Dynamical Simulations and Flavour Singlets

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Motivation

Lattice QCD is a (the) non-perturbative method
for *ab-initio* computations of

- hadron spectrum
- meson decay constants
- chiral condensate $\langle \bar{q} q \rangle$
- string breaking
- ...

and therefore fundamental for testing QCD as the theory for strong interactions

The Goal: Precision Lattice QCD Results

- For given parameters lattice calculations are exact (up to statistical errors)...
- ... but we need to control the systematic artifacts:
  - lattice artifacts $\Rightarrow$ continuum limit, lattice spacing $a \to 0$,
  - finite size effects $\Rightarrow$ thermodynamic limit, physical volume $L^3 \to \infty$,
  - chiral effects $\Rightarrow$ chiral limit, $m_{\mathrm{PS}} \to m_\pi$,

$\Rightarrow$ subtle interplay of limits

- We need

$$\begin{aligned} a &< 0.1\,\mathrm{fm}, \\ L &> 2\,\mathrm{fm}, \\ m_{\mathrm{PS}} &< 300\,\mathrm{MeV}. \end{aligned}$$

and non-perturbative renormalisation

Outline

Introduction
Lattice Regularisation
$\mathcal{O}(a)$ Improvement

Results
Flavour Singlets

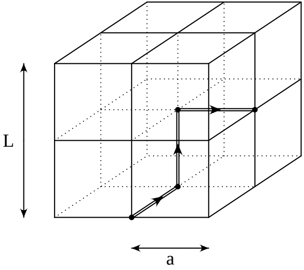
QCD on the Lattice

Quantum Chromodynamics is formally described by the Lagrange density:

$$\mathcal{L}_{\mathrm{QCD}} = \bar{\psi}(i\not{D} - m_q)\psi - \frac{1}{4}G_{\mu\nu}G^{\mu\nu}$$

Lattice regularisation: discretise Euclidean space-time

- hyper-cubic $L^3 \times T$-lattice with lattice spacing a
- derivatives $\Rightarrow$ finite differences
- integrals $\Rightarrow$ sums
- gauge potentials A_μ in $G_{\mu\nu}$ $\Rightarrow$ link matrices U_μ (' ')



Wilson Formulation

Wilson Dirac Operator

$$D_{\mathrm{W}}[U] + m_0 = \frac{1}{2}\sum_{\mu}\left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) \qquad\qquad \right] + m_0$$

- with the covariant difference operators:

$$\nabla_\mu\psi(x) = \frac{1}{a}\left[U(x,\mu)\psi(x + a\hat{\mu}) - \psi(x)\right]$$
$$\nabla^*_\mu\psi(x) = \frac{1}{a}\left[\psi(x) - U(x,-\mu)\psi(x - a\hat{\mu})\right]$$

- suffers from a fermion doubling problem.

Wilson Formulation

Wilson Dirac Operator

$$D_{\mathrm{W}}[U] + m_0 = \frac{1}{2}\sum_{\mu}\left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] + m_0$$

- Wilson Term $-a\nabla^*_\mu\nabla_\mu$
  - solves the fermion doubling problem,
- but:
  - chiral symmetry is explicitly broken, $\{D_{\mathrm{W}}, \gamma_5\} \neq 0$,
  - therefore m_0 renormalises additively (and multiplicatively)

$$m_q = m_0 - m_{\mathrm{crit}} \ ,$$

  - leading lattice artifacts are $\mathcal{O}(a)$,
  - unphysically small eigenvalues of $D_{\mathrm{W}}[U] + m_0$.

Why is it so expensive?

- we need to compute:

$$\mathcal{Z}_{\mathrm{QCD}} = \int \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, e^{-\bar{\psi}(\gamma_\mu D_\mu + m_0)\psi} \propto \det(\gamma_\mu D_\mu + m_0)$$

- determinant can be represented by bosonic fields:

$$\det(\gamma_\mu D_\mu + m_0) \propto \int \mathcal{D}\phi^\dagger\, \mathcal{D}\phi\, e^{-\phi^\dagger(\gamma_\mu D_\mu + m_0)^{-1}\phi}$$

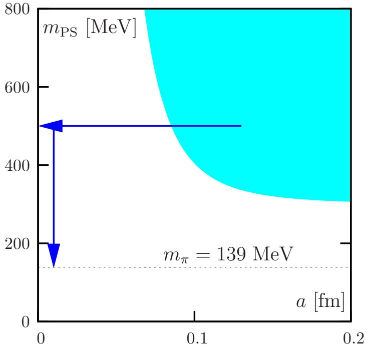
- solving

$$\varphi = (\gamma_\mu D_\mu + m_0)^{-1}\phi$$

  for φ becomes very expensive for small quark mass and large lattice extent L/a.

