Lattice QCD: fundamental parameters of Quantum Chromodynamics from non-perturbative methods

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December 24, 2009

Content

QCD

- Commonly accepted theory of strong interaction
  → **Quantum Chromodynamics**

- QCD Lagrangian density (Euclidean: $t \to -ix_4$)

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

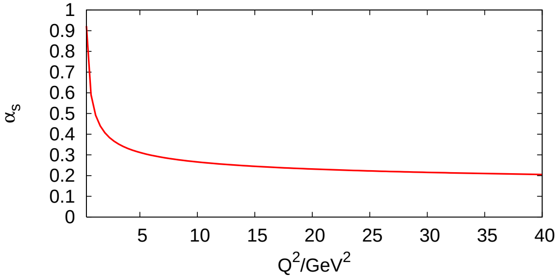
$$S = \int d^4x \, \mathcal{L}_{QCD}$$

- No free parameters other than:
  - gauge coupling g
  - quark masses m_u, m_d, ...

- **Note:** bare parameters → scale dependence!!

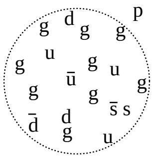
QCD

- Two extremal regimes:
  - low energy $\longrightarrow$ quarks confined into hadrons
  - high energy $\longrightarrow$ quarks essentially free: asymptotic freedom
- At low energy/momentum transfer: perturbation theory methods fail!



- Non-perturbative methods needed: lattice QCD

Problems not accessible by perturbation theory



- Chiral symmetry breaking
  - Explicit: Not-zero quark masses
  - Spontaneous: The pion is a Goldstone boson
- Confinement and the low energy properties of hadrons:
  - Hadron masses
  - Low energy parameters (decay constants, current quark masses, LEC of Chiral Perturbation Theory)
  - Form factors, matrix elements, structure functions

Functional Integral Formalism

- Feynman's QM Path Integral $\rightarrow$ Quantum Field Theory
- Each specific field configuration:

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

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

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

Regularization: The Lattice

- Divergencies in continuum QCD $\longrightarrow$ **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 ($\int d^4x \ \longrightarrow \ a^4 \sum_n$)
- Computable with the help of Monte Carlo techniques

Lattice discretization

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

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

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

- Discretization prescription:

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

Naive Lattice Fermion Action

- $S_F^0\left[\psi,\overline{\psi}\right] = \int d^4x\ \overline{\psi}(x)\ \left(\gamma_\mu \partial_\mu + m\right)\ \psi(x)$

- Symmetrically discretized partial derivative:

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

- Naive lattice ansatz for free fermion action:

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

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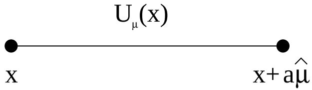
- **Let us examine gauge invariance** $\rightarrow$

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

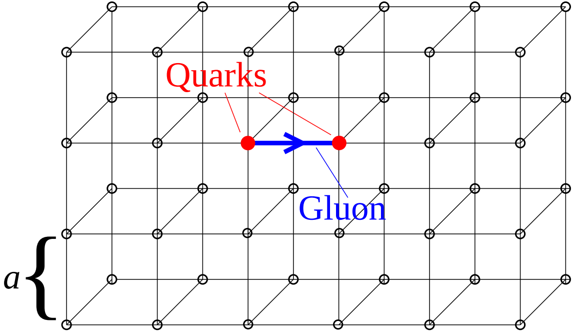


- Introduce **link variables $\mathbf{U}_\mu(\mathbf{n})$**:

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

- $U_\mu(n) \;\rightarrow\;$ 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 $\sim U_{\mu}(n) = e^{iagA_{\mu}}$

The three limits of Lattice QCD

- Continuum limit: $a \;\longrightarrow\; 0$

  Lattice artifacts should become small

  $\longrightarrow$ Improvement program

- Thermodynamic limit: $N \;\longrightarrow\; \infty \quad (L = Na = const)$

  Hadron physics in a box of few fm

  $\longrightarrow$ Finite volume effects can be utilized (Part 2)

- Chiral limit: $m_q \;\longrightarrow\; 0$

  Physical u,d quark masses are small

  $\longrightarrow$ We want to understand chiral symmetry breaking

Continuum limit: $a \to 0$

- Continuum limit of the lattice theory

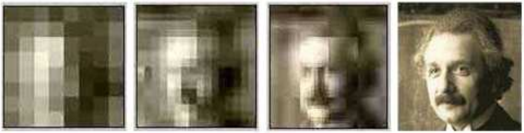
  $\to$ a possible definition of a renormalized continuum theory

  $\to$ $\Lambda_{cut} \sim \frac{1}{a}$ $\to \Lambda_{cut} \to \infty \iff a \to 0$

- Predictions for experiments:

  $\to$ obtained only from the continuum limit of the lattice theory!

