Lattice QCD at the Exascale

The 2nd R-CCS International Symposium
K to Fugaku
RIKEN Center for Computational Science

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Columbia University
Outline

• Overview of Lattice QCD
• Algorithms and architectures
• Recent calculations
  – Muon $g-2$
  – $K_L \rightarrow \mu^+ \mu^- / \pi^0 \rightarrow e^+ e^-$
  – $K_L-K_S$ mass difference
• Exascale plans
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- Tobias Tsang
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Particle Physics – Overview

• Search for new phenomena at the highest energies.
• Goal of the Large Hadron Collider at CERN.

• High precision results at lower energies may have greater reach: Belle II at KEK.
• To compare with Standard Model need lattice QCD predictions: HPC plays a critical role
• $\gamma$ (photon), $g$ (gluon) and $W^+$ (weak) exchange
Standard Model

- Proton and neutron in atomic nucleus composed for \( u \) and \( d \) quarks.
- These are bound by the exchange of gluons \( g \).

<table>
<thead>
<tr>
<th>Quarks</th>
<th>Mass (MeV/c^2)</th>
<th>Charge</th>
<th>Spin</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u )</td>
<td>( \frac{1}{2} )</td>
<td>( +\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>up</td>
</tr>
<tr>
<td>( d )</td>
<td>( -\frac{1}{2} )</td>
<td>( +\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>down</td>
</tr>
<tr>
<td>( c )</td>
<td>( \frac{2}{3} )</td>
<td>( +\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>charm</td>
</tr>
<tr>
<td>( s )</td>
<td>( -\frac{1}{3} )</td>
<td>( +\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>strange</td>
</tr>
<tr>
<td>( t )</td>
<td>( \frac{4}{3} )</td>
<td>( +\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>top</td>
</tr>
<tr>
<td>( b )</td>
<td>( -\frac{1}{3} )</td>
<td>( -\frac{1}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>bottom</td>
</tr>
</tbody>
</table>

- \( u \) and \( d \) quarks nearly massless and highly relativistic
- Copious virtual pair creation → many body problem
Lattice QCD
Lattice QCD

• Introduce a space-time lattice
• Evaluate the Euclidean Feynman path integral
  – Study $e^{-H_{QCD}t}$
  – Precise non-perturbative formulation

\[
\sum_n \langle n | e^{-H(T-t)} \mathcal{O} e^{-Ht} | n \rangle = \int d[U_\mu(n)] e^{-A[U]} \det(D+m) \mathcal{O}[U](t)
\]

• Use Monte Carlo importance sampling with hybrid, MD/Langevin evolution
• ~40 samples give sub-percent errors
Challenges

• Numerical control of the path integral
  – $96^3 \times 192$ lattice $\rightarrow$ $5 \times 10^9$ dimensional integral
  – Long autocorrelation times $\rightarrow$ misleading errors

• Extend Schrodinger quantum mechanics into Euclidean time
  – Unphysical time evolution
  – Time-like processes challenging

• Fermion sign problem
  – $\mu_{\text{baryon}} \neq 0$ $\rightarrow$ path integral weight not positive
  – Poor signal to noise ratio in baryon correlators

\[
\left| |q(x)\overline{q}(y)|^2 \right| \sim e^{-|x-y|m_{\pi}} \quad \left( (q(x))^3 B \ (\overline{q}(y))^3 B \right) \sim e^{-|x-y|B m_N}
\]
Historical overview

- **1974** Gauge-invariant lattice theory formulated. [Ken Wilson]
- **1980** String tension computed with physical dependence on the gauge coupling. [Mike Creutz]
- **1990** Fermion loops routinely included.
- **1992** Fermion doubling problem solved. [David B. Kaplan]
- **2002** Routine use of chiral quarks.
- **2014** Routine calculation with physical $u$, $d$ and $s$ quark masses.
Lattice QCD – 2020

• Physical quark masses (ChPT not needed)
• Chiral quarks (doubling problem solved)
• Large physical volumes: (6 -10 fm)$^3$
• Small lattice spacing: $1/a = 2.774$ GeV
• Some quantities with $\sim 0.1\%$ precision
• Now an essential tool for many standard model tests.
Algorithms and Architectures
Architecture

- Regular lattice problem: easy for parallel computer.
- Difficulty scales as $\sim L^6$.
- Weak scaling not sufficient
- Large demand on network bandwidth:
  - Local 4D volume grows with node flops
  - Off-node bandwidth grows as $(\text{node flops})^{3/4}$
  - Mira $\rightarrow$ Summit
    - 0.2 TF/s / 20 GB/s $\rightarrow$ 42 TF/s / 25 GB/s
- Serious algorithm challenge

