., ASK, hep-lat/0205021

- lattice $N_S^3 \times N_4$, spacing $a$
- memory $\propto N_S^3 N_4 = L_S^3 L_4 / a^4$
- $\tau_g \propto a^{-(4+z)}$, $z = 1$ or 2
- $\tau_q \propto (m_q a)^{-p}$, $p = 1$ or 2
- Imaginary time, $x_4 = it$:
  - static quantities 😛
  - size $L_S = N_S a$, $L_4 = N_4 a$
  - dimension of spacetime = 4
  - critical slowing down
  - especially dire w/ sea quarks
  - thermodynamics: $\Theta = 1/N_4 a$

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D} \psi \mathcal{D} \bar{\psi} \exp(-S)[\bullet] = \text{Tr}\{\bullet e^{-\hat{H}/\Theta}\} / \text{Tr}\{e^{-\hat{H}/\Theta}\}$$
Computing Hadronic Matrix Elements

- Find masses and “legs” from two-point correlation functions:

\[ \langle B(x_4)B^\dagger(0) \rangle = \sum_n |\langle B_n | \hat{B}^\dagger | 0 \rangle|^2 e^{-M_{Bn}x_4} \]

\[ \langle A_4(x_4)B^\dagger(0) \rangle = \sum_n \langle 0 | \hat{A}_4 | B_n \rangle \langle B_n | \hat{B}^\dagger | 0 \rangle e^{-M_{Bn}x_4} \]

where \( x_4 = it \) is “Euclidean time”. Then get matrix elements from three-point functions:

\[ \langle B^\dagger(x_4) \mathcal{O}_i(0)B^\dagger(-x'_4) \rangle = \sum_{m,n} \langle 0 | \hat{B}^\dagger | B_m \rangle \langle \tilde{B}_m | \hat{O}_i | B_n \rangle \langle B_n | \hat{B}^\dagger | 0 \rangle e^{-M_{Bn}(x_4+x'_4)} \]

in which desired matrix element lies in the middle (of leading term).

- Use supercomputer to generate LHS; hire superhumans to analyze RHS.
The Steps

• Use random number generator to create lattice gauge fields distributed with the weight $e^{-S}$.

• Solve $(\mathbf{D} + m)_{xz}G_{zy} = b_x$ for quark propagators in these gauge fields.

• Fit correlation functions to get masses and matrix elements.

• Repeat several times while varying bare gauge coupling and bare masses.

• Find a trajectory with constant pion, kaon, $D_s, B_s$, masses (one for each quark) in dimensionless but physical units and obtain the continuum limit.

• Convert units to MeV.
Software (USQCD Example)
The problem naturally splits into two parts:

- generating $\{U^{(c)}\}$ requires capability machines, e.g., BlueGene/Q or Cray XK7;

- working out the $\bullet'$ and the curve fitting requires capacity machines.
Heterogenous Platforms

- Lattice QCD runs on everything: Intel/AMD in your laptop (i.e., clusters), GPUs, Xeon Φ, Knight’s Landing, BlueGene/Q, Cray XK7, etc.

- Lowest-level computations:

\[
\begin{pmatrix}
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\end{pmatrix}
\times
\begin{pmatrix}
\cdot \\
\cdot \\
\cdot \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\end{pmatrix}
\times
\begin{pmatrix}
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot \\
\end{pmatrix}
\]

optimize these, and a few other things, on any chip.
Remarks

• Lattice QCD was the(?) first community to use GPUs:
  • by now, a few lattice-QCD algorithm experts work for NVIDIA.

• Software development (in US) supported by SciDAC (essential) & industry.

• Other notable efforts (presumably a partial list):
  • European Twisted-Mass Collab: tmLQCD and related packages;
  • Martin Lüscher et alia: openQCD (∃ branch for C-periodic boxes)
  • Guido Cossu et alia (KEK): Irolro++;
  • Peter Boyle: BAGEL code generator; multithreading Grid library.
Generating Lattice Gauge Fields
Functional Integral

• Objective is to compute many integrals of the form

\[
\langle \bullet \rangle = \frac{1}{Z} \int D U \text{Det}(\mathcal{D} + m) \exp(-S_{\text{gauge}})[\bullet']
\]

with billions and billions of integration variables.

• Action is “extensive”, so the integrand varies over a huge range.