  $\to$ universality classes of operators on the lattice.



The same physical image represented on lattices of linear extent 8, 16, 32 and 128 corresponding to lattice spacings of 4cm, 2cm, 1cm and 1/4cm.

Lattice Fermion Action

- 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

$$D_W(n,m) = \left(m + \frac{4}{a}\right)\delta_{n,m} - \frac{1}{2a}\sum_{\mu=\pm1}^{\pm4}\left(1-\gamma_\mu\right)U_\mu(n)\,\delta_{n+\hat{\mu},m}$$

- Wilson term: shifting the mass of the doublers to infinity, as $a \longrightarrow 0$
- 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

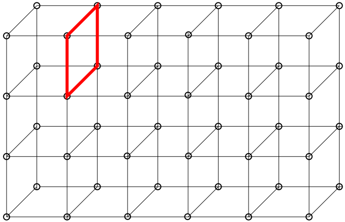
Lattice Gauge Action - shortly

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

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

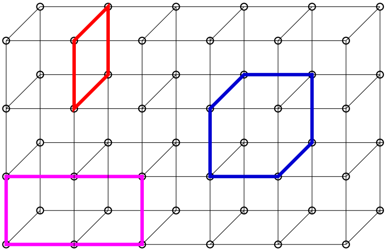
- **Wilson gauge action:**

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



Lattice Gauge Action II

- Improvement: taking into account larger Wilson loops



- All in the same universality class:

  $\longrightarrow$ converge to $\mathrm{Tr}\left[F_{\mu\nu}(x)F_{\mu\nu}(x)\right]$ 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]

Lattice and Symmetries

- Local gauge symmetry:
  Explicitly obeyed.
- Translational symmetry:
  Broken to discrete symmetry, but nicely restored in 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.
- Chiral symmetry:
  Explicitly broken if doublers are removed. Restoration possible but expensive.

2. Nonperturbative renormalization of QCD

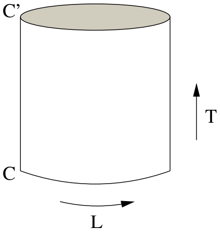
- Parameters of QCD: $g, m_u, m_d, m_s \ldots \longrightarrow$ scale dependent!
- Lattice QCD - purely NP definition of QCD $\longrightarrow$ need NP renormalization!
- Connection between the low energy sector and the perturbative regime
- Compute renormalization factors without directly relying on perturbation theory
  - Match the low energy sector with an intermediate non-perturbative renormalization scheme
  - Pass to the perturbative scheme ($\overline{MS}$) in the high energy region

Nonperturbative renormalization of QCD

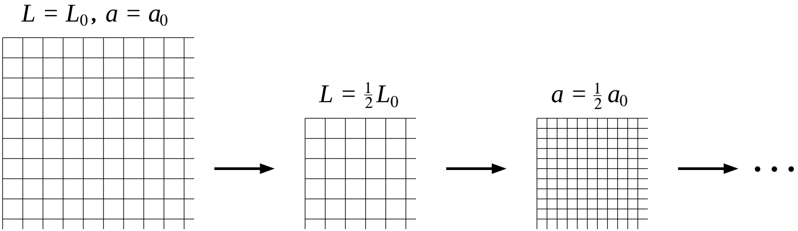
- Conditions to be satisfied:
  - Compute $\alpha(\mu)$ at energy scales of $\mu \gtrsim 10 GeV$
    $\longrightarrow$ controlled connection to the perturbative regime!
  - Keep μ removed from the lattice cutoff $\frac{1}{a}$
    $\longrightarrow$ to avoid large discretization effects
  - Keep the box size L large compared to the confinement scale
    $\longrightarrow$ to avoid finite size effects in the simulations
- Summary: $L \gg \frac{1}{0.14 GeV} \gg \frac{1}{\mu} \sim \frac{1}{10 GeV} \gg a$
- Outcome: lattice $N \equiv \frac{L}{a} \gg 70$
- Possible to compute: lattices max $N \equiv \frac{L}{a} \sim 70$

Finite-size scaling

- Solution: $\mu \equiv \frac{1}{L}$
- Finite size effect: physical observable
- Schrödinger Functional scheme:
  - QCD on a space-time cylinder $L^3 \times T$
  - periodic b.c. in spatial direction
  - fixed (Dirichlet) b.c. in time direction
- [Lüscher, Weisz, Wolff], ALPHA Collaboration



General Strategy



- Step scaling function:

$$\sigma(u) = \bar{g}^2(2L)|_{u=\bar{g}^2(L), m_i=0}$$

- Describes a finite jump in the scale evolution (here: $L \rightarrow 2L$)

