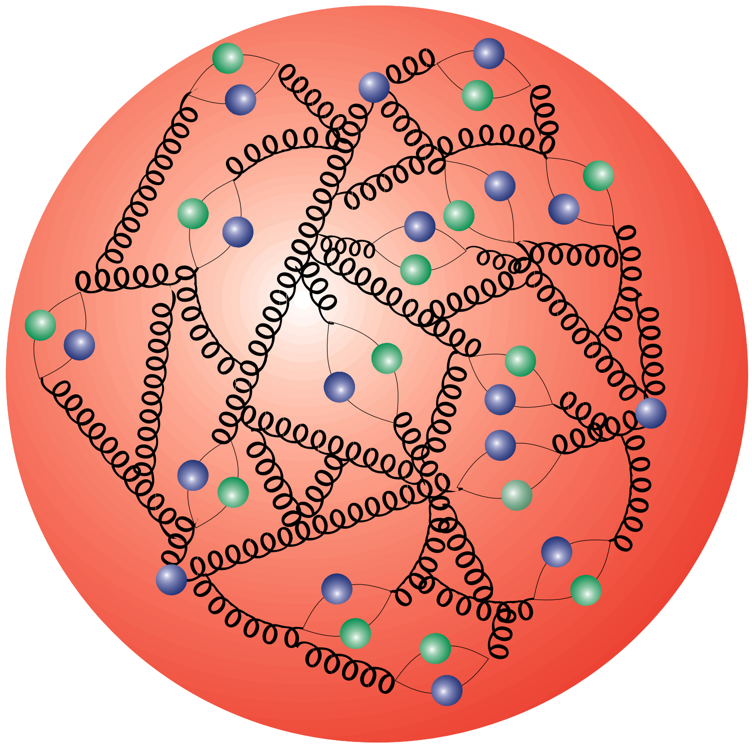
The Quest for Solving QCD: Recent Advances on the Lattice

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

$\rightarrow$ QuantumChromoDynamics

asymptotic freedom		confinement
distances $\ll 1\mathrm{fm}$		distances $\gtrsim 1\mathrm{fm}$
world of quarks and gluons		world of hadrons and glue balls
perturbative description		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.

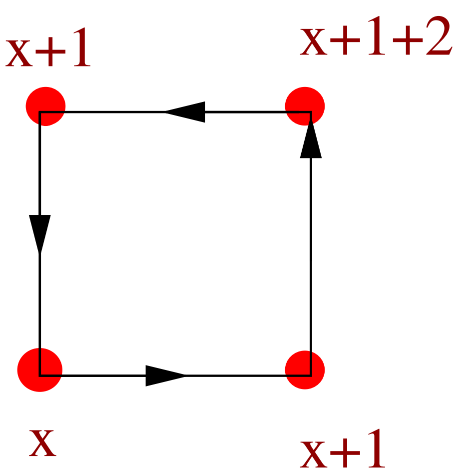
Wilson, Cargese Lecture notes 1976

Lattice Action

$$\mathcal{Z} = \int_{\text{fields}} e^{-S}$$

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

$$S = a^4 \sum_x \left\{ \beta \left[1 - \mathrm{Re}(U_{(x,p)}) \right] + \bar{\psi} \left[m_0 + \tfrac{1}{2} \{ \gamma_\mu (\partial_\mu + \partial_\mu^\star) - a \partial_\mu^\star \partial_\mu \} \right] \psi \right\}$$



lattice derivatives

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

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

$$U(x,\mu) = e^{iaA_\mu(x)}$$

Physical Observables

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

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

$\downarrow$ lattice discretization

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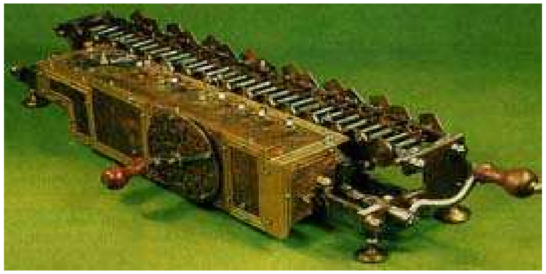
$\downarrow$



Monte Carlo Method

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

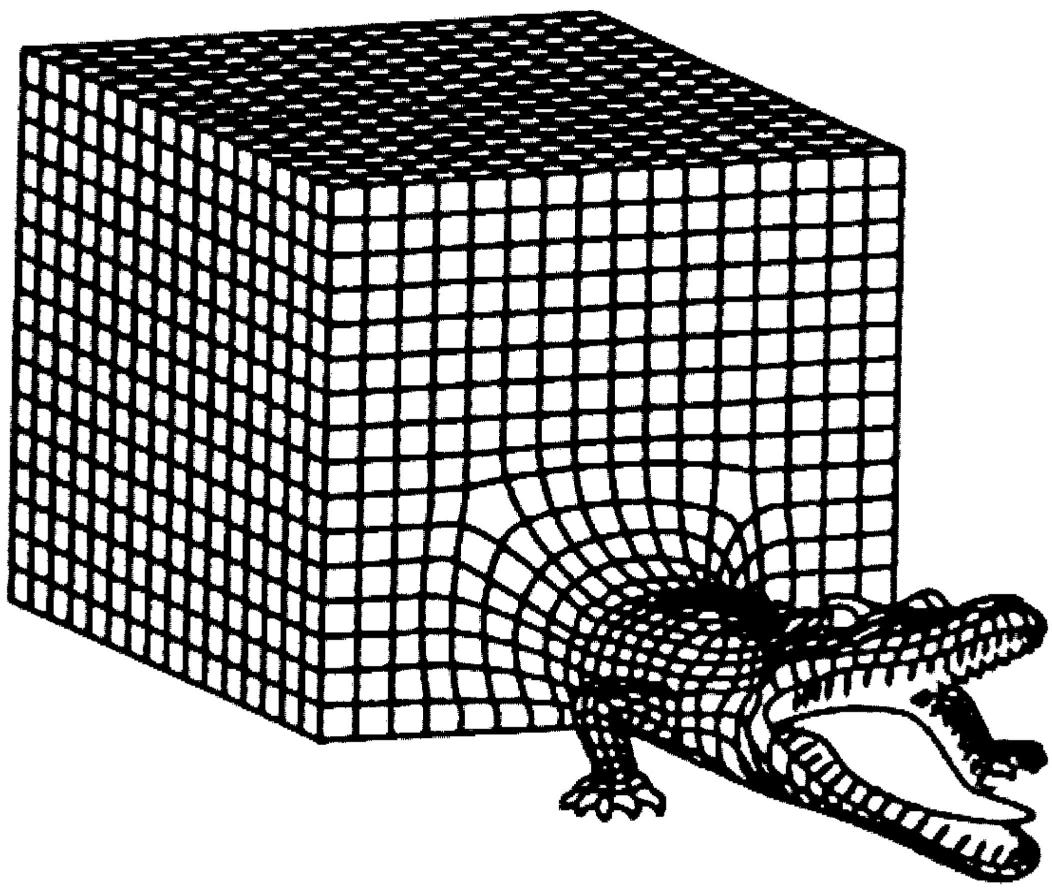
$\rightarrow$ importance sampling:
select points $x_i, i = 1, \cdots N$ with x_i Gaussian random number

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

Quantum Field Theory/Statistical Physics:

- sophisticated methods to generate the Boltzmann distribution e^{-S}
- x_i become *field configurations*
- $\langle . \rangle$ become physical observables

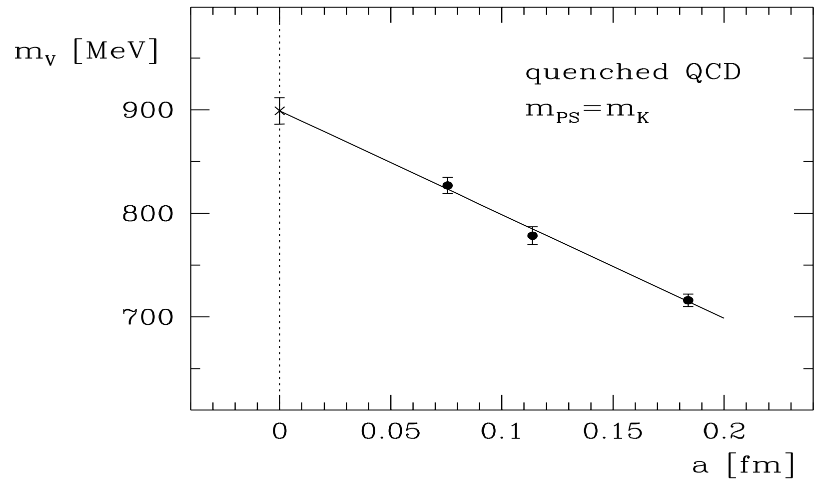
There are dangerous lattice animals



Wilson's Lattice Quantum Chromodynamics

$$S = \underbrace{S_{\mathrm{G}}}_{\mathrm{O}(a^2)} + \underbrace{S_{\mathrm{naive}}}_{\mathrm{O}(a^2)} + \underbrace{S_{\mathrm{wilson}}}_{\mathrm{O}(a)}$$

lattice artefacts appear linear in a



$\longrightarrow$ possibly large lattice artefacts
$\Rightarrow$ need of fine lattice spacings
$\Rightarrow$ large lattices
(want $L = N \cdot a = 1\mathrm{fm}$ fixed)
$\longrightarrow$ simulation costs $\propto 1/a^{6-7}$

present solutions:

- clover-improved Wilson fermions
- maximally twisted Wilson fermions
- staggered fermions
- overlap/domainwall fermions $\longleftarrow$ exact (lattice) chiral symmetry

Realizing $\mathrm{O}(a)$-improvement

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

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

changes only the mass term:

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

$\longrightarrow$ 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 ω : smooth change between both actions

Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

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

quark mass parameter m_q , twisted mass parameter μ

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

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

$$\lim_{a\rightarrow 0}: \quad p_\mu^2 + m_q^2 + \mu^2 + \underbrace{am_q\sum_\mu p_\mu}_{{\rm O}(a)}$$

- setting $m_q = 0$ $(\omega = \pi/2)$: no ${\rm O}(a)$ lattice artefacts
- quark mass is realized by twisted mass term alone

O(a) improvement

Symanzik expansion

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

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

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

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

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

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

$$\Rightarrow \langle \mathcal{O} \rangle|_{m_q=0,r} = \langle \mathcal{O} \rangle|^{\mathrm{cont}}_{m_q} + O(a^2\ )$$

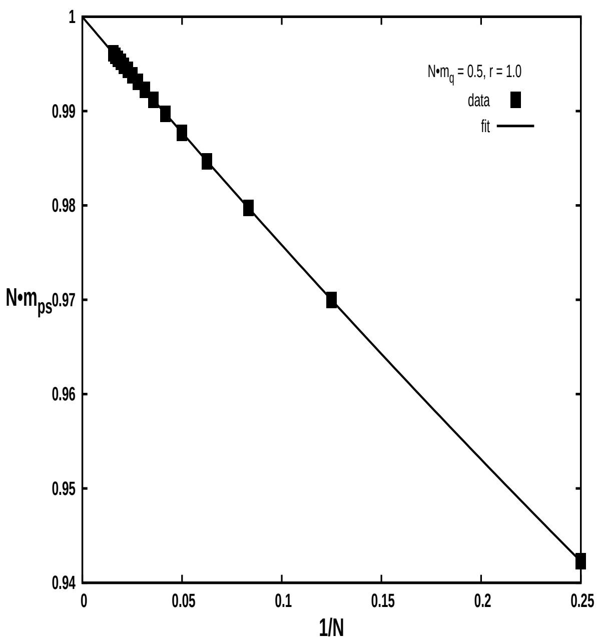
A demonstration in the free theory

(K. Cichy, J. Gonzales Lopez, A. Kujawa, A. Shindler, K.J.)

