ETH zürich

Institute for Theoretical
Physics, HPCP lab

Introduction to Lattice QCD

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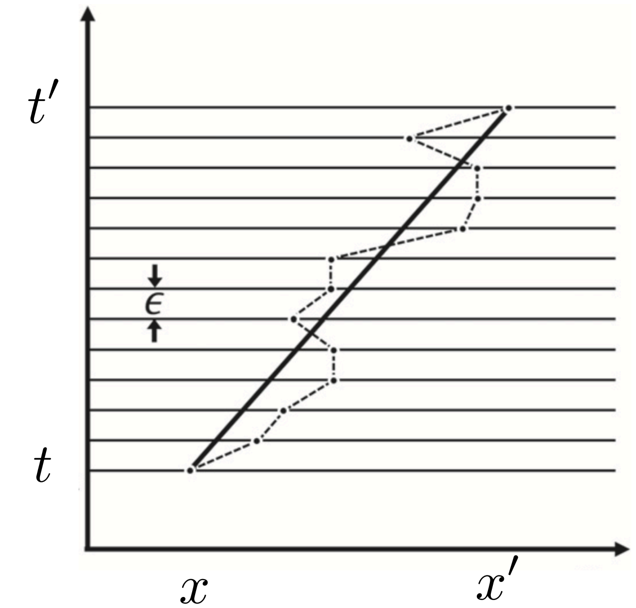
11-22 July 2022, NNPSS, MIT

Part 2:
Quantum Chromodynamics on the lattice: numerical simulations

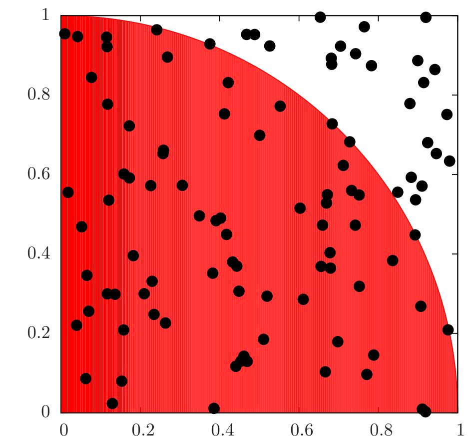
In yesterday's lecture:

- We have learned/reminded ourselves how to quantize:



  - ➡ Quantum Mechanics
  - ➡ Scalar Field Theory

- Mapping to Classical Statistical Mechanics

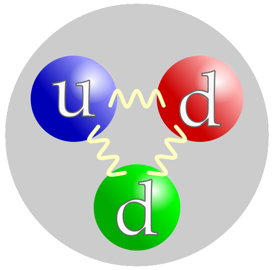


- Monte Carlo Sampling of Spin Systems $\longrightarrow$ Quantum Fields

- Monte Carlo Errors vs. Numerical Integration

In today's lecture:

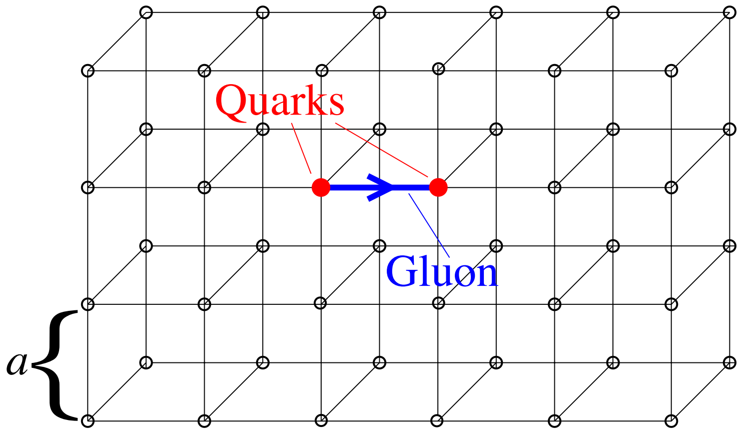
- We shall generalize this approach to Quantum Chromodynamics (QCD)



- We shall see how the numerical sampling is done in practice
  - for Scalar Field Theory
  - for QCD

- Why is QCD numerically so expensive?

- Practical examples



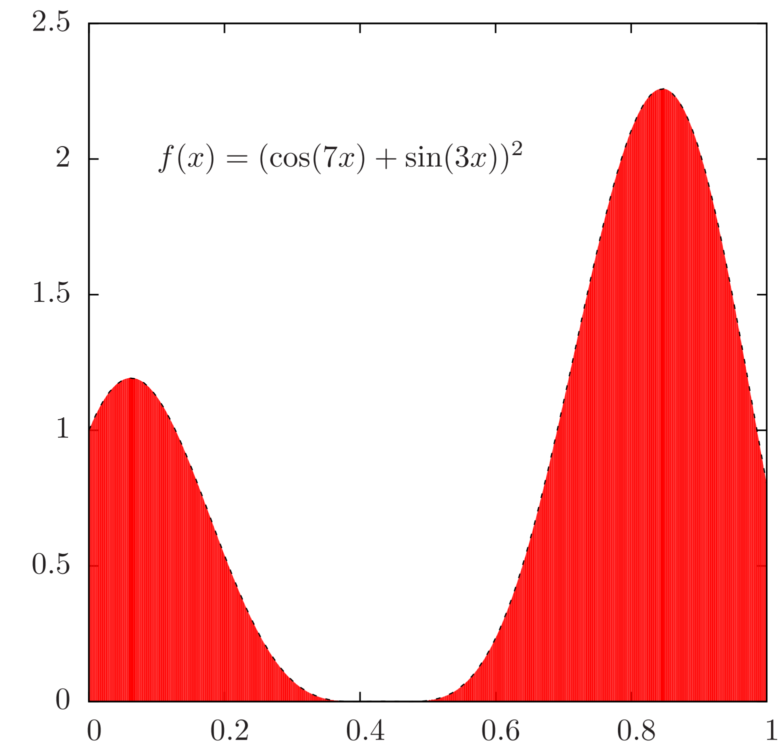
A tool for Lattice Simulations: Monte Carlo methods

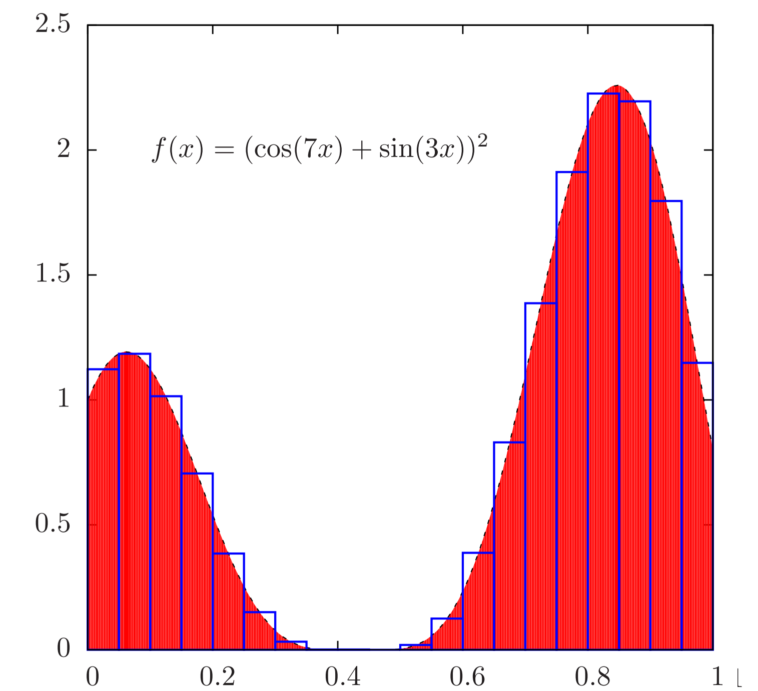
- **Calculating 1-dim integral:**

  ➡ $$I = \int_0^1 f(x)dx$$

- **Again, throw N random points on the rectangular surface:**
- **Count those under the value of the function** $f(x)$
- **Then the value of the integral is obtained by:**

  $$I \approx \langle I \rangle_N = 2.5 \times 1 \times \frac{N_{inside}}{N}$$





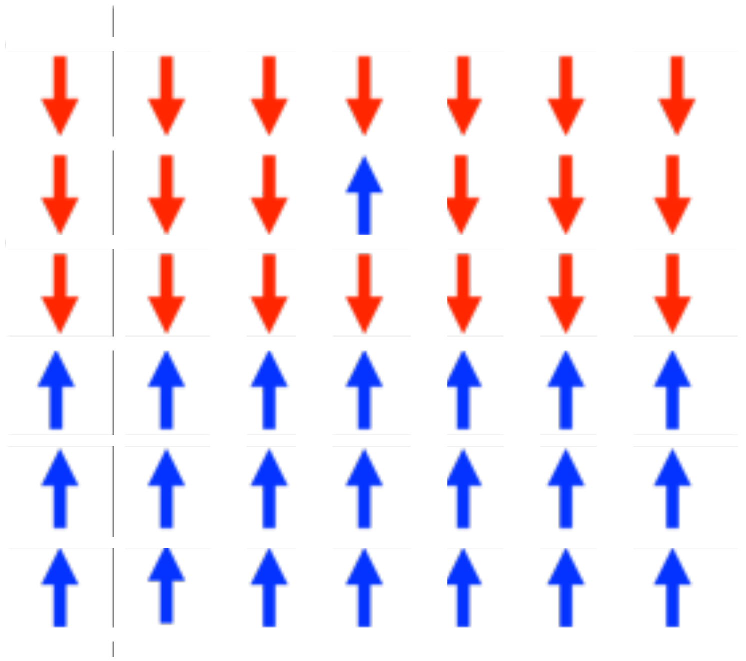
- **For larger N, better and better approximation of the integral**
- **Monte Carlo error in d-dim:** $\approx \frac{1}{\sqrt{N}}$
- **Numerical integration error (midpoint rule) in d-dim:** $\approx \frac{1}{N^{2/d}}$
- **For d>4, Monte Carlo is better than Numerical Integration!**

