Numerical Lattice QCD Using Parallel Supercomputers

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The Standard Model = Two kinds of matter and three kinds of force known:

\begin{tabular}{ll}
  matter & force (interaction) \\
  leptons ($\nu$, $e$, ...) & gravity + electro-weak \\
  hadrons ($\pi$, $p$, ...) & gravity + electro-weak + strong \\
\end{tabular}

All the interactions are described by gauge theories.

\textbf{QCD} = Quantum Chromodynamics = gauge theory of strong interaction:
- perturbative calculations: Feynman diagrams,
- non-perturbative calculations: \textit{lattice},

both require computers, often exceeding TFLOPS.
Numerical lattice has brought QCD theoretical calculations to about 10% accuracy,

- using 100 GFLOPS super computers.

Newer research projects were formed to bring us to 3-5% accuracy for calculations such as

- hadron mass spectrum,
- light quarks and chiral symmetry,
- hadron electroweak interactions,
- high-temperature QCD phase structure.

We will soon need 1% accuracy to go beyond the standard model:

- 10 TFLOPS super computer will be used soon.
1 Gauge Theory

Gauge theories: modeled after Maxwell theory of electromagnetism:

\[
\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}, \quad \vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{j}, \quad \vec{\nabla} \cdot \vec{D} = \rho, \quad \vec{\nabla} \cdot \vec{B} = 0.
\]

- Vector potential \( A_\mu = (\phi, \vec{A}) \): \( \vec{E} = -\vec{\nabla} \phi - \frac{\partial \vec{A}}{\partial t}, \vec{B} = \vec{\nabla} \times \vec{A} \).

- Gauge invariance: \( \phi \mapsto \phi - \frac{\partial \lambda}{\partial t}, \vec{A} \mapsto \vec{A} + \vec{\nabla} \lambda \), with arbitrary scalar \( \lambda(x) \).

QED (Quantum Electrodynamics): quantum theory of electromagnetism

- quantum gauge field theory of photon \((A_\mu)\) and electron \((\psi)\)

\[
\mathcal{L}_{\text{QED}} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} + \bar{\psi} (i\gamma^\mu D_\mu - m) \psi,
\]

\[-ie F_{\mu\nu} = [D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu, \quad D_\mu = \partial_\mu - ie A_\mu,\]

- accurate calculations using perturbative method of Tomonaga, Schwinger, Feynman and Dyson.
QCD (Quantum Chromodynamics): quantum theory of strong interaction

- quantum gauge field theory of gluon ($A_\mu^a$) and quark ($q^a$)

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{2} \text{Tr} G^{\mu\nu} G_{\mu\nu} + \bar{q} (i\gamma^\mu D_\mu - m) q,$$

$$-ig G_{\mu\nu} = [D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu], \quad D_\mu = \partial_\mu - ig A_\mu,$$

$$A_\mu = \sum_{a=1}^{8} A_\mu^a T_a, \quad [T_a, T_b] = if_{abc} T_c, \quad \text{Tr}(T_a T_b) = \frac{1}{2} \delta_{ab}.$$  

- asymptotic freedom (infrared slavery): $\beta_{\text{CS}}(g) \equiv \mu \frac{dg}{d\mu} = b_0 g^3 + b_1 g^5 + \mathcal{O}(g^7) < 0$,

$$b_0 = -\frac{1}{(4\pi)^2} \left( \frac{11N_c}{3} - \frac{2N_f}{3} \right),$$

$$b_1 = -\frac{1}{(4\pi)^4} \left( \frac{34N_c^2}{3} - \frac{10N_cN_f}{3} - \frac{(N_c^2 - 1)N_f}{N_c} \right).$$

**perturbative:** $g \to 0$ as $\mu \to \infty$, works for above $\sim 10$ GeV/c reactions, but

**non-perturbative:** $g \gg 1$ as $\mu$ decreases below $\sim 10$ GeV/c, needs lattice formulation.
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Interaction changes: $g = g(r)$

\[ r \to \infty: \; g(r) \to \infty, \text{ Confinement} \]
\[ r \to 0: \; g(r) \to 0, \text{ Asymptotic Freedom} \]

\[ r \to \infty: \; e(r) \to \text{Finite electron charge } e \]
2 Path Integral

Quantum mechanics = probability amplitude $\langle x | e^{-iHt} | y \rangle$,

- Hamiltonian $H = T + V = \frac{p^2}{2m} + V(x)$:

- Free particle ($V = 0$):

$$\int dp \langle x | p \rangle e^{-itp^2/(2m)} \langle p | y \rangle = \int dp \frac{1}{2\pi} \exp\left(-\frac{it}{2m}p^2 + ip(x-y)\right) = \sqrt{\frac{m}{2\pi it}} \exp \left[i \frac{m}{2t} (x-y)^2 \right].$$
• For interacting case in general, $V \neq 0$, introduce a lattice in time by dividing the interval

$$t_0 = 0, \quad t_1 = \epsilon, \quad t_2 = 2\epsilon, \quad \ldots, \quad t_{N-1} = (N-1)\epsilon, \quad t = N\epsilon,$$

and the amplitude is described by $U_\epsilon = e^{-i\epsilon(T+V)}$ as

$$\langle x|e^{-iHt}|y\rangle = \langle x|U_\epsilon^N|y\rangle.$$
• In the coordinate \((x)\) basis
\[
W_\epsilon = e^{-iV/2} e^{-i\epsilon T} e^{-iV/2}
\]
is more convenient, because
\[
\langle x|W_\epsilon|y \rangle = \sqrt{\frac{m}{2\pi i \epsilon}} \exp \left\{ i \frac{m}{2\epsilon} (x - y)^2 - i \frac{\epsilon}{2} [V(x) + V(y)] \right\}.
\]

• \(W_\epsilon\) and \(U_\epsilon\) differ only infinitesimally: \(W_\epsilon = U_\epsilon + O(\epsilon^3)\), hence
\[
\lim_{N \to \infty} W_\epsilon^N = \exp(-it(T + V)).
\]