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

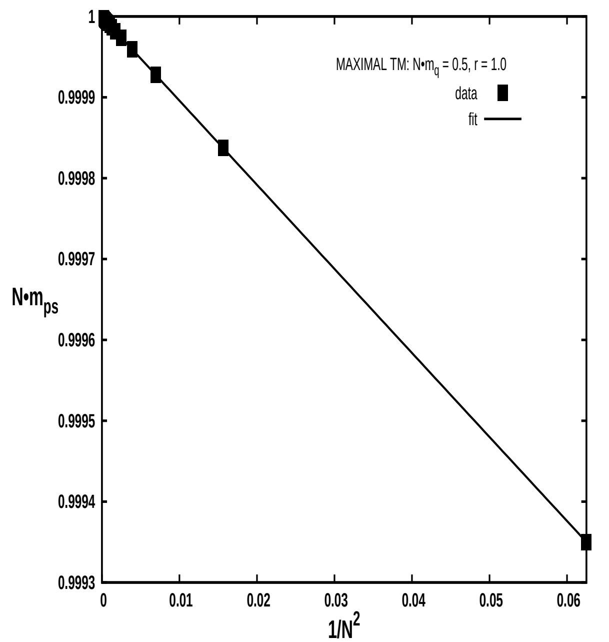
$\Rightarrow \quad L = N \cdot a \quad \rightarrow a \rightarrow 0 \leftrightarrow N \rightarrow \infty$

Wilson fermions at $m_q = 0.5$



$N \cdot m_\pi$ versus $\mathbf{1/N = a}$

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



$N \cdot m_\pi$ versus $\mathbf{1/N^2 = a^2}$

Overlap fermions: exact lattice chiral symmetry

starting point: **Ginsparg-Wilson relation**

$$\boxed{\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D} \qquad \Rightarrow D^{-1}\gamma_5 + \gamma_5 D^{-1} = 2a\gamma_5$$

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

$$\boxed{\delta\psi = \gamma_5(1 - \tfrac{1}{2}aD)\psi \;, \qquad \delta\bar{\psi} = \bar{\psi}(1 - \tfrac{1}{2}aD)\gamma_5}$$

$\Rightarrow$ almost continuum like behaviour of fermions

one <u>local</u> (Hernández, Lüscher, K.J.) solution: overlap operator $D_{\rm ov}$ (Neuberger)

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

with $A = 1 + s - D_{\rm w}(m_q = 0)$; 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

V, m_π	Overlap	Wilson TM	rel. factor
$12^4, 720$Mev	48.8(6)	2.6(1)	18.8
$12^4, 390$Mev	142(2)	4.0(1)	35.4
$16^4, 720$Mev	225(2)	9.0(2)	25.0
$16^4, 390$Mev	653(6)	17.5(6)	37.3
$16^4, 230$Mev	1949(22)	22.1(8)	88.6

timings in seconds on Jump

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

Why are fermions so expensive?

- need to evaluate

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}\{D_{\rm lattice}^{\rm Dirac}\}\psi} \propto \det[D_{\rm lattice}^{\rm Dirac}]$$

- bosonic representation of determinant

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

- need vector $X = D_{\rm lattice}^{-1}\Phi$

- solve linear equation $D_{\rm lattice}X = \Phi$

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

- number of such "inversions": $O(100)$ for one field configuration

- want: $O(1000 - 10000)$ such field configurations

Cost of fermions

- Situation: $a = 0.1$fm, $M_\pi \approx 350$MeV
- orginal Hybrid Monte Carlo Algorithm
  Duane, Kennedy, Pendleton, Rowet, Phys.Lett.B195:216-222,1987

– application of $D^{\mathrm{Dirac}}_{\mathrm{lattice}}$ on one lattice site: **1400flops**

– 16^4 lattice: **270Gigaflops**

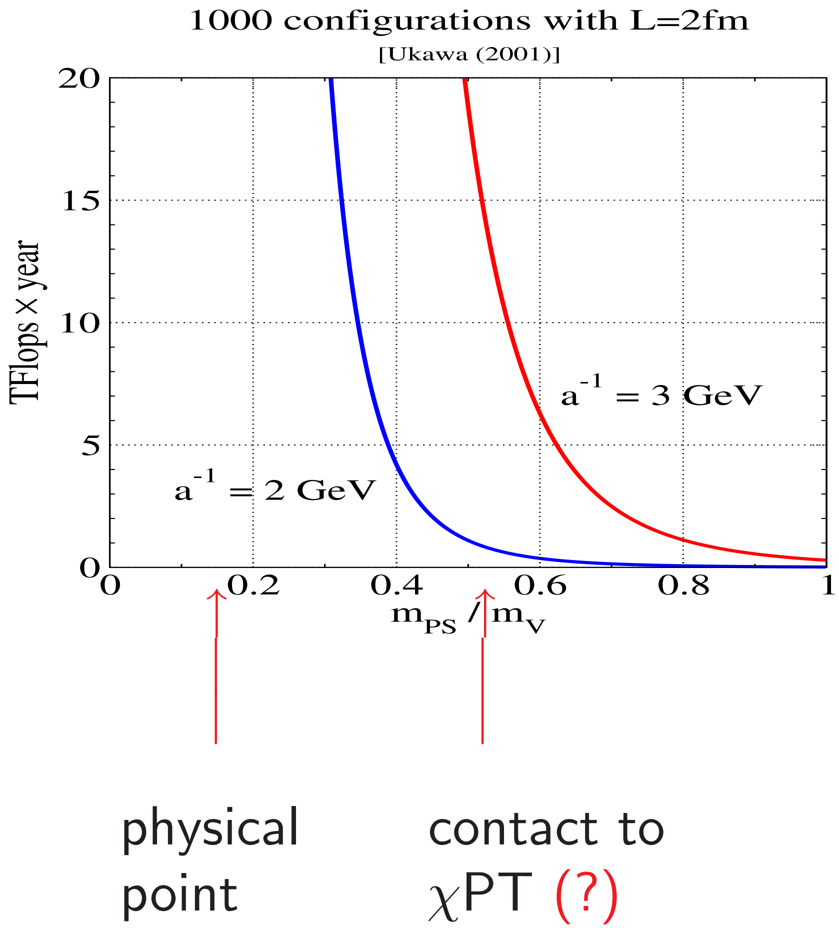
– 1500 CG iterations, 200 steps: **54Teraflops**

– 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



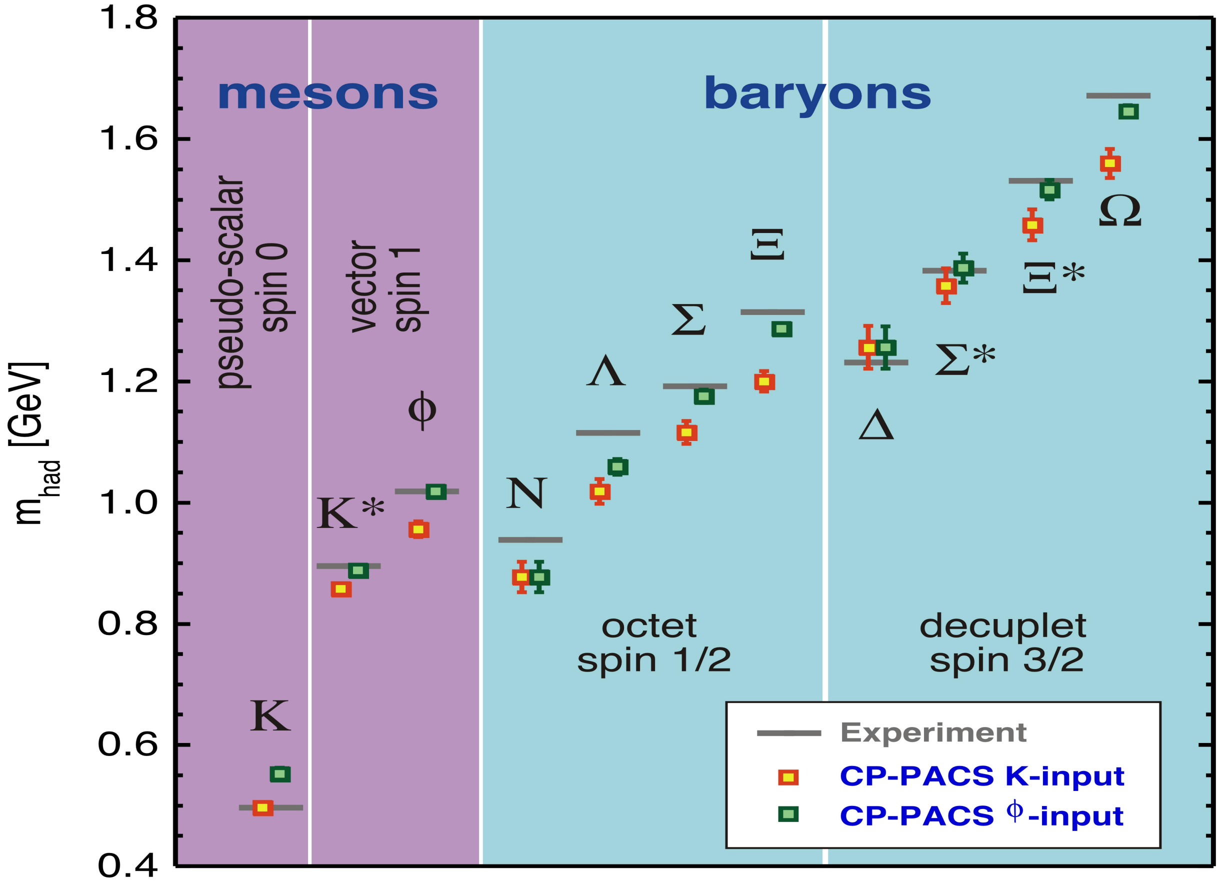
formula $C \propto \left(\frac{m_\pi}{m_\rho}\right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$

$$z_\pi = 6, \;\; z_L = 5, \;\; z_a = 7$$

"both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place."
(Wilson, 1989)

$\Rightarrow$ need of **Exaflops Computers**

Quenched approximation



CP-PACS collaboration, 2000

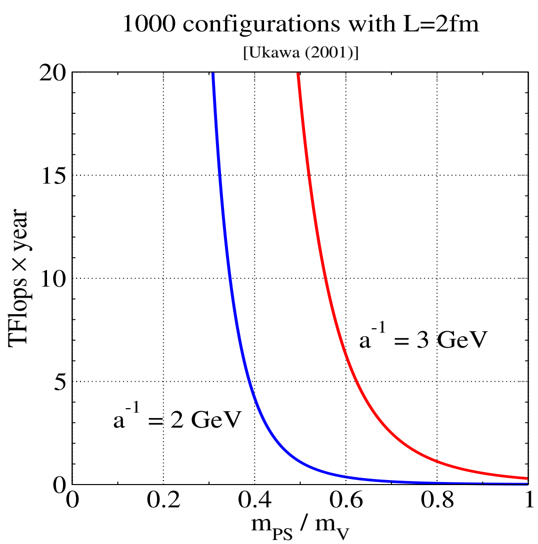
Solution of QCD?