Continuum and Chiral Extrapolation

Cost of a simulation $\propto (m_{\mathrm{PS}})^{-6} L^5 a^{-7}$ [Ukawa, 2001]



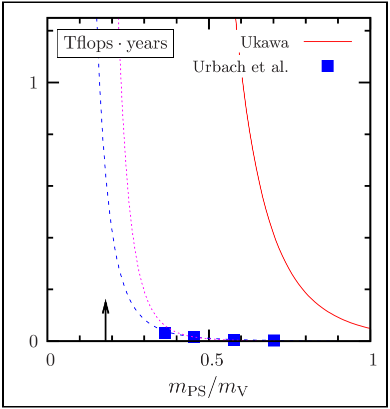
- continuum extrapolation.: remove leading lattice artifacts! ($\mathcal{O}(a)$ improvement)
- extrapolation. to m_π: $\Rightarrow$ chiral perturbation theory $m_{\mathrm{PS}} \lesssim 300$ MeV necessary!

$\Rightarrow$ Use bigger computers . . .

. . . and better algorithms!

Algorithmic Improvements

Cost for 1000 independent configurations, $a = 0.08$ fm,
Wilson fermions

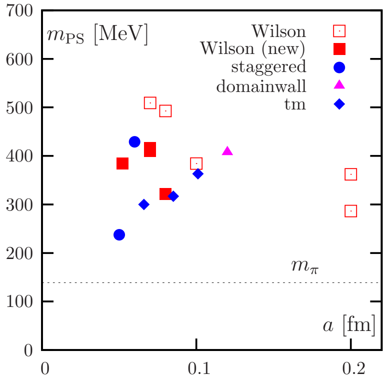


- much faster than standard HMC
- scales better in m_{PS}/m_V
- similar developments by other groups

  [Lüscher; QCDSF; Peardon et al.; Clark, Kennedy]

Simulation Landscape

- Wilson/Wilson twisted mass and staggered:
  - $a < 0.1$ fm
  - $m_{\text{PS}} \sim 250$ MeV
  - $L > 2$ fm
- domainwall and overlap
  - much more expensive
  - results for $a \sim 0.11$ fm available
  - (almost) exact chiral symmetry



Why not going to the physical point

Use formula [Del Debbio et al., 2006] for Wilson fermions as rough estimate for 1000 independent configurations:

$$0.3 \frac{20\mathrm{MeV}}{m_q} \left(\frac{L}{3\mathrm{fm}}\right)^5 \left(\frac{0.1\mathrm{fm}}{a}\right)^6$$

- $m_q^{\overline{\mathrm{MS}}}(\mu = 2\ \mathrm{GeV}) = 4\ \mathrm{MeV}$, $L = 3\ \mathrm{fm}$, $a = 0.1\ \mathrm{fm}$:

$$1.5\ \mathrm{TFlops} \cdot \mathrm{years}$$

- $m_q^{\overline{\mathrm{MS}}}(\mu = 2\ \mathrm{GeV}) = 4\ \mathrm{MeV}$, $L = 4.8\ \mathrm{fm}$, $a = 0.1\ \mathrm{fm}$:

$$15.8\ \mathrm{TFlops} \cdot \mathrm{years}$$

- $m_q^{\overline{\mathrm{MS}}}(\mu = 2\ \mathrm{GeV}) = 4\ \mathrm{MeV}$, $L = 4.8\ \mathrm{fm}$, $a = 0.05\ \mathrm{fm}$:

$$1006\ \mathrm{TFlops} \cdot \mathrm{years}$$

Further improvements needed: deflation!?

Outline

$\mathcal{O}(a)$ Improvement

- can be obtained in different ways, e.g.
- Symanzik improvement programme
  - add suitable counter-term to lattice action (clover term)
  - operator specific improvement coefficients needed (many)
- formulations with exact chiral symmetry on the lattice are $\mathcal{O}(a)$ improved, but costly (overlap, domainwall)
- or use maximally twisted mass formulation...