• Only feasible approach is Monte Carlo integration with importance sampling:

\[
\langle \bullet \rangle = \frac{1}{C} \sum_{0}^{C-1} \bullet' \left[ \{U\}^{(c)} \right]
\]

with each field \(\{U\}^{(c)}\) generated with probability \(\text{Det}(\mathcal{D} + m) \exp(-S_{\text{gauge}})\).
Field Theory is Local

• … so local MCMC (Metropolis, heat-bath, ...) algorithms work with $S_{\text{gauge}}$:
  • order variables in some nice way, $U_n^{(c)} \rightarrow U_n^{(c+1)}$, $\forall \ n = 0, \ldots, N - 1$.
  • But $\text{Det}(\mathcal{D} + m) = \exp[-\text{Tr} \ln(\mathcal{D} + m)]$ leads to nonlocal $S_F = \text{Tr} \ln(\mathcal{D} + m)$.
  • Led (mid 1980s) to search for global algorithms, $\{U\}^{(c)} \rightarrow \{U\}^{(c+1)}$:
    • molecular dynamics: use Hamilton’s equations—$z = 1$, but ergodic?;
    • Langevin equation: use random noise $\oplus$ diffusion—ergodic but $z = 2$;
    • hybrid molecular dynamics: noise $\oplus$ Hamilton—$z = 1$ (?), ergodic.
Hybrid Molecular Dynamics (HMD)

- These algorithms, or variants, are used in machine learning, for example to examine a posterior probability distribution.

- Consider a potential QFT action, energy, cost function, ... \( V(\phi) = \ln \mathbb{P}(\phi) \).

- Stat mech of real molecules actually needs \( H(\phi, \pi) = \frac{1}{2} \pi \cdot \pi + V(\phi) \):

\[
\dot{\pi}_i = -\frac{\partial H}{\partial \phi_i} \quad \Rightarrow \quad \pi_i^{(t+1)} = \pi_i^{(t)} - \delta \frac{\partial V^{(t)}}{\partial \phi_i} \\
\dot{\phi}_i = +\frac{\partial H}{\partial \pi_i} \quad \Rightarrow \quad \phi_i^{(t+1)} = \phi_i^{(t)} + \delta \pi_i^{(t)}
\]

- For our purpose, a danger arises for nearly periodic modes.
• Introduce Gaussian random noise $\xi_i$ into momenta every so often:

$$
\pi_i^{(\lambda,0)} = \xi_i
$$

$$
\pi_i^{(\lambda,1/2)} = \pi_i^{(\lambda,0)} - \frac{1}{2} \delta \frac{\partial V}{\partial \phi_i}^{(\lambda,0)}
$$

$$
\phi_i^{(\lambda,n+1)} = \phi_i^{(\lambda,n)} + \delta \pi_i^{(\lambda,n+1/2)}
$$

$$
\pi_i^{(\lambda,n+1/2)} = \pi_i^{(\lambda,n-1/2)} - \delta \frac{\partial V}{\partial \phi_i}^{(\lambda,n)}
$$

$$
\phi_i^{(\lambda,N)} = \phi_i^{(\lambda,N-1)} + \delta \pi_i^{(\lambda,N-1/2)}
$$

$$
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$$

\begin{align*}
\text{refresh &} \\
\text{half step} &
\end{align*}

\begin{align*}
N - 1 \text{ steps} &
\end{align*}

\begin{align*}
\text{finish } \phi & \text{ &} \\
\text{half step } \pi &
\end{align*}
• Introduce Gaussian random noise $\xi_i$ into momenta every so often:

\[ \pi_i^{(\lambda,0)} = \xi_i \]

\[ \pi_i^{(\lambda,1/2)} = \pi_i^{(\lambda,0)} - \frac{1}{2} \delta \frac{\partial V^{(\lambda,0)}}{\partial \phi_i} \]

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\[
\begin{align*}
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\phi_i^{(\lambda,n+1)} &= \phi_i^{(\lambda,n)} + \delta \pi_i^{(\lambda,n+1/2)} \\
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$$
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\pi_i^{(\lambda,1/2)} &= \pi_i^{(\lambda,0)} - \frac{1}{2} \delta \frac{\partial V}{\partial \phi_i}^{(\lambda,0)}
\end{align*}
$$

Hybrid (aka Hamiltonian) Monte Carlo:
accept $\phi_i^{(\lambda,N)} \rightarrow \phi_i^{(\lambda+1,0)}$ à la Metropolis w/ $e^{-\Delta H}$

$$
\begin{align*}
\phi_i^{(\lambda,N)} &= \phi_i^{(\lambda,N-1)} + \delta \pi_i^{(\lambda,N-1/2)} \\
\pi_i^{(\lambda,N)} &= \pi_i^{(\lambda,N-1/2)} - \frac{1}{2} \delta \frac{\partial V}{\partial \phi_i}^{(\lambda,N)}
\end{align*}
$$

finish $\phi$ & half step $\pi$
Step-size Errors

- The discrete Hamiltonian evolution conserves energy only up to \( O(\delta^2) \), but “shadow Hamiltonian” [\textit{e.g.}, Kennedy, Silva, Clark (2012)] is conserved:

\[
\tilde{H} = H - \frac{\delta^2}{24} (\{V, \{V, T\}\} - 2\{T, \{T, V\}\}) + O(\delta^4)
\]

where \( \{,\} \) is a Poisson bracket (last seen in undergrad mechanics).

