Understanding the Strong Interactions through large scale simulations

C. Alexandrou
University of Cyprus and Cyprus Institute
Outline

1 Introduction
   - Strong Interaction Phenomena
   - QCD on the lattice
   - Computational cost

2 Recent results
   - Hadron masses
   - Nucleon form factors
   - Origin of the spin of the Nucleon
   - On the shape of hadrons
   - Nuclear forces
   - QCD phase diagram

3 Computational resources

4 Conclusions
Standard model of Elementary Particles

The Standard Model (SM) is a synthesis of three of the four forces of nature described by gauge theories with coupling constants:

- **Strong Interactions:** $\alpha_s \sim 1$
- **Electromagnetic interactions:** $\alpha_{em} \approx 1/137$
- **Weak interactions:** $G_F \approx 10^{-5} \text{ GeV}^{-2}$

Basic constituents of matter:

- Six quarks, $u, d, s, c, b, t$, each in 3 colors, and six leptons $e, \nu_e, \mu, \nu_\mu, \tau, \nu_\tau$
- The quarks and leptons are classified into 3 generations of families.
- The interactions between the particles are mediated by vector bosons: the 8 gluons mediate strong interactions, the $W^\pm$ and $Z$ mediate weak interactions, and the electromagnetic interactions are carried by the photon $\gamma$.
- The weak bosons acquire a mass through the Higgs mechanism.
- The SM is a local gauge field theory with the gauge group $SU(3) \times SU(2) \times U(1)$ specifying the interactions among these constituents.

### Masses in the Standard Model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Number</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Masses of quarks</td>
<td>6</td>
<td>$u, d, s$ light $c, b$ heavy $t = 175 \pm 6 \text{ GeV}$</td>
</tr>
<tr>
<td>Masses of leptons</td>
<td>6</td>
<td>$e, \mu, \tau$ $M_{\nu_e, \nu_\mu, \nu_\tau}$ non-zero</td>
</tr>
<tr>
<td>Mass of $W^\pm$</td>
<td>1</td>
<td>80.3 GeV</td>
</tr>
<tr>
<td>Mass of $Z$</td>
<td>1</td>
<td>91.2 GeV</td>
</tr>
<tr>
<td>Mass of gluons, $\gamma$</td>
<td>0 (Gauge symmetry)</td>
<td></td>
</tr>
<tr>
<td>Mass of Higgs</td>
<td>1</td>
<td>Not yet seen</td>
</tr>
</tbody>
</table>

C. Alexandrou (Univ. of Cyprus & Cyprus Inst.)

Strong Interactions through simulations

DEISA/PRACE, Helsinki, 2011
QCD – Gauge theory of the strong interaction

- Lagrangian: formulated in terms of quarks and gluons

\[
\mathcal{L}_{\text{QCD}} = -\frac{1}{4} F^a_{\mu\nu} F^{a \mu\nu} + \sum_f \bar{\psi}_f (i \gamma^\mu D_\mu - m_f) \psi_f, \quad f = u, d, s, c, b, t
\]

\[
D_\mu = \partial_\mu - ig(\frac{1}{2} \lambda^a) A_\mu^a
\]

Harald Fritzsch  Murray Gell-Mann  Heinrich Leutwyler
Properties of QCD

Asymptotic freedom: $g(\mu)$

![Graph showing $g(\mu)$ vs $\mu$ GeV with data points and curves.]

[Yao et al., PDG 2006]

Confinement

![Graph showing $[V(r) - V(r_0)]/r_0$ vs $r/r_0$ with data points and curves.]


Nobel Prize in Physics 2004

“...for the discovery of asymptotic freedom in the theory of the strong interaction”

David Gross  Frank Wilczek  David Politzer
QCD versus QED

Quantum Electrodynamics (QED): The interaction is due to the exchange of photons. Every time there is an exchange of a photon there is a correction in the interaction of the order of 0.01.