Classical statistical Mechanics: Ising Model

→ CLASSICAL HAMILTON FUNCTION:

$$\mathcal{H}[s] = -J \sum_{\langle x y \rangle} s_x s_y - \mu B \sum_x s_x$$

* $J > 0$; FERROMAGNETIC COUPLING CONST.
* μ COUPLING TO AN EXTERNAL MAG. FIELD B



Classical statistical Mechanics: Ising Model

- CLASSICAL PARTITION F-ON:

$$Z = \int \mathcal{D}s \, e^{-\mathcal{H}[s]/T}$$

$$= \prod_x \sum_{s_x=\pm 1} e^{-\frac{1}{T}\mathcal{H}[s]}$$

- THERMAL AVERAGES:

* MAGNETIZATION: $\langle s_x \rangle = \frac{1}{Z} \prod_x \sum_{s_x=\pm 1} s_x \, e^{-\frac{\mathcal{H}[s]}{T}}$

* SPIN CORRELATION F-ON:

$$\langle s_x s_y \rangle = \frac{1}{Z} \prod_x \sum_{s_x=\pm 1} s_x s_y \, e^{-\frac{\mathcal{H}[s]}{T}}$$

Expectation values in the MC approach: spin systems

- **Ising model Hamiltonian (without external magnetic field):**

$$H = -J \sum_{\langle x,y \rangle} s_x s_y; \qquad \langle x, y \rangle - \text{nearest neighbours}$$

- **Generate configurations of spins with probability** $\sim e^{-\frac{H}{T}}$ **(importance sampling)**

- **Expectation value of the observables as averages over ensemble of spin configurations**

$$\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{k=1}^{N_{cnfg}} O[\bar{s}_k] + \mathcal{O}\left(\frac{1}{\sqrt{N_{cnfg}}}\right)$$

- **How do we generate the ensemble** $\{\bar{s}_k\}$ **?**

Expectation values in the MC approach: QFT

- Numerical approach exploits the analogy:

Euclidean QFT ⟷ **Statistical Mechanics**

$$\langle O[\phi] \rangle = \frac{1}{Z} \int \mathcal{D}\phi \; e^{-S_E[\phi]} \; O[\phi]$$

- Path integrals are computed by importance sampling

$$\mathcal{P}[\phi_i] \propto e^{-S_E[\phi]}$$

- Generate ensemble of field configurations $\{\phi_i\}$

- Expectation values $\langle O[\phi] \rangle$ are averages over the ensemble

$$\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[\phi] + \mathcal{O}\left(\frac{1}{\sqrt{N_{cnfg}}}\right)$$

- How do we generate ensemble $\{\phi_i\}$ with the correct probability distribution?

Markov processes

- **Recursive procedure that generates $\{\phi_i\}$ with specific algorithm s.t. aimed distribution is asymptotically obtained**

$$\{\phi_0\} \longrightarrow \{\phi_1\} \longrightarrow \{\phi_2\} \longrightarrow \cdots \longrightarrow \{\phi_i\} \longrightarrow \{\phi_{i+1}\} \longrightarrow \ldots$$

- **Markov chains that converge exponentially to the equilibrium distr.**

- **The configurations $\{\phi_i\}$ are correlated by construction**

$$Var\,[\bar{O}] \;=\; Var[O]\,(\frac{2\tau_O}{N_{cnfg}})$$

— integrated autocorrelation time

- **The error of the estimator scales as $\frac{1}{\sqrt{N_{cnfg}}}$ (Monte Carlo)**

- **The variance of the actual observable**

$$Var\,[O] \;=\; \langle\big(O - \langle O\rangle\big)^2\rangle$$

→ **property of QFT itself, should not depend of the Markov chain.**

Detailed Balance

- **Probability for a random transition $\phi \to \phi'$:**

$$R(\phi' \leftarrow \phi)$$

- **Sequence of probabilities in Markov chain, $P^{k+1}(\phi')$ depends only on $P^k(\phi)$**

$$P^{k+1}(\phi') = \int [d\phi]\, P^k(\phi)\, R(\phi' \leftarrow \phi)$$

- **Probabilities of ϕ' being initial or final configuration in a random update are equal**

$$\sum_{\phi} R(\phi' \leftarrow \phi) P(\phi) = \sum_{\phi} R(\phi \leftarrow \phi') P(\phi')$$

- **The above is known as a "balance equation"**

Detailed Balance

- **Calculate the sum using normalization of R**

$$0 \leq R(\phi \leftarrow \phi') \leq 1, \qquad \sum_{\phi} R(\phi \leftarrow \phi') = 1$$

- **Obtain that equilibrium distribution $P(\phi')$ is a fixed point of the Markov Process**

$$\sum_{\phi} R(\phi' \leftarrow \phi) P(\phi) = P(\phi')$$

- **The solution of the balance equation can be obtained if *detailed balance* is fulfilled**

$$R(\phi' \leftarrow \phi) P(\phi) = R(\phi \leftarrow \phi') P(\phi')$$

The MR^{2}T^2 algorithm

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- **The Metropolis Algorithm:**
- **Given ϕ, propose ϕ' in a reversible, area-preserving way**
- **Accept the proposal as new entry with probability p, otherwise add ϕ to the chain again.**
- $\mathrm{p} = \min(1, \frac{\pi(\phi')}{\pi(\phi)})$




The MR²T² algorithm

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- **Accept the proposal as new entry with probability p, otherwise add ϕ to the chain again.**
- $\mathrm{p} = \min\left(1, \frac{\pi(\phi')}{\pi(\phi)}\right)$

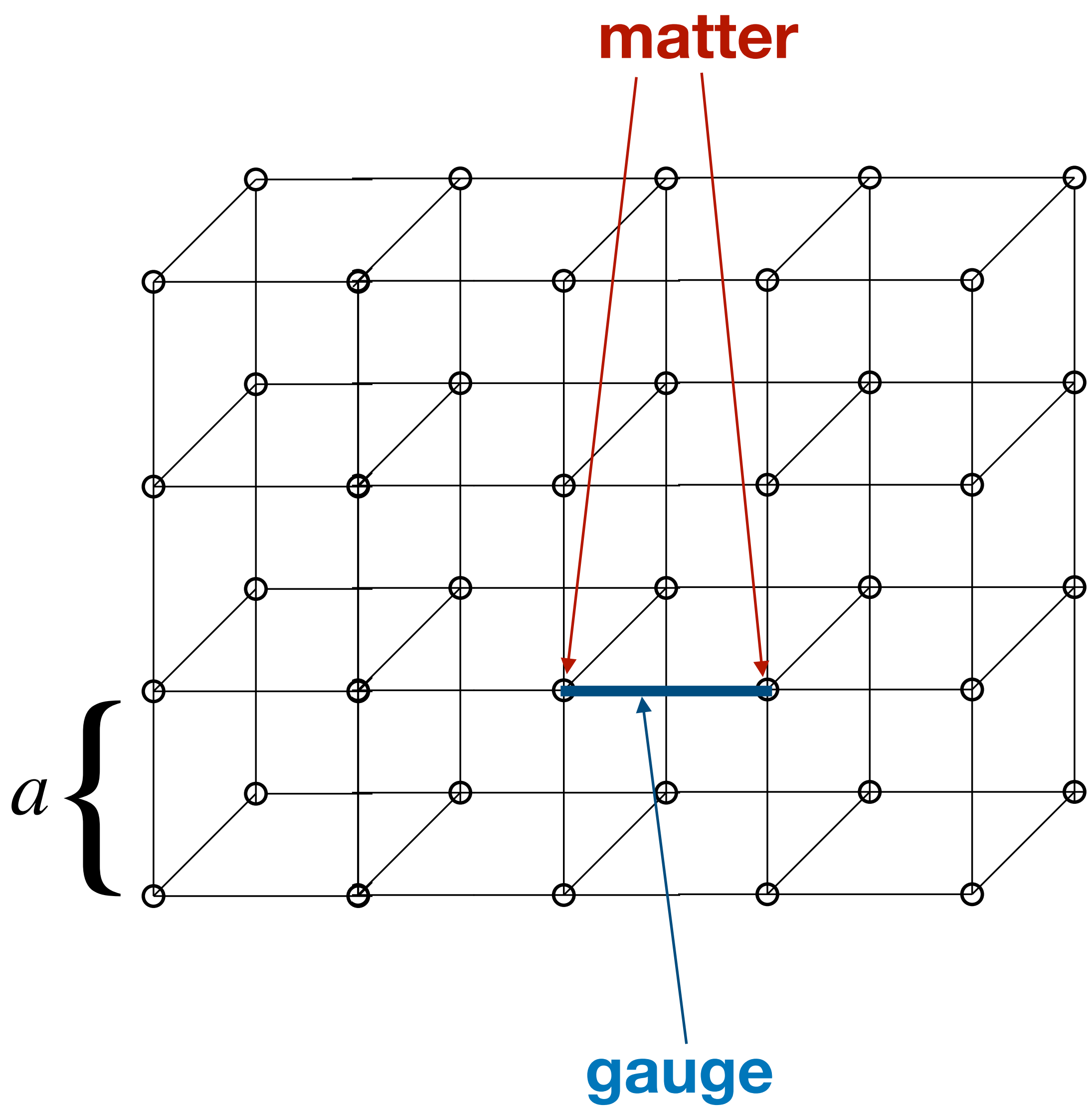
- **The Metropolis Algorithm for Scalar F.T.:**
- **Given ϕ propose ϕ'**
- **Choose a random number $r \in [0,1]$**
- **If $S_E(\phi') < S_E(\phi)$, always accept, otherwise add ϕ' to the chain again if**

$$e^{-\Delta S} > r;$$
$$\Delta S = S_E(\phi') - S_E(\phi)$$

QFT on the lattice: symmetries

- **Translational Symmetry:**
  Broken to discrete symmetry, but nicely restored in the continuum limit

