Current methods for QCD on the lattice

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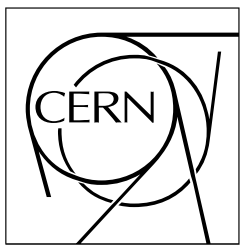


MC2013

Introduction **Q**uantum **C**hromo**D**ynamics

- Best theory of strong interactions.
- *Quarks* and *gluons* are the constituents of nuclear matter.
- Strongly interacting field theory.
  Pen and paper methods only answer a limited set of questions.
- Numerical computations needed.

QCD

	name	mass	q_{em}/e
u	up	2.3(7) MeV	2/3
d	down	4.8(7) MeV	-1/3
s	strange	95(5)MeV	-1/3
c	charm	1.275(25)GeV	2/3
b	bottom	4.18(3)GeV	-1/3
t	top	174.5(1)GeV	2/3

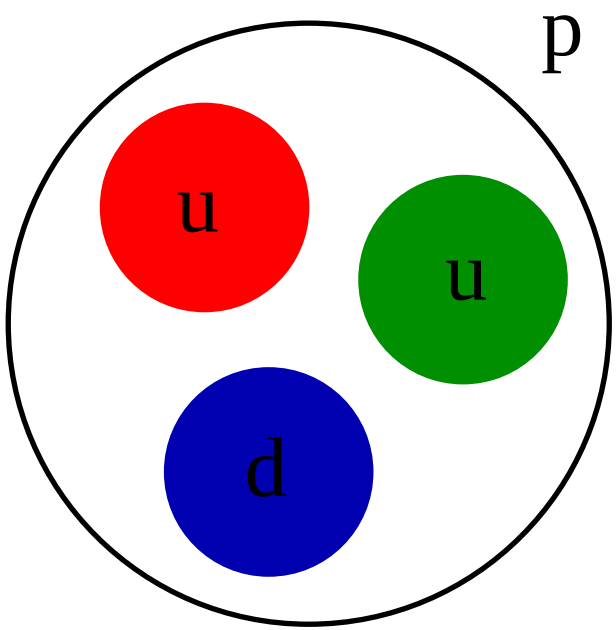
$$m_{\text{electron}} = 0.5\text{MeV}$$
$$m_{\text{proton}} = 938\text{MeV}$$

+ anti-quarks + gluons

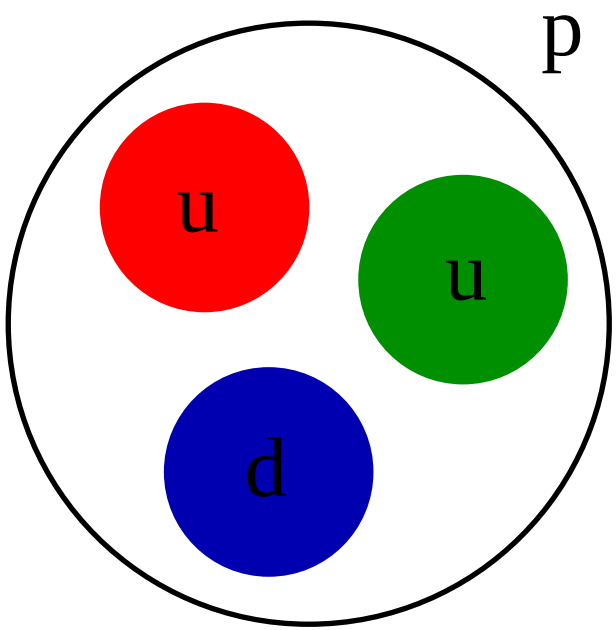
Large range of scales

$\rightarrow$ problem for numerical computations

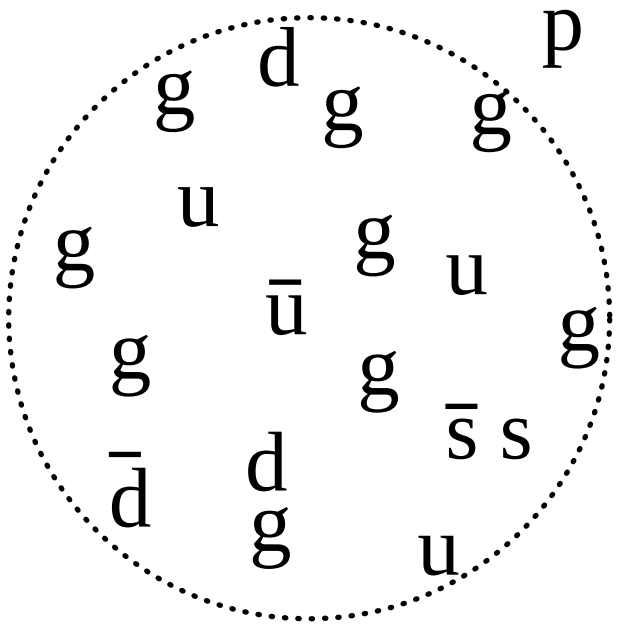
Naive view



Naive view



the reality is complicated



No good picture of structure.