→ a number of systematic errors

A generic improvement for Wilson type fermions

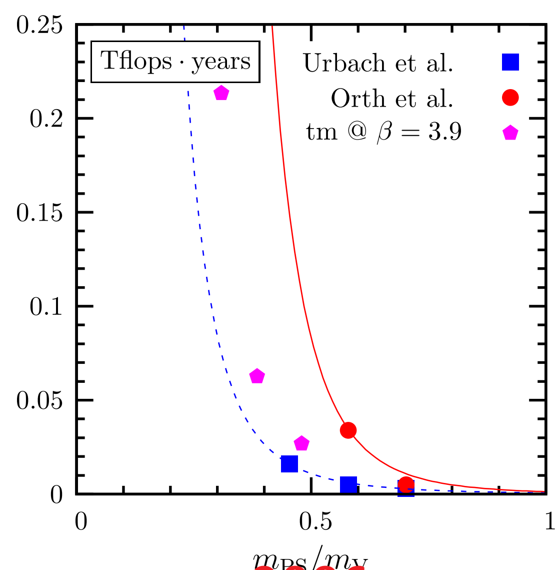
New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

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



2001

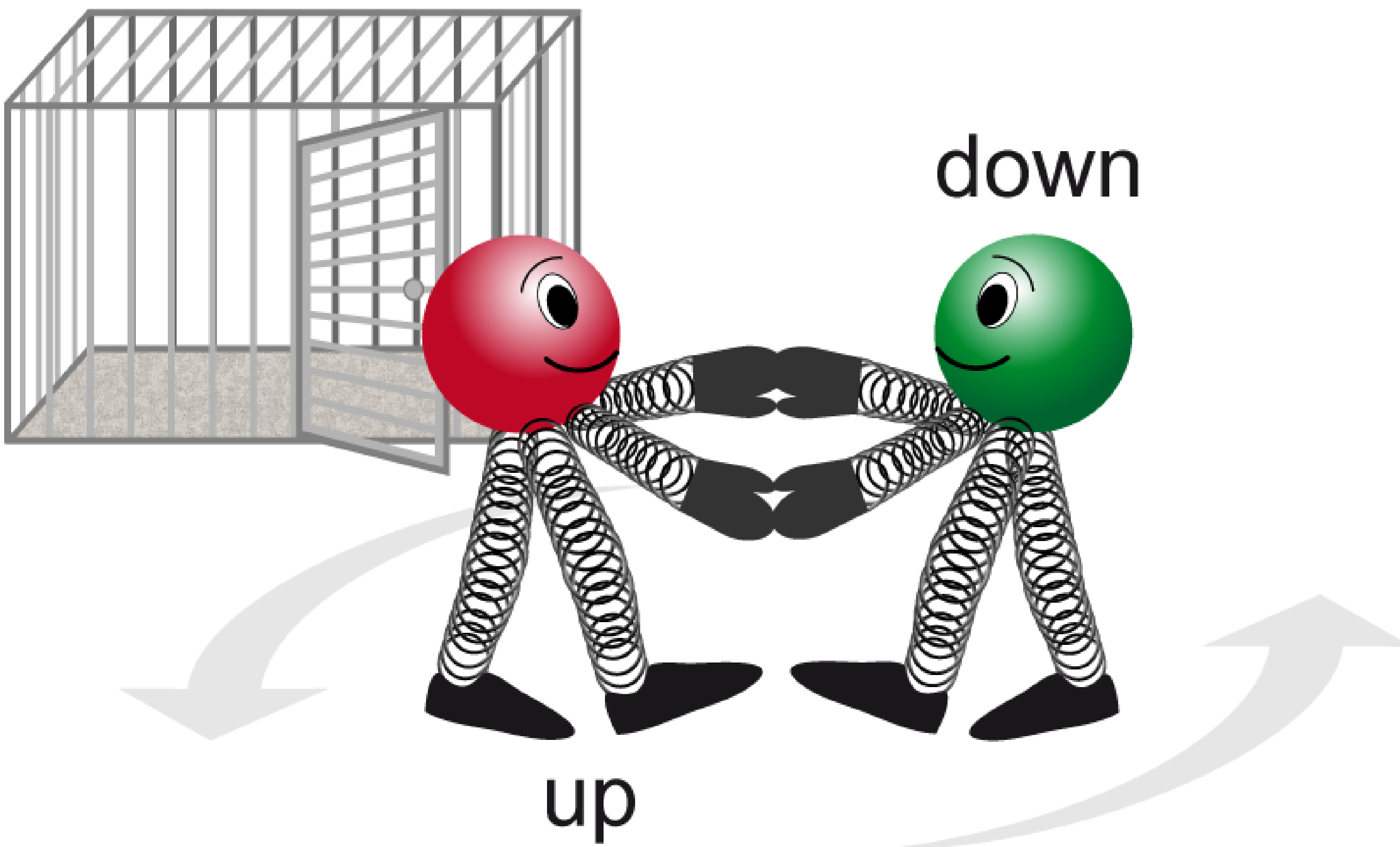
⟶



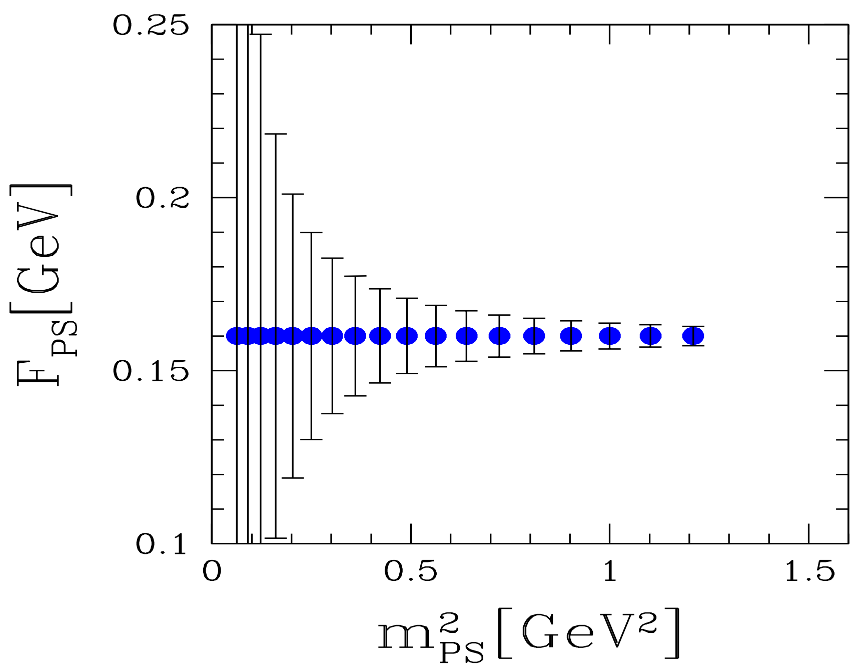
2006

– comparable to staggered
– reach small pseudo scalar masses ≈ 300MeV

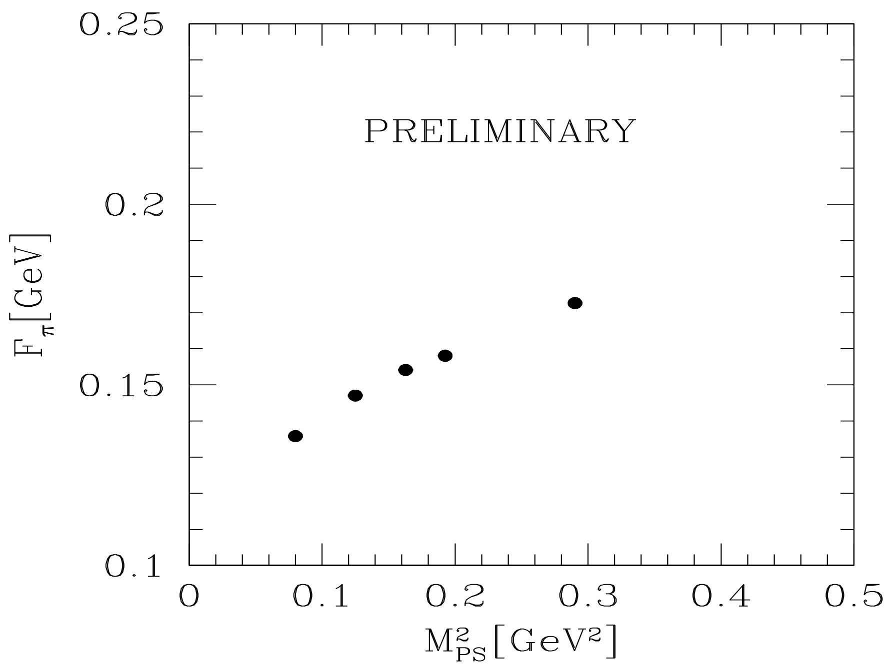
$N_f = 2$ **dynamical flavours**



A computation of F_π in 2002 and now
for up and down quarks ($N_f = 2$)