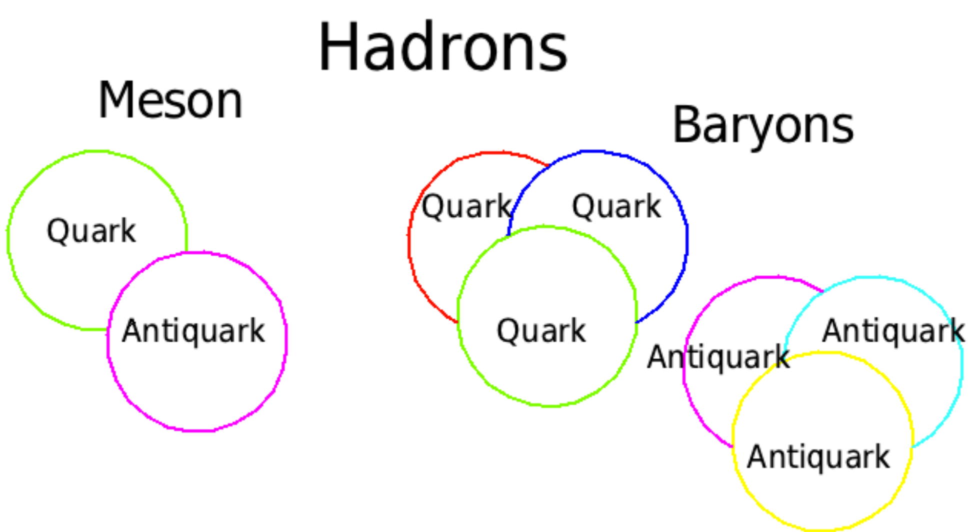
- **Rotational Symmetry:**
  Similar to translational symmetry. Finite number of irreducible representations (quantum numbers) instead of spin, but correct states are obtained in the continuum limit



Strong interaction

$\longrightarrow$ quarks ($q_i = u, d, s, c, b, [t]$) elementary constituens of:

- mesons ($q\bar{q}$)
- barions (qqq),($\bar{q}\bar{q}\bar{q}$)



Quark / Antiquark	Symbol		Charge/e		Baryon number, B		Strangeness, S	
up	u	$\bar{u}$	+2/3	-2/3	1/3	-1/3	0	0
down	d	$\bar{d}$	-1/3	+1/3	1/3	-1/3	0	0
charm	c	$\bar{c}$	+2/3	-2/3	1/3	-1/3	0	0
strange	s	$\bar{s}$	-1/3	+1/3	1/3	-1/3	-1	1
top	t	$\bar{t}$	+2/3	-2/3	1/3	-1/3	0	0
bottom	b	$\bar{b}$	-1/3	+1/3	1/3	-1/3	0	0

revisionworld

COLOUR: SU(3) symmetry

Quantum Chromodynamics

- QCD Lagrangian

$$\mathcal{L}_{QCD} = -\frac{1}{4}\, F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f \left\{ \, i\gamma_\mu \left(\partial_\mu - i g_s A^a_\mu T^a\right) - m_f \, \right\} \psi_f$$

$$S = \int d^4x \, \mathcal{L}_{QCD}$$

- Covariant derivative: $D_\mu = \partial_\mu - i g_s A_\mu$

Quantum Chromodynamics

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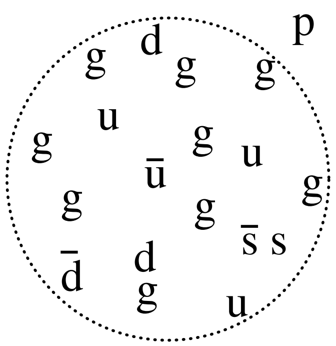
$$\mathcal{L}_{QCD} = -\frac{1}{4}\, F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f \left\{ i\gamma_\mu \left(\partial_\mu - i g_s A^a_\mu T^a\right) - m_f \right\} \psi_f$$

$$S = \int d^4x \; \mathcal{L}_{QCD}$$

- Covariant derivative: $D_\mu = \partial_\mu - i g_s A_\mu$

- Bare QCD parameters ($N_f + 1$)
  - gauge coupling g_s
  - quark masses m_u, m_d, . . .



Quantum Chromodynamics

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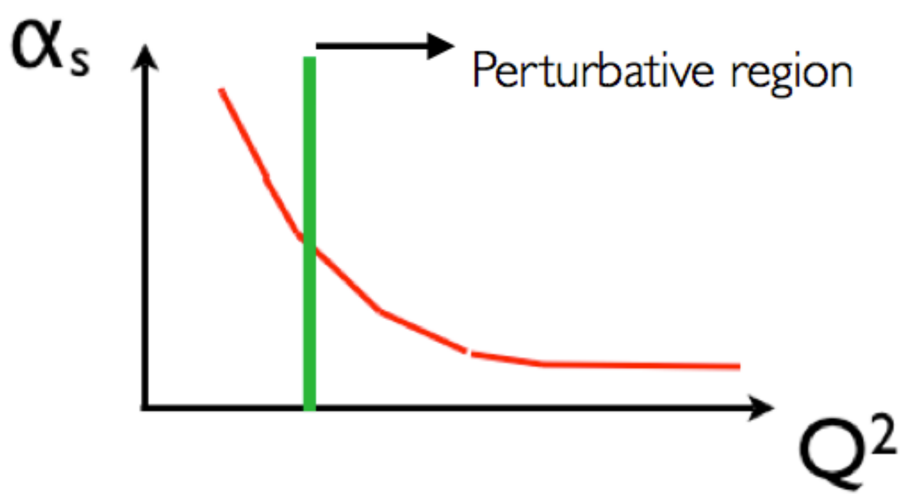


- Euclidean QCD Lagrangian ($t \equiv x^E \leftrightarrow -ix_0$)

$$\mathcal{L}_{QCD} = \frac{1}{2g^2} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_{f=u,d,s,\ldots} \overline{\psi}_f \left\{ \gamma_\mu \left(\partial_\mu + i A^a_\mu T^a\right) + m_f \right\} \psi_f$$

$$S_{QCD} = \int d^4x \, \mathcal{L}_{QCD}$$

Path Integrals in Quantum Chromodynamics

- Each specific field configuration:

$$P(\psi, \overline{\psi}, A) \sim e^{-S(\psi, \overline{\psi}, A)}$$

- Expectation value of an operator $O(\psi, \overline{\psi}, A)$:

$$\begin{aligned} \langle O(\psi, \overline{\psi}, A) \rangle &= \langle \langle O(\psi, \overline{\psi}, A) \rangle_F \rangle_G \\ &= \frac{1}{Z} \int \mathcal{D}[A] \mathcal{D}[\overline{\psi}, \psi] \, e^{-S(\psi, \overline{\psi}, A)} O(\psi, \overline{\psi}, A) \\ Z &= \int \mathcal{D}[A] \mathcal{D}[\overline{\psi}, \psi] \, e^{-S(\psi, \overline{\psi}, A)} \end{aligned}$$

Lattice regularization of QCD

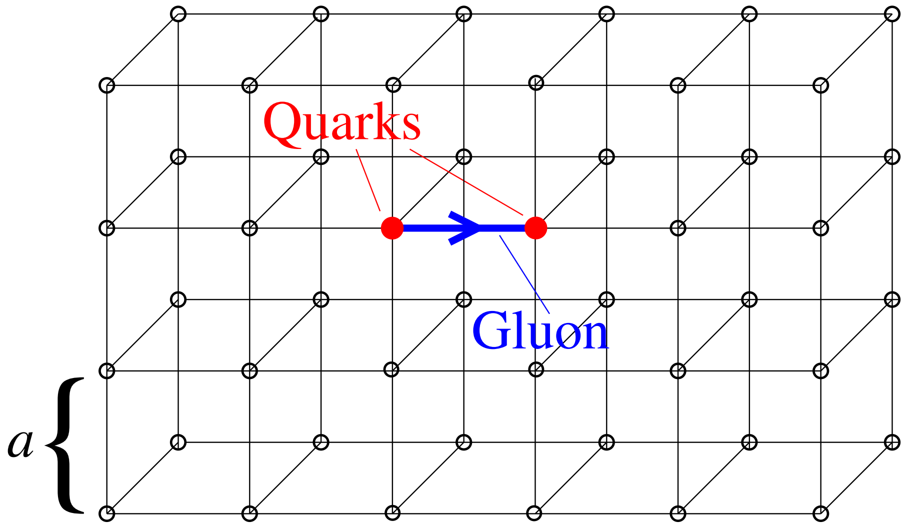
- Divergencies in continuum QCD $\rightarrow$ **regularization** is necessary!
- One possible regularization:
  Introduce **momentum ultraviolet-cutoff** $\Leftrightarrow$ minimum distance (FT)
- If required also: **local gauge symmetry** $\rightarrow$ **Lattice QCD**
- Finite number of integrals over fields ($\int d^4x \ \rightarrow \ a^4 \sum_n$)
- Computable with the help of Monte Carlo techniques

Lattice regularization of QCD

$$S_{QCD}[\psi, \bar{\psi}, A] = S_G + S_F$$
$$= \tfrac{1}{2g} F_{\mu\nu}F_{\mu\nu} + \int d^4x\ \bar{\psi}(x)\ [\gamma_\mu\ (\partial_\mu + iA_\mu(x)) + m]\ \psi(x)$$

- Discretization prescription:

$$x \longrightarrow n = (n_1, n_2, n_3, n_4)\ n_1 = 0, \ldots, N-1$$
$$\psi(x), \bar{\psi}(x) \longrightarrow \psi(n), \bar{\psi}(n)$$
$$\int d^4x \ldots \longrightarrow a^4 \sum_n \ldots$$
$$\partial_\mu\ \psi(x) \longrightarrow \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} + \mathcal{O}(a^2)$$



Naive Lattice Fermion Action

- Simple example - free fermion field ($A_\mu = 0$):

  $S_F^0[\psi, \bar{\psi}] = \int d^4x \; \bar{\psi}(x) \; (\gamma_\mu \; \partial_\mu + m) \; \psi(x)$

- Symmetrically discretized partial derivative:

$$\partial_\mu \psi(na) = \frac{\psi((n+\hat{\mu})) - \psi((n-\hat{\mu}))}{2a} + \mathcal{O}(a^2)$$

- Naive lattice ansatz for free fermion action:

$$S_F\left[\psi, \overline{\psi}\right] = a^4 \sum_{n \in \Lambda} \overline{\psi}(n) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{\psi(n+\hat{\mu}) - \psi(n-\hat{\mu})}{2a} + m\psi(n) \right)$$