- Discrete form of β function

- Lattice effects of order a:

  $\rightarrow$ extrapolated away by repeating the calculation for several values of $\frac{L}{a}$

Nonperturbative renormalization of QCD

Running of the coupling/mass, $N_f = 2$

[Della Morte et al (ALPHA Collab.),2004]

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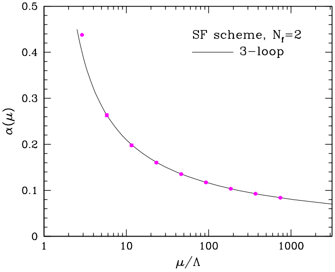
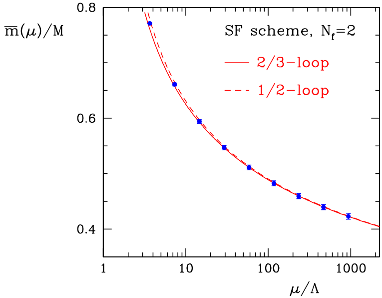
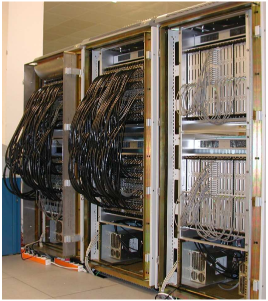




Goal: include more flavours ($N_f = 4$), $m_c \neq 0 \longrightarrow$ even more precise $\alpha_s \dots$

Lattice simulations



- typical lattice sizes: ~ 3 *fm*
- 32ˆ3 x 64 lattice $\longrightarrow$ 2100000 points
- lattice spacings a: $0.05 - 0.1$ *fm*
- advanced algorithms
- large computer resources

Why is it so expensive?

- We need to compute:

$$Z = \int \mathcal{D}\,\overline{\psi}\mathcal{D}\psi\; e^{-\overline{\psi}\;(\gamma_\mu D_\mu + m)\;\psi}$$
$$\approx \; det\;(\gamma_\mu D_\mu + m)$$

- Determinant can be represented by bosonic fields → "pseudofermions"

$$det\;(\gamma_\mu D_\mu + m) \propto \int \mathcal{D}\Phi^\dagger\;\mathcal{D}\Phi\; e^{\;\Phi^\dagger\;(\gamma_\mu D_\mu + m)^{-1}\;\Phi}$$

- Effective action:

$$S_{eff} = \Phi^\dagger\;(\gamma_\mu D_\mu + m)^{-1}\;\Phi$$

- Solving:

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

  very expensive for:
  - small quark mass m
  - large lattice extent $\frac{L}{a}$

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

Hybrid Monte Carlo

[Duane, Kennedy, Pendleton, Roweth, 1987]

- Most used algorithm for lattice QCD
- Introduce momenta $P_\mu(n)$ conjugate to fundamental fields $U_\mu(n)$ and the Hamiltonian:

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

- **Molecular dynamics (MD)** evolution of P and U

  $\longrightarrow$ by numerical integration of the corresponding e. o. m.

$$(P, U) \quad \rightarrow \quad (P', U')$$

- **Metropolis accept/reject step**

  $\longrightarrow$ to correct for discetization errors of the numerical integration

$$P_{acc} = min\{1, exp(-\Delta\mathcal{H} = \mathcal{H}(P', U') - \mathcal{H}(P, U))\}$$

Multiple Time Scale Integration

- Assume: $\mathcal{H} = \frac{1}{2}\sum_{n,\mu} P_{n,\mu}^2 + S_0 + S_1$

- Define ($j = 0, 1$):

$$\begin{aligned} T_U(\Delta\tau) &: \quad U \rightarrow U' = exp(i\Delta\tau P)U, \\ T_{S_j}(\Delta\tau) &: \quad P \rightarrow P' = P - i\Delta\tau\delta S_j \end{aligned}$$

- Recursively define integration scales:

$$\begin{aligned} T_0 &= T_{S_0}(\Delta\tau_0/2)\ T_U(\Delta\tau_0)\ T_{S_0}(\Delta\tau_0/2) \\ T_1 &= T_{S_1}(\Delta\tau_1/2)\ [T_U]^{N_0}\ T_{S_1}(\Delta\tau_1/2) \end{aligned}$$

- Trajectory of length τ: $[T_1]^{N_1}$

Preconditioning

- Most expensive part: fermion determinant
- Precondition by factorization (suitable C and E)

  $$det Q^2 = det(C) \cdot det(E)$$

  $\rightarrow$ C and E better "behaved" than Q^2
- Different preconditioning approaches:
  - mass preconditioning [Hasenbusch]
  - polynomial filtering [Peardon, Sexton]
  - domain decomposition [Lüscher]
  - n^{th}-root trick [Clark, Kennedy]
- Often is the case:
  - C is cheap
  - E is expensive

n^{th}-root Trick

- Use the following factorization:

$$detQ^2 = \sqrt{detQ^2} \cdot \sqrt{detQ^2}$$

- In terms of condition numbers:

$$k \quad \rightarrow \quad 2 * \sqrt{k}$$

- Generalization:

$$detQ^2 = \left[\, \left(detQ^2\right)^{1/n} \, \right]^n$$

- Saves large factors!

