Numerical Lattice QCD Using Parallel Supercomputers

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

matter	force (interaction)
lepton (ν, e, ...)	gravity + electro-weak
hadron (π, p, ...)	gravity + electro-weak + strong

All the interactions are described by gauge theories.

QCD = Quantum Chromodynamics = gauge theory of strong interaction:

- perturbative calculations: Feynman diagrams,
- non-perturbative calculations: 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:

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

- Vector potential $A_\mu = (\phi, \vec{A})$: $\vec{E} = -\vec{\nabla}\phi - \dfrac{\partial \vec{A}}{\partial t}$, $\vec{B} = \vec{\nabla} \times \vec{A}$.
- Gauge invariance: $\phi \mapsto \phi - \dfrac{\partial \lambda}{\partial t}$, $\vec{A} \mapsto \vec{A} + \vec{\nabla}\lambda$, with arbitrary scalar $\lambda(x)$.

QED (Quantum Electrodynamics): quantum theory of electromagnetism

- quantum gauge field theory of photon (A_μ) and electron (ψ)

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

$$-ieF_{\mu\nu} = [D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu, \qquad D_\mu = \partial_\mu - ieA_\mu,$$

- accurate calculations using perturbative method of Tomonaga, Schwinger, Feynman and Dyson.

QCD (Quantum Chromodynamics): quantum theory of strong interaction

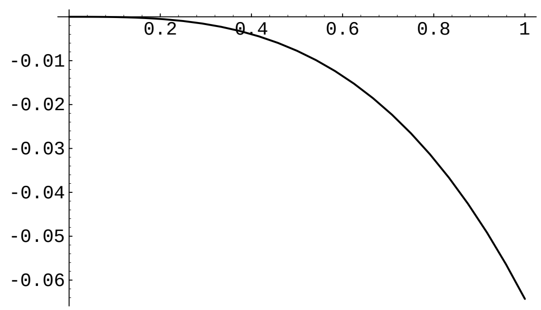
- quantum gauge field theory of gluon (A_μ^a) and quark ((q^a)

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

$$-igG_{\mu\nu} = [D_\mu, D_\nu] = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu], \qquad D_\mu = \partial_\mu - igA_\mu,$$

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

- asymptotic freedom (infrared slavery): $\beta_{\mathrm{CS}}(g) \equiv \mu\dfrac{\mathrm{d}g}{\mathrm{d}\mu} = b_0g^3 + b_1g^5 + \mathcal{O}(g^7) < 0,$



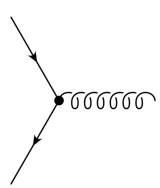
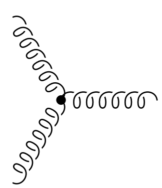
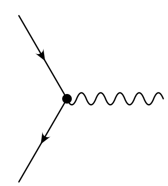
$$b_0 = -\frac{1}{(4\pi)^2}\left(\frac{11N_c}{3} - \frac{2N_f}{3}\right),$$

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

perturbative: $g \to 0$ as $\mu \to \infty$, works for above ~ 10 Gev/c reactions, but

non-perturbative: $g \gg 1$ as μ decreases below $\simeq 10$ GeV/c, needs lattice formulation.

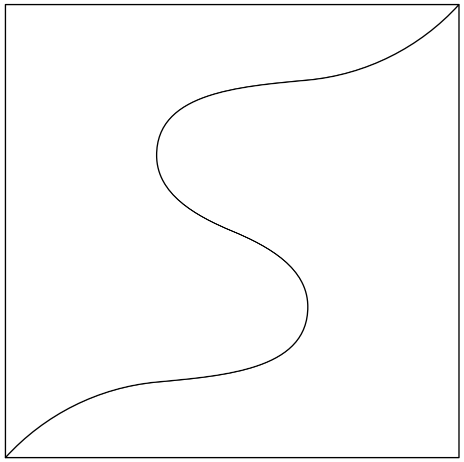
Quantum Gauge Field Theories

QCD	QED
Quantum Theory of Strong Interaction	Quantum Theory of Electromagnetic Interaction
$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{2}\mathrm{Tr}G^{\mu\nu}G_{\mu\nu} + \bar{q}(i\gamma^{\mu}D_{\mu} - m)q,$	$\mathcal{L}_{\mathrm{QED}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \bar{\psi}(i\gamma^{\mu}D_{\mu} - m)\psi,$
Non-Linear Interaction	Linear Interaction
 	