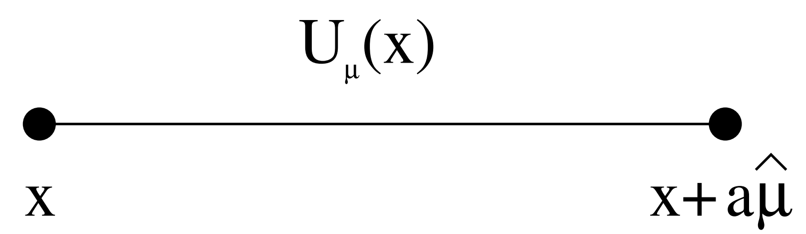
- **Let us examine gauge invariance** $\rightarrow$

Gauge Invariance

- $\Omega(n) \in SU(3)$:

$$\begin{aligned} \psi'(n) &= \Omega(n)\psi(n) \\ \overline{\psi}'(n) &= \overline{\psi}(n)\Omega(n)^\dagger \\ \overline{\psi}'(n)\psi'(n+\hat{\mu}) &= \overline{\psi}(n)\Omega(n)^\dagger\Omega(n+\hat{\mu})\psi(n+\hat{\mu}) \quad (!) \end{aligned}$$

- (!) not gauge invariant

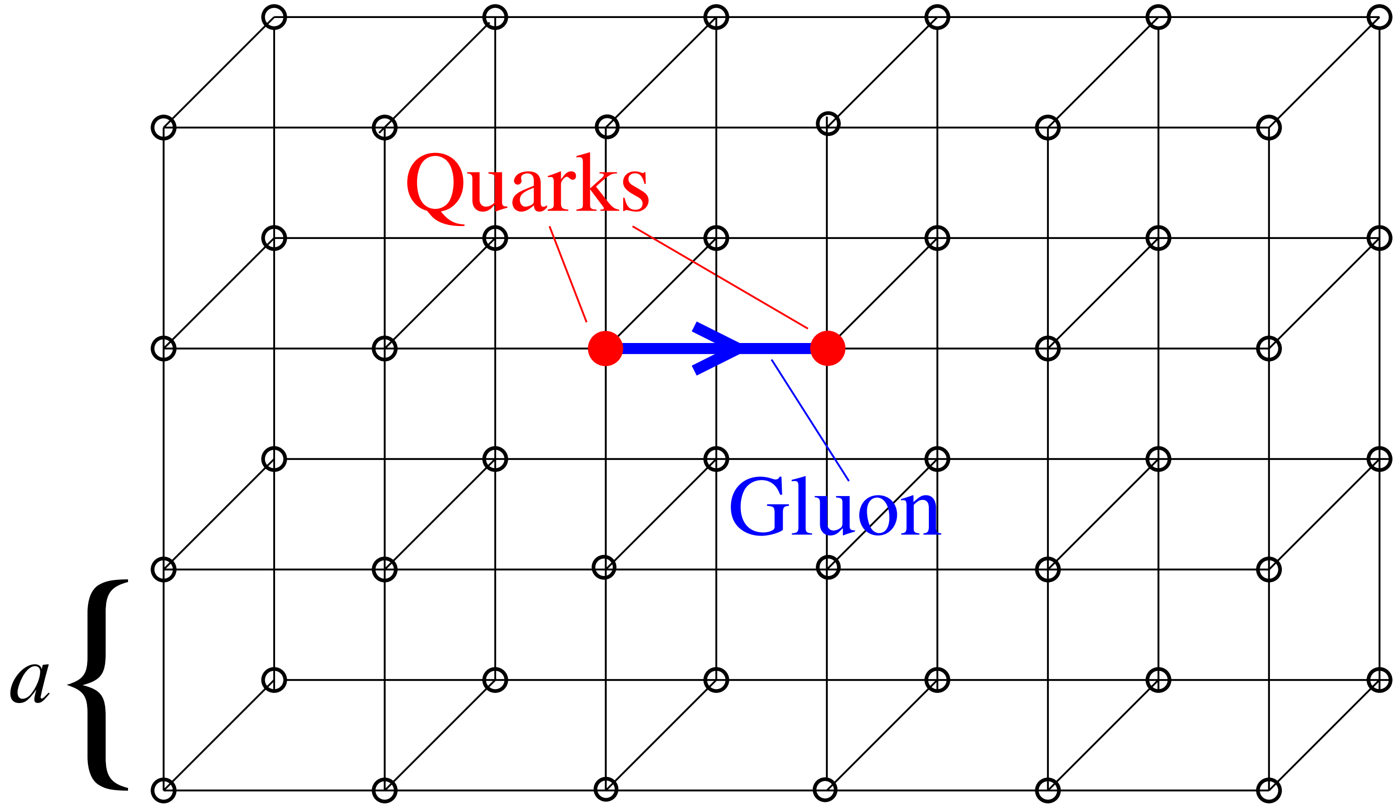


- Introduce **link variables $\mathbf{U_\mu(n)}$**:

$$\begin{aligned} U'_\mu(n) &= \Omega(n)U_\mu(n)\Omega(n+\hat{\mu})^\dagger \\ \overline{\psi}'(n)U'_\mu(n)\psi'(n+\hat{\mu}) &= \overline{\psi}(n)U_\mu(n)\psi(n+\hat{\mu}) \end{aligned}$$

- $U_\mu(n) \rightarrow$ fundamental gluonic variables on the lattice

Quark and gluon fields on the lattice



Quarks $\sim \overline{\psi}(n), \psi(n)$

Gluons $\sim$ "Link variables" $\sim$ Parallel transporter $\sim U_\mu(n) = e^{iagA_\mu}$

Lattice fermion action (I)

- Fermionic action: $S_F = a^4 \sum_f \overline{\psi}(n)\, D(n,m)\, \psi(m)$
- Naive fermion action

$$D(n,m) = m\delta_{n,m} + \frac{1}{2a} \sum_{\mu=\pm 1}^{\pm 4} \gamma_\mu U_\mu(n)\, \delta_{n+\hat{\mu},m}$$

- Propagator in momentum space:

$$\tilde{D}(p)^{-1} = \frac{m\mathbf{1} - ia^{-1} \sum_{\mu=\pm 1}^{\pm 4} \gamma_\mu sin(p_\mu a)}{m^2 + a^{-2} \sum_{\mu=\pm 1}^{\pm 4} sin(p_\mu a)^2}$$

- Important: case of massless fermions, $m = 0$:

$$\tilde{D}(p)^{-1}|_{m=0} = \frac{-ia^{-1} \sum_\mu \gamma_\mu sin(p_\mu a)}{a^{-2} \sum_\mu sin(p_\mu a)^2}$$

- Unphysical poles at $p_\mu = \frac{\pi}{a}$
- Unwanted **doublers**: obtainded 16 instead of 1 fermionic particles!

Lattice fermion action (II)

- **Wilson Dirac matrix** D_W

$$D_W(n,m) = \left(m + \tfrac{4}{a}\right)\delta_{n,m} - \tfrac{1}{2a}\sum_{\mu=\pm 1}^{\pm 4}\left(1-\gamma_\mu\right)U_\mu(n)\,\delta_{n+\hat{\mu},m}$$

- Wilson term: shifting the mass of the doublers to infinity, as $a \to 0$
- Only the physical pole, no doublers!
- Problem: Additional term **breaks chiral symmetry** explicitly
- **No-Go Theorem** on the lattice [Nielsen & Ninomiya, 1981]: simple action without doublers $\leftrightarrow$ broken chiral symmetry
- Different choices of lattice derivatives
  $\rightarrow$ $O(a), O(a^2), \ldots$ discretization errors
  $\rightarrow$ different rates to approach continuum limit

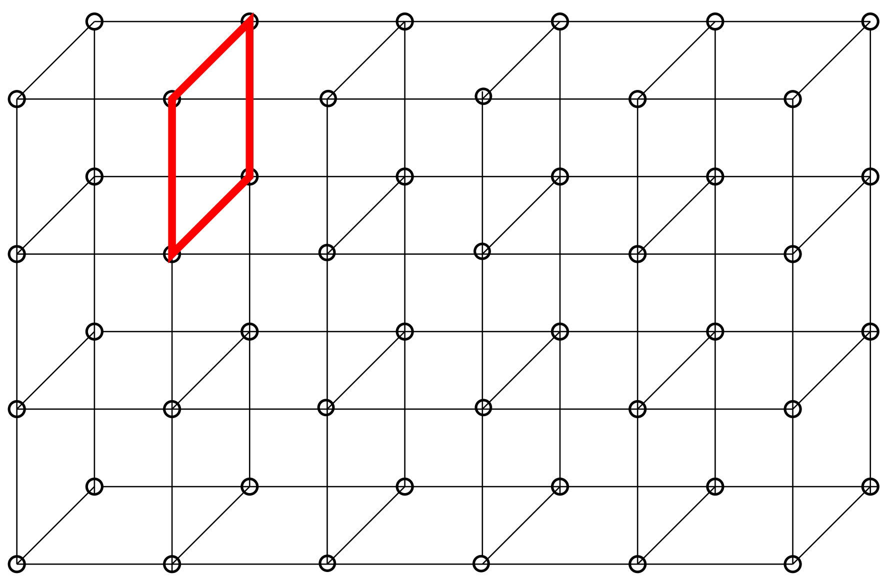
Lattice gauge action (I)

- $S_G = \frac{1}{2g} Tr\ F_{\mu\nu}(x)\ F_{\mu\nu}(x)$
- Need gauge invariant object: trace over closed loop of gauge links
- Smallest possible closed loop: **Plaquette**

$$U_{\mu\nu}(n) = U_\mu(n) U_\nu(n+\hat{\mu}) U_{-\mu}(n+\hat{\mu}+\hat{\nu}) U_{-\nu}(n+\hat{\nu})$$
$$= U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu(n+\hat{\nu})^\dagger U_\nu(n)^\dagger$$