→ we can apply perturbation theory reaching whatever accuracy we like

QCD: Interaction due to exchange of gluons. In the energy range of ~ 1 GeV the coupling constant is ~ 1

→ We can no longer use perturbation theory
QCD versus QED

- Conventional perturbative approach cannot be applied for hadronic process at scales \( \lesssim 1 \text{ GeV} \) \( \Rightarrow \) we cannot calculate the masses of mesons and baryons from QCD even if we are given \( \alpha_s \) and the masses of quarks.

- Bound state in QCD very different from QED e.g. the binding energy of a hydrogen atom is to a good approximation the sum of its constituent masses. Similarly for nuclei the binding energy is \( \mathcal{O}(\text{MeV}) \). For the proton almost all the mass is attributed to the strong non-linear interactions of the gluons.

\[
\begin{align*}
\text{QED} & \quad \text{Hydrogen Atom} \\
\text{QCD} & \quad \text{Proton}
\end{align*}
\]

**QED**
- \( e^- + p^+ = 13.6 \text{ eV} \)
- \( M_e = 0.5 \text{ MeV} \)
- \( M_p = 938 \text{ MeV} \)
- \( E_{\text{binding}} = 13.6 \text{ eV} \) (EM force)

**QCD**
- \( M_u \sim 3 \text{ MeV} \)
- \( M_d \sim 6 \text{ MeV} \)
- \( M_p = 938 \text{ MeV} \) (Strong force)

C. Alexandrou (Univ. of Cyprus & Cyprus Inst.)

Strong Interactions through simulations

DEISA/PRACE, Helsinki, 2011
Strong Interaction Phenomena

The Strong Interactions describe the evolution from the big-bag to the present Universe and beyond.

- QCD phase diagram relevant for Quark-Gluon Plasma: $t \sim 10^{-32}$ s and $T \sim 10^{27}$, studied in heavy ion collisions at RHIC and LHC
- Hadron structure: $t \sim 10^{-6}$ s, experimental program at JLab, Mainz.
  - Momentum distribution of quarks and gluons in the nucleon
  - Hadron form factors e.g. the nucleon axial charge $g_A$
- Matter-antimatter asymmetry: $t \sim 10^{-6}$ s

Exa-scale machines are required to go beyond hadrons to nuclei
K. Wilson: 1974 formulated Euclidean gauge theories on the lattice as a tool for the study of confinement and non-perturbative properties of QCD.

M. Creutz: 1980 performed the first numerical implementation of the path integral formulation for gauge theories.

The set-up for the numerical evaluation requires:
- Discretization of space-time in 4 Euclidean dimensions → simplest isotropic hypercubic grid:
  - Rotation into imaginary time is the most drastic modification
  - Lattice acts as a non-perturbative regularization scheme with the lattice spacing $a$ providing an ultraviolet cutoff at $\pi/a$ → no infinities
- Gauge fields are links and fermions are anticommuting Grassmann variables
- Construction of an appropriate action such that when $a \to 0$ (and Volume $\to \infty$) gives the continuum theory
- Construction of the appropriate operators with their renormalization to extract physical quantities

Why Lattice QCD?
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems in terms of the fundamental quark and gluon degrees of freedom.
- Like continuum QCD, lattice QCD has as unknown input parameters the coupling constant $\alpha_s$ and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).
- Lattice QCD provides a well-defined approach to calculate a set of observables non-perturbatively starting directly from the QCD Lagrangian.
K. Wilson: 1974 formulated Euclidean gauge theories on the lattice as a tool for the study of confinement and non-perturbative properties of QCD.

M. Creutz: 1980 performed the first numerical implementation of the path integral formulation for gauge theories.

Why Lattice QCD?

- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems in terms of the fundamental quark and gluon degrees of freedom.
- Like continuum QCD, lattice QCD has as unknown input parameters the coupling constant $\alpha_s$ and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).

$$U_{\mu}(n) = e^{igaA_{\mu}(n)}$$
K. Wilson: 1974 formulated Euclidean gauge theories on the lattice as a tool for the study of confinement and non-perturbative properties of QCD.