Complicated Vacuum	Simple Vacuum
Interaction changes: $g = g(r)$ $r \to \infty$: $g(r) \to \infty$, Confinement $r \to 0$: $g(r) \to 0$, Asymptotic Freedom	$r \to \infty$: $e(r) \to$ Finite electron charge e

2 Path Integral

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

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

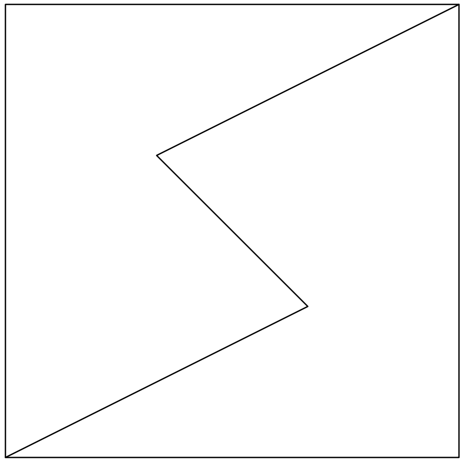


- Free particle ($V = 0$):

$$\int dp \langle x|p\rangle e^{-itp^2/(2m)}\langle p|y\rangle = \int dp \frac{1}{2\pi}\exp(-\frac{it}{2m}p^2 + ip(x-y)) = \sqrt{\frac{m}{2\pi it}}\exp\left[i\frac{m}{2t}(x-y)^2\right].$$

- For interacting case in general, $V \neq 0$, introduce a lattice in time by dividing the interval

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



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

- W_ϵ and U_ϵ 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

$$Dx = \lim_{N\to\infty} \left(\frac{m}{2\pi i\epsilon}\right)^{N/2} dx_1 ... dx_{N-1}.$$

- 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

$$\langle x|e^{-H\tau}|y\rangle = \int Dxe^{-S_E},$$

  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 ϕ_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 ϕ_i defined on discretized space-time points i.

Fermion fields (1): each fermion state requires a pair of Grassmann variables (ξ, ξ^+),

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

$$\int d\xi_1 d\xi_1^+ d\xi_2 d\xi_2^+ ... d\xi_N d\xi_N^+ F(\xi^+,\xi) = (-1)^N \int d\xi_1^+ d\xi_1 d\xi_2^+ d\xi_2 ... d\xi_N^+ d\xi_N F(\xi^+,\xi) = F^{(NN)},$$

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

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

further, taking derivatives of $(\partial_{\eta_i} \partial_{\eta_j^+})$ and setting $\eta = \eta^+ = 0$,

$$\int d\xi_1^+ d\xi_1 ... d\xi_N^+ d\xi_N \exp(-\xi_j^+ A_{ji}\xi_i) \xi_{j_1}^+ \xi_{i_1} ... \xi_{j_n}^+ \xi_{i_n} = (\det A) \epsilon_{j_1 \cdots j_n}^{k_1 \cdots k_n} A_{k_1 i_1}^{-1} ... A k_n i_n{}^{-1},$$

where $\epsilon_{j_1 \cdots j_n}^{k_1 \cdots k_n}$ takes value ± 1 for even/odd permutations and 0 otherwise.