Twisted Mass Fermions

- Consider the continuum 2-flavour fermionic action

  [Frezzotti, Grassi, Sint, Weisz, '99]

$$S_F = \int d^4x\ \bar{\psi}\ [D + m_q + i\mu\gamma_5\tau_3]\ \psi$$

  with
  - twisted mass parameter μ
  - τ_3 third Pauli matrix acting in flavour space

- S_F is form invariant under a change of variables with angle ω:

$$\psi \to e^{i\omega\gamma_5\tau_3/2}\psi, \qquad \bar{\psi} \to \bar{\psi}e^{i\omega\gamma_5\tau_3/2}.$$

Wilson Twisted Mass Fermions

Wilson Twisted Mass Dirac operator [Frezzotti, Grassi, Sint, Weisz, '99]

$$D_{\mathrm{tm}} = \frac{1}{2}\sum_{\mu}\left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu\right] + m_0 + i\mu\gamma_5\tau_3$$

- spectrum of $(\gamma_5 D_{\mathrm{tm}})(\gamma_5 D_{\mathrm{tm}})^\dagger$ bounded from below
- when $m_0 = m_{\mathrm{crit}}$ (maximal twist)
  physical observables are $\mathcal{O}(a)$ improved

  [Frezzotti, Rossi, 2003]

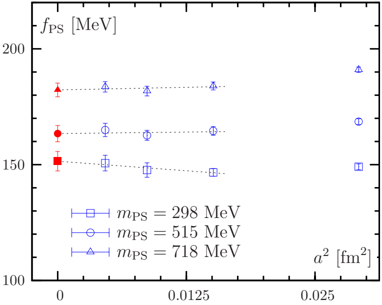
  (proof basically by Parity symmetry of continuum action in Symanzik expansion)

Drawback:

- flavour symmetry explicitly broken

$\mathcal{O}(a)$ Improvement at Maximal Twist

- shown to work in practise
  in the quenched approximation
  [Jansen et al., 2004, 2005]
  [Abdel-Rehim et al., 2004, 2005]
- twisted mass μ relates directly
  to physical quark mass
  only multiplicative renormalisation



- only one parameter $m_0 \to m_{\mathrm{crit}}$ must be tuned
  no additional operator improvement!
- many mixings under renormalisation are simplified
- flavour symmetry breaking appears at $\mathcal{O}(a^2)$
  in practise only important for neutral pion mass $\to$ see later!

Tuning to Maximal Twist

- Choose a Parity odd operator O
- tune m_0 such that O has vanishing expectation value for each lattice spacing at fixed physical situation e.g. $\mu_{\mathrm{ref}} = r_0 Z_\mu \mu$ fixed

$\Rightarrow$ this guarantees $\mathcal{O}(a)$ improvement,

- possible choice:

$$m_{\mathrm{PCAC}} \equiv \frac{\langle \partial_0 A_0^a(x) P^a(y) \rangle}{2\langle P^a(x) P^a(y) \rangle}\Big|_{\mu=\mu_{\mathrm{ref}}} = 0 \quad a = 1, 2$$

- optimal choice: $\mu_{\mathrm{ref}} \longrightarrow 0$ [Frezzotti et al., 2005; Aoki, Bär, 2005; Sharpe, Wu, 2005]
- Our choice: $\mu_{\mathrm{ref}} \approx \mu_{\mathrm{min}}$

Outline

European Twisted Mass Collaboration

Members from all over Europe:
Cyprus, France, Germany, Great Britain, Italy, Spain, Switzerland

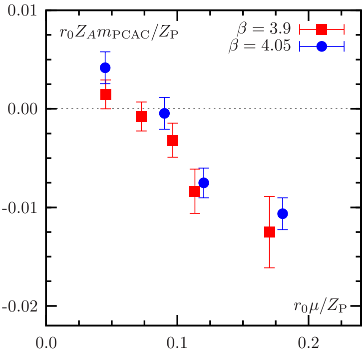
C. Alexandrou, O. Bär, R. Baron, B. Blossier,
Ph. Boucaud, M. Brinet, J. Carbonell,
T. Chiarappa, P. Dimopoulos, V. Drach,
F. Farchioni, R. Frezzotti, V. Gimenez, I. Hailperin,
G. Herdoiza, K. Jansen, J. Gonzalez Lopez,
T. Korzec, G. Koutsou, Z. Liu, V. Lubicz,
G. Martinelli, C. McNeile, C. Michael, I. Montvay,
G. Münster, A. Nube, D. Palao, M. Papinutto,
O. Pène, J. Pickavance, C. Richards, G.C. Rossi,
S. Schäfer, L. Scorzato, A. Shindler, S. Simula,
T. Sudmann, C. Tarantino, C. Urbach, A. Vladikas,
M. Wagner, U. Wenger