• Insert \(N - 1\) complete sets of position eigenstates,
\[
\langle x|e^{-iHt}|y \rangle = \lim_{N \to \infty} \int dx_1...dx_{N-1} \langle x|W_\epsilon|x_1\rangle...\langle x_{N-1}|W_\epsilon|y \rangle.
\]
we obtain an expression for the amplitude
\[
\lim_{N \to \infty} \left( \frac{m}{2\pi i \epsilon} \right)^{N/2} \int dx_1...dx_{N-1} \exp \left\{ i \frac{m}{2\epsilon} [(x - x_1)^2 + ...] - i \epsilon \left[ \frac{1}{2} V(x) + V(x_1) + ... \right] \right\}.
\]
• We abbreviate this “path integral” as
\[ \langle x | e^{-iHt} | y \rangle = \int Dx e^{iS}. \]
where for each “path” \( x(t) \) the “action” is given by
\[ S = \int_0^t dt' (T - V) \]
and the path integral measure is
\[ Dx = \lim_{N \to \infty} \left( \frac{m}{2\pi i} \right)^{N/2} dx_1 \ldots dx_{N-1}. \]

• Usually the action \( S \) is real, making
  
  – the factor \( e^{iS} \) to oscillate,
  – the path integral hard to calculate.
Euclidean path integral:

- By choosing \( t = -i\tau \) \((\tau > 0)\), we obtain a better-behaving expression

\[
\langle x | e^{-H\tau} | y \rangle = \int Dx e^{-S_E},
\]

with

\[
S = \int_0^\tau d\tau'(T_E + V),
\]

which is the same as \( iS_E \) if \( t \) is substituted by \( i\tau \).

- Again this is actually an abbreviation for

\[
\lim_{N \to \infty} \left( \frac{m}{2\pi\epsilon} \right)^{N/2} \int dx_1...dx_{N-1} \exp \left\{ -\frac{m}{2\epsilon}[(x - x_1)^2 + ...] - \epsilon \left[ \frac{1}{2}V(x) + V(x_1) + ... \right] \right\}.
\]

So far only the time coordinate is “latticized” (discretized).

In the following we shall “latticize” (discretize) all the space-time coordinates.
Quantum field theory:

- The probability amplitude is given by
  \[
  \langle \phi_i(x) | e^{-iHT} | \phi_f(x) \rangle = \int D[\phi] e^{iS[\phi]}.
  \]

- For each field configuration \( \phi(x) \) is associated the "action"
  \[
  S[\phi] = \int_0^T dt \int d^3x \mathcal{L}(\phi, \partial \phi) = \int_0^T dt (T[\phi] - V[\phi]).
  \]

- Any relevant field correlation or observable is described like
  \[
  \langle T \phi' \phi'' \rangle = Z \int D[\phi] \phi' \phi'' e^{iS[\phi]},
  \]
  with \( Z \) defined to make \( \langle 1 \rangle = 1. \)

These are actually abbreviations for more complicated but accurate space-time discretized formulae with \( D[\phi] \) meaning integral over \( \phi_i \) defined on discretized space-time points \( i \).
Euclidean quantum field theory: a better-behaving version with $x^0 = t = -i\tau = -ix^4$,

- The “action” for a field configuration $\phi(x)$ is
  \[
  S[\phi] = \int_0^T d\tau \int d^3x \mathcal{L}_E(\phi, \partial\phi) = \int_0^T d\tau (T_E[\phi] + V[\phi]).
  \]

- Any observable is described as
  \[
  \langle O \rangle = Z \int D[\phi] O[\phi] e^{-S_E[\phi]},
  \]
  with $Z$ defined to make $\langle 1 \rangle = 1$.

These are actually abbreviations for more complicated but accurate space-time discretized formulae with $D[\phi]$ meaning integral over $\phi_i$ defined on discretized space-time points $i$. 
Fermion fields (1): each fermion state requires a pair of Grassmann variables $(\xi, \xi^+)$,

- anticommutate: $\{\xi^+, \eta\} = \{\xi, \eta\} = \{\xi, \eta^+\} = 0$,

- any function is a polynomial: $F(\xi^+, \xi) = F^{(00)} + F^{(01)}\xi + F^{(10)}\xi^+ + F^{(11)}\xi^+\xi$,

- integral: $\int d\xi d\xi^+ F(\xi^+, \xi) = -\int d\xi^+ d\xi F(\xi^+, \xi) = F^{(11)}$, eg,

\[
\int d\xi^+ d\xi e^{-\lambda\xi^+\xi} = \int d\xi^+ d\xi (1 - \lambda\xi^+\xi) = \lambda,
\]

- derivative: $\partial_{\xi^+} = F^{(10)} + F^{(11)}\xi$ and $\partial_{\xi} = F^{(01)} - F^{(11)}\xi^+$ so that

\[
\partial_{\xi}\partial_{\xi^+}F = F^{(11)} = -\partial_{\xi^+}\partial_{\xi}F = \int d\xi d\xi^+ F,
\]
generalizing,
\[
\int d\xi_1 d\xi_2^+ d\xi_2^+ ... d\xi_N^+ d\xi_N^+ F(\xi^+, \xi) = (-1)^N \int d\xi_1^+ d\xi_2^+ d\xi_2^+ ... d\xi_N^+ d\xi_N^+ F(\xi^+, \xi) = F^{(NN)},
\]

eg
\[
\int d\xi_1^+ d\xi_1^+ d\xi_2^+ d\xi_2^+ ... d\xi_N^+ d\xi_N^+ \exp(-\xi_j^+ A_{ji} \xi_i) = \det A,
\]

and
\[
\int d\xi_1^+ d\xi_1^+ d\xi_2^+ d\xi_2^+ ... d\xi_N^+ d\xi_N^+ \exp(-\xi_j^+ A_{ji} \xi_i + \xi_i^+ \eta_i + \eta_i^+ \xi_i) = (\det A) \exp(\xi_j^+ A_{ji} \eta_i),
\]