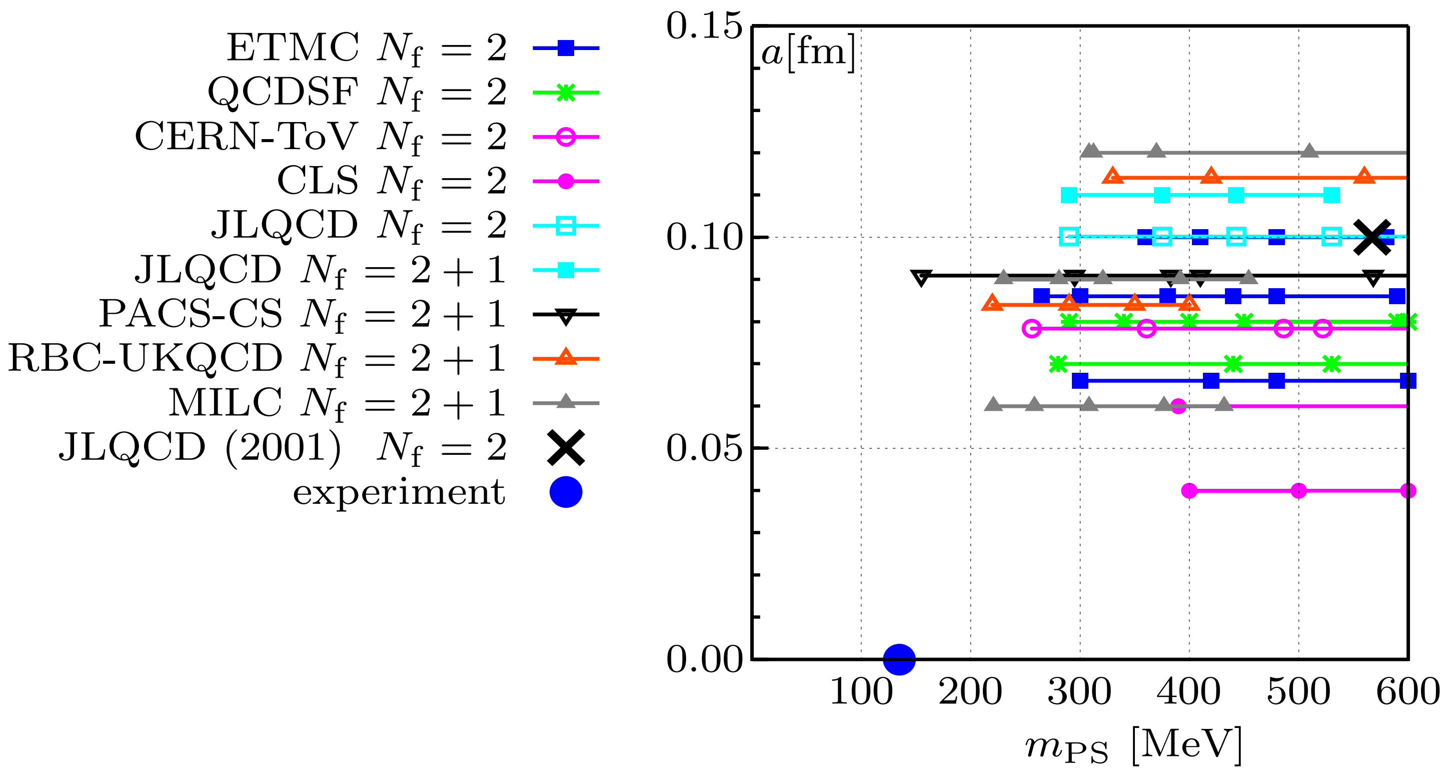


2002



2006

Simulation landscape

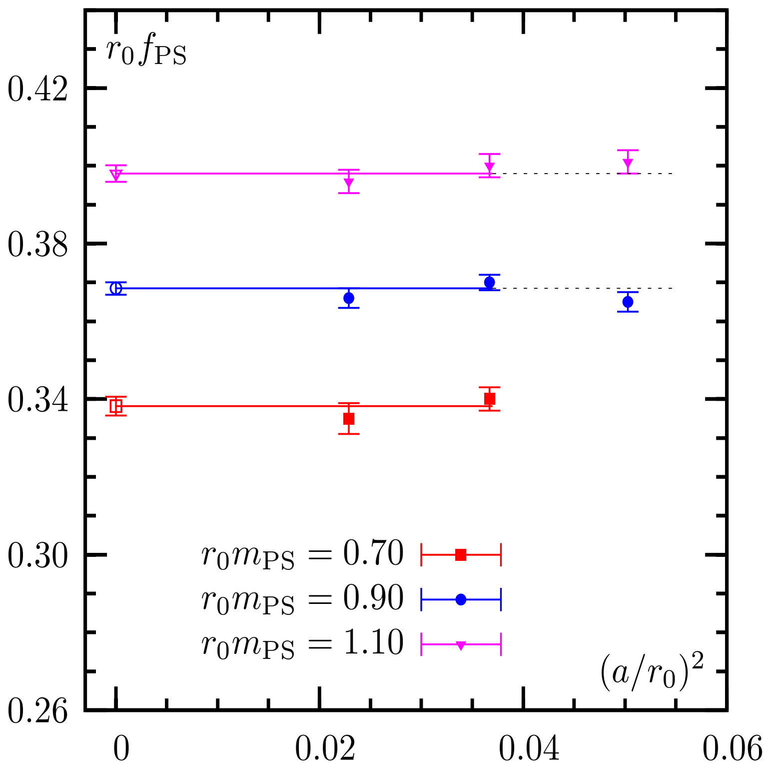


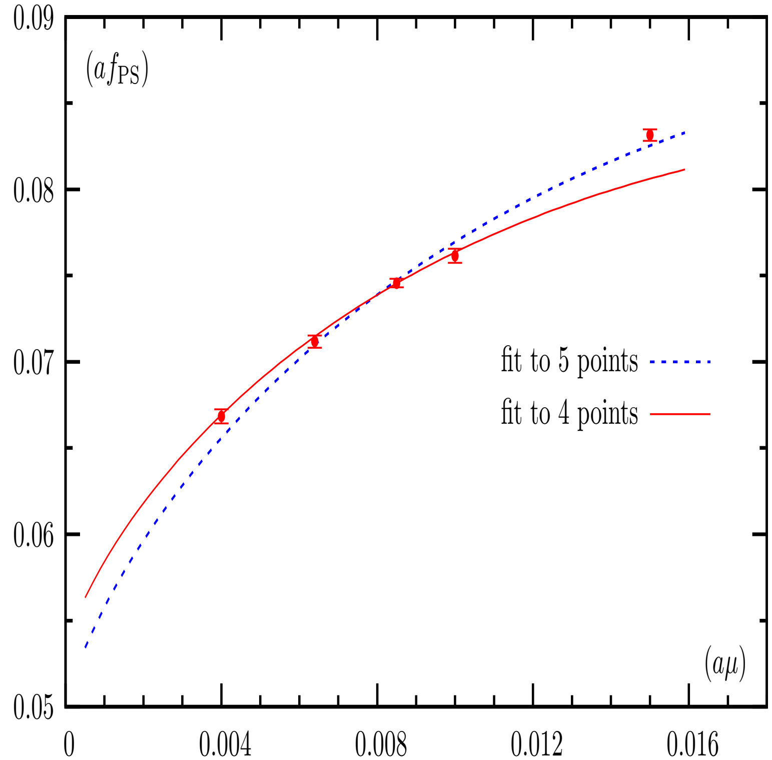
European Twisted Mass Collaboration

- 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





$\Rightarrow$ excellent description by chiral perturbation theory

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

$a^2\bar{l}_3^{\,2} \equiv \log(a^2\Lambda_3^2) = -1.93(10), \quad a^2\bar{l}_4^{\,2} \equiv \log(a^2\Lambda_4^2) = -1.06(4)$

Comparison to other determinations

- ETMC:
  $\bar{l}_3 = 3.65 \pm 0.12$
  $\bar{l}_4 = 4.52 \pm 0.06$

- Other estimates Leutwyler, hep-ph/0612112

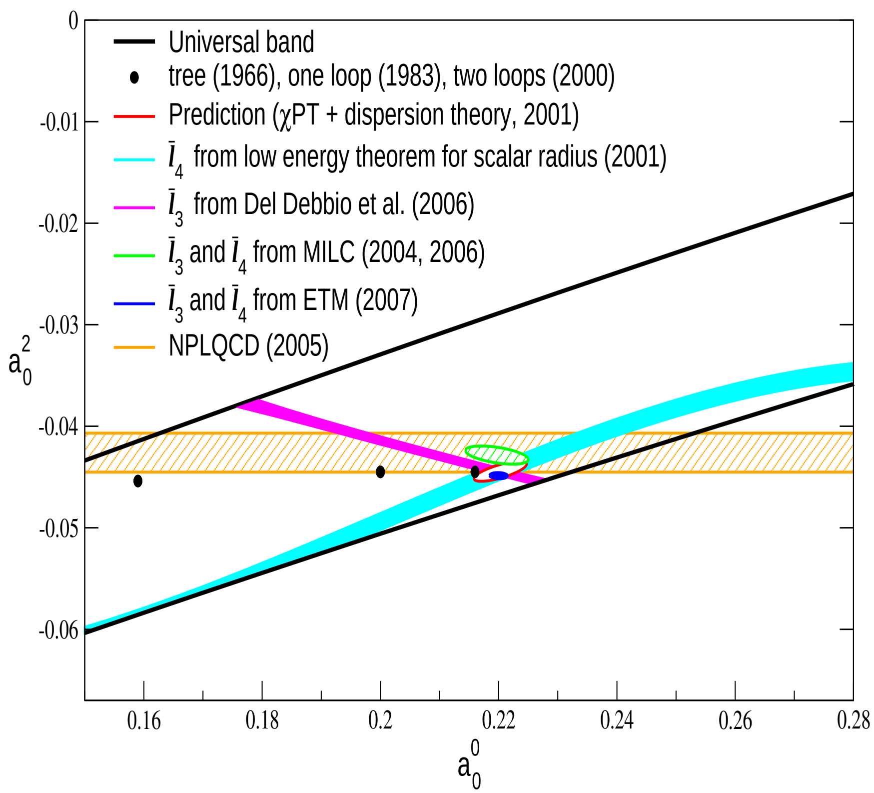
  phenomenological determinations

  $\bar{l}_3 = 2.9 \pm 2.4$ *from the mass spectrum of the pseudoscalar octet*
  $\bar{l}_4 = 4.4 \pm 0.2$ *from the radius of the scalar*

  other lattice determinations

  $\bar{l}_3 = 0.8 \pm 2.3$ from MILC (US-UK, staggered)
  $\bar{l}_3 = 3.0 \pm 0.6$ from lattice CERN group (Wilson)
  $\bar{l}_4 = 4.3 \pm 0.9$ from f_K/f_π *pion form factor*
  $\bar{l}_4 = 4.0 \pm 0.6$ *from MILC*

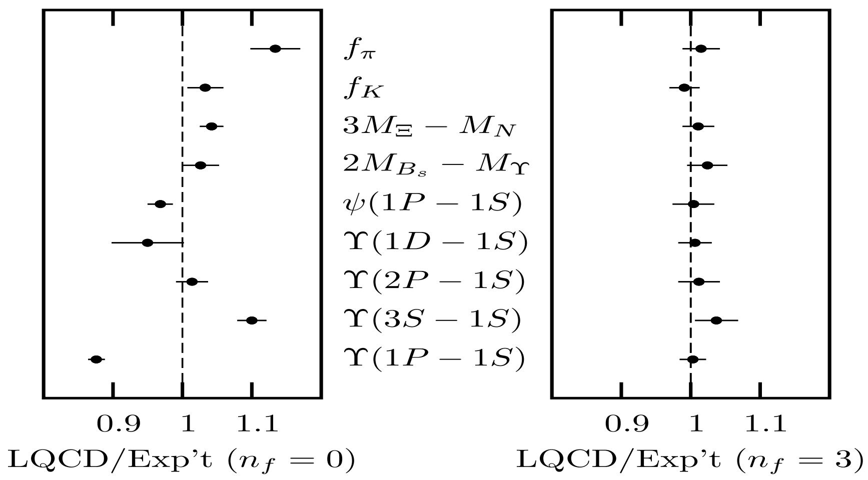
Narrowing scattering lengths (Leutwyler, private communication)



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

- scalar pion radius (ETMC): $< r^2 >= 0.637(26)\text{fm}^2$
  Colangelo, Gasser, Leutwyler: $< r^2 >= 0.61(4)\text{fm}^2$
- swave scattering lengths:
  $a_{00} = 0.220 \pm 0.002, \;\; a_{20} = -0.0449 \pm 0.0003$