QCDSP – 600 Gflops
- RIKEN/Columbia/BNL
- Gordon Bell Prize 1998
Numerical methods

- Use low eigenmodes to solve $\hat{D} G_n = h_n$ for multiple right-hand sides (deflation).
- $96^3 \times 192$ volume requires 5K eigenvectors (160 TB).
- Compress using local coherence: 30x (Clark, Jung & Lehner, arXiv:1710.06884)
- Use All-Mode-Averaging technique (Blum, Izubuchi & Shintani, arXiv:1208.4349 [hep-lat])
  - Loosen CG stopping condition $10^{-8} \rightarrow 10^{-4}$.
  - Obtain accurate result for 8 out of 128 time slices
  - $O(10^{-8})$ accurate result = $\langle G_{10^{-4}} \rangle_{124} + \langle G_{10^{-8}} - G_{10^{-4}} \rangle_8$
  - Achieve 5-20x speed-up.
Numerical methods - cont

- **Split-Grids** (Boyle and Jung)
  - Deflate multiple right-hand sides on full machine
  - Perform separate CG inversions on many subpartions
  - 4x speed-up on Cori at NERSC (Cray XC40/KNL)

- **Multi-splitting preconditioned conjugate gradient**
  (Tu, Guo, and Mawhinney, arXiv:180408593)
  - Precondition with Dirac operator without off-node comms.
  - Use many local inversions, exploit large node performance.
  - Use tensor cores on Summit
  and obtain 1.5x speedup
  - Must include halo sites in
  product $D_{pcond}^+ D_{pcond}$. 

[Diagram of a grid with arrows indicating halo sites and tensor cores usage]
New Directions

• Use machine learning to infer the results for complex quantities from those of simple ones. (Boram Yoon, LANL)

Correct small errors with a few exact results.

• Use machine learning to generate Markov samples. (Albergo, Kanwar and Shanahan, arXiv:1904.12072)
New Directions

• Use machine learning to simplify local MSPCG approximation (Jiqun Tu: Columbia → NVIDIA)

\[ M_{Ls}^{-1} \sim T^\dagger M_{Ls}^{-1} T + \mu I \]

• Learn optimal 1536 parameters in \( T \)

• Use Quantum Computing to generate real-time evolution?
Muon anomalous magnetic moment
$g - 2$ for the muon

- Anomalous moment: $a_\mu = (g_\mu - 2)/2$
- BNL E821 expt:
  $a_\mu = 11699208.9 \pm 6.3 \times 10^{-10}$
- $3\sigma$ difference between the
  standard model prediction and experiment:
  $a_\mu^{\text{EXP}} - a_\mu^{\text{SM}} = 27.4(2.7)(2.6)(6.3) \times 10^{-10}$
- Effects of quark and gluons enter at order $\alpha_{\text{EM}}^2$:

\[ q = p' - p, \nu \]

HVP

$692.5(2.7) \times 10^{-10}$

HLbL

$10.5(2.6) \times 10^{-10}$
Brookhaven, Columbia, Connecticut, Nagoya, RIKEN

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Norman Christ (Columbia)
Masashi Hayakawa (RIKEN & Nagoya)
Taku Izubuchi (BNL & RIKEN BNL)
Luchang Jin (Columbia → Connecticut)
Chulwoo Jung (Brookhaven)
Christoph Lehner (Regensburg & BNL)
Use lattice QCD to calculate HLbL

- Compute connected and leading disconnected parts.
  \[ \bar{\mu} = \frac{1}{2} \int d^3r \left( \vec{r} \times \vec{j}(\vec{r}) \right) \]

- Important challenge for lattice QCD
  - Treat E&M through an expansion in \( \alpha_{\text{EM}} \)
  - Massless photon introduces new problems

- Sum stochastically over \( x \) and \( y \)
Use lattice QCD to calculate HLbL

- Use Lattice QCD for quark loop and gluons
- Evaluate photons and muon parts analytically

\[ \mu = 7.20(3.98)_{\text{stat}}(1.65)_{\text{sys}} \times 10^{-10} \text{ from QED}_L \]

(arxiv:1911.081230)
$K_L \rightarrow \mu^+ \mu^-$

$\pi^0 \rightarrow e^+ e^-$
Physics of $K_L \rightarrow \mu^+ \mu^-$

- A second order weak, "strangeness changing neutral current"

(Cirigliano, et al., Rev. Mod. Phys., 84, 2012)

- $K_L \rightarrow \mu^+ \mu^-$ decay rate is known:
  - $\text{BR}(K_L \rightarrow \mu^+ \mu^-) = (6.84 \pm 0.11) \times 10^{-9}$

