The Quest for Solving QCD: Recent Advances on the Lattice

Karl Jansen

- Introduction
- Accelerating the Continuum limit: The examples of Overlap and Twisted Mass Fermions
- Dynamical Quarks: small quark masses and small lattice spacings
  - Breakthrough in Simulation Algorithm
  - Selected Results
  - Some open questions and challenges
- State of the art supercomputers
- Summary
Why Perturbation Theory fails for the Strong Interaction

- situation becomes incredibly complicated

- value of the coupling (expansion parameter)
  \[ \alpha_{\text{strong}}(1\text{fm}) \approx 1 \]

  \[ \Rightarrow \] need different ("exact") method

  \[ \Rightarrow \] has to be non-perturbative

- Wilson’s Proposal: Lattice Quantum Chromodynamics
Lattice Gauge Theory had to be invented

→ Quantum Chromo Dynamics

Asymptotic freedom

distances $\ll 1\text{fm}$

world of quarks and gluons

perturbative description

Confinement

distances $\gtrsim 1\text{fm}$

world of hadrons and glue balls

non-perturbative methods

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976
Lattice Action

\[ Z = \int_{\text{fields}} e^{-S} \]

Partition functions (pathintegral) with Boltzmann weight (action) \( S \)

\[ S = a^4 \sum_x \left\{ \beta \left[ 1 - \text{Re}(U(x,p)) \right] + \bar{\psi} \left[ m_0 + \frac{1}{2} \{ \gamma_\mu(\partial_\mu + \partial^*_\mu) - a\partial^*_\mu\partial_\mu \} \right] \psi \right\} \]

lattice derivatives

\[ \partial_\mu \Psi(x) = \frac{1}{a} [U(x, \mu)\Psi(x + \mu) - \Psi(x)] \]

\[ U_p = U(x, \mu)U(x + \mu, \nu)U^{-1}(x + \nu, \mu)U^{-1}(x, \nu) \]

\[ U(x, \mu) = e^{iaA_\mu(x)} \]
Physical Observables

expectation value of physical observables $\mathcal{O}$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\text{fields}} \mathcal{O} e^{-S}$$

↓ lattice discretization

01011100011100011110011
Monte Carlo Method

\[ \langle f(x) \rangle = \int dx f(x) e^{-x^2} \]

→ importance sampling:
   select points \( x_i, i = 1, \cdots N \) with \( x_i \) Gaussian random number

\[ \Rightarrow \langle f(x) \rangle \approx \frac{1}{N} \sum_i f(x_i) \]

Quantum Field Theory/Statistical Physics:

- sophisticated methods to generate the Boltzmann distribution \( e^{-S} \)
- \( x_i \) become field configurations
- \( \langle . \rangle \) become physical observables
There are dangerous lattice animals
Wilson’s Lattice Quantum Chromodynamics

\[ S = S_G + S_{\text{naive}} + S_{\text{wilson}} \]

\[ O(a^2) \quad O(a^2) \quad O(a) \]

lattice artefacts appear linear in \( a \)

\[\Rightarrow\] possibly large lattice artefacts

\[\Rightarrow\] need of fine lattice spacings

\[\Rightarrow\] large lattices

\( (\text{want} \ L = N \cdot a = 1 \text{fm fixed}) \)

\[\Rightarrow\] simulation costs \( \propto 1/a^{6-7} \)

present solutions:

- clover-improved Wilson fermions
- maximally twisted Wilson fermions
- staggered fermions
- overlap/domainwall fermions \( \leftrightarrow \) exact (lattice) chiral symmetry
Realizing $O(a)$-improvement

Continuum lattice QCD action $S = \bar{\Psi} \left[ m + \gamma_\mu D_\mu \right] \Psi$

an axial transformation: $\Psi \rightarrow e^{i \omega \gamma_5 \tau_3 / 2} \Psi$, $\bar{\Psi} \rightarrow \bar{\Psi} e^{i \omega \gamma_5 \tau_3 / 2}$

changes only the mass term:

$m \rightarrow m e^{i \omega \gamma_5 \tau_3} \equiv m' + i \mu \gamma_5 \tau_3$, $m = \sqrt{m'^2 + \mu^2}$, $\tan \omega = \mu / m$

→ generalized form of continuum action

• $\omega = 0$: standard QCD action

• $\omega = \pi / 2$: $S = \bar{\Psi} \left[ i \mu \gamma_5 \tau_3 + \gamma_\mu D_\mu \right] \Psi$

• general $\omega$: smooth change between both actions
Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

\[ D_{tm} = m_q + i \mu \tau_3 \gamma_5 + \frac{1}{2} \gamma_\mu \left[ \nabla_\mu + \nabla^*_\mu \right] - a \frac{1}{2} \nabla^*_\mu \nabla_\mu \]

quark mass parameter \( m_q \), twisted mass parameter \( \mu \)

difference to continuum situation:
Wilson term not invariant under axial transformations

\[ \Psi \rightarrow e^{i \omega \gamma_5 \tau_3 / 2} \Psi \quad \bar{\Psi} \rightarrow \bar{\Psi} e^{i \omega \gamma_5 \tau_3 / 2} \]

2-point function:

\[ \left[ m_q + i \gamma_\mu \sin p_\mu a + \frac{r}{a} \sum_\mu (1 - \cos p_\mu a) + i \mu \tau_3 \gamma_5 \right]^{-1} \]

\[ \propto (\sin p_\mu a)^2 + \left[ m_q + \frac{r}{a} \sum_\mu (1 - \cos p_\mu a) \right]^2 + \mu^2 \]

\[ \lim_{a \rightarrow 0} : \quad p^2_\mu + m^2_q + \mu^2 + am_q \sum_{\mu} p_\mu \]

\( O(a) \)

- setting \( m_q = 0 \) (\( \omega = \pi/2 \)) : no \( O(a) \) lattice artefacts

- quark mass is realized by twisted mass term alone
O(a) improvement

Symanzik expansion

$$\langle \mathcal{O} \rangle |_{(m_q,r)} = [\xi(r) + a m_q \eta(r)] \langle \mathcal{O} \rangle |_{m_q}^{\text{cont}} + a \chi(r) \langle \mathcal{O}_1 \rangle |_{m_q}^{\text{cont}}$$

$$\langle \mathcal{O} \rangle |_{(-m_q,-r)} = [\xi(-r) - a m_q \eta(-r)] \langle \mathcal{O} \rangle |_{-m_q}^{\text{cont}} + a \chi(-r) \langle \mathcal{O}_1 \rangle |_{-m_q}^{\text{cont}}$$

Using symmetry: $R_5 \times (r \rightarrow -r) \times (m_q \rightarrow -m_q)$, $R_5 = e^{i \omega \gamma_5 \tau^3}$

- **mass average:**
  $$\frac{1}{2} \left[ \langle \mathcal{O} \rangle |_{m_q,r} + \langle \mathcal{O} \rangle |_{-m_q,r} \right] = \langle \mathcal{O} \rangle |_{m_q}^{\text{cont}} + O(a^2)$$

- **Wilson average:**
  $$\frac{1}{2} \left[ \langle \mathcal{O} \rangle |_{m_q,r} + \langle \mathcal{O} \rangle |_{m_q,-r} \right] = \langle \mathcal{O} \rangle |_{m_q}^{\text{cont}} + O(a^2)$$

- **automatic O(a) improvement**
  → special case of mass average: $m_q = 0$

  $$\Rightarrow \langle \mathcal{O} \rangle |_{m_q=0,r} = \langle \mathcal{O} \rangle |_{m_q}^{\text{cont}} + O(a^2)$$
A demonstration in the free theory
(K. Cichy, J. Gonzales Lopez, A. Kujawa, A. Shindler, K.J.)

free fields: imagine study system for $L[\text{fm}] < \infty$

$\Rightarrow L = N \cdot a \quad \rightarrow a \rightarrow 0 \leftrightarrow N \rightarrow \infty$