further, taking derivatives of \((\partial_{\eta_i} \partial_{\eta_j}^+)\) and setting \(\eta = \eta^+ = 0\),
\[
\int d\xi_1^+ d\xi_1^+ d\xi_2^+ d\xi_2^+ ... d\xi_N^+ d\xi_N^+ \exp(-\xi_j^+ A_{ji} \xi_i) \xi_{j_1}^+ \xi_{j_1}^+ \xi_{j_n}^+ \xi_{i_n} = (\det A) \epsilon_{j_1...j_n}^{k_1...k_n} A_{k_1i_1}^{-1} ... A_{k_ni_n}^{-1},
\]

where \(\epsilon_{j_1...j_n}^{k_1...k_n}\) takes value \(\pm 1\) for even/odd permutations and 0 otherwise.
Fermion fields (2): coherent states are indispensable, defined as

\[ |\xi\rangle = |\xi_1, \xi_2, \ldots, \xi_N\rangle = \exp(\sum_{n=1}^{N} a_i^+ \xi_i)|0\rangle \]

and

\[ \langle 0|\xi\rangle = 1, \quad \text{and} \quad a_i|\xi\rangle = \xi_i|\xi\rangle, \]

describe completeness:

\[ 1 = \int d\xi^+ d\xi e^{-\xi^+\xi} |\xi\rangle \langle \xi|, \]

and matrix elements:

\[ \langle \xi|a_j^+ A_{ji} a_i|\xi'\rangle = \xi_j^+ A_{ji} \xi' e^{-\xi^+\xi'}, \]

or

\[ \langle \xi|\exp(a_j^+ A_{ji} a_i)|\xi'\rangle = \exp(\xi_j^+ (e^A)_{ji} \xi_i'), \]

so that

\[ \text{Tr} \exp(a_j^+ A_{ji} a_i) = \int d\xi^+ d\xi \exp(-\xi^+\xi) \langle +\xi| \exp(a_j^+ A_{ji} a_i)| -\xi\rangle. \]
3 Lattice QCD

Simplify from 4d Minkowski continuum to 4d Euclid discrete space-time: Easiest: 4d simple hyper-cubic lattice, $L_0L_1L_2L_3$,

**site:** $s = (n_0n_1n_2n_3)$, $0 \leq n_i \leq L_i - 1$ ($i = 0, 1, 2, 3$).

**link:** $l = (s, \mu)$, $\mu \in \{0, 1, 2, 3\}$, connects $s$ and $s + \hat{\mu}$.

constant separation (lattice constant) $a$ between neighboring sites. Taking $a \to 0$ should give continuum physics.
Dynamical variables:

**quark:** $q(s)$, defined on site and forms basis of fundamental (3) representation of SU(3),

**gluon:** $U(s, \mu) = \exp(ig \int_s^{s+\mu} A_\mu(y)dy_\mu) \in SU(3)$, now a group element defined on link.

Gauge transformation: $G(s) \in SU(3)$, defined on site, maps quarks and gluons

$$q(s) \mapsto G(s)q(s)$$

and

$$U(s, \mu) \mapsto G(s)U(s, \mu)G(s + \mu)^{-1}.$$  

There are many other ways to define lattice, eg:

- random lattice,

with different advantages, but the way $q$, $U$ and $G$ are defined is basically the same.
Action: $S_{\text{QCD}}[U, q, \bar{q}] = S_{\text{gluon}}[U] + S_{\text{quark}}[U, q, \bar{q}]$, must respect gauge invariance:

**gluon part:** $S_{\text{gluon}}[U] = \frac{6}{g^2} \sum_s \sum_{\mu < \nu} \Box(s, \mu, \nu),$

- where the plaquette, $\Box(s, \mu, \nu) = 1 - \frac{1}{3} \text{Re} \text{Tr} U(s, \mu)U(s + \hat{\mu}, \nu)U(s + \hat{\nu}, \mu)^{-1}U(s, \nu)^{-1},$
- gives $-\frac{1}{2} \text{Tr} G^{\mu\nu} G_{\mu\nu}$ as $a \to 0$ and $g \to 0,$

**quark part:** $S_{\text{quark}}[U, q, \bar{q}] = \sum_{s, s'} \bar{q}(s) M[U](s, s') q(s'),$

- with $M[U](s, s')$ describing quark propagation between sites $s$ and $s'$,
- which should give $\bar{q}(i\gamma^\mu D_\mu - m)q$ as $a \to 0$ and $g \to 0,$
- but there is a serious problem, which will be discussed later,

Gauge invariance is preserved.
Expectation values of any gauge-invariant observable:

\[ \langle O \rangle = N^{-1} \int [dU][dq][d\bar{q}] O[U, q, \bar{q}] \exp(-S_{\text{QCD}}[U, q, \bar{q}]), \]

or by integrating over the quark Grassmann variables,

\[ N'^{-1} \int [dU] (\det M[U]) \exp(-S_{\text{gluon}}[U]) \]

where \( N \) or \( N' \) is defined by \( \langle 1 \rangle = 1 \).

Finite lattice and compact SU(3) assures finite \( \langle O \rangle \).

Since

\[ (\det M[U]) \exp(-S_{\text{gluon}}[U]) = \exp(-S_{\text{gluon}}[U] + \text{Tr} \log M[U]), \]

it is often convenient to use effective action

\[ \tilde{S}[U] = S_{\text{gluon}}[U] - \text{Tr} \log M[U], \]
Continuum limit is well defined because of the asymptotic freedom.