- Large "background" from two-photon process:
Calculation $\pi^0 \rightarrow e^+ e^-$

- Avoid Euclidean calculation
- Evaluate in Minkowski space
- Wick rotate internal time integral:

\[
A_{\pi^0 \rightarrow e^+ e^-} \rightarrow \int d^4w \widetilde{L}(k_-, k_+, w)_{\mu\nu} \langle 0 | T \left\{ J^\mu_\nu \left( \frac{W}{2} \right) J^\nu_\nu \left( -\frac{W}{2} \right) \right\} |\pi^0 (\vec{P} = 0) \rangle
\]
Lattice Results for $\pi^0 \rightarrow e^+ e^-$

(Yidi Zhao)

$$A_{\pi^0 \rightarrow e^+ e^-} \rightarrow \int d^4w \tilde{L}(k_-, k_+, w)_{\mu \nu} \langle 0 | T \left \{ J_\mu \left ( -\frac{w}{2} \right ) J_\nu \left ( -\frac{w}{2} \right ) \right \} | \pi^0 (\vec{P} = 0) \rangle$$

- Lattice result is complex:
  - Exponentially small FV corrections
  - Physical kinematics, $1/a \leq 1.73$ GeV:
    - $\text{Im}(A) = 35.94(1.01)(1.09)$ [Expt: 35.07(37)]
    - $\text{Re}(A) = 20.39(72)(70)$. [Expt: 21.51(2.02)]

- First step in predicting $K_L \rightarrow \mu^+ \mu^-$
  - Lattice QCD calculation needed to remove two-photon background.
  - Would allow ~10% test of standard model prediction for rare, 2nd order weak decay
$K_L - K_s$

mass difference
$K^0 - \bar{K}^0$ system

- $K^0 - \bar{K}^0$ are distinct anti-particles: $(\bar{s}d)$ and $(\bar{d}s)$ bound states
- These are mixed by the strangeness-violating weak couplings:

\[
M_{KL} - M_{KS} = 3.483(6) \times 10^{-12} \text{ MeV}
\]
- Sensitive to 1000 TeV energy scale, 1000 x LHC energies
- Evidence for charm quark energy scale first found here.
- Effects of QCD can now be computed from first principles!
Lattice Version

- Evaluate standard, Euclidean, 2\textsuperscript{nd} order $\bar{K}^0 - K^0$ amplitude:

$$\mathcal{A} = \langle 0 | T \left( K^0(t_f) \frac{1}{2} \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_b} dt_1 H_W(t_2) H_W(t_1) K^0(t_i) \right) | 0 \rangle$$
\( \Delta M_K \) **Preliminary Results**

(Bigeng Wang)

<table>
<thead>
<tr>
<th></th>
<th>( \Delta M_K x 10^{+12} \text{ MeV} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta M_K )</td>
<td>6.7(0.6)</td>
</tr>
<tr>
<td>( \Delta_{FV} )</td>
<td>0.27(18)</td>
</tr>
<tr>
<td>Expt.</td>
<td>3.483(6)</td>
</tr>
</tbody>
</table>

- Physical light, strange and charm masses
- \( 64^3 \times 128, \ 1/a = 2.36 \text{ GeV} \)
- Integrate: \( 0 \leq \delta \leq 10 \)
- 152 configurations
- \( a^2 \) errors 20% ?

\( t_2 - t_1 \)
Many new lattice results

• Study two-nucleon problem (S. Aoki, et al. HAL QCD)
• Use Euclidean lattice data to constrain spectral functions in inclusive decays (S. Hashimoto, et al.)
• Results for $Kl3$ decay on largest lattice to date (K.-I. Ishikawa, et al., PACS Collaboration)
• Calculate long-distance part (5%) of direct CP violation in $K \rightarrow \pi\pi$ decay: $\varepsilon_K$ (J. Karpie):
  • $K \rightarrow \pi\pi$ decay and direct CP violation (RBC/UKQCD)
    $\text{re } (\varepsilon'/\varepsilon) = (1.38 \pm 7) \times 10^{-4}$ (lattice)
    $(16.6 \pm 0.23) \times 10^{-4}$ (Expt)
Lattice QCD at the Exascale

• Important opportunities to discover new physics beyond the standard model.

• Much work still needed to compensate for the increasingly weak inter-node network.

• Target smaller lattice spacing
  – Increase accuracy of charm quark physics
  – Use open boundary conditions (Luscher & Schaefer)
  – Fourier accelerate: HMC → RMHMC (Girolami & Calderhead)
  – Studying QCD at $\beta = 100$: 

![Graph](image.png)