Hasenbusch trick

- Precondition the fermion determinant ($Q = \gamma_5 D(m)$, $N_f = 2$)

$$det Q^2 = det\big[Q^2 + \mu^2\big] \cdot det\big[\frac{Q^2}{Q^2 + \mu^2}\big]$$

- Corresponding effective action:

$$S_{eff} = S_G + \Phi_1^\dagger \frac{1}{Q^2 + \mu^2} \Phi_1 + \Phi_2^\dagger \frac{Q^2 + \mu^2}{Q^2} \Phi_2$$

- Can be extended to $N_{PF} > 2$ pseudo-fermion fields
- Saves large factors!

Why does preconditioning help?

Tune preconditioner such that:

- the most expensive part (S1) contributes the least to the total force

  $\rightarrow$ can be integrated with large $\Delta\tau$

- the cheaper the action part, the smaller $\Delta\tau$

- different parts can be integrated on different time scales chosen according to their force magnitude:

  $$\Delta\tau_j ||F_j|| = const$$

  as a tuning guidline

- Force corresponding to action contribution S_j: $\delta S_j = F_j \delta U$

Literature

Books:

- **"Quarks, gluons and lattices"**,
  M. Creutz, "Cambridge Univ. Pr.", 1983, **0-521-31535-2**
- **"Introduction to Quantum Fields on a Lattice"**,
  J. Smith, Cambridge Univ. Pr., 2002, **0-521-89051-9**
- **"Quantum fields on a lattice"**,
  I. Montvay and G. Münster, Cambridge Univ. Pr., 1994, **0-521-40432-0**
- **"Lattice gauge theories"**,
  H.J. Rothe, World Scientific, 2005, **981-256-168-4**
- **"Lattice methods for quantum chromodynamics"**,
  T. DeGrand and C. DeTar, World Scientific, 2006, **981-256-727-5**
- **"Quantum Chromodynamics on the Lattice: An introductory presentation"**
  C. Gattringer. C.B. Lang, Springer, Berlin Heidelberg 2010, **978-3-642-01850-3**

Lecture notes:

- **"Introduction to lattice QCD"**",
  Rajan Gupta, 1997, **arXiv:hep-lat/9807028**
- **"Advanced lattice QCD"**,
  Martin Lüscher, Les Houches 1997, **arxiv:hep-lat/9802029**bg
- **"Non-perturbative renormalization of QCD"**,
  Rainer Sommer, Schladming winter school, 1997, **hep-ph/9711243**

Download and simulate

Publicly available packages for lattice qcd simulations and measurements:

- **"The MIMD lattice computation"**,
  MILC Collaboration, USA, **www.physics.utah.edu/ detar/milc/** (Version 7)
- **"DD-HMC algorithm for two-flavour QCD"**,
  Martin Lüscher, CERN - Theory Division, **http://luscher.web.cern.ch/luscher/DD-HMC/index.html** (DD-HMC-1.2.2)
- **"tmLQCD - A program suite to simulate Wilson twisted mass lattice QCD"**,
  ETMC, K. Jansen, C. Urbach **http://www.sciencedirect.com/science/journal/00104655**
- **"The CHROMA Library for Lattice Field Theory"**,
  US Lattice Quantum Chromodynamics, **http://usqcd.jlab.org/usqcd-docs/chroma/**

All above (and other codes) are mainly based on HMC algorithm, with one or more different kind of preconditioning of the Dirac matrix implemented.

Different approach(es) to the discretization of the Dirac operator are used.

Summary

- QCD can be formulated on a Euclidean space-time lattice
- Quantization amounts to summing over all gauge configurations; this can be approximated by Monte Carlo sums
- Different discretizations give different lattice artefacts
  $\rightarrow$ **universal in continuum limit!**
- Fundamental QCD parameters: determined from low energy hadron data
- Non-perturbative renormalization
- Finite size scaling $\rightarrow$ high precision data with limited resources
- Expensive calculations, many tricks in algorithms need to be applied

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- Expensive calculations, many tricks in algorithms need to be applied
- . . . and a lot more to come :)

HVALA NA PAŽNJI !