M. Creutz: 1980 performed the first numerical implementation of the path integral formulation for gauge theories.

The set-up for the numerical evaluation requires:

- Discretization of space-time in 4 Euclidean dimensions → simplest isotropic hypercubic grid:
  - Rotation into imaginary time is the most drastic modification
  - Lattice acts as a non-perturbative regularization scheme with the lattice spacing $a$ providing an ultraviolet cutoff at $\pi/a$ → no infinities
- Gauge fields are links and fermions are anticommuting Grassmann variables
- Construction of an appropriate action such that when $a \rightarrow 0$ (and Volume $\rightarrow \infty$) gives the continuum theory
- Construction of the appropriate operators with their renormalization to extract physical quantities

Why Lattice QCD?

- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems in terms of the fundamental quark and gluon degrees of freedom.
- Like continuum QCD, lattice QCD has as unknown input parameters the coupling constant $\alpha_s$ and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).

$Lattice QCD provides a well-defined approach to calculate a set of observables non-perturbatively starting directly from the QCD Lagrangian.
Computational cost

Simulation cost: \( C_{\text{sim}} \propto \left( \frac{300 \text{MeV}}{m_\pi} \right)^{c_m} \left( \frac{L}{2 \text{fm}} \right)^{c_L} \left( \frac{0.1 \text{fm}}{a} \right)^{c_a} \)

Coefficients \( c_m, c_L \) and \( c_a \) depend on the discretized action used for the fermions. State-of-the-art simulations use improved algorithms:
- Multiple time scales in the molecular dynamics updates

\[ \implies \text{for twisted mass fermions: } c_m \sim 4, \ c_L \sim 5 \text{ and } c_a \sim 6. \]

- Simulations at physical quark masses, \( a \sim 0.1 \text{ fm} \) and \( L \sim 5 \text{ fm} \) require \( \mathcal{O}(1) \text{ Pflop.Years.} \)
- The analysis to produce physics results requires \( \mathcal{O}(0.1) \text{ Pflop.Year.} \)
- After post-diction of well measured quantities the goal is to predict quantities that are difficult or impossible to measure experimentally.

\[ \implies \text{progress depends crucially on access to Tier-0 machines} \]

L=2.1 fm, \( a=0.089 \text{ fm} \), K. Jansen and C. Urbach, arXiv:0905.3331
Mass of low-lying hadrons


\( N_F = 2 \) twisted mass fermions, ETM Collaboration, C. Alexandrou et al. PRD (2008)

- **BMW with** \( N_F = 2 + 1 \):
  - 3 lattice spacings: 
    \( a \sim 0.125, 0.085, 0.065 \) fm set by \( m_\Xi \)
  - Pion masses: \( m_\pi \gtrsim 190 \) MeV
  - Volumes: \( m_\pi^{\text{min}} L \gtrsim 4 \)

- **ETMC with** \( N_F = 2 \):
  - 3 lattice spacings: 
    \( a = 0.089, 0.070, a = 0.056 \) fm, set my \( m_N \)
  - \( m_\pi \gtrsim 260 \) MeV
  - Volumes: \( m_\pi^{\text{min}} L \gtrsim 3.3 \)

Good agreement between different discretization schemes

\( \Rightarrow \) Significant progress in understanding the masses of low-lying mesons ans baryons
Mass of low-lying hadrons


$N_F = 2$ twisted mass fermions, ETM Collaboration, C. Alexandrou et al. PRD (2008)

BMW with $N_F = 2 + 1$:
- 3 lattice spacings: $a \approx 0.125, 0.085, 0.065$ fm set by $m_\Xi$
- Pion masses: $m_\pi \gtrsim 190$ MeV
- Volumes: $m_\pi^{\text{min}} L \gtrsim 4$

ETMC with $N_F = 2$:
- 3 lattice spacings: $a = 0.089, 0.070, 0.056$ fm, set my $m_N$
- $m_\pi \gtrsim 260$ MeV
- Volumes: $m_\pi^{\text{min}} L \gtrsim 3.3$

Good agreement between different discretization schemes

⇒ Significant progress in understanding the masses of low-lying mesons ans baryons
Nucleon form factors

Experimental measurements of electromagnetic form factors since the 50’s but still open questions
→ high-precision experiments at JLab.