Fermion fields (2): coherent states are indispensable, defined as

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

and

$$\langle 0|\xi\rangle = 1, \qquad \text{and} \qquad a_i|\xi\rangle = \xi_i|\xi\rangle,$$

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

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

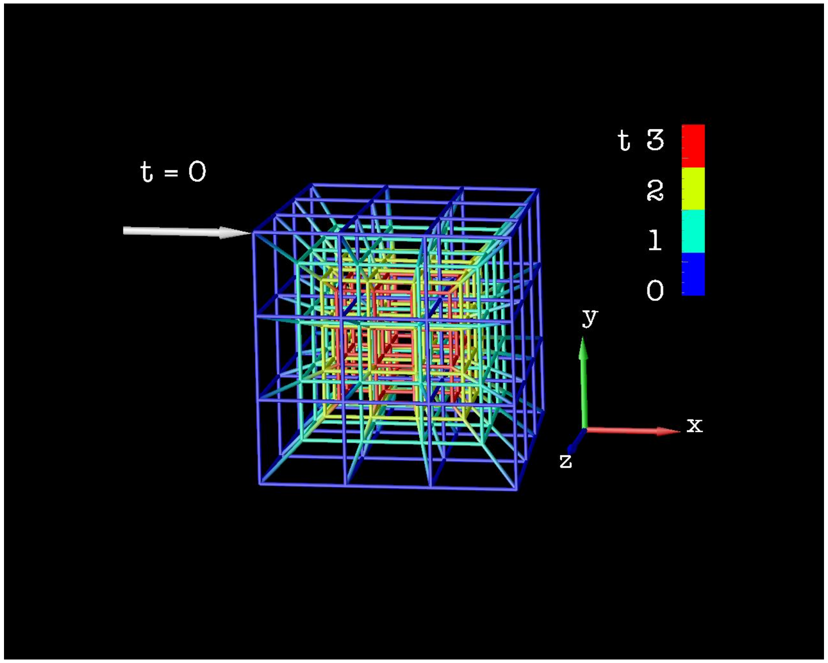
so that

$$\mathrm{Tr}\exp(a_j^+ A_{ji} a_i) = \int d\xi^+ d\xi \exp(-\xi^+\xi)\langle +\xi|\exp(a_j^+ A_{ji} a_i)| - \xi\rangle.$$

3 Lattice QCD

Simplify from 4d Minkowski continuum to 4d Euclid discrete space-time:

Easiest: 4d simple hyper-cubic lattice, $L_0 L_1 L_2 L_3$,



site: $s = (n_0 n_1 n_2 n_3)$, $0 \le n_i \le L_i - 1$ $(i = 0, 1, 2, 3)$.

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 $a \longrightarrow 0$ should give continuum physics.

Dynamical variables:

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

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

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

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

and

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

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

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 $a \longrightarrow 0$ and $g \longrightarrow 0$,
- but there is a serious problem, which will be discussed later,

Gauge invariance is preserved.

Expectation values of any gauge-invariant observable:

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

or by integrating over the quark Grassmann variables,

$$N'^{-1} \int [\mathrm{d}U] (\det M[U]) \exp(-S_{\mathrm{gluon}}[U])$$

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

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

Since

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

it is often convenient to use effective action

$$\tilde{S}[U] = S_{\mathrm{gluon}}[U] - \mathrm{Tr} \log M[U].$$

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

$$\frac{d\langle O\rangle}{da} \longrightarrow 0$$

as $a \longrightarrow 0$, or

$$f(g) - f'(g)\left(a\frac{dg}{da}\right) = \beta(g)f'(g) + f(g) \longrightarrow 0.$$