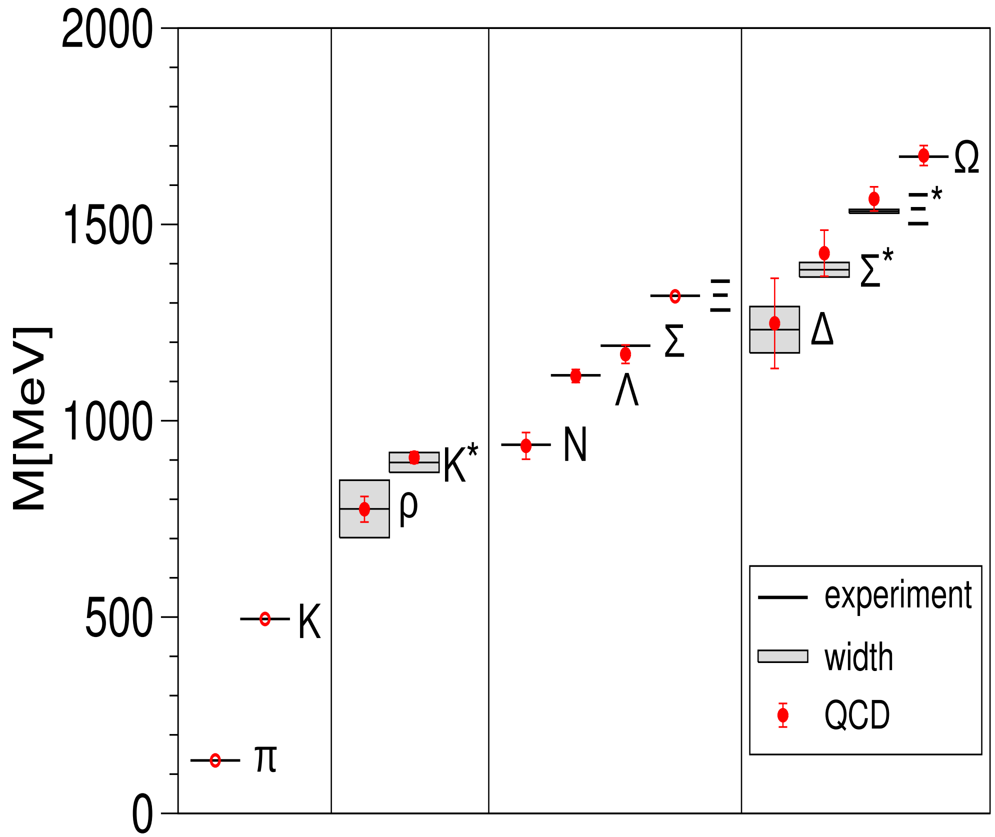
Lattice QCD and experiment



UKQCD, HPQCD
MILC
Collaborations, 2004

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

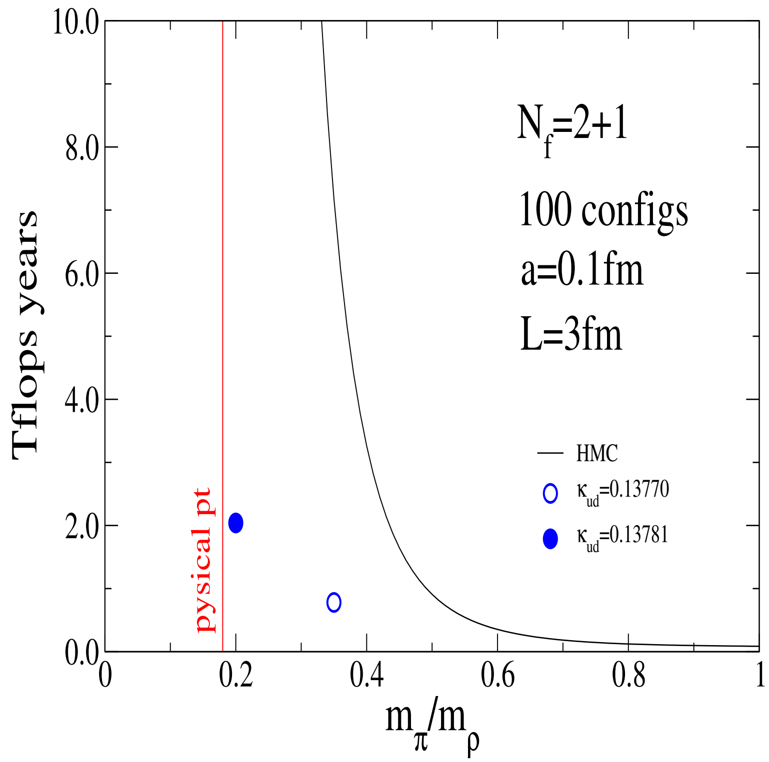
The Baryon spectrum, $N_f = 2 + 1$

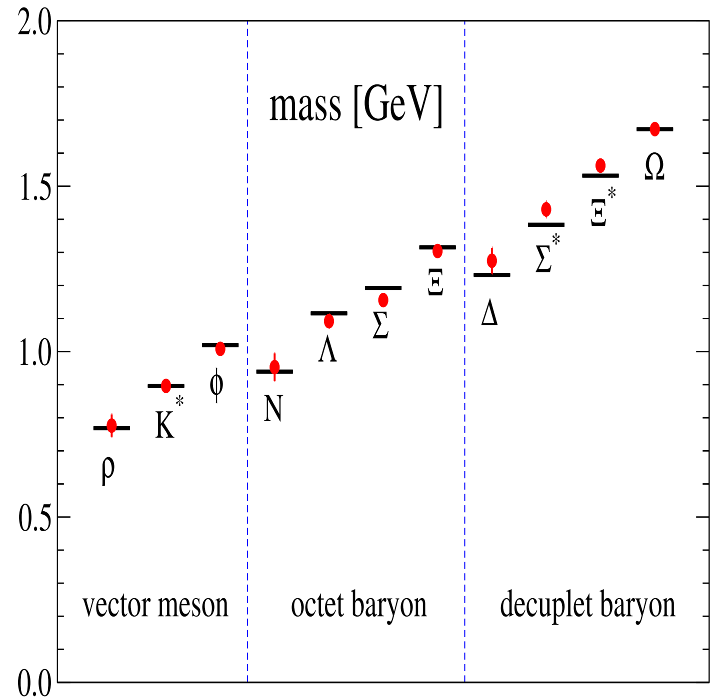


Budapest
Marseille
Wuppertal
Collaboration, 2008

- question of extrapolation to physical point
- e.g. ρ and Δ are resonances
- need second calculation and check at physical point

The Baryon spectrum towards the physical point from PACS-CS



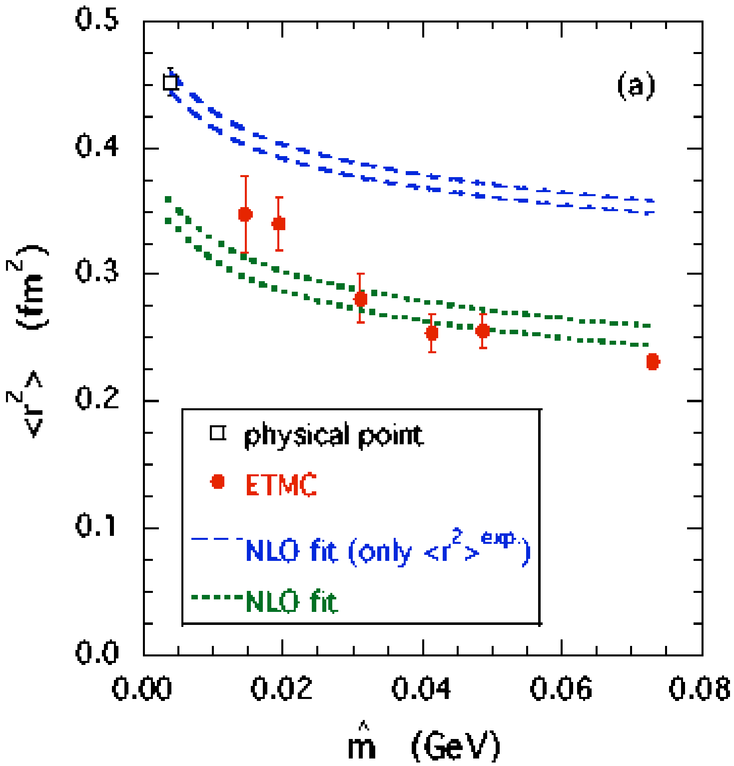


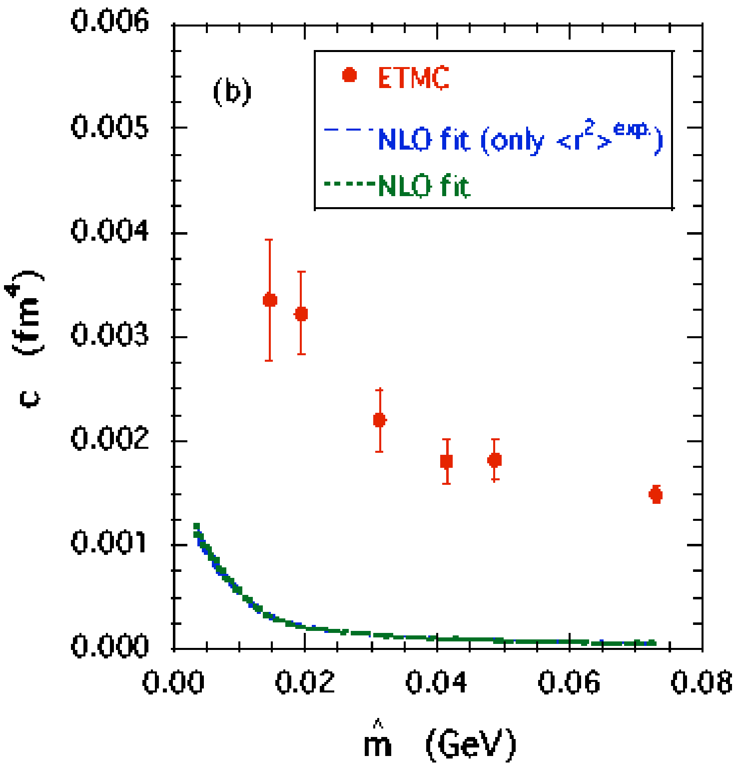
published July, 2008

- so far: only one value of the lattice spacing

Pion form factor (Lubicz, Simula, ETMC)

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

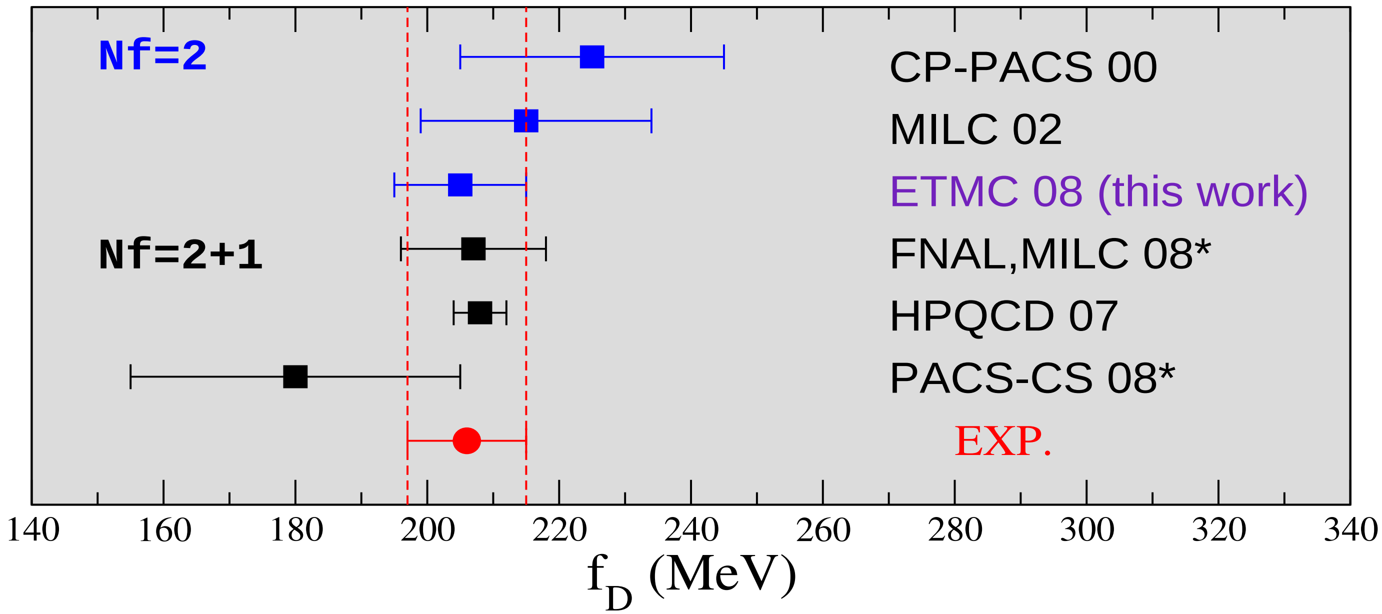




$$\langle r^2\rangle_{\rm NLO} = -\frac{2}{F^2}\left(6l_6 + L(\mu) + \frac{1}{(4\pi)^2}\right) \qquad c_{\rm NLO} = \frac{32\pi^2}{60F^4x_2}$$

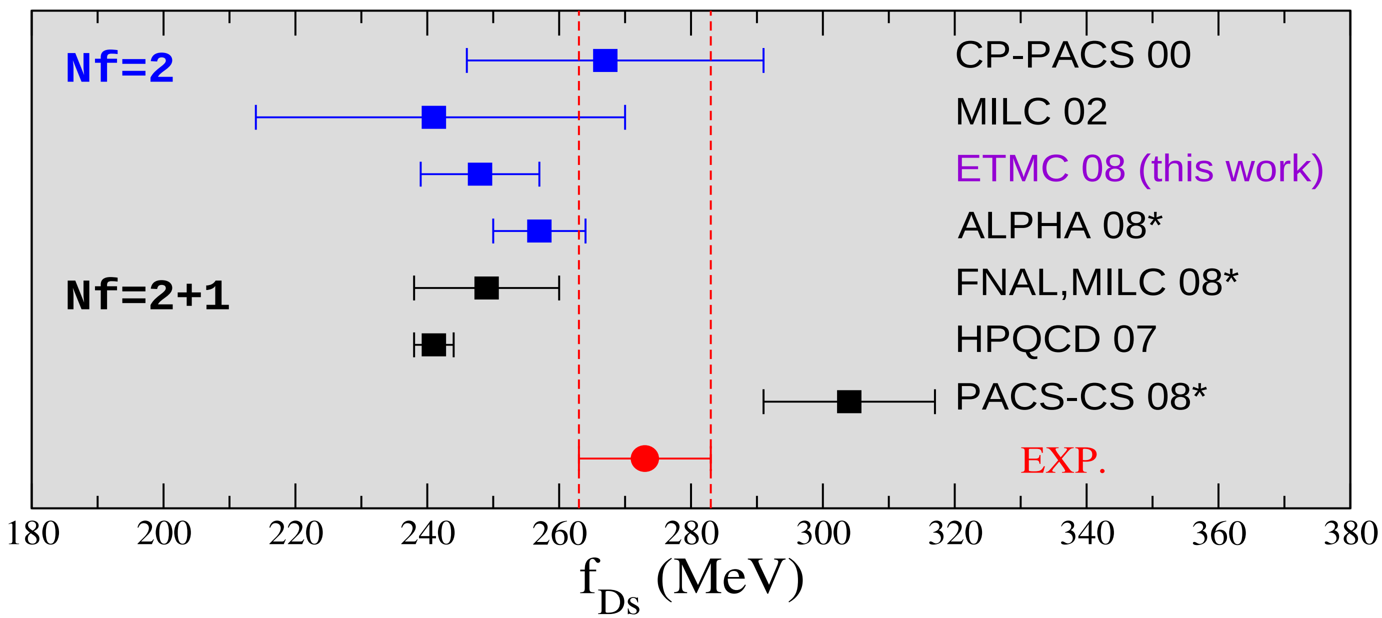
$$x_2 = 2Bm/F^2\ ,\quad L(\mu) = 16\pi^2 \log\left(2Bm/\mu^2\right)$$

f_D a compilation (ETMC)