- Assume all the relevant quarks are massless.
- Then any observable with mass dimension must be described as
  \[ \langle O \rangle = a^{-1} f(g) \]
  with some dimensionless function \( f(g) \) of dimensionless coupling \( g \).
- Renormalizability of the theory means the cutoff dependence should vanish
  \[ \frac{d\langle O \rangle}{da} \to 0 \]
  as \( a \to 0 \), or
  \[ f(g) - f'(g) \left( a \frac{dg}{da} \right) = \beta(g)f'(g) + f(g) \to 0. \]
- This \( (df/f = -dg/\beta) \) is easily solved to give:
  \[ \langle O \rangle a \propto \exp \left( - \int^g \frac{dh}{\beta(h)} \right), \]
  or
  \[ \langle O \rangle a \propto (g^2b_0)^{-b_1/(2b_0^2)} \exp(-1/(2b_0g^2))[1 + O(g^2)], \]
  where \( \beta(g) \equiv -a \frac{dg}{da} = -b_0g^3 - b_1g^5 + O(g^7) \) is perturbatively well known.
In practice quarks are massive: so

- instead of solving
  \[
  \left[-a \frac{\partial}{\partial a} + \beta(g) \frac{\partial}{\partial g}\right] f(a, g) = O(a),
  \]

- work with
  \[
  \left[\mu \frac{\partial}{\partial \mu} + \beta(g) \frac{\partial}{\partial g} - \gamma(g) m_i \frac{\partial}{\partial m_i}\right] f(a, g, m) = 0
  \]
  at some prescribed kinematic condition,

- the coefficient \( \gamma(g) = c_0 g^2 + O(g^4) \) is perturbatively calculable again,
  \[
  c_0 = \frac{1}{(4\pi)^2} \frac{3(N^2 - 1)}{N},
  \]

- two independent solutions,
  \[
  \Lambda = \mu(b_0 g^2)^{-b_1/(2b_0^2)} \exp \left[ - \int^g dh \left( \frac{1}{\beta(h)} + \frac{1}{b_0 h^3} - \frac{b_1}{b_0^2} \right) \right],
  \]
  and
  \[
  M = m(2b_0 g^2)^{-c_0/(2b_0)} \exp \left[ \int^g dh \left( \frac{\gamma(h)}{\beta(h)} + \frac{c_0}{b_0 h} \right) \right],
  \]

- because \( b_0, b_1 \) and \( c_0 \) are independent of regularization scheme, \( M \) is also.

Thus we can work with fixed mass ratio.
Chiral symmetry: invariance under global transformation

\[ q \rightarrow e^{\alpha \gamma_5}q \quad \text{and} \quad \bar{q} \rightarrow \bar{q}e^{\alpha \gamma_5}. \]

- preserved in the absence of \( m\bar{q}q \), like

\[ U(N_f)_L \times U(N_f)_R = SU(N_f)_V \times SU(N_f)_A \times U(1)_V \times U(1)_A \]

- spontaneously broken for light normal quarks, \( m_u \sim m_d \sim 0 \), but is fairly good \( (SU(2)_V \times SU(2)_A) \)

- important for Nambu-Goldstone pion, PCAC, etc,

- might be still good with strange quark, \( m_s \sim 100 \text{ MeV} \),

- but is hard to maintain on regular lattices.
Naive (and free and massless) lattice fermion action,

\[ M_{xy} = \frac{1}{2} a^{D-1} \sum_{\mu} \gamma_\mu [\delta_{x+\mu,y} - \delta_{x-\mu,y}], \]

leads to a propagator

\[ \Delta(p) = a(\gamma_\mu \sin(p_\mu a))^{-1}, \]

which has \(2^D\) poles at \(p_\mu = 0\) or \(\pi/a\):

- for \(D = 4\) there appear \(2^4 = 16\) flavors instead of 1,
- shifting of one component of \(p_\mu\), such as \(\tilde{p}_\mu = p_\mu - \pi/a\), acts like

\[ \gamma_\mu \sin(p_\mu a) = -\gamma_\mu \sin(\tilde{p}_\mu a)\]

so the chirality \(\pm\) states are paired.
Nielsen and Ninomiya proved that for a fermionic system with

- a regular lattice and

- local,

- hermitian,

- and translationally invariant action,

chirality ± states are paired.
Three traditional ways to alleviate this fermion doubling problem:

- move away from regular lattice, like random lattice approach,
- explicitly break the chiral symmetry, like Wilson approach,

\[ M_{xy} = a^D \left( m + \frac{Dr}{a} \right) \delta_{xy} + \frac{1}{2} a^{D-1} \sum_{\mu} [(r + \gamma_\mu)U_{x\mu} \delta_{x+\hat{\mu},y} + (r - \gamma_\mu)U^\dagger_{y\mu} \delta_{x-\hat{\mu},y}], \]

or by rescaling the fields,

\[ M_{xy} = \delta_{xy} + K \sum_{\mu} [(r + \gamma_\mu)U_{x\mu} \delta_{x+\hat{\mu},y} + (r - \gamma_\mu)U^\dagger_{y\mu} \delta_{x-\hat{\mu},y}], \]

with “hopping parameter” \( K = 1/2(ma + Dr) \).

- propagation from a site \( x \) to \( x \pm \hat{\mu} \) projects chirality:

\[ \left( \frac{1 \pm \gamma_\mu}{2} \right)^2 = \left( \frac{1 \pm \gamma_\mu}{2} \right), \]

- propagator becomes

\[ a\{\sum_{\mu} [\gamma_\mu \sin p_\mu a + r(1 - \cos p_\mu a)]\}^{-1} \]

giving a mass \( m + 2dr/a \) to the doublers.
• dilute the doubling and keep part of the chiral symmetry, like Kogut-Susskind (staggered) approach

- Assume even sites in all the lattice directions, \( L_\mu = 2K_\mu \),

- single-component Grassmann site variable \( \chi_x, (x_\mu = 0, 1, \ldots, L_\mu - 1) \),

- action \( S_{KS} = \bar{\chi}_x M_{xy} \chi_y \) with propagation matrix

\[
M_{xy} = a^D m \delta_{xy} - \frac{1}{2} a^{D-1} \sum_\mu \eta_{x,\mu} [\delta_{x+\hat{\mu},y} U_{x\mu} - \delta_{x-\hat{\mu},y} U_{y\mu}^\dagger ]
\]