Set-up

- $n_f = 2$ mass-degenerate Wilson quarks at maximal twist
- Gauge action: tree level Symanzik improved [Weisz, 1983]
- three lattice spacings:
  - coarse: $\beta = 3.80$, $a \sim 0.10\ \mathrm{fm}$
    still preliminary and under analysis
  - intermediate: $\beta = 3.9$, $a \sim 0.09\ \mathrm{fm}$
  - fine: $\beta = 4.05$, $a \sim 0.07\ \mathrm{fm}$
- values for m_{PS} range from 300 to 600 MeV
- ≥ 5000 equilibrated trajectories ($\tau = 1/2$) per ensemble
  1500 equilibration trajectories

Tuning to Maximal Twist $\beta = 3.9$ and $\beta = 4.05$

Tuning to full twist was possible with modest computer resources!



- needed to be done on the target lattice volume
- at $\beta = 3.9$ and $\beta = 4.05$ the PCAC mass is zero at reference point
- we see deviations for the other μ-values (as expected)
- μ-dependence is a $\mathcal{O}(a)$ cut-off effect modifying the $\mathcal{O}(a^2)$ artifacts in physical observables.

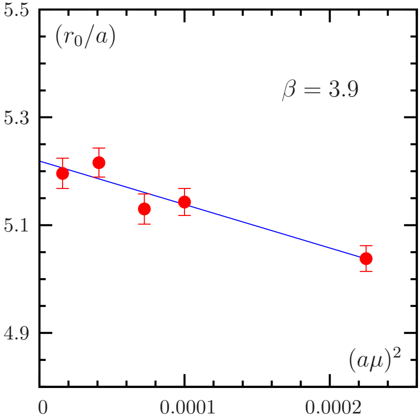
Setting the Scale

- Lattice spacing a is the only dimensionful quantity in the game,
- so the translation to physical units needs some input, e.g. a meson mass, decay constant, etc.
- One possibility is the Sommer parameter r_0, defined via the force between two static quarks [Sommer '94]

$$r^2 F(r)|_{r=r(c)} = c\,, \quad r_0 = r(1.65)$$

- r_0/a can be measured with high accuracy
- $r_0 \approx 0.5\mathrm{fm}$ is only known approximately.

Sommer Parameter r_0



- statistical accuracy of less than 0.5%,
- compatible with μ^2 dependence (but also with a linear one)
- μ-dependence is rather weak unlike Wilson / Wilson clover

$\Rightarrow$ at $\mu \to 0$:
$\beta = 3.8$: $r_0/a = 4.46(3)$
$\beta = 3.9$: $r_0/a = 5.22(2)$
$\beta = 4.05$: $r_0/a = 6.61(3)$

Sommer Parameter Compared

Group	n_f	Method	r_0 fm
Sommer	-	quark model	0.49^{+0}_{-5}
Morningstar/Peardon	0	quenched sum.	0.48(2)
UKQCD	2	K/K*	0.55
JLQCD	2	m_ρ	0.497 (-9)(13)
JLQCD	0	m_ρ	0.5702(75)(50)
QCDSF	2	m_{N}	0.47(3)
QCDSF	2	$\frac{f_\pi}{g_A}$	0.45(1)
ETMC	2	f_π	0.454(7)
HPQCD/MILC/FNAL	2+1	Upsilon & ratio plot	0.469(7)

Taken from C. McNeile, Lat07 plenary talk

Pion Sector: m_{PS} and f_{PS}

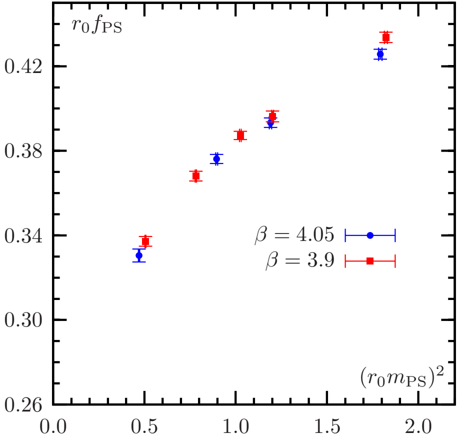
- m_{PS} from exponential decay
  of appropriate correlation functions
- f_{PS} can be extracted at maximal twist from

$$f_{\mathrm{PS}} = \frac{2\mu}{m_{\mathrm{PS}}^2} |\langle 0 | P^1(0) | \pi \rangle|$$