Possible questions

- What is the mass of the proton?
- How is it build from quarks and gluons? $\rightarrow$ structure
- How about the masses of other hadrons?
- Masses of the quarks.
- Value of the coupling constant.
- Matrix elements to interpret HEP data.
- ...

One goal of lattice QCD investigations:
Essential input for particle physics analysis

QCD: A **quantum** field theory

Quantum field theory: All field values contribute

- Need to integrate over all possible field configurations.
- Weight of a field configuration given by theory.

Partition sum

$$Z = \int [dU]\, e^{-S[U]}$$

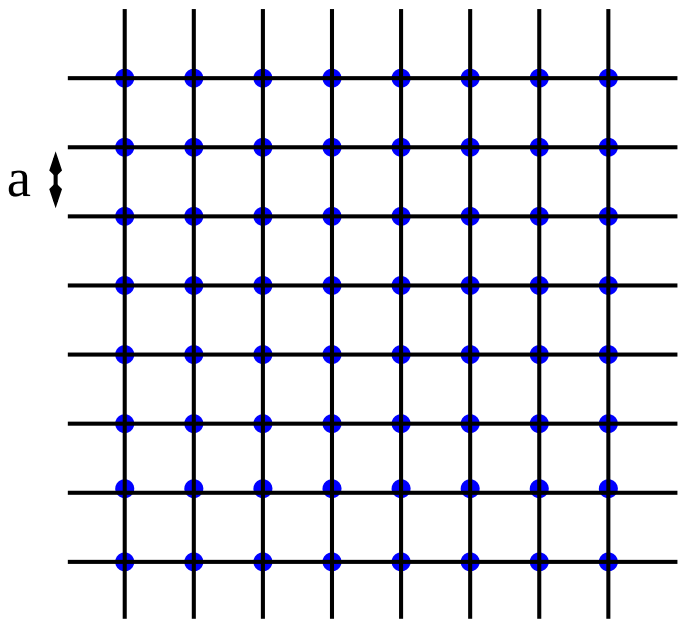
Path Integral over all possible values of gluon field U
$\rightarrow$ continuum definition problematic

Lattice

Discrete space time

WILSON'74

- continuous fields $\rightarrow$ values at discrete points
- Path integral $\rightarrow$ high-dimensional integral
- lattice spacing a
  $\rightarrow$ need to take continuum limit $a \rightarrow 0$



Monte Carlo

QCD: Monte Carlo view

Task

Compute integrals of the type

$$\langle O \rangle = \frac{1}{Z} \int \prod_{x,\mu} \mathrm{d}U_{x,\mu}\, e^{-S[U]}\, O[U]$$

- $\mathrm{O}(10^8)$ integration variables
- Importance sampling
  generate field configurations with large contribution
- Probability

$$P[U] \propto \frac{1}{Z} e^{-S[U]}$$

- Action $S[U]$ given by theory

Task is to update this many variables.

QCD: Monte Carlo view

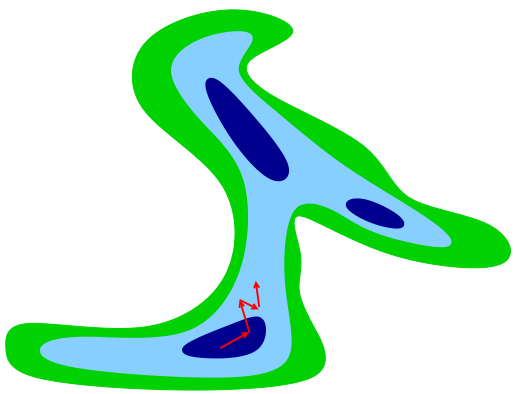
Markov Chain Monte Carlo

Sequence of field configurations

$$U_1 \to U_2 \to U_3 \to \cdots \to U_N$$

With transition matrix T

$$P[U] = \int dU' \, T[U \leftarrow U'] \, P[U']$$



Measurements

Sequence of field configurations

$$U_1 \rightarrow U_2 \rightarrow U_3 \rightarrow \cdots \rightarrow U_N$$

Measurements of observables

$$A_1 \rightarrow A_2 \rightarrow A_3 \rightarrow \cdots \rightarrow A_N$$

Estimates

$$\langle A \rangle \approx \frac{1}{N} \sum_{i=1}^{N} A_i$$

- **Subsequent measurements are correlated.**
- Need methods to deal with autocorrelations

  SOKAL'99, WOLFF'03
- Deal with slow modes

  ALPHA'11

Two basic types

Local updates

- Change one field on one lattice site at a time.
- Fast in simple situations.
  Inefficient for non-local actions (fermions).