- phase factor \( \eta_{x,\mu} \) satisfies \( \eta_{\Box} = -1 \),

- to form a spinor, use a \( 2^D \) hypercube,

\[
x_\mu = 2u_\mu + v_\mu,
\]

with \( u_\mu = 0, 1, \ldots, K_\mu - 1 \) and \( v_\mu = 0, 1 \),

- \( 2^D = 16 \) components in each hypercube are combined to form Dirac spinors of 4 flavors,
- define $\Gamma_v = \gamma_1^{v_1} \gamma_2^{v_2} \gamma_3^{v_3} \gamma_4^{v_4}$ and

$$q_v^{sf} = \frac{1}{8} \sum_v \Gamma_v^{sf} \chi_{2u+v} \quad \text{and} \quad \bar{q}_v^{sf} = \frac{1}{8} \sum_v \bar{\chi}_{2u+v} \Gamma_v^{+sf},$$

$$- \frac{1}{4} \text{Tr} \Gamma_v^+ \Gamma_w = \delta_{vw} \quad \text{and} \quad \frac{1}{4} \sum_v (\Gamma_v^+)^{sf} (\Gamma_v)^{tg} = \delta^{st} \delta^{fg}$$

lead to

$$\chi_{2u+v} = 2\text{Tr}(\Gamma_v^+ q_u) \quad \text{and} \quad \bar{\chi}_{2u+v} = 2\text{Tr}(\bar{q}_u \Gamma_v),$$

- with $\sum = \sum' \sum$, the mass term becomes

$$\sum_x \bar{\chi}_x \chi_x = 16 \sum' (\bar{q}_u 1_\gamma \times 1_t q_u)$$

where $1_\gamma$ acts on Dirac indices $s$ and $1_t$ acts on flavor indices $f$. 
relations like

$$\gamma_\mu \Gamma_\nu = \delta_{0,v_\mu} \eta_{v_\mu} \Gamma_{v+\hat{\mu}} + \delta_{1,v_\mu} \eta_{v_\mu} \Gamma_{v-\hat{\mu}}, \quad \text{and} \quad \gamma_5 \Gamma_\nu \gamma_5 = (-1)^{v_1+v_2+v_3+v_4} \Gamma_v,$$

and difference operators for $a \partial_\mu f_u$ and for $a^2 \partial_\mu^2 f_u$

$$\Delta_\mu f_u = \frac{1}{4} (f_{u+\hat{\mu}} - f_{u-\hat{\mu}}) \quad \text{and} \quad \delta_\mu f_u = \frac{1}{4} (f_{u+\hat{\mu}} + f_{u-\hat{\mu}} - 2f_u)$$

are used to obtain the kinetic term

$$16 \sum_u' \sum_\mu \bar{q}_u [(\gamma_\mu \times 1_i) \Delta_\mu - (\gamma_5 \times t_5 t_\mu) \delta_\mu] q_u$$

with flavor matrices given by $t_\mu = \gamma_\mu^T = t_\mu^+$,
\(- O(a) \) part \((\gamma_\mu \times 1_t) \Delta_\mu \) gives back ordinary Dirac fermions with \(U(4) \times U(4)\) flavor symmetry,

\(- \) while \(O(a^2)\) part, \((\gamma_5 \times t_5 t_\mu) \delta_\mu\), a lattice artifact, breaks the symmetry,

\(- \) yet a continuous subgroup \(U(1)_e \times U(1)_o\)

\[ q_u \mapsto (U_e P_e + U_o P_o)q_u \quad \text{and} \quad \bar{q}_u \mapsto \bar{q}_u(P_e U^+_o + P_o U^+_e) \]

survives, with even- and odd-site projections defined by

\[ P_e = \frac{1}{2}(1_\gamma \times 1_t + \gamma_5 \times t_5) \quad \text{and} \quad P_o = \frac{1}{2}(1_\gamma \times 1_t - \gamma_5 \times t_5), \]

\(- \) mass term \((1_\gamma \times 1_t\) further breaks the symmetry down to diagonal \(U(1)_e = U(1)_o,\)
- propagator:

$$a \over 8[ (\gamma_\mu \times 1_t) \sin k_\mu a + (\gamma_5 \times t_5 t_\mu)(1 - \cos k_\mu a)]'$$

- physical momentum is $p_\mu = k_\mu/2$, and with

$$- \pi \over a < k_\mu \leq \pi \over a \quad \text{or} \quad - \pi \over 2a < p_\mu \leq \pi \over 2a,$$

the propagator has only one pole near $p = 0$ for $a \to 0$ as the $\gamma_5 \times t_5 t_\mu$ part drops out,

- at finite $a$ we have a continuous symmetry that allows studying Nambu-Goldstone pion,

- in continuum limit $a \to 0$ the full $U(4) \times U(4)$ symmetry should be restored.
Domain-wall fermions: promising new method by Kaplan, ..., Shamir, ...

- use 5d lattice, \((x_\mu, s)\), with the breaking exponentially suppressed in the 5th dimension.
- Dirac operator \(D^5 = \gamma_\mu \partial_\mu + \gamma_5 \partial_s + m(s)\) with standard Dirac matrices and
  - \(m(s)\): monotonously increasing from \(m(-\infty) = m_-\) to \(m(0) = 0\) to \(m(+\infty) = m^+\),

\[ \begin{array}{c}
\end{array} \]

- has a zero-mode solution \(D\psi_\pm = 0\):
  - \(\psi_\pm = e^{ipx} \phi_\pm u_\pm\),
  - chiral eigen mode \(\gamma_5 u_\pm = \pm u_\pm\),
- localized to the \(m(0) = 0\) defect \((\pm \partial_s + m(s))\phi_\pm = 0\), ie \(\phi_\pm \propto \exp(\mp \int^s m(s')ds')\).

Needs wall-anti-wall in a finite periodic lattice, yet works well for QCD.
Hadron spectroscopy

- Quark propagator $Q(s, s')$: inverse of the propagation matrix, $M[U]^{-1}(s, s')$.
- Hadron propagator $H(s, s')$: color-singlet combination of quark propagators.
- Hadron mass:
  - pole, in the real Minkowski world,
  - decay constant in time in the Euclidean world,
  \[ H(s, s') \propto \sum_n c_n \exp(-E_n t) \sim \exp(-mt) \quad \text{for large } t = |s_0 - s'_0|. \]
  - $t$ is finite (not $\infty$) on the lattice:
    - instead look at effective mass
    \[ m_{\text{eff}}(t) \equiv -\ln(H(t + 1)/H(t)) \]
    - $m_{\text{eff}}(t)$ should show a plateau ($\to m$ as $t \to \infty$).
- Don’t forget to project onto fixed momentum, usually 0.
- Structure and decay parameters are calculable with appropriate insertions of current operators in the plateau.
Light hadron spectrum is well within reach:

Need:

- full-QCD with light-quark mass and its chiral symmetry controlled by DWF,
- hadron matrix elements (Belle, BaBar, KTeV, etc),
- nucleon structure (RHIC Spin, SuperK, etc),
- quark mass ,
- $\alpha_s(M_Z) = 0.117 \pm 0.003$,
- thermodynamics (RHIC, LHC, etc),
- ...
Hadronic matrix elements:

- $K$ physics (AGS, KTeV): explain
  - $\Delta I=1/2$ rule, $\mathcal{A}(K \to \pi\pi(I=0))/\mathcal{A}(K \to \pi\pi(I=2)) \sim 22$, through
    \[ V_{ud}V_{us}^*(G_F/\sqrt{2})[C^+(\mu)O^+(\mu) + C^-(\mu)O^-(\mu)], \quad O^\pm = [(\bar{s}d)_L(\bar{u}u)_L \pm (\bar{s}u)_L(\bar{u}d)_L] - [u \leftrightarrow c], \]
    where $O^-$ is $\Delta I=1/2$ and $O^+$ is mixed with $3/2$,
  - $\epsilon'/\epsilon=28(4) \times 10^{-4}$, where $\eta_+=\epsilon+\epsilon'$, $\eta_0=\epsilon-2\epsilon'$, $\eta=\mathcal{A}(K_L \to \pi\pi)/\mathcal{A}(K_S \to \pi\pi)$, through
    \[ B_K = 3\langle \bar{K}^0|\bar{s}d\rangle^2\rangle K^0\rangle / 8\langle \bar{K}^0|\bar{s}d\rangle\langle 0|\bar{s}d\rangle\langle K^0\rangle, \]
    etc.

- $B$ physics (Belle, BaBar): similar to $K$.

- Nucleon (spin) structure (... , HERMES, RHIC-Spin, LHC, ...).

- Nucleon decay (Kamiokande, SuperK, ...).

Correct treatise of quark mass and chiral symmetry is crucial: DWF.
QCD Thermodynamics: phase transition or cross-over is expected at $T \sim 200\text{MeV}$

- from confined to deconfined, or
- from chiral-broken to chiral-symmetric

Look at canonical partition at temperature $T$

$$Z = \text{tr} \exp(-H/T)$$

which can be described by a lattice path integral

$$\text{tr} \exp(-H/T) = \int D[\phi] e^{-S(T)}$$

with

$$S(T) = \int_0^{1/T} dt \int_V d^3x \mathcal{L}_E(\phi, \partial \phi)$$

and periodic [anti-periodic] boundary condition in time is imposed on bosonic [fermionic] fields.
Order parameters:

- for chiral symmetry \((m_q \sim 0)\), chiral condensate
  \[
  \chi = \langle \bar{q} q \rangle,
  \]
  calculable as \(\propto \text{tr} M^{-1}\):
  - in spontaneously broken phase \(\chi \neq 0\) and \(m_\pi^2 f_\pi^2 = m_q \chi\)
  - in symmetric phase \(\chi = 0\).

- for confinement \((m_q \sim \infty)\), Polyakov line
  \[
  P = \langle \text{Tr} \prod_{t=0}^{N_t-1} U(x,t;\mu = \hat{t}) \rangle
  \]
  which measures the free energy of a heavy color charge \(e^{-F/T} = \langle ce^{-H/T} c^+ \rangle = \langle c(1/T)c^+(0) \rangle\):
  - confined: \(F \to \infty\) and \(P = 0\),
  - deconfined: \(P \neq 0\)
  Related to center \((Z_3)\) symmetry: \(P \mapsto \omega P, \omega^3 = 1\).

Other thermodynamic quantities are calculated too.
Exotica: $N_c \neq 3$, $N_f \neq 2+1$, ...

- $T \neq 0$ QCD phase structure is easier to understand if SU($N_c$) quenched is second order for $N_c \geq 4$
- Hagedorn temperature, $\frac{T_c}{\sqrt{\sigma}} = \sqrt{\frac{3}{\pi(d-2)}}$?
- New developments in M/string theory starting from Maldacena’s duality conjecture.
  - Glueball spectrum at large $N_c$ and large $g^2$ can be obtained.
  - Ratio between different string tensions can be obtained,
    * classified by $Z(N_c)$ $N_c$-ality and string tension:
    * naive SU($N_c$) strong coupling, $\sigma_k \propto \min\{k, N - k\}$
    * Strassler SU($N_c$) strong coupling, $\sigma_k \propto k(N_c - k)$
    * Strassler super-SU($N_c$) strong coupling, $\sigma_k \propto \sin \frac{k\pi}{N_c}$.
  - $N_c = 4$ is the first example with different string tensions,
    * 3-3* and 6-6* tensions are the same in SU(3) pure-gauge theory.
4 Computational Method

In practice, there are too many degrees of freedom for analytic computation:

- modest $10^4$ lattice means $4 \times 10^4$ link variables,
- or $32 \times 10^4$ real degrees of freedom for gauge field alone,
- even when restricted to $U_{x\mu} = \pm 1$, the path integral is a sum over $2^{40000} \sim 10^{12000}$ configurations usually impossible to perform analytically.

Lattice QCD action $S_{\text{QCD}}[U, q, \bar{q}]$, is real (for most of the interesting cases):

- “Boltzman factor” $\exp(-S_{\text{QCD}}[U, q, \bar{q}])$ is positive definite,
- Monte Carlo technique is useful.