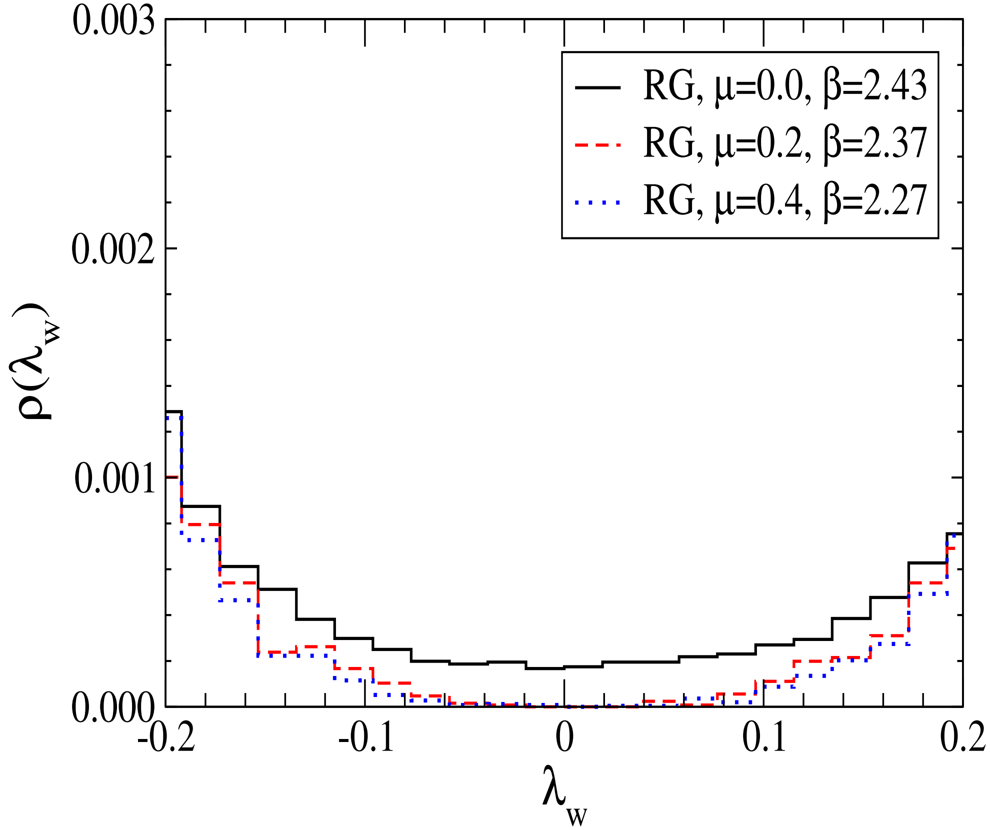
- perfect match with experiment

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:

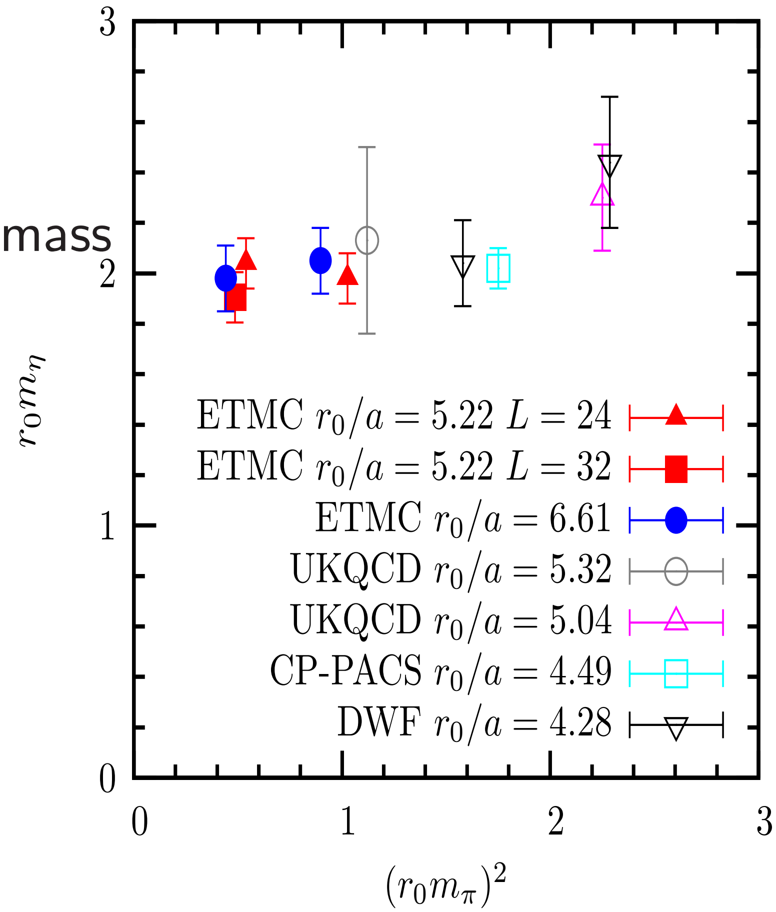
$$\frac{\det(D_W^2(-m_0))}{\det(D_W^2(-m_0)+\mu^2)}$$

- study of topological finite size effects
- ergodicity of simulation

The η' Mass

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

mass



- 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 **(tm-example, arXiv:0709.4574)**

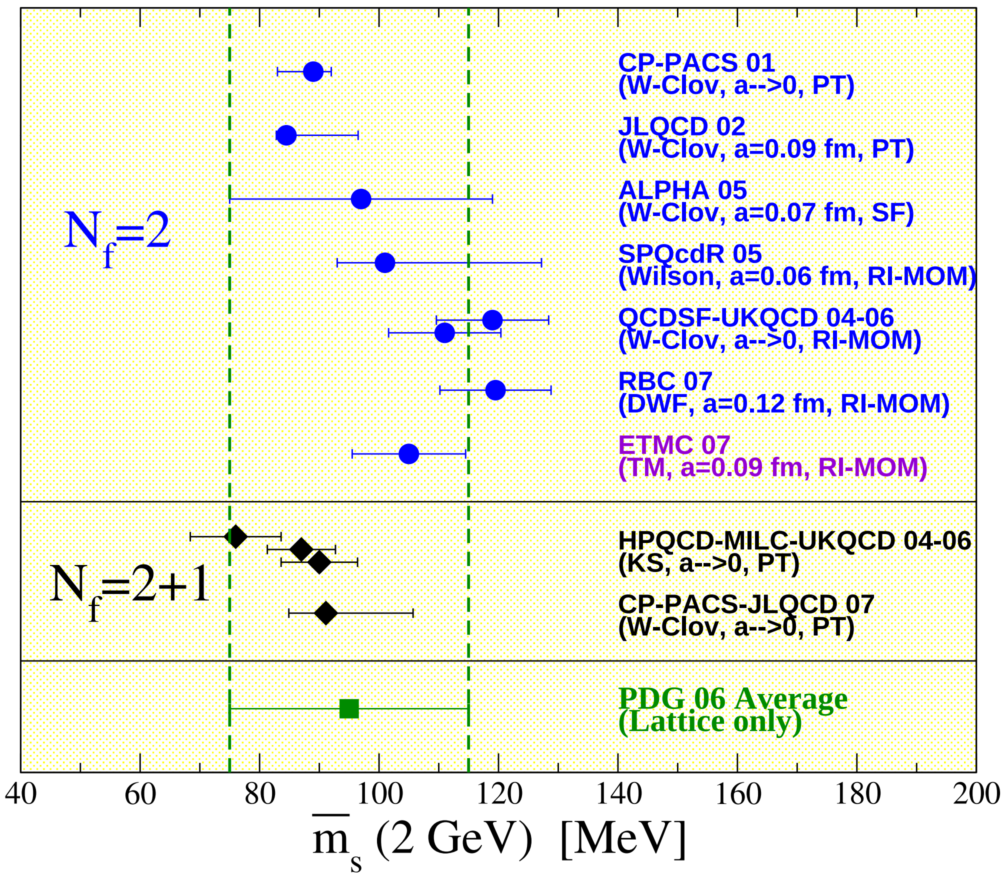
$Z_P^{\mathrm{RI-MOM}}(1/a) = 0.39(1)(2)$ $\leftarrow$ non-perturbative RI-MOM method

$Z_P^{\mathrm{BPT}}(1/a) \simeq 0.57(5)$ $\leftarrow$ one-loop boosted perturbation theory

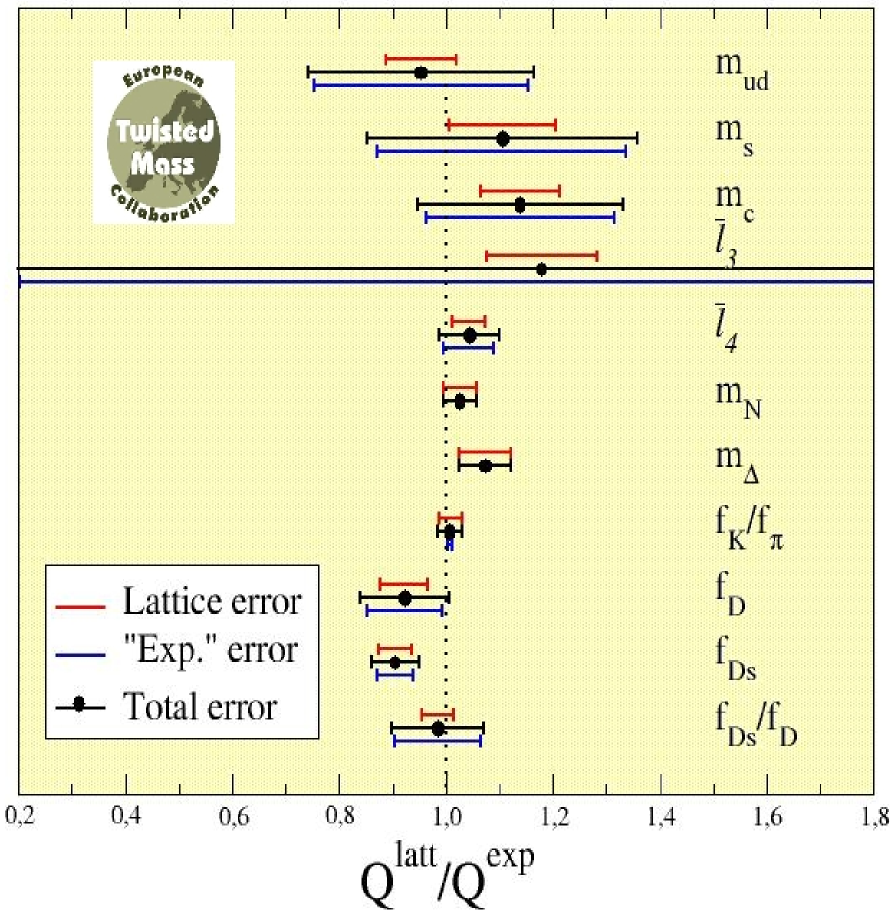
$m_q^{\overline{\mathrm{MS}}}(2\mathrm{GeV})\mathrm{MeV}$	perturbative	non-perturbative
m_s	$72 \pm 2 \pm 9$	$105 \pm 3 \pm 9$
m_s (PACS-CS)	72.7 ± 0.8	