Global updates

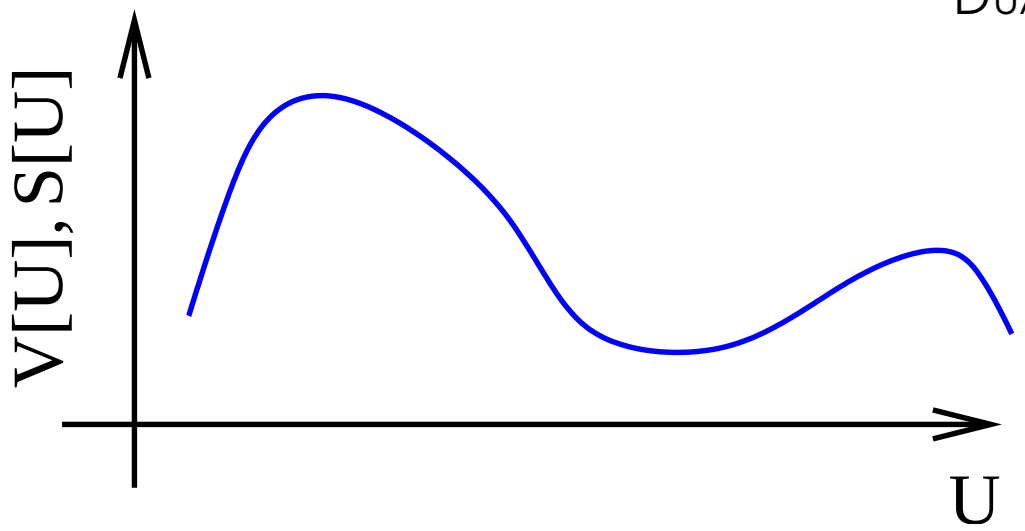
- Based on differential equations.
- Viable for virtually all actions.

Will be discussed in the following.

Hybrid Monte Carlo

Hybrid Monte Carlo

DUANE ET AL, '86



HMC: rough idea

- **Introduce momentum** π, conjugate to U
- Solve classical equations of motion

$$\dot{\pi} = -\frac{\delta S[U]}{\delta U} \qquad \dot{U} = \pi$$

- Randomize momentum at fixed intervals.

Hybrid Monte Carlo

Extended phase space

$$Z = \int [dU][d\pi]\, e^{-\frac{1}{2}\pi^2 - S[U]}$$

- Expectation values of observables $A[U]$ remain the same.
- Momenta Gaussian random numbers.

Microcanonical updates in this extended phase space.

$\Rightarrow$

Updates for U fields.

Momentum Heatbath

Refresh momenta $\pi \rightarrow$ only source of randomness

Molecular Dynamics

Solve numerically MD equations for some MC time τ (trajectory) deriving from Hamiltonian $H = \frac{1}{2}|\pi|^2 + S[U]$.

Acceptance Step

Correcting for inaccuracies in integration.

Numerical integration

Equations of motion cannot be solved analytically
$\rightarrow$ Need numerical methods
$\rightarrow$ Solution of differential equation never exact

Acceptance step

Metropolis test, acceptance probability

$$P_{\mathrm{acc}} = \min\left(1, e^{-\Delta H}\right)$$

Total energy violation must be max. $\mathrm{O}(1)$

H extensive quantity
$\rightarrow$ difficult for large volume
Computation of forces expensive
$\rightarrow$ requires solution of linear equations

Improvements

Progress over last decade

Status 2000

- Quarks 16$\times$ heavier than in nature.
  No perspective even with 2012 computers.
- Coarse lattices $a \approx 0.1$fm
  (the typical length scale is 1fm)

Cost of a simulation (Ukawa Lattice 2001)

$$\text{Cost} = C \left[\frac{\#conf}{1000}\right] \cdot \left[\frac{m_q}{16 m_{\text{phys}}}\right]^{-3} \cdot \left[\frac{L}{3\text{fm}}\right]^{5} \cdot \left[\frac{a}{0.1\text{fm}}\right]^{-7}$$

- $C \approx 2.8$ Tflops year

Comparison to 2012

Quarks at physical masses $L = 3$ fm box,
lattice spacing 0.1 fm (**coarse**)

2001 — Ukawa 2001

$$\text{cost} = 5.5\,\text{Pflops} \cdot \text{years}$$

Needs to be taken with grain of salt.

2012 — Lüscher, S.S.'12

$$\text{cost} = 0.1\,\text{Tflops} \cdot \text{years}$$

Fruit of community effort over many years.
Quark mass scaling much milder.