Wilson fermions at $m_q = 0.5$

twisted mass at $m_q = 0.0$, $\mu_q = 0.5$

$N \cdot m_\pi$ versus $1/N = a$

$N \cdot m_\pi$ versus $1/N^2 = a^2$
Overlap fermions: exact lattice chiral symmetry

starting point: **Ginsparg-Wilson relation**

\[
\gamma_5 D + D \gamma_5 = 2a D \gamma_5 D \quad \Rightarrow \quad D^{-1} \gamma_5 + \gamma_5 D^{-1} = 2a \gamma_5
\]

Ginsparg-Wilson relation implies an **exact lattice chiral symmetry** (Lüscher):

for any operator \( D \) which satisfies the Ginsparg-Wilson relation, the action

\[ S = \bar{\psi} D \psi \]

is invariant under the transformations

\[
\delta \psi = \gamma_5 (1 - \frac{1}{2} a D) \psi , \quad \delta \bar{\psi} = \bar{\psi} (1 - \frac{1}{2} a D) \gamma_5
\]

\[ \Rightarrow \text{almost continuum like behaviour of fermions} \]

one **local** (Hernández, Lüscher, K.J.) solution: overlap operator \( D_{ov} \) (Neuberger)

\[
D_{ov} = \left[ 1 - A (A^\dagger A)^{-1/2} \right]
\]

with \( A = 1 + s - D_w (m_q = 0) \); \( s \) a tunable parameter, \( 0 < s < 1 \)
The “No free lunch theorem”
A cost comparison
T. Chiarappa, K.J., K. Nagai, M. Papinutto, L. Scorzato,
A. Shindler, C. Urbach, U. Wenger, I. Wetzorke

<table>
<thead>
<tr>
<th>$V, m_\pi$</th>
<th>Overlap</th>
<th>Wilson TM</th>
<th>rel. factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>$12^4, 720\text{MeV}$</td>
<td>48.8(6)</td>
<td>2.6(1)</td>
<td>18.8</td>
</tr>
<tr>
<td>$12^4, 390\text{MeV}$</td>
<td>142(2)</td>
<td>4.0(1)</td>
<td>35.4</td>
</tr>
<tr>
<td>$16^4, 720\text{MeV}$</td>
<td>225(2)</td>
<td>9.0(2)</td>
<td>25.0</td>
</tr>
<tr>
<td>$16^4, 390\text{MeV}$</td>
<td>653(6)</td>
<td>17.5(6)</td>
<td>37.3</td>
</tr>
<tr>
<td>$16^4, 230\text{MeV}$</td>
<td>1949(22)</td>
<td>22.1(8)</td>
<td>88.6</td>
</tr>
</tbody>
</table>

*timings in seconds on Jump*

- nevertheless chiral symmetric lattice fermions can be advantageous
  - e.g., Kaon Physics, $B_K, K \to \pi\pi$
  - $\epsilon$-regime of chiral perturbation theory
  - topology
  - use in valence sector
Why are fermions so expensive?

– need to evaluate

\[ Z = \int D\bar{\psi} D\psi e^{-\bar{\psi}\{D_{\text{Dirac}}\}\psi} \propto \text{det}[D_{\text{Dirac}}] \]

– bosonic representation of determinant

\[ \text{det}[D_{\text{Dirac}}] \propto \int D\Phi^\dagger D\Phi e^{-\Phi^\dagger\{D_{\text{lattice}}^{-1}\}\Phi} \]

– need vector \( X = D_{\text{lattice}}^{-1} \Phi \)

– solve linear equation \( D_{\text{lattice}} X = \Phi \)

\( D_{\text{lattice}} \) matrix of dimension \( 1\text{million} \otimes 1\text{million} \) (however, sparse)

– number of such “inversions”: \( O(100) \) for one field configuration

– want: \( O(1000 - 10000) \) such field configurations
Cost of fermions

- Situation: $a = 0.1\text{fm}$, $M_\pi \approx 350\text{MeV}$

- orginal Hybrid Monte Carlo Algorithm

- application of $D_{\text{Dirac lattice}}$ on one lattice site: 1400flops

- $16^4$ lattice: 270Gigaflops

- 1500 CG iterations, 200 steps: 54Teraflops

- 5000 configurations: 270 Petaflops

- $32^3 \cdot 64$ lattice: 8500Petaflops
Costs of dynamical fermions simulations, the “Berlin Wall”

see panel discussion in Lattice2001, Berlin, 2001

formula \(C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}\)

\(z_\pi = 6, \quad z_L = 5, \quad z_a = 7\)

“both a \(10^8\) increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place.”