- 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

$$\langle O\rangle a \propto (g^2 b_0)^{-b_1/(2b_0^2)} \exp(-1/(2b_0 g^2))[1 + O(g^2)],$$

where $\beta(g) \equiv -a\dfrac{dg}{da} = -b_0 g^3 - b_1 g^5 + O(g^7)$ 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 $\gamma(g)=c_0g^2+O(g^4)$ is perturbatively calculable again,
$$c_0=\frac{1}{(4\pi)^2}\frac{3(N^2-1)}{N},$$
- two independent solutions,
$$\Lambda=\mu(b_0g^2)^{-b_1/(2b_0^2)}\exp\left[-\int^g dh\left(\frac{1}{\beta(h)}+\frac{1}{b_0h^3}-\frac{b_1}{b_0^2}\right)\right],$$
and
$$M=m(2b_0g^2)^{-c_0/(2b_0)}\exp\left[\int^g dh\left(\frac{\gamma(h)}{\beta(h)}+\frac{c_0}{b_0h}\right)\right],$$
- 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

$$q \mapsto e^{\alpha\gamma_5} q \qquad \text{and} \qquad \bar{q} \mapsto \bar{q} e^{\alpha\gamma_5}.$$

- 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, $m_s \sim 100$ MeV,
- but is hard to maintain on regular lattices.

Naive (and free and massless) lattice fermion action,

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

leads to a propagator

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

which has 2^D poles at $p_\mu = 0$ or π/a:

- for $D = 4$ there appear $2^4 = 16$ flavors instead of 1,
- shifting of one component of p_μ, 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 $\pm$ 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 χ_x, $(x_\mu = 0, 1, ..., L_\mu - 1)$,
  - action $S_{\mathrm{KS}} = \bar{\chi}_x M_{xy} \chi_y$ with propagation matrix

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

  - 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 $u_\mu = 0, 1, ..., K_\mu - 1$ 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

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

– $\frac{1}{4}\mathrm{Tr}\Gamma_v^+\Gamma_w = \delta_{vw}$ and $\frac{1}{4}\sum_v (\Gamma_v^+)^{sf}(\Gamma_v)^{tg} = \delta^{st}\delta^{fg}$ lead to

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

– with $\sum_x = \sum_u{}' \sum_v$, the mass term becomes

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

where 1_γ acts on Dirac indices s and 1_t acts on flavor indices f,

– relations like

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

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

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

are used to obtain the kinetic term

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

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 $U(1)_e \times U(1)_o$

$$q_u \mapsto (U_e P_e + U_o P_o) q_u \qquad \text{and} \qquad \bar{q}_u \mapsto \bar{q}_u (P_e U_o^+ + P_o U_e^+)$$

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

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

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

– propagator:

$$\frac{a}{8[(\gamma_\mu \times 1_t)\sin k_\mu a + (\gamma_5 \times t_5 t_\mu)(1 - \cos k_\mu a)]},$$

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

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

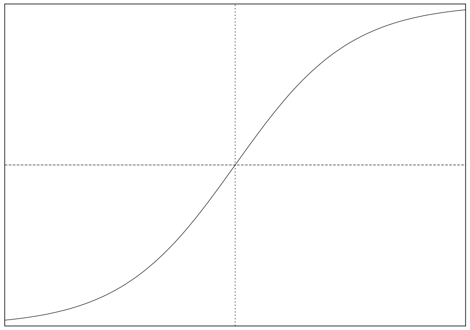
the propagator has only one pole near $p = 0$ for $a \longrightarrow 0$ as the $\gamma_5 \times t_5 t_\mu$ part drops out,

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

– in continuum limit $a \longrightarrow 0$ the full $U(4) \times U(4)$ symmetry should be restored.

Domain-wall fermions: promising new method by Kaplan, ..., Shamir, ...