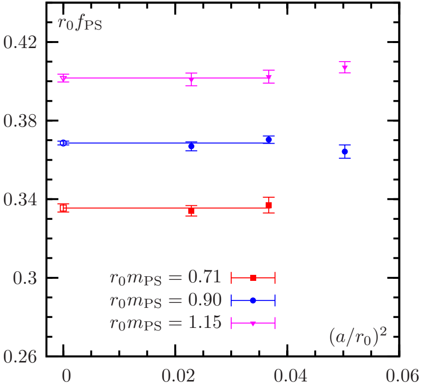
  [Frezzotti, Grassi, Sint, Weisz]
  due to an exact lattice Ward identity
- no renormalisation factor needed!
  - since $Z_\mu = 1/Z_P$
  - similar to overlap fermions (exact chiral symmetry)
  - unlike pure Wilson

$r_0 f_{\mathrm{PS}}$ as a Function of $(r_0 m_{\mathrm{PS}})^2$ in Finite Volume

- lattice artifacts seem to be small
- high statistical accuracy
- no renormalisation needed



Continuum Extrapolation f_{PS} in Finite Volume



- finite volume $L/r_0 \sim 5.0$
- linear interpolation to reference points
  $r_0 m_{\mathrm{PS}} = \mathrm{const}$
- constant extrapolation $a \to 0$
  $\beta = 3.8$ not included

$\Rightarrow$ Only small lattice artifacts!

Comparing f_{PS}

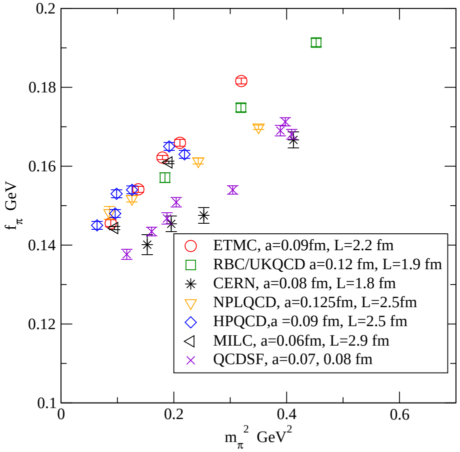
- data finite size corrected

  [Colangelo, Dürr, Haefeli, 2005]

- Caution: results need to agree only in the continuum

- Thanks to C. McNeile for this plot

- scale set by $r_0 = 0.469$ from HPQCD/MILC



Outline

Flavour Singlet Pseudo-Scalar Mesons

- η' acquires mass through QCD vacuum structure and anomaly: not a Goldstone boson
- $2+1$ flavours of quarks:
  mixing between light and strange interpolating operators

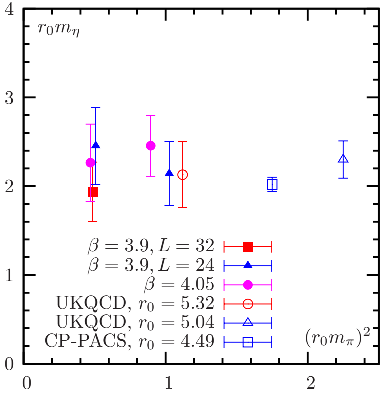
$$\eta \approx 0.58(\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) - 0.57\bar{s}\gamma_5 s$$

$$\eta' \approx 0.40(\bar{u}\gamma_5 u + \bar{d}\gamma_5 d) + 0.82\bar{s}\gamma_5 s$$

- 2 flavours of quarks:
  only one singlet state (η_2) which is related to the “real world” $\eta'(958)$
- η_2 should have mass around 800 MeV [McNeile, Michael, 2000]

Flavour Singlet Pseudo-Scalar Meson η_2

Comparison of results for η_2 with $a < 0.1$ rm and $r_0/a > 4.5$



- consistent
  with constant behaviour
  in the chiral limit
- $m_{\eta_2} \approx 880$ MeV
- this is important:
  linked to topological charge
  fluctuations