(Wilson, 1989)

⇒ need of Exaflops Computers

physical contact to \(\chi\)PT (?)
Quenched approximation
CP-PACS collaboration, 2000

Solution of QCD?

→ a number of systematic errors
A generic improvement for Wilson type fermions

New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps

- comparable to staggered
- reach small pseudo scalar masses \( \approx 300\text{MeV} \)
$N_f = 2$ dynamical flavours
A computation of $F_\pi$ in 2002 and now for up and down quarks ($N_f = 2$)

**2002**

![Graph 1](#)

**2006**

![Graph 2](#)
Simulation landscape

ETMC $N_f = 2$
QCDSF $N_f = 2$
CERN-ToV $N_f = 2$
CLS $N_f = 2$
JLQCD $N_f = 2$
JLQCD $N_f = 2 + 1$
PACS-CS $N_f = 2 + 1$
RBC-UKQCD $N_f = 2 + 1$
MILC $N_f = 2 + 1$
JLQCD (2001) $N_f = 2$

$m_{PS}$ [MeV]

$0.15$
$0.10$
$0.05$
$0.00$
$0.00$
$100$ $200$ $300$ $400$ $500$ $600$

$a[fm]$
European Twisted Mass Collaboration

- Cyprus (Nicosia)
- France (Orsay, Grenoble)
- Italy (Rome I, II, III, Trento)
- Netherlands (Groningen)
- Poland (Poznan)
- Spain (Valencia)
- Switzerland (Zurich)
- United Kingdom (Glasgow, Liverpool)
- Germany (Berlin, Zeuthen, Hamburg, Münster)
European Twisted Mass Collaboration
Fits to chiral perturbation theory formulae

⇒ excellent description by chiral perturbation theory

\[ 2aB_0 = 4.99(6), \quad aF = 0.0534(6) \]

\[ a^2l_3^2 \equiv \log(a^2\Lambda_3^2) = -1.93(10), \quad a^2l_4^2 \equiv \log(a^2\Lambda_4^2) = -1.06(4) \]
Comparison to other determinations

● ETMC:
  \[ \bar{\ell}_3 = 3.65 \pm 0.12 \]
  \[ \bar{\ell}_4 = 4.52 \pm 0.06 \]

● Other estimates Leutwyler, hep-ph/0612112

phenomenological determinations
  \[ \bar{\ell}_3 = 2.9 \pm 2.4 \text{ from the mass spectrum of the pseudoscalar octet} \]
  \[ \bar{\ell}_4 = 4.4 \pm 0.2 \text{ from the radius of the scalar} \]

other lattice determinations
  \[ \bar{\ell}_3 = 0.8 \pm 2.3 \text{ from MILC (US-UK, staggered)} \]
  \[ \bar{\ell}_3 = 3.0 \pm 0.6 \text{ from lattice CERN group (Wilson)} \]
  \[ \bar{\ell}_4 = 4.3 \pm 0.9 \text{ from } f_K/f_\pi \text{ pion form factor} \]
  \[ \bar{\ell}_4 = 4.0 \pm 0.6 \text{ from MILC} \]
Narrowing scattering lengths (Leutwyler, private communication)

- Lattice calculations: only statistical errors
  → systematic effects under systematic investigation

- scalar pion radius (ETMC): $< r^2 > = 0.637(26)\text{fm}^2$

Colangelo, Gasser, Leutwyler: $< r^2 > = 0.61(4)\text{fm}^2$

- s-wave scattering lengths:
  $a_{00} = 0.220 \pm 0.002, \quad a_{20} = -0.0449 \pm 0.0003$
Lattice QCD and experiment