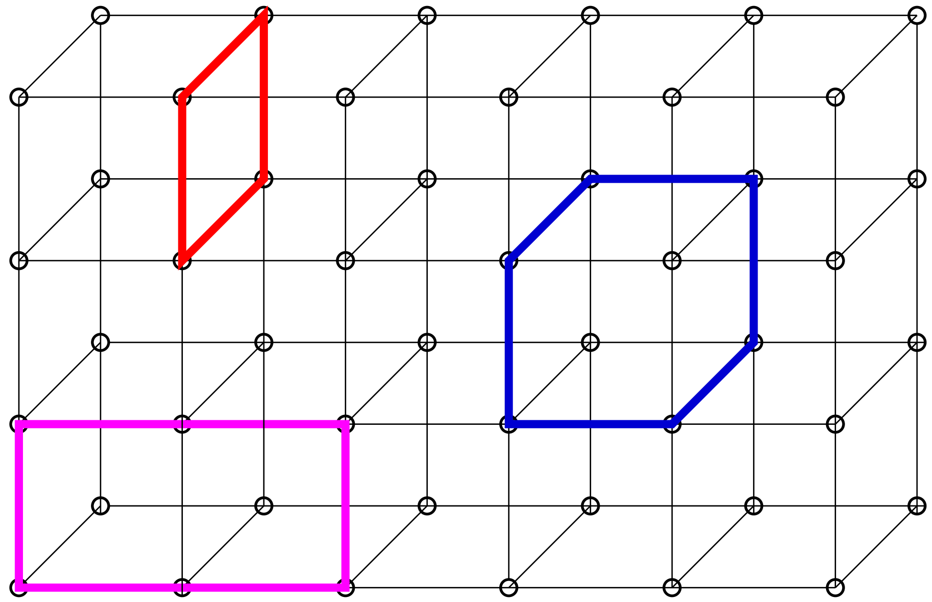
- **Wilson gauge action:**

$$S_g \sim \sum_n \sum_{\mu<\nu} \text{Re tr} \left[1 - U_{\mu\nu}(n)\right]$$



Lattice gauge action (II)

- Improvement: taking into account larger Wilson loops



- All in the same universality class:

  $\longrightarrow$ converge to tr $\left[F_{\mu\nu}(x)F_{\mu\nu}(x)\right]$ in the continuum limit

  $\longrightarrow$ improvement reduces the discretization errors!

- Lattice artefacts in scaling behaviour:

  $\longrightarrow$ Wilson gauge action: $O(a^2)$

  $\longrightarrow$ Luscher-Weisz: $O(a^4)$ [K. Symanzik, 1981; Luscher and Weisz, 1985]

Recipe for Lattice QCD Computation

(1) Generate ensembles of field configurations using Monte Carlo

(2) Average over a set of configurations: $\langle O \rangle \approx \bar{O} = \frac{1}{N_{cnfg}} \sum_{i=1}^{N_{cnfg}} O[U] + \mathcal{O}(\frac{1}{\sqrt{N_{cnfg}}})$

- Compute correlation function of fields, extract Euclidean matrix elements or amplitudes
- Computational cost dominated by quarks: inverses of large, sparse matrix

(3) Extrapolate to continuum, infinite volume, physical quark masses (now directly accessible)

- Lattice QCD path integrals are computed by **importance sampling**: $\mathcal{P}[U_i] \propto e^{-S_E[U]}$
- Markov chain: $\{U_0\} \longrightarrow \{U_1\} \longrightarrow \{U_2\} \longrightarrow \cdots \longrightarrow \{U_i\} \longrightarrow \{U_{i+1}\} \longrightarrow \ldots$
- The configurations are correlated by construction: $Var\,[\bar{O}] = Var[O]\,(\frac{2\tau_O}{N_{cnfg}})$

The cost of dynamical fermions

$$S^E_{QCD} = S_G[U] + S_f[U, \psi, \overline{\psi}]$$

$$\langle O[\psi, \overline{\psi}, U] \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\overline{\psi} e^{-S_G[U] - S_f[U,\psi,\overline{\psi}]} O[\psi, \overline{\psi}, U]$$

$$\int \mathcal{D}\,\psi\ \mathcal{D}\,\overline{\psi}\ e^{-\overline{\psi}\,(\gamma_\mu D_\mu + m_q)\,\psi} \quad \approx \quad det\,(\gamma_\mu D_\mu + m_q)$$

classical

- Fermions represented by Grassmann variables in P.I: expensive to manipulate on a computer

- Easy to evaluate integral over fermionic (anti-commuting) fields: $\eta_i \eta_j = -\,\eta_j \eta_i$

- Integration rules: $\int d\eta = 0;\quad \int d\eta\,\eta = 1$

The cost of dynamical fermions

$$\langle O[\psi,\overline{\psi},U]\rangle = \frac{1}{Z}\int \mathcal{D}\,U\;e^{-S_G[U]}\,\left[det\,(\gamma_\mu D_\mu + m_q)\right]^{N_f}\,O[\psi,\overline{\psi},U]$$

$$\int \mathcal{D}\,\phi\,\mathcal{D}\,\phi^\dagger\;e^{-\phi^\dagger\,(D^\dagger(m_q)D(m_q))^{-1}\,\phi} \quad\propto\quad \left[det\,(\gamma_\mu D_\mu + m_q)\right]^2$$

- Determinant: non-local object on the lattice —> virtually impossible to compute exactly!

- Computational cost of solving:

$$\chi = (\gamma_\mu D_\mu + m_q)^{-1}\Phi$$

grows for: small quark masses m_q, and large $\frac{L}{a}$

- $k = \text{cond}\,(M) \;\propto\; \frac{\lambda_{max}}{\lambda_{min}}$

The cost of dynamical fermions

$$\langle O[\psi,\overline{\psi},U]\rangle = \frac{1}{Z}\int \mathcal{D}\,U\,\mathcal{D}\,\phi\,\mathcal{D}\,\phi^\dagger\; e^{-S_G[U]-\phi^\dagger\,(D^\dagger(m_q)D(m_q))^{-\frac{N_f}{2}}\,\phi}\,O[U,\phi,\phi^\dagger]$$

$$\int \mathcal{D}\,\phi\,\mathcal{D}\,\phi^\dagger\; e^{-\phi^\dagger\,(D^\dagger(m_q)D(m_q))^{-1}\,\phi} \quad\propto\quad [det\,(\gamma_\mu D_\mu + m_q)]^2$$

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$$\chi = (\gamma_\mu D_\mu + m_q)^{-1}\Phi$$

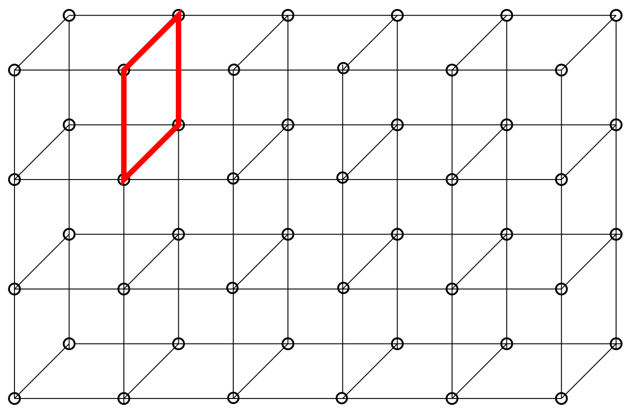
grows for: small quark masses m_q, and large $\frac{L}{a}$

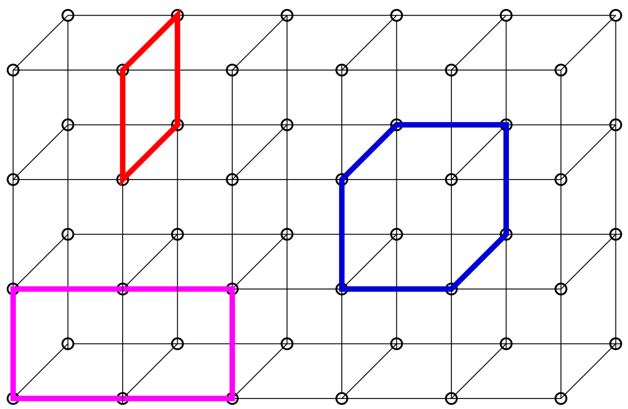
- $k = \text{cond}\,(M) \;\propto\; \frac{\lambda_{max}}{\lambda_{min}}$

The cost of dynamical fermions

$$\langle O[\psi,\overline{\psi},U]\rangle = \frac{1}{Z}\int \mathcal{D}\,U\; e^{-S_G[U]}\,[det\,(\gamma_\mu D_\mu + m_q)]^{N_f}\; O[\psi,\overline{\psi},U]$$