- use 5d lattice, (x_μ, 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 $m(+\infty) = m^+$,



- 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,

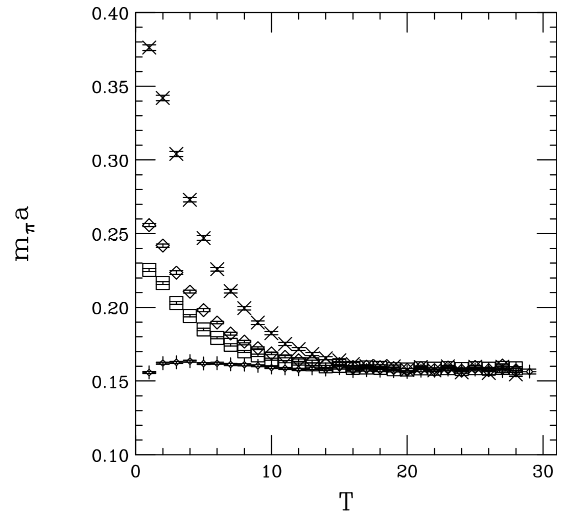
$$H(s, s') \propto \sum_n c_n \exp(-E_n t) \sim \exp(-mt) \qquad \text{for large } t = |s_0 - s_0'|.$$

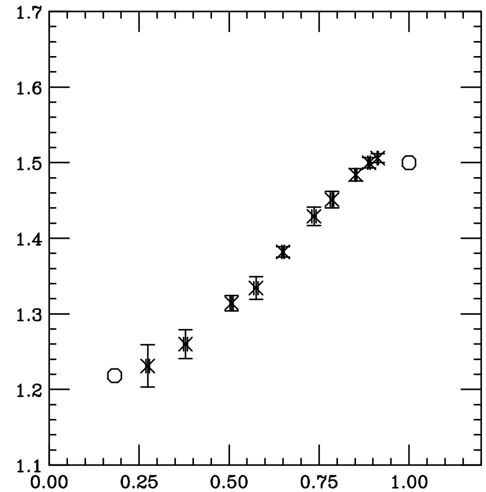
  - t is finite (not ∞) on the lattice:
  - instead look at effective mass

$$m_{\text{eff}}(t) \equiv -\ln(H(t+1)/H(t))$$

  - $m_{\text{eff}}(t)$ 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 th 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
  - ΔI=1/2 rule, $\mathcal{A}(K \to \pi\pi(I=0))/\mathcal{A}(K \to \pi\pi(I=2)) \sim$22, through

    $$V_{\rm ud}V_{\rm us}^*(G_F/\sqrt{2})[C^+(\mu)O^+(\mu)+C^-(\mu)O^-(\mu)], \quad O^\pm = [(\bar{s}d)_L(\bar{u}u)_L \pm (\bar{s}u)_L(\bar{u}d)_L] - [u \leftrightarrow c],$$

    where O^- is ΔI=1/2 and O^+ is mixed with 3/2,
  - ϵ'/ϵ=28(4) $\times$ 10^{-4}, where $\eta_\pm$=ϵ+ϵ', η_0=ϵ-2ϵ', η=$\mathcal{A}(K_L \to \pi\pi)/\mathcal{A}(K_S \to \pi\pi)$, through

    $$B_K = 3\langle \bar{K}^0|(\bar{s}d)_L^2|K^0\rangle/8\langle \bar{K}^0|(\bar{s}d)_A|0\rangle\langle 0|(\bar{s}d)_A|K^0\rangle, \qquad \text{etc.}$$

- 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

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

which can be described by a lattice path integral

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

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 $\propto \mathrm{tr} M^{-1}$:

  – 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

$$P = \langle \mathrm{Tr} \prod_{t=0}^{N_t - 1} U(x, t; \mu = \hat{t}) \rangle$$

  which measures the free energy of a heavy color charge $e^{-F/T} = \langle c e^{-H/T} c^+ \rangle = \langle c(1/T) c^+(0) \rangle$:

  – confined: $F \longrightarrow \infty$ 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, $\dfrac{T_c}{\sqrt{\sigma}} = \sqrt{\dfrac{3}{\pi(d-2)}}$?
- 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, $\sigma_k \propto \sin \dfrac{k\pi}{N_c}$.
  - $N_c = 4$ 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 4×10^4 link variables,
- or 32×10^4 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 $S_{\mathrm{QCD}}[U, q, \bar{q}]$, is real (for most of the interesting cases):