$\pi, K, 3M_\Xi - M_N, 2M_{Bs} - M_\Upsilon, \psi(1P - 1S), \Upsilon(1D - 1S), \Upsilon(2P - 1S), \Upsilon(3S - 1S), \Upsilon(1P - 1S)$

LQCD/Exp't ($n_f = 0$)

LQCD/Exp't ($n_f = 3$)

- systematic error from taking fourth root?
- non-local lattice action for $a > 0$

UKQCD, HPQCD
MILC
Collaborations, 2004
The Baryon spectrum, $N_f = 2 + 1$

- Question of extrapolation to physical point
- E.g. $\rho$ and $\Delta$ are resonances
- Need second calculation and check at physical point

Budapest
Marseille
Wuppertal
Collaboration, 2008
The Baryon spectrum towards the physical point from PACS-CS

\[ N_f = 2 + 1 \]

100 configs
\( a = 0.1 \text{fm} \)
\( L = 3 \text{fm} \)

\( \kappa_u = 0.13770 \)
\( \kappa_d = 0.13781 \)

\( N_f = 2 + 1 \)
100 configs
\( a = 0.1 \text{fm} \)
\( L = 3 \text{fm} \)

so far: only one value of the lattice spacing

published July, 2008
Pion form factor (Lubicz, Simula, ETMC)

\[ F_\pi(q^2) = 1 + sq^2 + cq^4 + O(q^6) \, , \, s = r^2/6 \, , \, c = s^2 \]

\[ \langle r^2 \rangle_{\text{NLO}} = -\frac{2}{F^2} \left( 6l_6 + L(\mu) + \frac{1}{(4\pi)^2} \right) \]

\[ c_{\text{NLO}} = \frac{32\pi^2}{60F^4x_2} \]

\[ x_2 = 2Bm/F^2 \, , \, L(\mu) = 16\pi^2\log \left( 2Bm/\mu^2 \right) \]
• perfect match with experiment
$f_{D_s}$ a compilation (ETMC)

- tension with experiment weakened but remains
Simulations at fixed topology and exact chiral symmetry

JLQCD

modified gauge action, add:

\[ \frac{\det(D_W^{2}(-m_0))}{\det(D_W^{2}(-m_0)+\mu^2)} \]

- study of topological finite size effects
- ergodicity of simulation
The $\eta'$ Mass

(Michael, Urbach, K.J., ETMC)

- mysterious particle
- quark content: mass similar to pion
- $m_{\eta} \approx 150\text{MeV}$
- find: $m_{\eta} \approx 865\text{MeV}$
- explanation: additional mass of
- purely topological origin
Importance of non-perturbative renormalization

• strange quark mass \((\text{tm-example, arXiv:0709.4574})\)

\[
Z_{\text{RI-MOM}}^{\mathcal{P}}(1/a) = 0.39(1)(2) \quad \text{← non-perturbative RI-MOM method}
\]

\[
Z_{\text{BPT}}^{\mathcal{P}}(1/a) \simeq 0.57(5) \quad \text{← one-loop boosted perturbation theory}
\]

<table>
<thead>
<tr>
<th>(m_{\overline{\text{MS}}}^q(2\text{GeV})\text{MeV})</th>
<th>perturbative</th>
<th>non-perturbative</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_s)</td>
<td>72 ± 2 ± 9</td>
<td>105 ± 3 ± 9</td>
</tr>
<tr>
<td>(m_s) (PACS-CS)</td>
<td>72.7 ± 0.8</td>
<td></td>
</tr>
</tbody>
</table>

• RI-MOM and Schrödinger functional schemes
  UK expertise Dublin (Sint), Liverpool (Shindler)
Strange quark mass

N_f=2

N_f=2+1

CP-PACS 01
(W-Clov, a-->0, PT)

JLQCD 02
(W-Clov, a=0.09 fm, PT)

ALPHA 05
(W-Clov, a=0.07 fm, SF)

SPQcdR 05
(Wilson, a=0.06 fm, RI-MOM)

QCDSF-UKQCD 04-06
(W-Clov, a-->0, RI-MOM)

RBC 07
(DWF, a=0.12 fm, RI-MOM)