S_G Wilson Luscher-Weisz

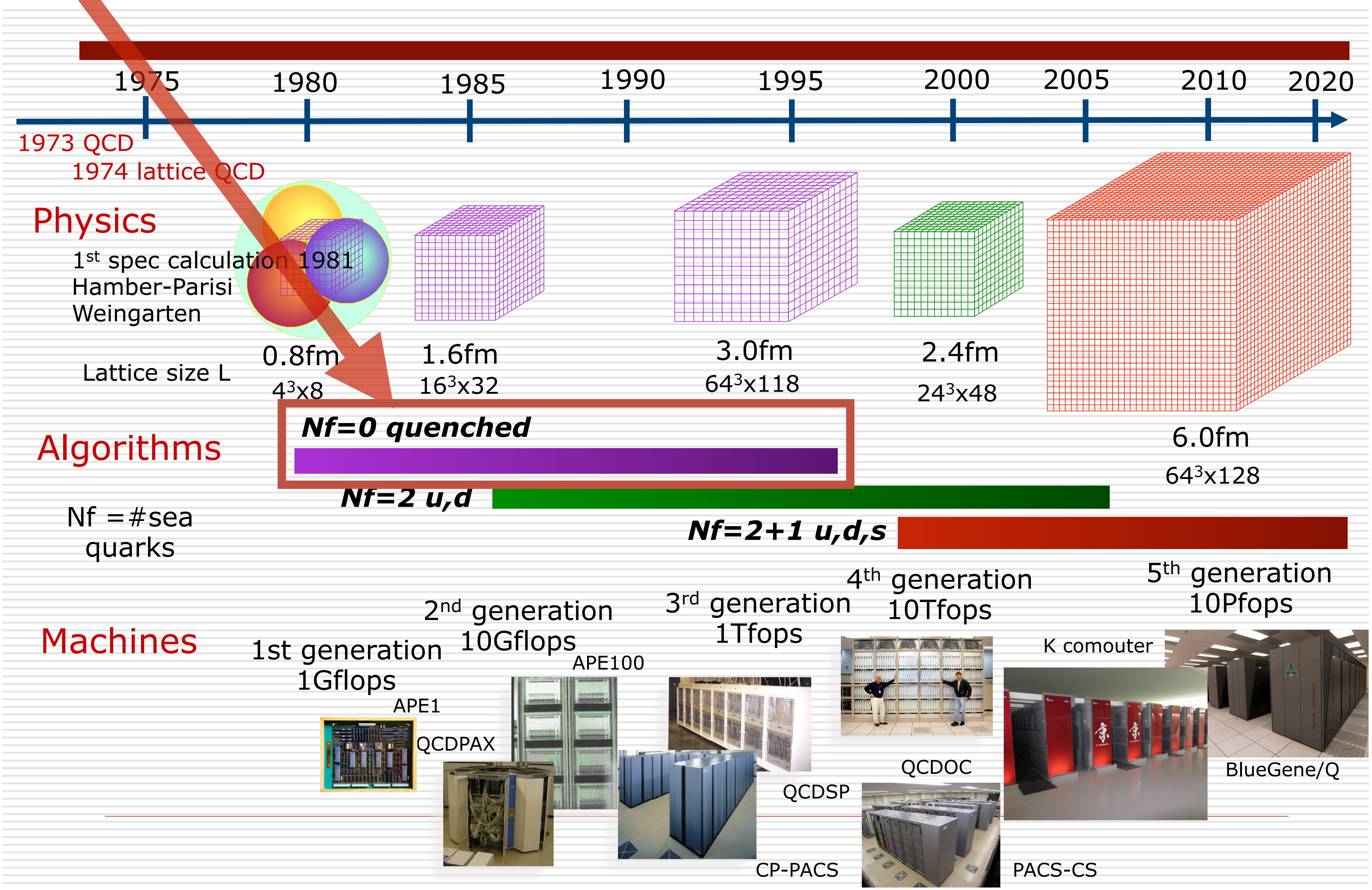




- Local objects: plaquettes, extended plaquettes (rectangles, chairs …)
- Rate of convergence towards continuum limit: $O(a), O(a^2), \ldots$
- Monte Carlo algorithms with local updates sufficient in the approximation: $\det(\gamma_\mu D_\mu + m_q) \equiv 1$

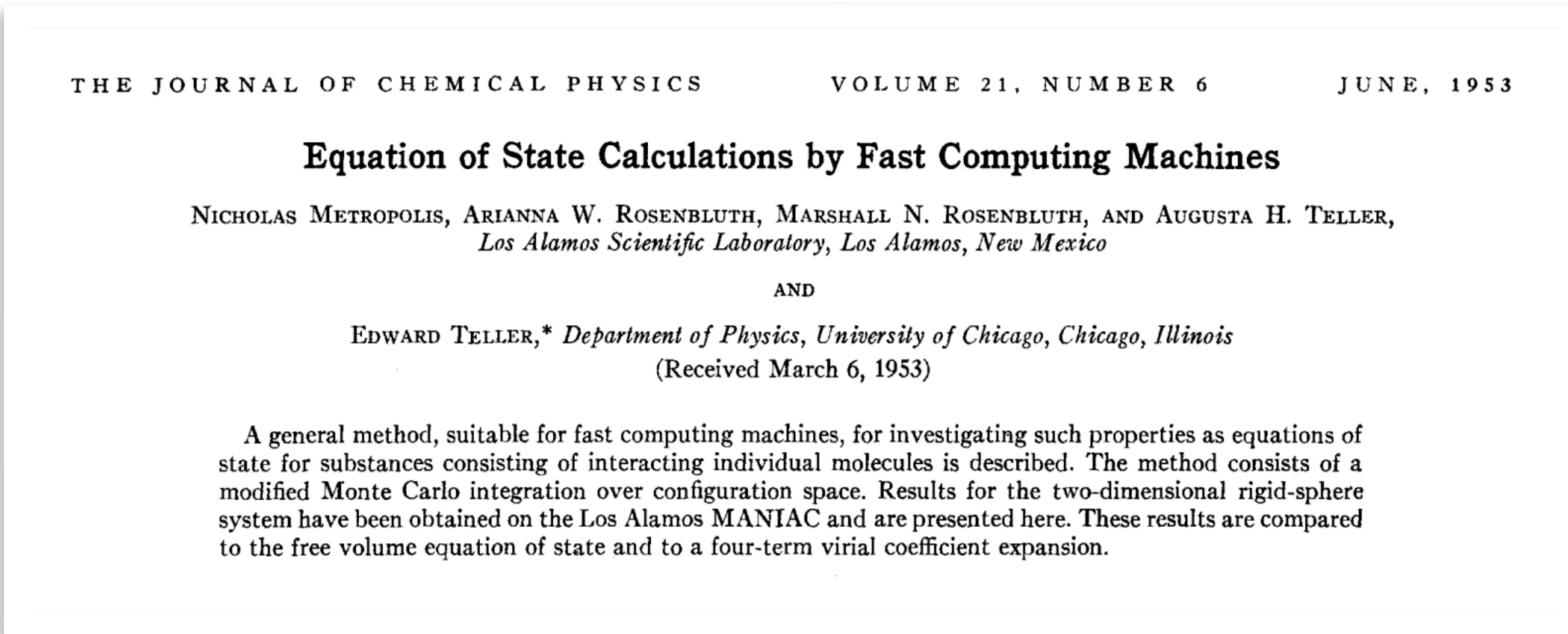
Development of Lattice QCD

$$\det(\gamma_\mu D_\mu + m_q) \equiv 1$$



[Credit: A. Ukawa, HPC Summer School (2013)]

The Metropolis algorithm


THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*
(Received March 6, 1953)

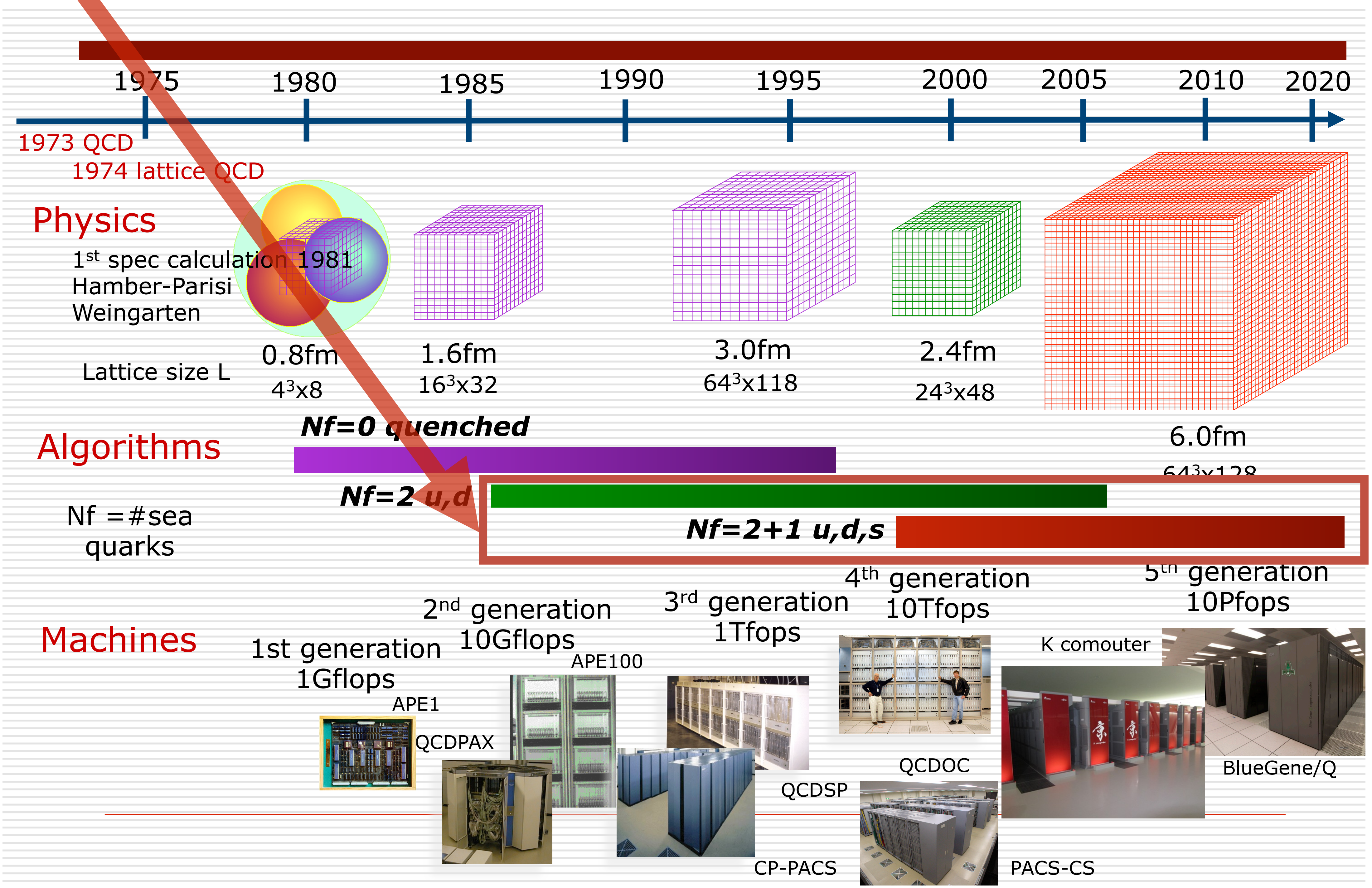
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

- The Metropolis Algorithm:
- Given $\{U\}$, propose $\{U'\}$ in a reversible, area-preserving way
- Accept the proposal as new entry with probability p,

  otherwise add $\{U\}$ to the chain again.
- $$p = \min\left(1, \frac{\pi(U')}{\pi(U)}\right)$$

Development of Lattice QCD

$$\det(\gamma_\mu D_\mu + m_q) \neq 1$$



[Credit: A. Ukawa, HPC Summer School (2013)]