Currently largest computer in Germany (JUQUEEN):
~ 5 Pflops

Hybrid Monte Carlo

Improvements

- Methods to solve molecular dynamics equations of motion.
- Solvers for Dirac equation (system of linear equations)
- Changed boundary conditions to avoid problems with ergodicity $\rightarrow$ connected field space
- Interplay between physics and MD solver.

2000: General purpose algorithms

$\rightarrow$

2012: Physics informed algorithms

Hybrid Monte Carlo

Improvements

- Methods to solve molecular dynamics equations of motion.
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- Changed boundary conditions to avoid problems with ergodicity $\rightarrow$ connected field space
- **Interplay between physics and MD solver.**

2000: General purpose algorithms

$\rightarrow$

2012: Physics informed algorithms

Fermions

Example: Integrators

Molecular Dynamics

Solve numerically MD equations for some MC time τ (trajectory) deriving from Hamiltonian $\boldsymbol{H} = \frac{1}{2}|\pi|^2 + \boldsymbol{S}[\boldsymbol{U}]$.

Long time favorite: Verlet/Leapfrog integrator

$$\mathcal{I} = [\boldsymbol{T}_U(\epsilon/2)\, \boldsymbol{T}_\pi(\epsilon)\, \boldsymbol{T}_U(\epsilon/2)]^n$$

OMELYAN ET AL

Currently improved 2nd and 4th order schemes
$\rightarrow$ savings of factor 2 and more

Fermions

The inclusion of dynamical quarks is difficult.

$$P[U] \propto \det M[U]$$

- Fermion matrix M large, sparse matrix of dim $\mathrm{O}(10^7)$
- Impossible to compute directly.

Pseudofermions — Petcher-Weingarten'81

Fermions introduced by stochastic, unbiased estimator.

$$\det M = \frac{1}{Z_0} \int [d\phi][d\phi^\dagger] \exp[-\phi^\dagger \frac{1}{M} \phi]$$

Expensive because of solution of system of lin. equations

This approximation was source of problem up to 2000.

Solution

Large amount of possible modifications

$$P[U] \propto \det M[U] = \prod_{i=1}^{N} \det A_i[U]$$

Algorithms based on factorizations of M

- Physics ideas: IR/UV filtering, ...

  HASENBUSCH'01, LÜSCHER'03, CLARK&KENNEDY'03, ...
- A lot of heuristics $\rightarrow$ large speed-up.
- Theoretical guidance needed.

Need to take integrator for MD into consideration.

4D physics $\rightarrow$ 5D = 4D+simulation time

Theory of symplectic integrators

Well known, but need to connect to simulations.

Integrators

Shadow Hamiltonian E.G. CLARK&KENNEDY'07-'12

- Numerical integration does not conserve H exactly.
- For each symplectic integrator, there is a $\tilde{H}$ which is conserved.
- Construct in a power series in step size.

$$\tilde{H} = H + (c_1\, \partial_a S \partial_a S - c_2\, \pi_a \pi_b \partial_a \partial_b S)\delta\tau^2 + \dots$$

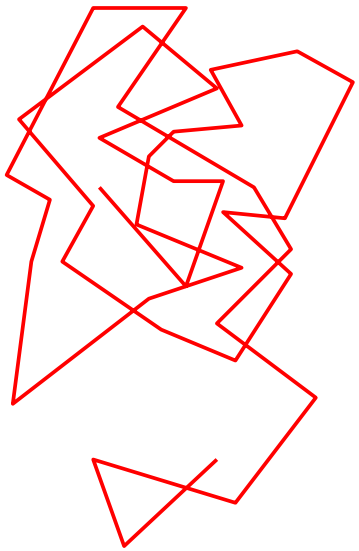
- Can compute energy violation.
- Understanding of determinant factorization S.S.'12

Gives a criterion for a good setup.

HMC vs. Langevin

HMC should outperform random walk

HMC



Langevin

- HMC: directed motion, Langevin: random walk
- Free field analysis supports this statement.
- Does not carry over to interacting theory.
- Langevin and HMC in same dynamical universality class.

LÜSCHER, S.S.'11

Summary

Physics

- Lattice QCD is the *ab-initio* approach to QCD.
- Computation of strong interaction observables, needed in high energy physics.
- Controlled simulations with realistic physics underway.

Methods

- Hybrid Monte Carlo algorithm of choice.
- Based on differential equations.

Summary

Improvements

- Solvers for Dirac equation.
  mild scaling towards criticality
- Improvements from better MD integrators.
- Determinant factorization.

$\rightarrow$ many orders of magnitude speed-up

Understanding of algorithms

- 5D perspective very fruitful.
- Scaling behavior towards the continuum.
- Useful to quantify ideas how to introduce fermions.