ETMC 07
(TM, a=0.09 fm, RI-MOM)

HPQCD-MILC-UKQCD 04-06
(KS, a-->0, PT)

CP-PACS-JLQCD 07
(W-Clov, a-->0, PT)

PDG 06 Average
(Lattice only)

m_s (2 GeV) [MeV]
A comparison to experiment
Universality

no ideal fermion action:

- $O(a)$-improved Wilson fermions: breaking of chiral symmetry, non-perturbative operator improvement;

- rooted staggered fermions: taste breaking, non-local lattice action;

- twisted mass fermions: breaking of chiral symmetry, isospin breaking;

- overlap fermion: expense of simulation;

- domain wall fermions: expense of simulation and breaking of chirality;

- fixed topology: topological finite size effects
Demonstrating universality

Example of the Schwinger model
(N. Christian, K. Nagai, B. Pollakowski, K.J.)

- $m_{\text{quark}}\sqrt{\beta}$ fixed
- observe $a^2$ scaling
- universality of continuum limit
- $\approx 10\%$ scaling violation

\begin{align*}
1 & \quad 1.0 \quad 0.8 \quad 0.6 \quad 0.4 \quad 0.2 \quad 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \quad \frac{1}{\beta} \\
0.74 & \quad 0.76 & \quad 0.78 & \quad 0.80 & \quad 0.82 & \quad 0.84 & \quad 0.86 & \quad 0.88 \\
0 & \quad \frac{1}{\beta} = a^2
\end{align*}
Universality: a challenge for lattice QCD

- nucleon mass
- nice scaling
- pseudo scalar decay constant
- no common scaling visible
More challenges: glueball spectrum, $\chi$PT at the strange quark

quenched glueball spectrum
Morningstar and Peardon

chiral perturbation theory
JLQCD collaboration
$N_f = 2 + 1 + 1$ flavours

$N_f = 2 + 1 + 1$
Kaon and Nucleon mass (ETMC)

\[ (a m_{\pi})^2 \]

\[ (a m_K)^2 \]

\[ M_K \]

\[ M_{\text{nucleon}} \]

→ no effect of strange quark
State of the art supercomputers

- **BG/P**

Blue Gene/P system structure

- **Node Card**
  - 32 chips 4x4x2
  - 32 compute, 0-1 IO cards
  - 435 GF/s, 64 GB

- **System**
  - 72 Racks, 72x32x32
  - 1 PF/s, 144 TB

- **Rack**
  - 32 Node Cards
  - Cabled 8x8x16
  - 13.9 TF/s, 2 TB

- **Chip**
  - 4 processors
  - 13.6 GF/s

- **Compute Card**
  - 1 chip
  - 13.6 GF/s
  - 2.0 GB DDR2
  - (4.0GB optional)
State of the art supercomputers

- **QPACE**
  - based on cell processor
  - 3-d torus network
  - low power consumption 1.5W/Gflop

- **Videocards (NVIDIA G80)**
  - CUDA programming language (C extension)
Selection of Supercomputers

- MareNostrum, IBM, Barcelona
  40 Teraflops peak performance

- Earth Simulator, NEC, Yokohama, 2002
  40 Teraflops peak performance

- BlueGeneP, NIC, FZ-Jülich
  223 Teraflops peak performance

- BlueGeneL, IBM, Los Alamos,
  367 Teraflops peak performance, Nov. 2007
  (application area: not specified)

- IBM, Roadrunner, LANL,
  1.2 Petaflops peak performance, Top 1

- 2005 Workshop on Zetaflop Computing

remark: often only part of the machines available for basic science, often poor efficiency
Summary

- Progress in solving QCD with lattice techniques
  - $O(a)$-improved fermion actions
  - dramatic algorithm improvements
  - new supercomputer architectures
- offers possibility to
  - reach continuum limit
  - perform chiral limit
  - control finite volume effects
    - have computed the baryon spectrum
    - have determined low energy constants
    - decay constants
- challenges
  - understand better systematic effects
  - glueball spectrum, $\chi$PT at the kaon and heavy baryons
  - resonances, scattering processes
  - simulations at physical point