Consider the matrix of the electromagnetic current: \( j_{\mu} = \sum_f q_f \bar{\psi}^f \gamma_{\mu} \psi^f \)

\[
\langle N(\vec{p}') | j_\mu | N(\vec{p}) \rangle \sim u_N(\vec{p}') \left[ \gamma_\mu F_1(q^2) + \frac{i\sigma_{\mu\nu} q^\nu}{2m} F_2(q^2) \right] u_N(\vec{p})
\]

The Dirac \( F_1 \) and Pauli \( F_2 \) are related to the electric and magnetic Sachs form factors:

\[
G_E(q^2) = F_1(q^2) - \frac{q^2}{(2m)^2} F_2(q^2), \quad G_M(q^2) = F_1(q^2) + F_2(q^2)
\]
Nucleon form factors

Experimental measurements of electromagnetic form factors since the 50’s but still open questions → high-precision experiments at JLab.

PQCD: \( F_i(Q^2) \rightarrow \frac{1}{Q^2(i+1)} \left[ \ln \left( \frac{Q^2}{Q_0^2} \right) \right]^{-\gamma} , \ i = 1, 2. \)

Consider the matrix of the electromagnetic current: \( j_\mu = \sum_f q_f \bar{\psi}_f \gamma_\mu \psi_f \)

\[ \Rightarrow \langle N(\vec{p}') | j_\mu | N(\vec{p}) \rangle \sim u_N(\vec{p}') \left[ \gamma_\mu F_1(q^2) + \frac{i\sigma_{\mu \nu} q^\nu}{2m} F_2(q^2) \right] u_N(\vec{p}) \]

The Dirac \( F_1 \) and Pauli \( F_2 \) are related to the electric and magnetic Sachs form factors:

\[ G_E(q^2) = F_1(q^2) - \frac{q^2}{(2m)^2} F_2(q^2), \quad G_M(q^2) = F_1(q^2) + F_2(q^2) \]
Nucleon axial charge

The nucleon axial charge $g_A$ probes nucleon structure in neutron $\beta$-decay. Its value determines the rate of proton-proton fusion that enters in thermonuclear reaction chains that determine hydrogen burning in stars like the sun.

It is given by the $Q^2 = 0$ value of the nucleon matrix of the axial-vector current: $A_{\mu}^a = \bar{\psi} \gamma_{\mu} \gamma_5 \frac{\tau^a}{2} \psi(x)$

$$
\langle N(p') \mid A_{\mu}^a \mid N(p) \rangle \sim u_N(p') \left[ \gamma_{\mu} \gamma_5 G_A(q^2) + \frac{q_{\mu} \gamma_5}{2m} G_P(q^2) \right] \frac{\tau^a}{2} u_N(p) \mid_{Q^2=0} \sim g_A
$$

C. Alexandrou (Univ. of Cyprus & Cyprus Inst.)

Strong Interactions through simulations

DEISA/PRACE, Helsinki, 2011
Nucleon momentum fraction

Matrix of the one derivative vector current

\[ \mathbf{q} = \mathbf{p}' - \mathbf{p}_0 \Gamma \]

probes the momentum fraction carried by quarks

\[ \langle x \rangle_{u-d} \]

\[ m^2_{\pi} \ (\text{GeV}^2) \]

\[ \langle x \rangle_{u-d} \]
Origin of the spin of the Nucleon

Results using $N_F = 2$ TMF for $270 \text{ MeV} < m_\pi < 500 \text{ MeV}$, C. Alexandrou et al. (ETMC), arXiv:1104.1600

Total spin for u-quarks $J^u \sim 0.25$ and for d-quark $J^d \sim 0 \implies$ Where is the other half?