Numerically generate configurations $\{C\}$ with probability distribution $\propto e^{-S(C)}$:

- Metropolis,
- (pseudo) heatbath,
- Langevin,
- molecular dynamics,
- hybrid Monte Carlo...
Use Markov chain $C \rightarrow C'$ specified by a probability distribution $P(C, C')$

- to achieve equilibrium:
  
  $$e^{-S(C)} = \sum_{C'} P(C, C') e^{-S(C')}$$

  is the necessary and sufficient condition:

- distance between two ensembles $E$ and $E'$ of configurations:
  
  $$||E - E'|| = \sum_{C} |p(C) - p'(C)|$$

  $p(C)$ and $p'(C)$ are probability distributions for $E$ and $E'$ respectively,

- suppose $E'$ resulted from the Markov chain starting from $E$:
  
  $$p'(C) = \sum_{C'} P(C, C') p(C')$$

- since $P(C, C') \geq 0$ and $\sum_{C'} P(C, C') = 1$,
  
  $$||E' - E_{eq.}|| = \sum_{C} |\sum_{C'} P(C, C')(p(C') - p_{eq.}(C'))| \leq \sum_{C,C'} P(C, C')|p(C') - p_{eq.}(C')| = ||E - E_{eq.}||$$

  or the algorithm reduces the distance,

- if $P(C, C') > 0$ then the inequality is exact,

- easy way to implement: the detailed balance
  
  $$P(C', C)e^{-S(C)} = P(C, C')e^{-S(C')}.$$
Metropolis:

1. choose arbitrary candidate $U'$ to replace a link $U$ that satisfies $P(U, U') = P(U', U)$
   eg $U' = UV$ with some $p(V)$, $p(V) = p(V^{-1})$, (peaked at $p(1)$),
2. evaluate $S(U')$,
3. if $S(U') < S(U)$, accept $U'$,
4. otherwise, accept $U'$ with a probability of $\exp(-\Delta S)$:
   - generate a uniform random number $0 < x < 1$ and accept if $x < \exp(-\Delta S)$
5. fail safe, but efficiency depends on $p(V)$.

(Pseudo) Heatbath:

- given the environment, solve for $p(U') \propto e^{-S(U')}$,
- easy for Ising, like $p(+) = e^{-S(+)} / (e^{-S(+)} + e^{-S(-)})$,
- practical for SU(2) QCD (see Creutz),
- not so for SU(3) QCD: use pseudo heatbath (use combination of SU(2) subgroups to cover SU(3).)

Over relaxation

- used to accelerate decorrelation for the above two,
- choose $V$ to minimize $S(UV)$ and try $U' = UV^2$. 
Langevin

- Brownian motion in hypothetical time \( \tau \),
  \[
  \frac{dx}{d\tau} = -\frac{\delta S}{\delta x} + \eta \quad \text{or discretized} \quad x' = x - \epsilon \frac{\delta S}{\delta x} + \sqrt{\epsilon} \eta = x - f_\tau(x, \eta)
  \]
- Random noise \( \eta \) must be appropriately regularized, eg, by a measure like \( \propto \exp(-\eta^2/4) \) and satisfies
  \[
  \langle \eta(\tau) \rangle = 0 \quad \text{and} \quad \langle \eta(\tau)\eta(\tau') \rangle = 2\delta(\tau - \tau'),
  \]
- Probability distribution \( P(x, \tau) \) evolves according to
  \[
  P'(x') = \langle \int Dx P(x) \delta(x' - x + f_\tau(x, \eta)) \rangle_\eta,
  \]
  or to the first order
  \[
  \Delta P = \epsilon \frac{\partial}{\partial x} \left( \frac{\partial P(x)}{\partial x} + \frac{\delta S}{\delta x} P(x) \right) + O(\epsilon^2)
  \]
  which can be transformed into a Fokker-Planck equation
  \[
  -\frac{\partial}{\partial \tau} |P(\tau)\rangle = H_{FP} |P(\tau)\rangle
  \]
  where the positive semi-definite Fokker-Planck Hamiltonian has a zero-energy ground state
  \[
  H_{FP} |e^{-S(x)}\rangle = 0
  \]
  and usually finite energy gap, ie quick (exponential) convergence to \( \exp(-S) \),
- Conceptually simple but involves \( O(\epsilon) \) error.
Molecular dynamics (MD)

- follow a classical motion governed by a fictitious Hamiltonian
  \[ \frac{1}{2}p^2 + S(x) \]
- and appropriately (randomly) refresh momenta \( p \) to give \( \propto \exp(-S) \) distribution
- more efficient than Langevin (not a diffusion process)
- slightly more accurate also (usually \( O(\epsilon^2) \) error).

Hybrid Monte Carlo (HMC)

- follow a classical path, like in MD,
- accept or reject by a Metropolis test
- no discretization error in \( \epsilon \)
- applicability is limited.
Gauge part is easy, with local estimation of

\[ \Box = \text{Tr} UUUU. \]

Quark part must be integrated over Grassmann variables:

\[ \langle O \rangle = \tilde{N}^{-1} \int [dU] \tilde{O}[U] (\det M[U]) \exp(-S_{\text{gluon}}[U]) \]

leading to effective action,

\[ \tilde{S} = S_{\text{gluon}}[U] - \text{Tr} \ln M[U]. \]

Irrespective of L, MD or HMC, requires estimating

\[ \frac{\delta}{\delta U} \text{Tr} \ln M[U] = \text{Tr} \left( M[U]^{-1} \frac{\delta M[U]}{\delta U} \right), \]

often using noisy estimator and iterative methods: (bi)Conjugate Gradient (bCG), Conjugate Residua (CR), ...
In practice, \( L_i \approx 64 \):

- \( 4 \times 64^4 = 2^{26} = 64 \text{ million } U \)'s, each with 8 real degree's of freedom
- \( 512 \text{ M-dimensional integration, may require } 2^4 \text{ more.} \)

Needs a lot of \( U \times U \) and \( U \times q \) operations, eg, in a single update of a link are

**gluon part:** several \( 10^3 \) FLOP's, many \( (U \times U) \), to estimate plaquette \( \text{Tr}UUUU \),

**quark part:** several \( 10^5 \) FLOP's, many \( (U \times q) \) in CG-solving \( M[U]q = \xi \), to estimate \( \text{Tr ln } M[U] \).

Repeat a million times: \( \approx 64 \times (\text{million})^3 \approx 10^{20} \) FLOP's,

- takes months on \( O(10) \) GFLOPS computer.