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

Strange quark mass



A comparison to experiment



Universality

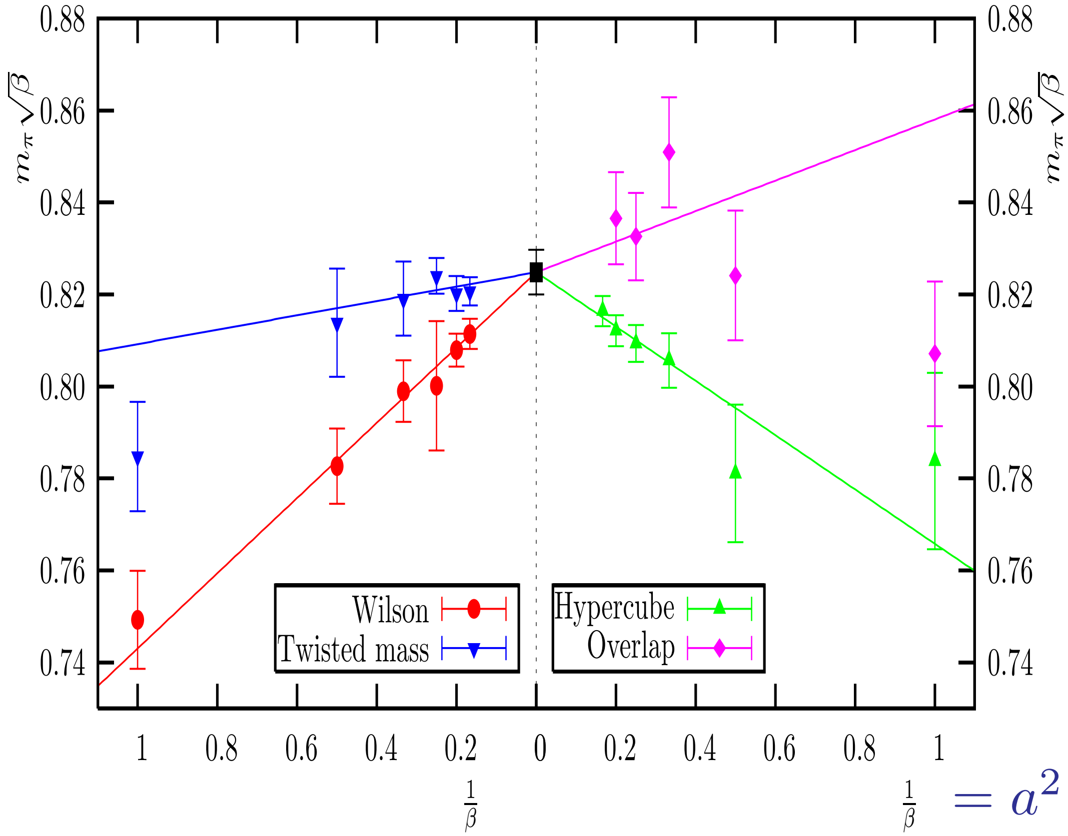
no ideal fermion action:

- $\mathrm{O}(a)$-*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

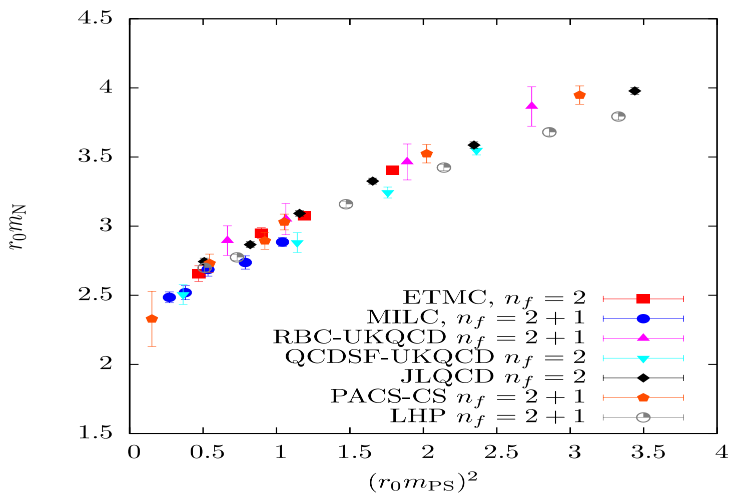
(N. Christian, K. Nagai, B. Pollakowski, K.J.)