In qualitative agreement with J. D. Bratt et al. (LHPC), PRD82 (2010) 094502
Origin of the spin of the Nucleon

Results using $N_F = 2$ TMF for $270 \text{ MeV} < m_\pi < 500 \text{ MeV}$, C. Alexandrou et al. (ETMC), arXiv:1104.1600


Disconnected contributions neglected
\( \langle \Delta(p', s')|j^\mu(0)|\Delta(p, s) \rangle = -\bar{u}_\alpha(p', s') \left\{ \left[ F_1^*(Q^2)g^{\alpha\beta} + F_3^*(Q^2) \frac{q^\alpha q^\beta}{(2M_\Delta)^2} \right] \gamma^\mu + \left[ F_2^*(Q^2)g^{\alpha\beta} + F_4^*(Q^2) \frac{q^\alpha q^\beta}{(2M_\Delta)^2} \right] i\sigma_{\mu\nu} q^\nu \right\} u_\beta(p, s) \)

with e.g. the quadrupole form factor given by: 
\[ G_{E2} = \left( F_1^* - \tau F_2^* \right) - \frac{1}{2} (1 + \tau) \left( F_3^* - \tau F_4^* \right) \]

where \( \tau \equiv Q^2/(4M_\Delta^2) \)

Construct an optimized source to isolate \( G_{E2} \rightarrow \) additional sequential propagators needed. Neglect disconnected contributions in this evaluation.

Transverse charge density of a \( \Delta \) polarized along the x-axis can be defined in the infinite momentum frame \( \rho_{T \frac{3}{2}}^\Delta (\vec{b}) \) and \( \rho_{T \frac{1}{2}}^\Delta (\vec{b}) \).

Using \( G_{E2} \) we can predict 'shape' of \( \Delta \).

\( \Delta \) with spin 3/2 projection elongated along spin axis compared to the \( \Omega^- \)

Shape of $\rho$-meson

Four-point functions $\rightarrow |\psi|^2$

The $\rho$-meson having spin=1 is cigar-like in the lab frame, C. A. and G. Koutsou, Phys. Rev. D78 (2008) 094506
Consider $\pi^+\pi^-$ in the $I = 1$-channel.

Estimate P-wave scattering phase shift $\delta_{11}(k)$ using finite size methods.

Use Lüscher's relation between energy in a finite box and the phase in infinite volume.

Use Center of Mass frame and Moving frame.

Use effective range formula:

$$\tan \delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E\left(m_R^2 - E^2\right)}, \quad k = \sqrt{E^2/4 - m^2_{\pi}}$$

To determine $M_R$ and $g_{\rho\pi\pi}$ and then extract $\Gamma_{\rho} = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m^2_R}, \quad k_R = \sqrt{m_R^2/4 - m^2_{\pi}}$

$m_{\pi} = 309$ MeV, $L = 2.8$ fm

$N_F = 2$ twisted mass fermions, Xu Feng et al., arXiv:0910:4891
Consider $\pi^+\pi^-$ in the $l = 1$-channel.

Estimate P-wave scattering phase shift $\delta_{11}(k)$ using finite size methods.

Use Lüscher's relation between energy in a finite box and the phase in infinite volume.

Use Center of Mass frame and Moving frame.

Use effective range formula:

$$\tan\delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E(m_R^2 - E^2)}, \quad k = \sqrt{E^2/4 - m_\pi^2}$$

determine $M_R$ and $g_{\rho\pi\pi}$ and then extract $\Gamma_\rho = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m_R^2}$, $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

$m_\pi = 309$ MeV, $L = 2.8$ fm

$N_F = 2$ twisted mass fermions, Xu Feng et al., arXiv:0910:4891
Shape of Nucleon

- 1/2-spin particles have vanishing quadrupole moment in the lab-frame
- Probe nucleon shape by studying transitions to its excited $\Delta$-state
- Difficult to calculate since quadrupole amplitudes are subdominant