- Consider spectrum \( \{\omega \mid \omega_{\text{min}} < \omega < \omega_{\text{max}}\} \sim \) gradients of \( V(\phi) = \ln \mathbb{P}(\phi) \).

- How fast is it? What is \( z \)?

- Trajectory length \( \tau = N\delta \): optimized at \( \tau_{\text{opt}} \sim \pi/2\omega_{\text{max}} \), in which case slow (not so steep) modes move only \( \tau \omega_{\text{min}} \sim \omega_{\text{min}}/\omega_{\text{max}} \):

- Need many trajectories to get anywhere and, effectively, \( z = 2 \) not 1 😞

\( O(\delta^{n>2}) \) methods: Omelyan, Mryglod, Folk
Stability

- Short trajectory length is needed because if $\tau > 2\pi/\omega_{\text{max}}$, then there are some modes that end up close to where they started (~cycle)
  - assumes $V$ has dense spectrum below $\omega_{\text{max}}$.
- Way out is known but usually forgotten: refresh with probability $\omega_{\text{min}}\delta$.
- Then some modes traverse a cycle sometimes, but none cycles always.
- Average trajectory has $\langle \tau \rangle \sim 1/\omega_{\text{min}}$, so all modes evolve rapidly; $z = 1$ 😊
Sea Quarks

• Remember QCD?

• And the nonlocal action of quarks on the gauge field $S_F = \text{Tr} \ln(\mathcal{D} + m)$.

• In the global-update algorithms, we need ($\partial$ in Lie groups, no worries):

$$\frac{\partial S_F}{\partial U_{\mu}(x)} = \text{Tr}[(\mathcal{D} + m)^{-1}] = \langle \xi^\dagger (\mathcal{D} + m)^{-1} \xi \rangle_{\xi}$$

so we only need to solve $(\mathcal{D} + m)G[\xi] = \xi$ for $G[\xi]$ [Batrouni et al. (1985)].

• This solve must be carried out at each time step along the way:

• thus, the most demanding part of lattice gauge theory.
Quark Propagators
Solvers

• Also need to solve $(D + m)G[b] = b$ for valence quarks with “source” $b$, out of which hadron correlation functions are constructed.

• All lattice formulations of $D$ yield a sparse matrix $\Rightarrow$ Krylov solvers.

• Solve slows down as $\omega_{\text{min}}/\omega_{\text{max}} \sim ma \to 0$.

• The lowest modes are very nonperturbative: (near) zero modes of $D$, associated with gauge-field topology.

• Solution called “deflation”: project out the first few-to-several modes:

$$
(D + m)^{-1} = \left[ D + m - \sum_{|\lambda|<\lambda_{\text{del}}} \lambda |\psi_{\lambda}\rangle\langle\bar{\psi}_{\lambda}| \right]^{-1} + \sum_{|\lambda|<\lambda_{\text{del}}} \lambda^{-1} |\psi_{\lambda}\rangle\langle\bar{\psi}_{\lambda}|
$$
Example: Multigrid

- Asaam
- Brannick et al. (2008)
- Babich et alia (2010)
- Frommer et al. (2013)
- Everything has to be gauge covariant.
- Slide from Brower at TUM Focal Period; graphic from Kahl (?)..

Adaptive Smooth Aggregations Algebraic MultiGrid

Slow convergence of Dirac solver is due small eigenvalues for vectors in near null subspace: $S$.

\[ D : S \simeq 0 \]

Spilt the vector space into near null space $S$ and the complement $S_{\perp}$.
Rampant Speculation

- HMC, in practice, has several adjustable choices:
  - trajectory length, details of integrator, etc.
- Quark solver also has adjustable choices:
  - various preconditioners (in any method);
  - how many modes to deflate (any methods);
  - smoothing & how to cycle in multigrid.
- Every Markov chain goes on for millions of iterations (lasting years): Can we learn how to accelerate the simulation while it runs?
Curve Fitting
Fitting Correlation Functions

• Our hired superhumans’ task is to fit a sum of exponentials:

\[ C_{ij}(x_4) = \left\langle B_i(x_4)B_j^\dagger(0) \right\rangle = \sum_{n=0} \langle 0|\hat{B}_i|B_n\rangle\langle B_n|\hat{B}_j^\dagger|0\rangle e^{-M_n x_4} + bc_4 \]

• Saved by the fact that the MC data are highly correlated:

  • roughly, principle components are height, slope, curvature, ….

  • Lowest-lying state dominates when \( x_4 \) is large, but …

  • … statistical errors grow (exponentially) with \( x_4 \) (except pion).