Hybrid Monte Carlo algorithm for QCD

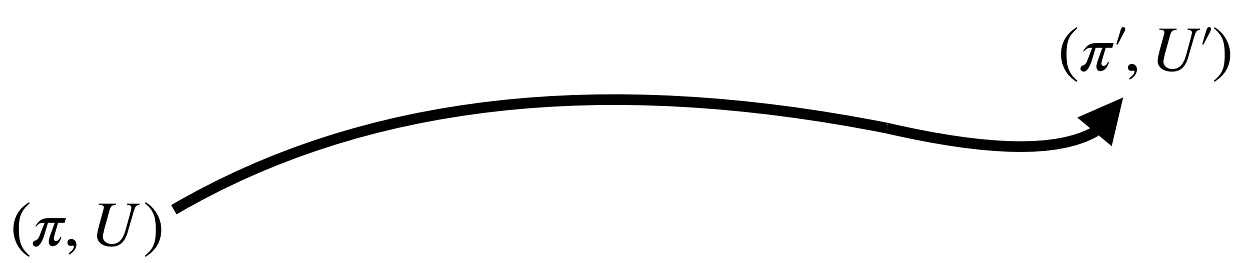
- Most widely used exact method for lattice QCD [Duane, Kennedy, Pendleton, Roweth, Phys. Lett. B, 195 (1987)]

- Introduce momenta $\pi_\mu(n)$ conjugate to fundamental fields $U_\mu(n)$ and the Hamiltonian

$$\mathscr{H} = \frac{1}{2}\sum_{n,\mu} \pi^2_{n,\mu} + S[U]$$

- **Momentum Heat-bath**: refresh momenta π (Gaussian random numbers)

- **Molecular Dynamics (MD)** evolution of π and U
  - ➡ numerically integrating the corresponding equations of motion (fictitious time τ):

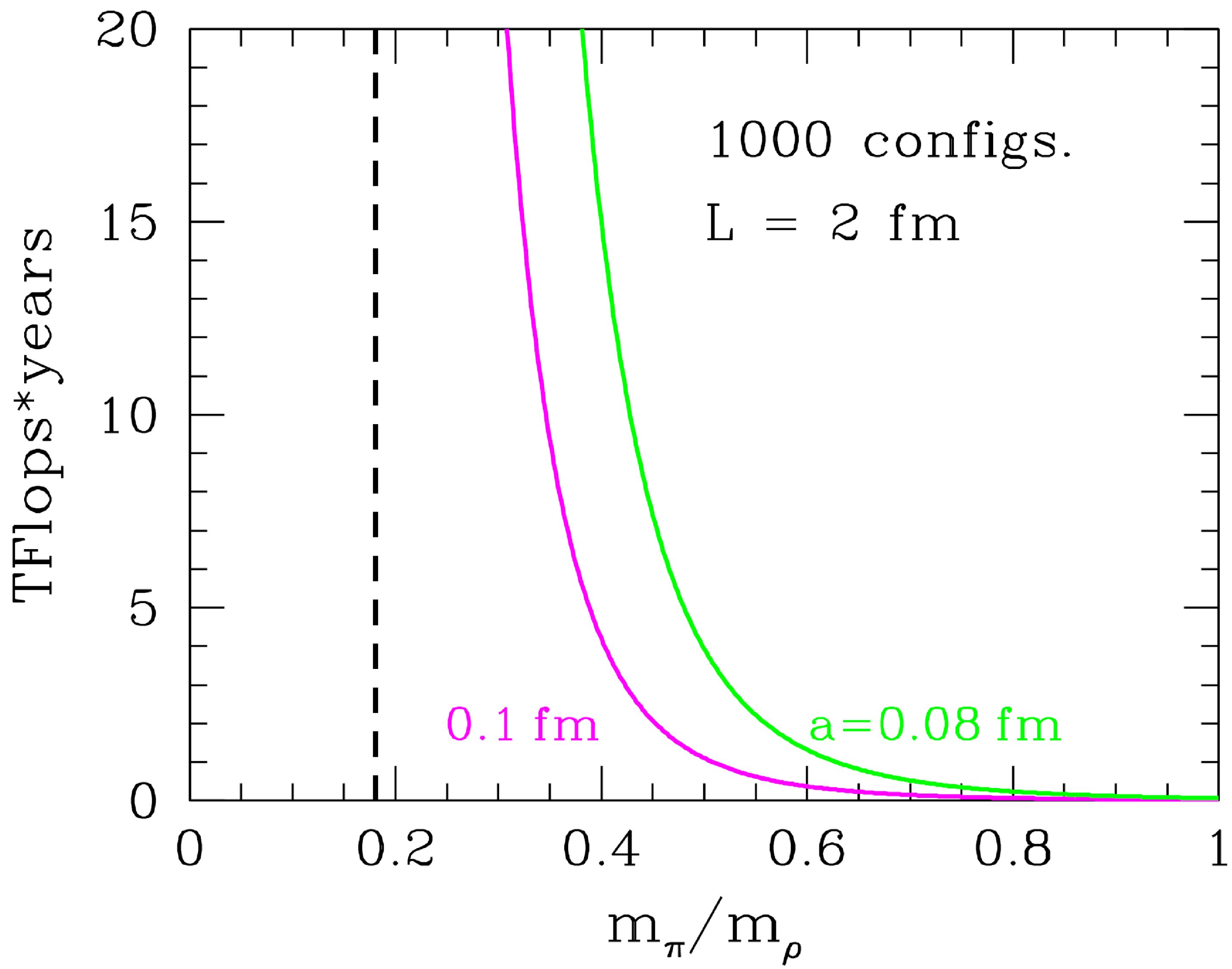


reversible, area-preserving scheme such as leap-frog, Omelyan…

- **Metropolis accept/reject step**
  - ➡ correcting for discretization errors of the numerical integration

$$P_{acc} = min\{1, e^{-(\mathscr{H}(\pi',U') - \mathscr{H}(\pi,U))}\}$$

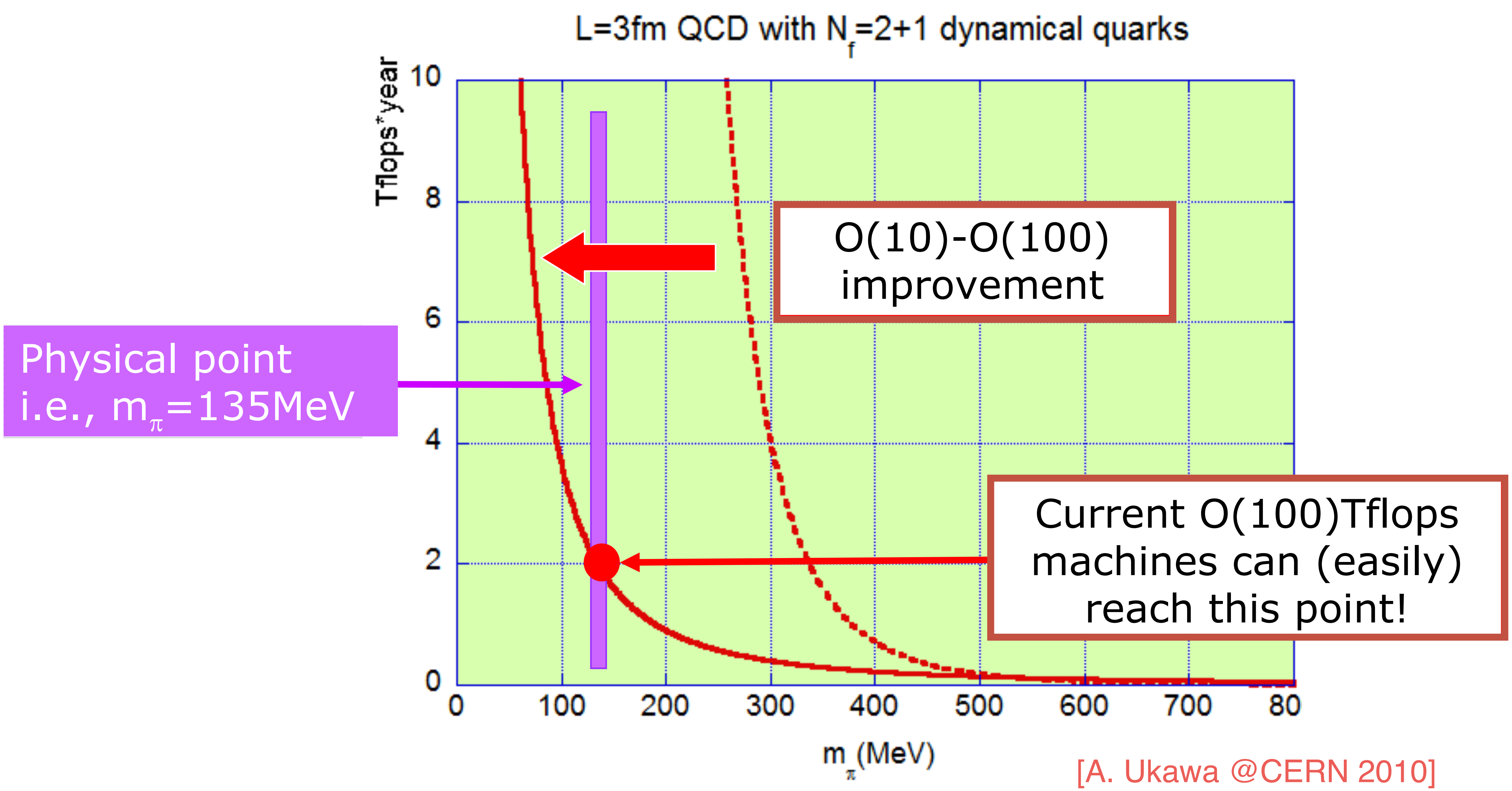
“Berlin Wall”



- Status in 2001: [A. Ukawa (2001)]
  - ➡ quarks 16x heavier than in nature; coarse lattices $a \approx 0.1$ fm (typical length scale is 1fm)
  - ➡ Cost of a simulation: $C\left[\frac{\#conf}{1000}\right]\left[\frac{m_q}{16m_{phys}}\right]^{-3}\left[\frac{L}{3\text{fm}}\right]^{5}\left[\frac{a}{0.1\text{fm}}\right]^{-7}; \quad C \approx 2.8$

Berlin Wall update

[2010, start of my PhD]



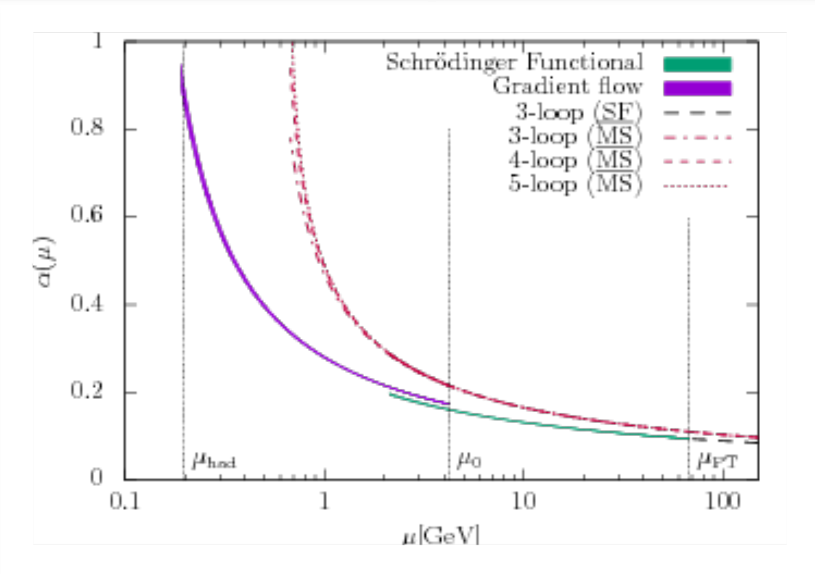
[A. Ukawa @CERN 2010]

Simulating physical quark masses becomes reality!