C. Alexandrou et al., PRL 94, 021601 (2005); PRD 83, 014501 (2011)
Nuclear forces

From the $q\bar{q}$ potential to the determination of nuclear forces

K. Schilling, G. Bali and C. Schlichter, 1995
Nuclear forces

From the $q\bar{q}$ potential to the determination of nuclear forces

K. Schilling, G. Bali and C. Schlichter, 1995

A.I. Signal, F.R.P. Bissey and D. Leinweber, arXiv:0806.0644
Nuclear forces

From the $q\bar{q}$ potential to the determination of nuclear forces

Determination of the nuclear force is essential for understanding the binding and stability of atomic nuclei, the structure of neutron stars and supernova explosions

S. Aoki et al. HAL QCD Collaboration
QCD phase diagram

Zero baryon density, phase transition extensively studied

- 1st order transition for large quark masses
- 1st order transition for small quark masses
- No transition for physical u-, d- and s- quarks
QCD phase diagram

Non-zero density action becomes complex → need new techniques
Computational resources


C. Alexandrou (Univ. of Cyprus & Cyprus Inst.)

Strong Interactions through simulations

DEISA/PRACE, Helsinki, 2011
Computational resources


- NNN interaction from LQCD
- Alpha particle

Deuteron axial-charge

Precision meson-meson interactions

- Baryon-baryon interactions
- Baryon-meson interactions

Energy

Sustained Petaflop-Years

0.01  0.1  1   10  100  1000
Ab initio structure in light nuclei

\[ ^{12}\text{C}(\alpha,\gamma)^{16}\text{O} \]
\[ ^{132}\text{Sn} \text{ structure} \]

\[ ^{8}\text{Be}(\alpha,\gamma)^{12}\text{C} \]

Sustained Petaflop-Years [0.01, 1, 10, 100, 1000]
Computational resources


- Continuum extrapolated results for EoS and $T_c$
- Universal properties of QCD at non-zero temperature

Phase transition and EoS from calculations with chiral fermions on coarse lattices

High temperature limit of the QCD EoS

Analysis of chiral properties of QCD transition using highly improved staggered fermions
Conclusions

- Large scale simulations using the underlying theory of the Strong Interactions have made spectacular progress
  - we now have simulations of the full theory at near physical parameters
- The low-lying hadron spectrum is reproduced
- Nucleon generalized form factors are being computed by a number of collaborations
- Finite temperature phase diagram of QCD established (at zero baryon density)
- Phase diagram, resonances, precise results on hadron form factors and GPDs, meson and baryon interactions are the next targets
Conclusions

- Large scale simulations using the underlying theory of the Strong Interactions have made spectacular progress
  - we now have simulations of the full theory at near physical parameters
- The low-lying hadron spectrum is reproduced
- Nucleon generalized form factors are being computed by a number of collaborations
- Finite temperature phase diagram of QCD established (at zero baryon density)
- Phase diagram, resonances, precise results on hadron form factors and GPDs, meson and baryon interactions are the next targets
Large scale simulations using the underlying theory of the Strong Interactions have made spectacular progress.

- We now have simulations of the full theory at near physical parameters.

- The low-lying hadron spectrum is reproduced.

- Nucleon generalized form factors are being computed by a number of collaborations.

- Finite temperature phase diagram of QCD established (at zero baryon density).

- Phase diagram, resonances, precise results on hadron form factors and GPDs, meson and baryon interactions are the next targets.
Conclusions

- Large scale simulations using the underlying theory of the Strong Interactions have made spectacular progress
  → we now have simulations of the full theory at near physical parameters
- The low-lying hadron spectrum is reproduced
- Nucleon generalized form factors are being computed by a number of collaborations
- Finite temperature phase diagram of QCD established (at zero baryon density)
- Phase diagram, resonances, precise results on hadron form factors and GPDs, meson and baryon interactions are the next targets
Conclusions

- Large scale simulations using the underlying theory of the Strong Interactions have made spectacular progress
  ⇒ we now have simulations of the full theory at near physical parameters
- The low-lying hadron spectrum is reproduced
- Nucleon generalized form factors are being computed by a number of collaborations
- Finite temperature phase diagram of QCD established (at zero baryon density)
- Phase diagram, resonances, precise results on hadron form factors and GPDs, meson and baryon interactions are the next targets
Thank you for your attention