- "Boltzman factor" $\exp(-S_{\mathrm{QCD}}[U, q, \bar{q}])$ 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 $C \to C'$ 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 $\sum_{C'} P(C, C') = 1$,

$$||E' - E_{\text{eq.}}|| = \sum_{C} |\sum_{C'} P(C, C')(p(C') - p_{\text{eq.}}(C'))| \leq \sum_{C,C'} P(C, C')|p(C') - p_{\text{eq.}}(C')| = ||E - E_{\text{eq.}}||$$

  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 τ,

$$\frac{dx}{d\tau} = -\frac{\delta S}{\delta x} + \eta \qquad \text{or discretized} \qquad x' = x - \epsilon \frac{\delta S}{\delta x} + \sqrt{\epsilon}\eta = x - f_\tau(x, \eta)$$

- random noise η must be appropriately regularized, eg, by a measure like $\propto \exp(-\eta^2/4)$ and satisfie

$$\langle \eta(\tau) \rangle = 0 \qquad \text{and} \qquad \langle \eta(\tau)\eta(\tau') \rangle = 2\delta(\tau - \tau'),$$

- probability distribution $P(x, \tau)$ evolves according to $P'(x') = \langle \int DxP(x)\delta(x' - x + f_\tau(x, \eta)) \rangle_\eta$, 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

$$-\frac{\partial}{\partial \tau} |P(\tau)\rangle = H_{\mathrm{FP}} |P(\tau)\rangle$$

where the positive semi-definite Fokker-Planck Hamiltonian has a zero-energy ground state

$$H_{\mathrm{FP}} |e^{-S(x)}\rangle = 0$$

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 ϵ
- applicability is limited.

Gauge part is easy, with local estimation of

$$\Box = \mathrm{Tr} UUUU.$$

Quark part must be integrated over Grassmann variables:

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

leading to effective action,

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

Irrespective of L, MD or HMC, requires estimating

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

often using noisy estimator and iterative methods: (bi)Conjugate Gradient (bCG), Conjugate Residua (CR), ...

In practice, $L_i \simeq 64$:

- $4 \times 64^4 = 2^{26} = 64$ million U's, each with 8 real degree's of freedom
- 512 M-dimensional integration, may require 2^4 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 $\mathrm{Tr}UUUU$,

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

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

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

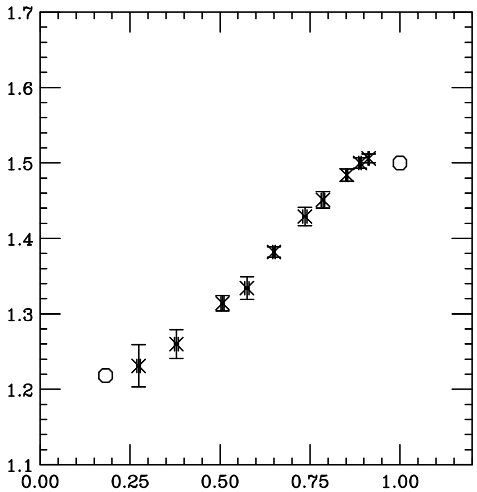
Needs better technology: parallel computing

- 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.



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

- partial success in hadron mass spectrum (π, ρ, 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