Needs better technology: **parallel computing**

- local interaction matches parallel computing.
5 QCD-dedicated Parallel Super-Computing

Requires a huge number of numerical calculations:

- 20 years ago: \( \sim \) MFLOPS on VAX‘en or CDC’s,
- 10 years ago: \( \sim \) GFLOPS using Columbia, APE, GF11, QCDPAX, CM2, etc,
- today: \( \sim \) TFLOPS using CP-PACS or QCDSP.

With about \( 10^{18-19} \) floating-point operations a year,

- partial success in hadron mass spectrum \((\pi, \rho, N, ...)\)
  - albeit with quenched approximation
- partial success in describing “deconfining/chiral” phase transition at about \( 10^{12} \) K,
  - investigated at RHIC and LHC experiments,
  - albeit with relatively heavy quarks.
Necessary to improve on

- systematic errors arising from finite lattice spacing $a$,
- systematic errors arising from finite lattice volume $La$,
- chiral symmetry,
- light-quark dynamics,
- understanding of hadronic electroweak interactions.

Requires TFLOPS supercomputers: RIKEN-BNL-Columbia QCD Project

QCDSP = QCD with DSP:

- a parallel super-computing project for QCD,
- made possible by passion and labor of many physicists.

DSP = Digital Signal Processor: inexpensive, but powerful.
QCDSP

- RIKEN-BNL Research Center: 600-GFLOPS,
  - one 150-GFLOPS,
  - four 100-GFLOPS,
  - one 50-GFLOPS partitions,
  - and some single-mother-board machines,
  - flexibly reconfigured for physics projects,
- Columbia University: 400-GFLOPS,
- Smaller configurations in SCRI (FSU), Ohio, Wuppertal (Germany).

CP-PACS Project of University of Tsukuba: 600-GFLOPS.
QCDSP at RIKEN-BNL Research Center

- 192 mother boards,
- one mother board = 64 daughter boards,
- one daughter board = 50-MFLOPS DSP + custom NGA + 2-MB memory,
- with single-precision arithmetic,

12K daughter boards form a uniform torus network with 4d nearest neighbor communications.

Design started in ’93:

- SCRI at Florida State University: Tony Kennedy, Robert Edwards,
- Trinity College, Dublin: Jim Sexton,
- Fermilab: Sten Hanson,
- Ohio State University: Greg Kilcup
Construction:

parallel computer is

- usable even before completion,
- so flexible,
  - as capable of 5d domain-wall fermion lattice calculations, not planned in the design stage,
  - as capable of Boltzmann Navier-Stokes, and other partial differential equation problems (nearest neighbor communication).
6 Research using QCDSP

Numerical lattice has brought QCD theoretical calculations to about 10% accuracy.

RIKEN-BNL-Columbia QCD Project was formed to bring us to 3-5% accuracy

- using 5d DWF method with correct chiral symmetry, and
- TFLOPS super computers,

for calculations such as

- hadron mass spectrum,
- light quarks and chiral symmetry,
- hadron electroweak interactions,
- high-temperature QCD phase structure.

Conventional 4d lattice calculations are kept alive too:

- in order to see all the different methods agree with each other.

We will soon need 1% accuracy to go beyond the standard model:

- 10 TFLOPS supercomputer will be used soon.
Hadron matrix elements: Blum + Soni (BNL),

- Good chiral behavior observed in three-point functions for $B_K$, $\epsilon'/\epsilon$ and $K\bar{K}$ mixing calculated from the first 11 configurations from QCDSP.

P. Vranas (Columbia → UIUC) contributed a lot too.
Quark mass: Lattice and sum-rule estimates do not agree,

- Lattice results are lighter by almost a factor of 2,
- After seeing that, sum-ruler has been busy revising their results:
  - especially with spectral function at medium energies,
  - and may be converging with the lattice results.

Lattice results are not perfect yet: (partially) quenched, Nielsen-Ninomiya.

DWF helps: Blum & Wingate + Soni,

- Lattice perturbation developed for DWF 1-loop $Z_m$,
- Tentative quenched result: $m_s(2\text{GeV}, \overline{\text{MS}}) \sim 82 \pm 15\text{MeV}$. 
$N_f$-dependence, staggered (ie with chiral symmetry):

- 2nd-order? for $N_f = 2$ and $m_q = 0$ with O(4) or O(2) exponents?
  - looks at susceptibility of $\chi$

- 1st-order for $N_f \geq 3$ and $m_q \to 0$
  - well established for $N_f \geq 4$,
  - not so for $N_f = 3$.

$N_f = 2 + 1$, staggered (ie realistic case):

the same unprintable figure

Need further investigation with larger $V$ and finer $T$. 
Pure-gauge SU(4) study: exploration of \((N_c, N_f)\) plane – Wingate + SO

- \(N_f=4\) and \(N_c=3\) is confining but chirally-symmetric at \(T = 0\) (parity doublet hadrons),
- Interesting M/string theory predictions for wider \((N_c, N_f)\) regions,
- Very weakly 1st-order \(N_c=3\) quenched deconfinement transition is hard to understand,
- 1st example with different string tensions (4 and 6).

- \(T \neq 0\): phase change is not stronger than weakly first-order SU(3).
- String tensions, at \(L_t = 6\), signals for different 4 and 6:
  - \(\sigma_4 \sim 0.068(3)\) and \(\sigma_6 \sim 0.11(2)\) or \(1 < \sigma_6/\sigma_4 < 2\),
  - \(T_c/\sqrt{\sigma_4(T = 0)} < T_c/\sqrt{\sigma_4(T \sim T_c)} \sim 0.64(1) < \sqrt{3/\pi(d - 2)}\), common with \(N_c=2\) and 3.
- Further investigation using QCDSP on larger and finer lattices and with general \((N_c, N_f)\) is being d
Numerical lattice has brought QCD theoretical calculations to about 10% accuracy,
  - using 100 GFLOPS super computers.
Newer research projects were formed to bring us to 3-5% accuracy for calculations such as
  - hadron mass spectrum,
  - light quarks and chiral symmetry,
  - hadron electroweak interactions,
  - high-temperature QCD phase structure.
We will soon need 1% accuracy to go beyond the standard model:
  - 10 TFLOPS super computer will be used soon.

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