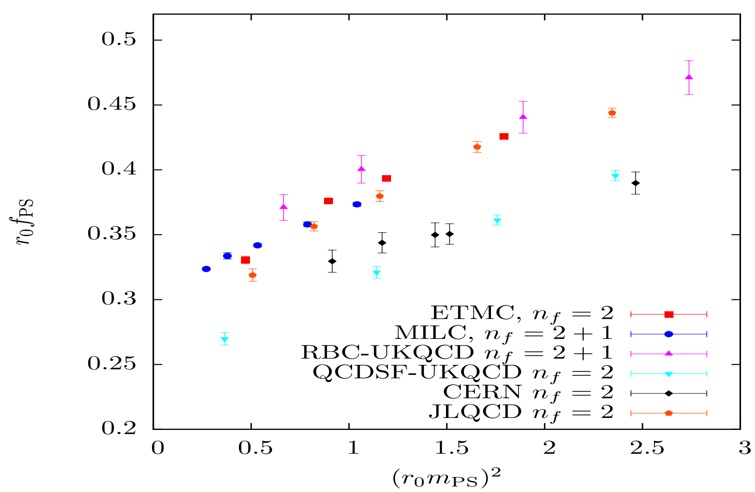


$\frac{1}{\beta} = a^2$

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

Universality: a challenge for lattice QCD





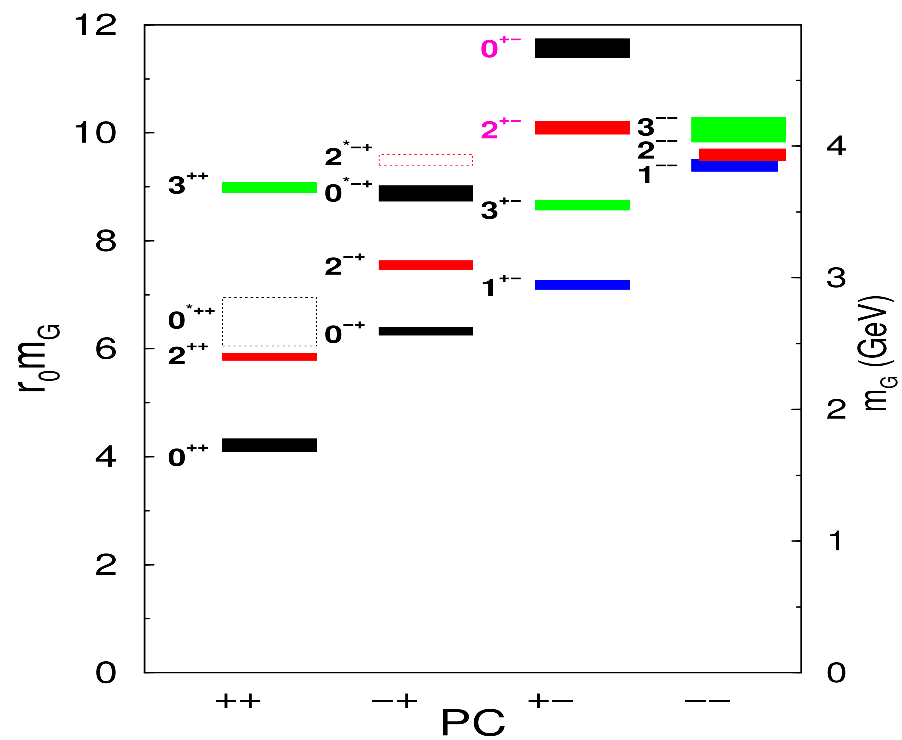
nucleon mass

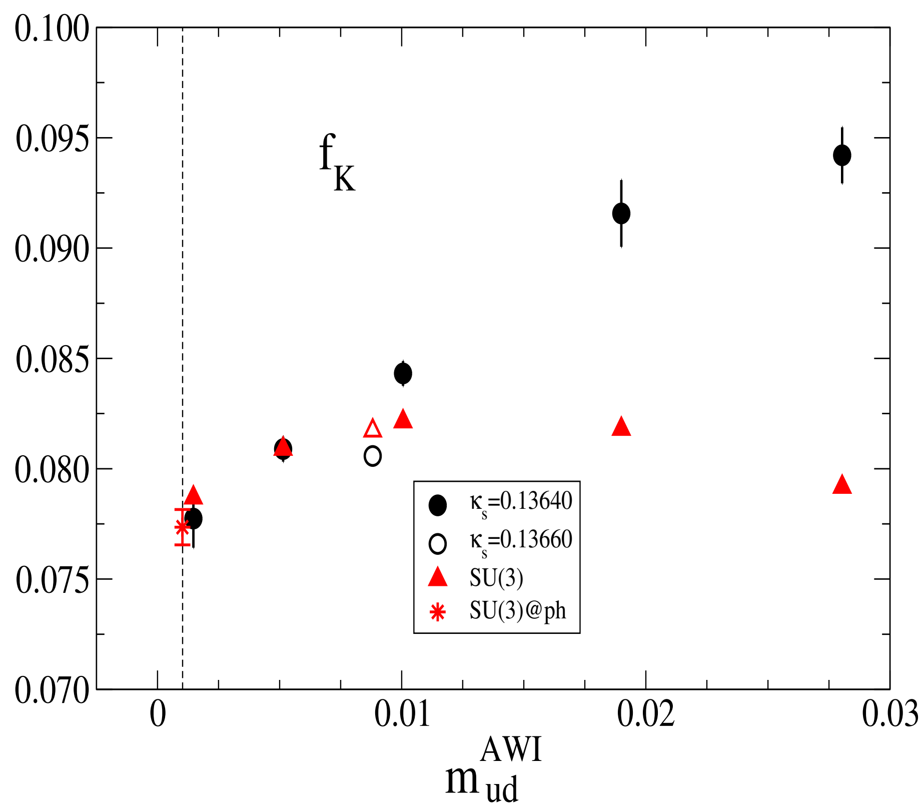
nice scaling

pseudo scalar decay constant

no common scaling visible

More challenges: glueball spectrum, χPT at the strange quark





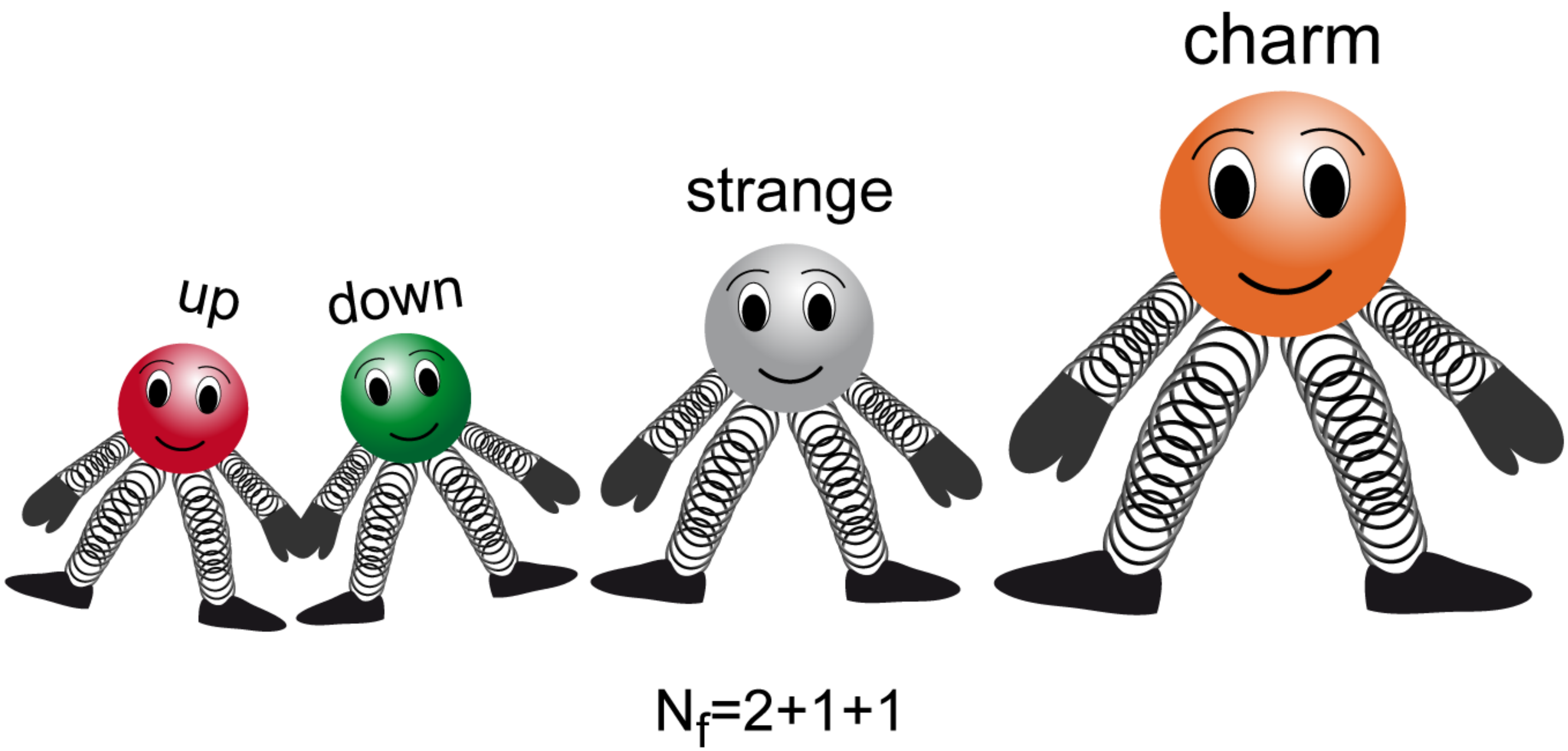
quenched glueball spectrum

Morningstar and Peardon

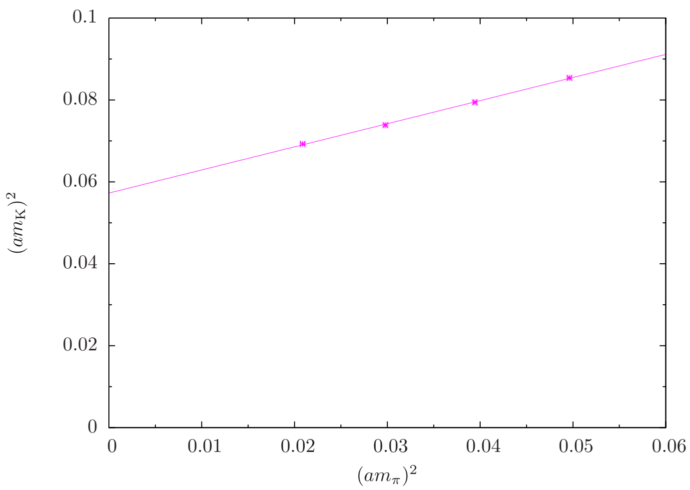
chiral perturbation theory

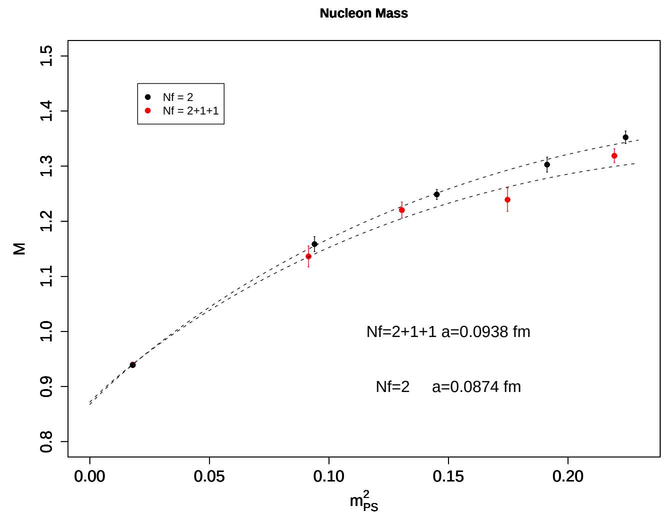
JLQCD collaboration

$N_f = 2+1+1$ flavours



Kaon and Nucleon mass (ETMC)





M_K

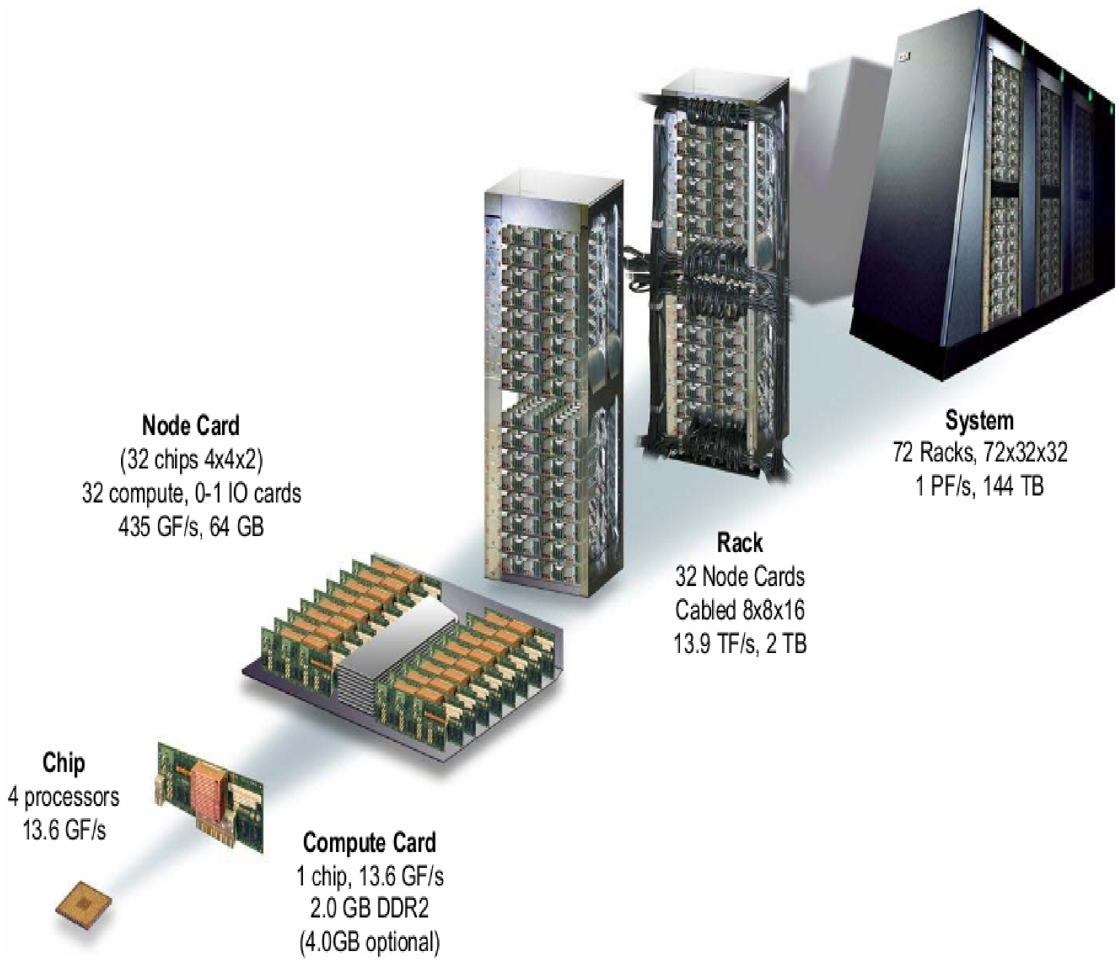
$M_{nucleon}$

$\longrightarrow$ no effect of strange quark

State of the art supercomputers

- **BG/P**

Blue Gene/P system structure

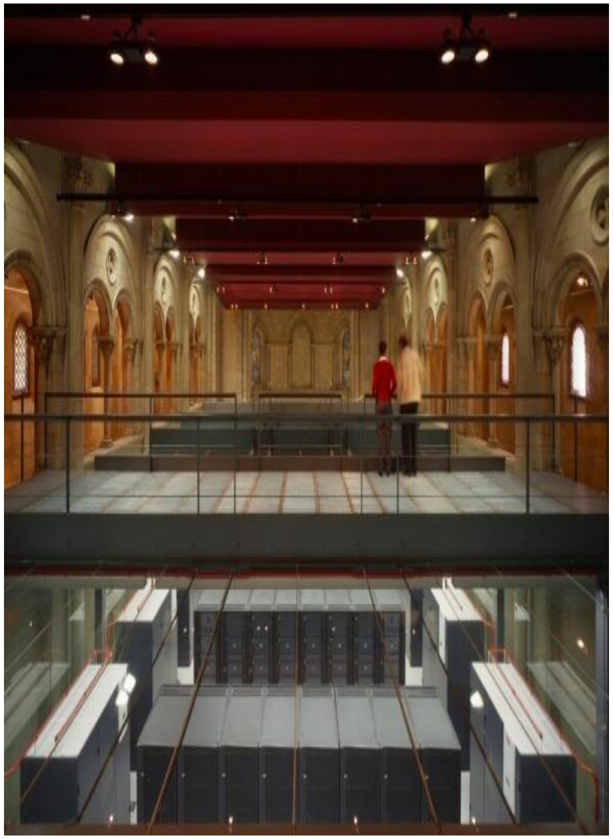


State of the art supercomputers

- **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

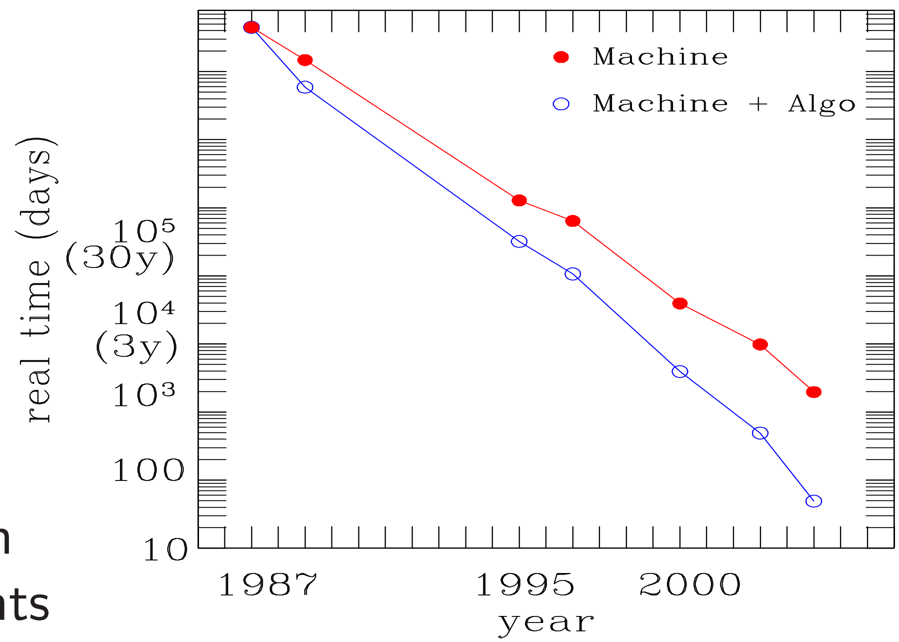


- MareNostrum, IBM, Barcelona
  40Teraflops peak performance
- Earth Simulator, NEC, Yokohama, 2002
  40Teraflops peak performance
- BlueGeneP, NIC, FZ-Jülich
  223Teraflops peak performance
- BlueGeneL, IBM, Los Alamos,
  367Teraflops peak performance, Nov. 2007
  (application area: not specified)
- IBM, Roadrunner, LANL,
  1.2Petaflops 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

  $\longrightarrow$ have computed the baryon spectrum
  $\longrightarrow$ have determined low energy constants
  $\longrightarrow$ decay constants

- challenges
  - understand better systematic effects
  - gluebal spectrum, χPT at the kaon and heavy baryons
  - resonances, scattering processes
  - simulations at physical point