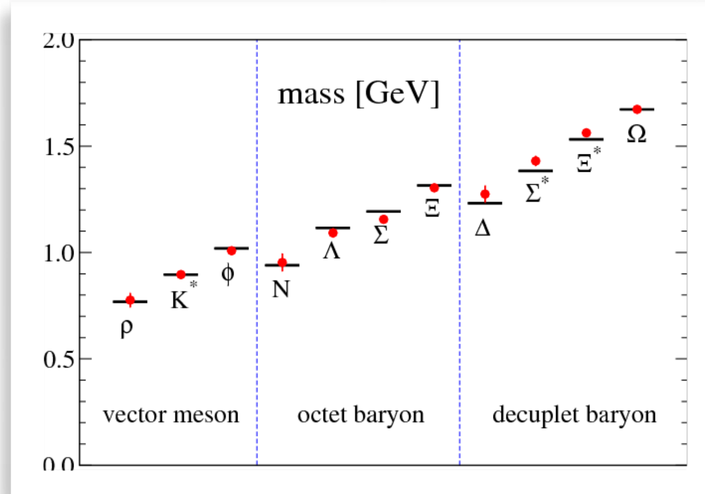
In today's lecture:

- QCD can be formulated on a Euclidean space time lattice
- Quantization amounts to summing over all gauge configurations; this can again be computed by Monte Carlo methods
- Different discretizations give different lattice artefacts
  - ➡ universal in continuum limit!
- Simulations with dynamical fermions computationally costly; many tricks in algorithms need to be applied
  - ➡ precise predictions of hadron spectrum, non-pert. renormalization, muon g-2, CKM matrix elements, QCD phase diagram etc.

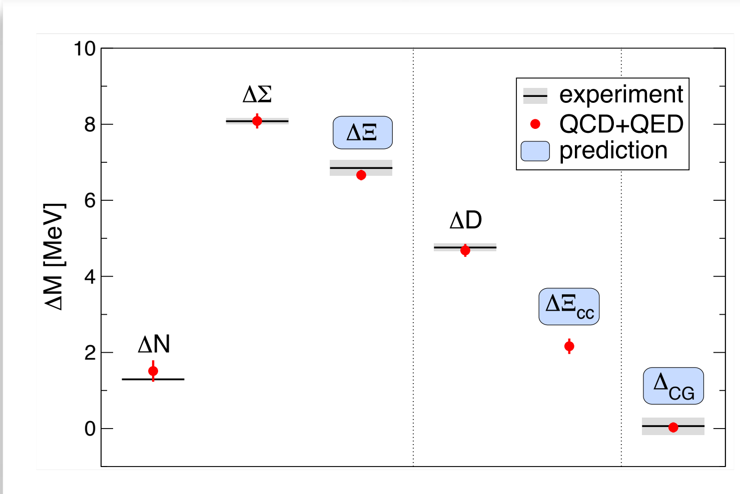
In tomorrow's lecture:



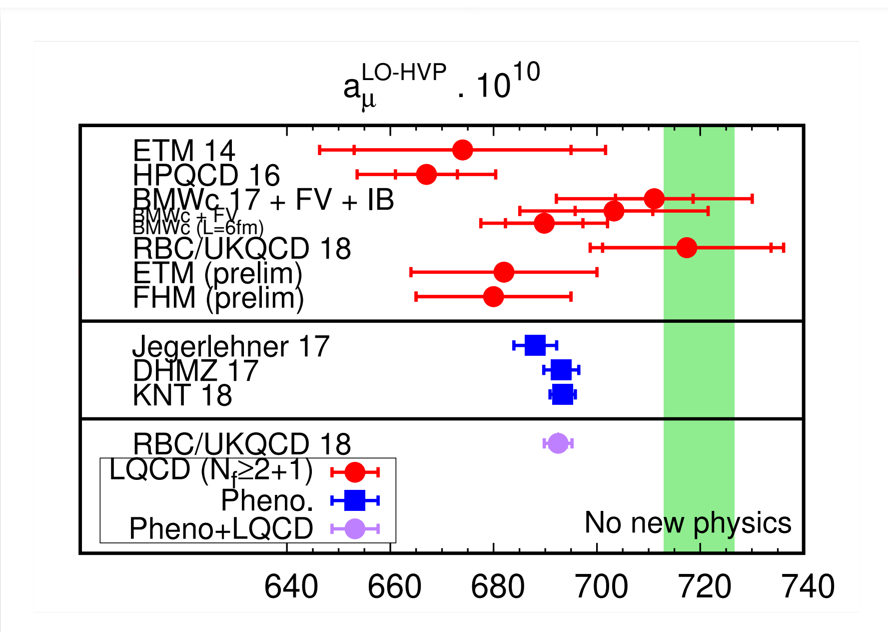
Strong coupling [Bruno et. al 2017]



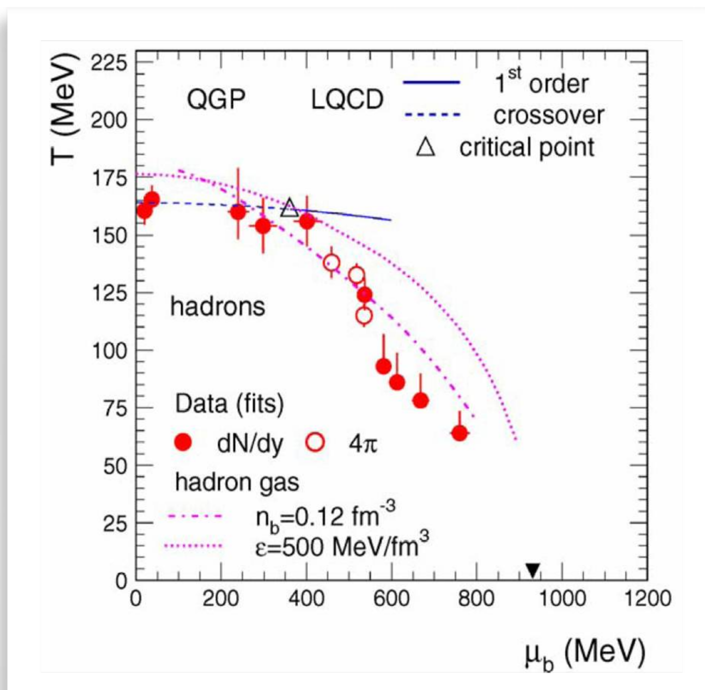
Hadron Spectrum [Aoki et. al 2008]



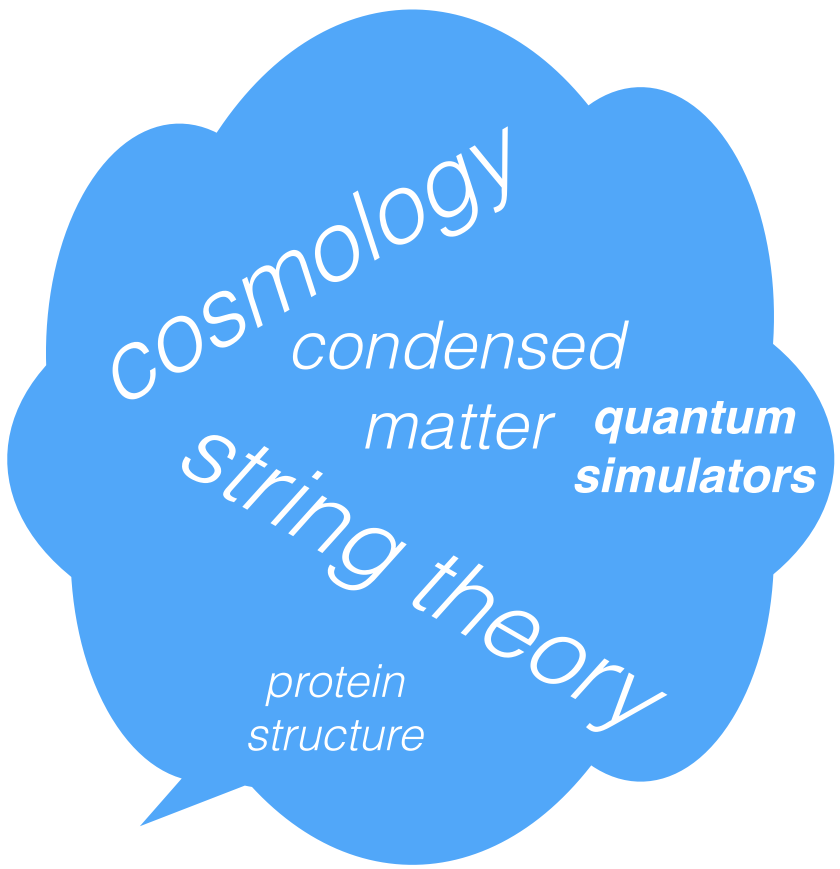
M_p-M_n [Borsanyi et. al 2014]



muon g-2: leading had. contib.
K. Miura @LATTICE2018



QCD Phase diagram
[Hohne et. al 2009]



Thank you!