• Augment least-squares cost function with Gaussian priors on \( M_0, \ln \Delta M_n, Z_n^{(i)} = \langle 0|B^{(i)}|B_n\rangle \).
Constrained Curve Fitting

• In principle, we cannot think about extracting more than $N \approx \frac{1}{2} N_4$ states.

• Thus, priors are necessary: e.g., truncate with $Z_n(i) \sim \delta(0)$, for $n$ too large.

• Less extreme is a Gaussian prior of sensible width:
  • we can look at large $x_4$ data (and then omit them from further analysis);
  • we know mass splittings are $400 \times \frac{1}{2}$ MeV.
Chiral-Continuum Limit

- After extracting masses & matrix elements for a range of the $1 + n_f (+ 1)$ parameters, the data are combined with effective field theories for
  - lattice-spacing dependence;
  - quark-mass dependence.
- More curve fitting.
- As before we know the model, just not where to truncate:
  - Gaussian priors again.
- Output is a curve!

---

form factor for $B \to \pi l \nu$

$$f_{\perp l}^{-1/2}$$

$$E_{\pi r_1}$$
Example Fit Function (Schematic)

\[ F_i = F_i^{\text{logs}} + F_i^{\text{analytic}} + F_i^{\text{HQ disc}} + F_i^{\alpha_s a^2 \text{ gen}} + F_i^\kappa + F_i^{\text{renorm}} \]

- **nonanalytic terms from NLO HMrS\(\chi\)PT aka “chiral logs”**
- **heavy-quark discretization effects (derived in HQET)**
- **fine tune \(c\)-quark hopping parameter**

- **analytic terms in \(N^n\)LO \(\chi\)PT:** base fit \(n = 2\)
- **gluon & light-quark cutoff effects \(\text{à la Symanzik}\)**
- **fit** \(\alpha_s^2 \rho_{ij}^{[2]}\) (alternatively \(\alpha_s^3 \rho_{ij}^{[3]}\))
Combining Lattice QCD with Experiment


- Fit curve from QCD with experimental data:

$$10^3 |V_{ub}| = 3.72(16)$$

- BTW, this superhuman is now in data science 😞
Future Physics Challenges in QCD
Scope and Precision

- The precision on some meson matrix elements is sub-percent:

\[ f_{B^+} = 186(4) \text{ MeV} \quad \Rightarrow 189.6(9) \text{ MeV} \quad \text{FLAG 2016} \quad \text{Fermilab-MILC} \]
\[ f_{B^+} = 224(5) \text{ MeV} \quad \Rightarrow 231.1(8) \text{ MeV} \quad \text{2017} \]

- Future work will need isospin effects: \( m_u \neq m_d \) & QCD+QED.

- Success attracts demands:
  - many new needs in particle physics;
  - even more in nuclear physics.
Nucleon Matrix Elements

- Hadron structure:
  - key in hadronic physics;
  - also in LHC physics;
  - and neutrino physics.

- Numerous nucleon form factors needed so experiment can confront nuclear models on sound footing.
Muons Anomalous Magnetic Moment

- Fermilab E989 is being mounted to explore a well-known tension between BNL E821 & SM.

\[ 10^{10} a_\mu = \begin{cases} 
11659208.9(6.3) \text{ \text{ expt}} \\
11659180.2(4.9) \text{ \text{ SM with HVP from } e^+ e^-} 
\end{cases} \]

28.7(6.3)(4.9) is a huge difference!

\[ a = \mu \frac{2m}{e\hbar} - 1 = \frac{1}{2}(g - 2) \]
Hadronic Contributions

- Two kinds of hadronic contributions:
  - vacuum polarization:
    - all gluons implied but quarks & photons are connected or disconnected
  - “light by light scattering”
HPQCD, arXiv:1601.03071

- Second full result from lattice QCD.
- Uses MILC’s 2+1+1 ensembles.
  - 3 lattice spacings;
  - 3 volumes;
  - 3 quark masses, including physical.
- $3\sigma$ from exp’t.
HLbL Progress from RBC

- Compute in coordinate space [arXiv: 1510.07100]

- finite-volume lattice QCD-QED [arXiv: 1610.04603]:
  \[ 10^{10} a_{\mu}^{HLbL} = 5.35(1.35) \]

- New idea: attach blob to infinite volume QED kernel: sum \( x, y \) randomly but wisely; sum \( x_{op}, y \) completely.

- Test with QED (instead of QCD) blob [arXiv: 1705.01067].
Conclusions and Outlook
Remarks

• Numerical lattice QCD could be a great element of this conference:
  • “machines and algorithms” sub-community is large & includes applied mathematicians;
  • pioneering work on algorithms (e.g., HMC);
  • pioneering work on hardware (e.g., GPUs);
  • probably also a lot for lattice-QCD practitioners to learn: How can advanced ML techniques help us?

• Our work is not going to get easier: success fosters expectations.
Thank you!