Flavour Singlet Mesons with $2 + 1$ Flavours

- Preliminary results from CP-PACS/JLQCD, [Aoki et al., 2006]
- $a \sim 0.12\ \mathrm{fm}$, Wilson clover action, $m_{\mathrm{PS}}/m_{\mathrm{V}} > 0.6$
- masses:

$$m_\eta = 0.545(16)\ \mathrm{GeV}\,, \qquad m_{\eta'} = 0.871(46)\ \mathrm{GeV}$$

- compare to experiment:

$$m_\eta = 0.548\ \mathrm{GeV}\,, \qquad m_{\eta'} = 0.958\ \mathrm{GeV}$$

Flavour Singlets: a Challenge

Why are the errors for m_{η_2} so large?

- we have around 900 measurements
- disconnected contributions needed:
  but errors for those are small
- only a small fraction of the configurations
  contributes 26% of the signal

$\Rightarrow$ much larger statistics needed!

- same phenomenon observed
  for staggered formulation [McNeile et al.]

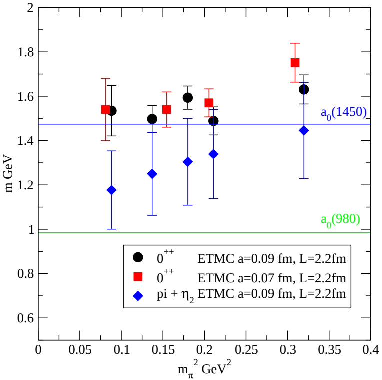
Flavour Singlet Scalar Meson

- hard to allocate experimental f_0 spectrum to specific content
rich spectrum with large uncertainties
- many states can contribute
also two body states in an S-wave ($\pi\pi$, $\bar{K}K$)
- we have preliminary results from mtmQCD
- in mtmQCD π^0 is the lightest state in the channel
- we have a clear signal for the the next state
but at the mass of two pions

$\Rightarrow$ emphasises the difficulty of studying scalar mesons:
light two body state will dominate the correlators

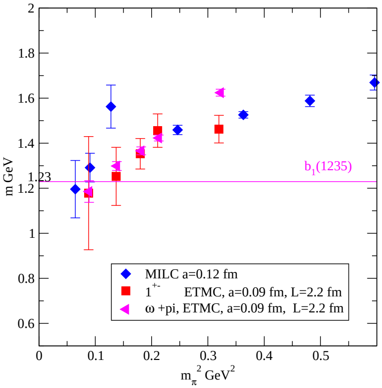
a_0 (0^{++}) Meson

- lightest state consistent with $a_0(1450)$
- only small lattice artifacts
- almost no mass dependence
- $\pi + \eta_2$ decay threshold included large errors



b_1 (1^{+-}) Meson

- b_1 dominantly decays to $\omega\pi$
- evidence for the decay $b_1 \to \omega\pi$?
- error bars still too large to be conclusive



Adding the strange in the sea... and a bit more

- with twisted mass $n_f = 2 + 1 + 1$ flavours are possible
  [Frezzotti, Rossi, 2003]
  flavour non-diagonal split-doublet for strange and charm quark
- determinant always positive [Frezzotti, Rossi, priv. comm.]
- $\mathcal{O}(a)$ improvement at maximal twist
- algorithms are ready [Montvay, Scholz, 2005; Chiarappa, Frezzotti, C.U., 2005]
- exploratory studies have been performed
  [Chiarappa, C.U., et al., 2006]
  - tuning possible
  - computational overhead about 20%
- jobs are in the queue...

Conclusion

- lattice QCD has entered a new regime of simulations
  - light pseudo-scalar masses
  - reasonably large volumes
  - results from many formulations become available
- maximally twisted mass QCD provides a sound setup
  - $\mathcal{O}(a)$ improvement works very well
  - contact to χPT with $300\ \mathrm{MeV} \lesssim m_{\mathrm{PS}} \lesssim 500\ \mathrm{MeV}$
    $a \lesssim 0.1\ \mathrm{fm}$ needed (see talk by Gregorio)
  - non-perturbative renormalisation important
  - ready to start with $2+1+1$ flavours of quarks
- preliminary results for flavour singlet states
  - encouraging, but we need to improve