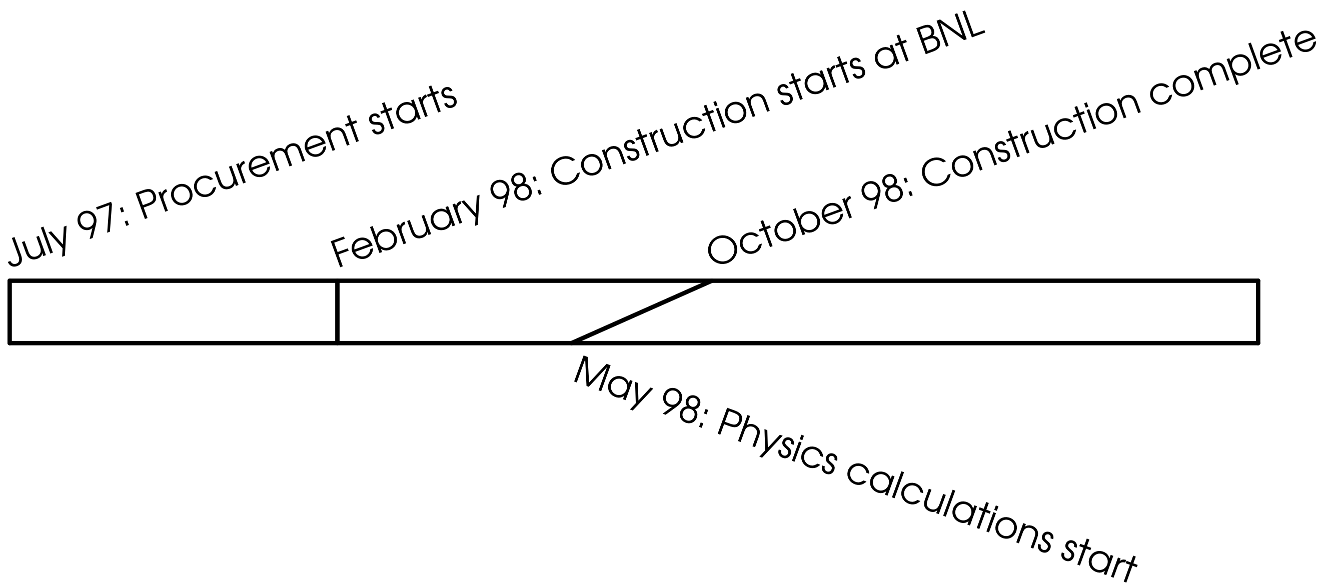
- 192 mother boards,
- one mother board = 64 daughter boards,
- one daughter board = 50-MFLOPS DSP + custom NGA + 2-MB memory,
- with single-precision arithmetic,

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

Design started in '93:

- Columbia University: Norman H. Christ, Robert D. Mawhinney, Pavlos Vranas, Dong Chen, Roy Luo, Chulwoo Jung, Adrian Kaehler, Catalin Malreanu, ChengZhong Sui, Alan Gara, John Parson (Nevis Labs),
- 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.

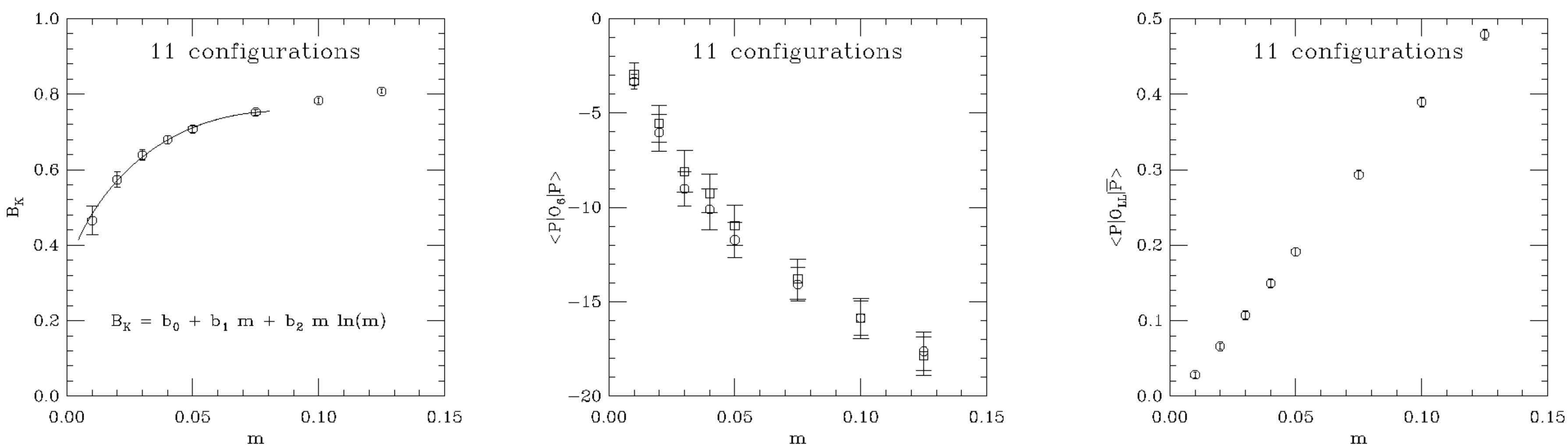
Conventional 4d lattice calculations are kept alive too:

- 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),



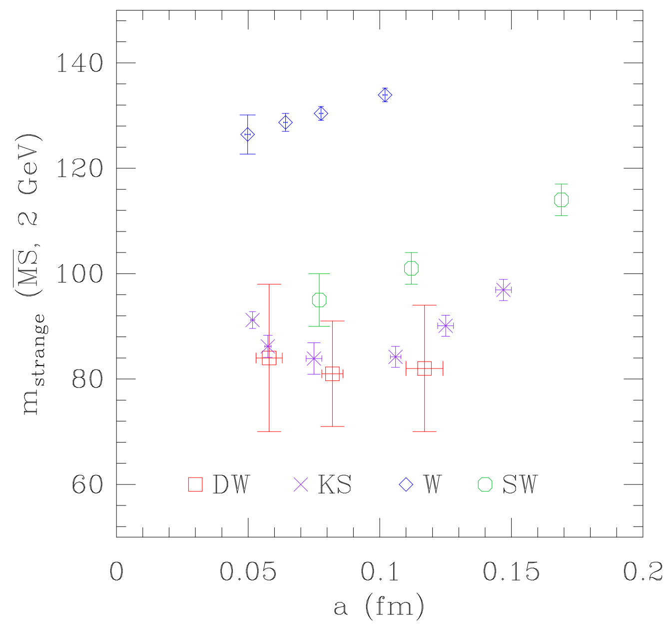
- Good chiral behavior observed in three-point functions for B_K, ϵ'/ϵ and $K\bar{K}$ mixing calculated from the first 11 configurations from QCDSP.

P. Vranas (Columbia $\rightarrow$ 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: $m_s(2\mathrm{GeV}, \overline{\mathrm{MS}}) \sim 82 \pm 15\mathrm{MeV}$.

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 χ
- 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):

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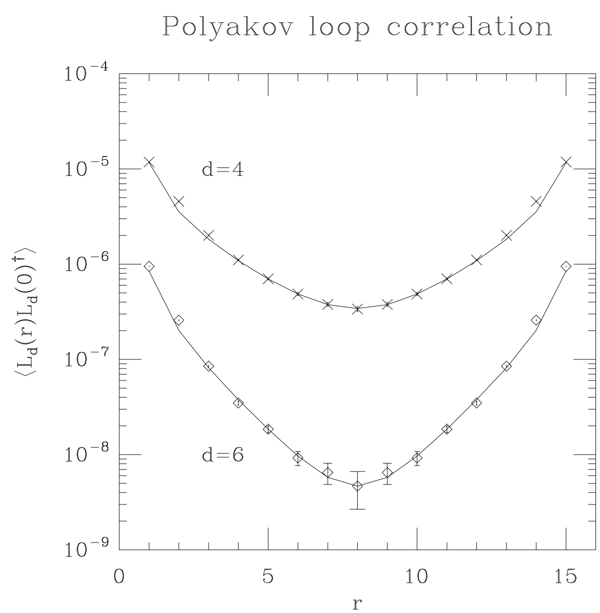
Need further investigation with larger V and finer T.

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.

Acknowledgement

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