Lattice QCD: from model to theory of strong interactions

Progress in unquenched simulations

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CERN-TH

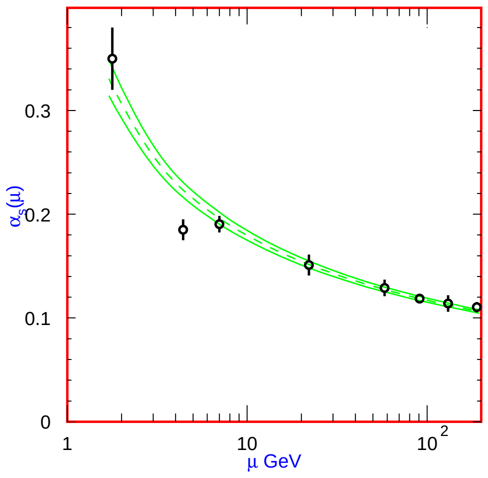
The QCD lagrangian

SU(3) gauge theory, matter in the fundamental representation

$$\mathcal{L} = -\frac{1}{4}G^2 + \bar{\psi}(D+m)\psi$$

large body of data with few params: 1 gauge coupling, quark masses

Asymptotically free:



[S. Eidelman et al., Phys. Lett. B592, 1 (2004)]

Running coupling

$$\alpha_s(\mu) = \frac{4\pi}{\beta_0 \log(\mu^2/\Lambda^2)}\left[1 + \ldots\right]$$

[Gross,Wilczek,Politzer 73]

At low-energy NP effects set in

NP effects

To study QFT beyond the usual framework of pert theory

♠ non-perturbative IR dynamics

(i) confinement and hadron spectrum (quark masses)
$\hookrightarrow$ to validate QCD as the theory of strong interactions

(ii) NP effects in SM phenomenology (hadronic matrix elements)
$\hookrightarrow$ to relate parameters of the SM to exp data

(iii) beyond QCD, new strong dynamics

Incorporate NP effects in models (symmetries, condensates, large N_c)

OR

$\boxed{\text{quantitative NP tool to compute field correlators}}$

Plan of the talk

- SM phenomenology: a few examples
  - masses and decay constants
  - form factors
  - B parameters
- lattice QCD: a NP definition of QCD
  - lattice regularization
  - choice of the action
- simulating lattice QCD
  - Monte Carlo methods
  - fermionic determinant
- quenched results
- unquenched simulations
  - algorithmic issues
  - Schwarz algorithm - preliminary results
- perspectives

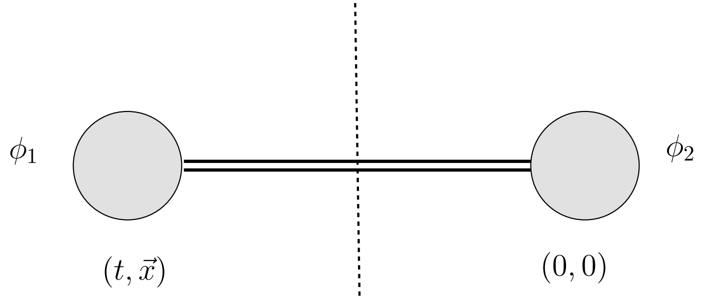
A simple example

Masses and decay constants

$$\begin{cases} M_{\rm PS} = E_{\rm PS}(\vec{p} = 0) \\ iF_{\rm PS}p_\mu = \langle 0|A_\mu(0)|\pi(p)\rangle \end{cases}$$

Extracted from a 2-pt correlator:

$$C_2(t,\vec{p}) = \int_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \langle \phi_1(t,\vec{x})\, \phi_2^\dagger(0)\rangle$$



Inserting a complete set of states:

$$C_2(t,\vec{p}) = \sum_S e^{-E_S(\vec{p})t} \langle 0|\phi_1(0)|S(\vec{p})\rangle \langle S(\vec{p})|\phi_2^\dagger(0)|0\rangle$$

A simple example

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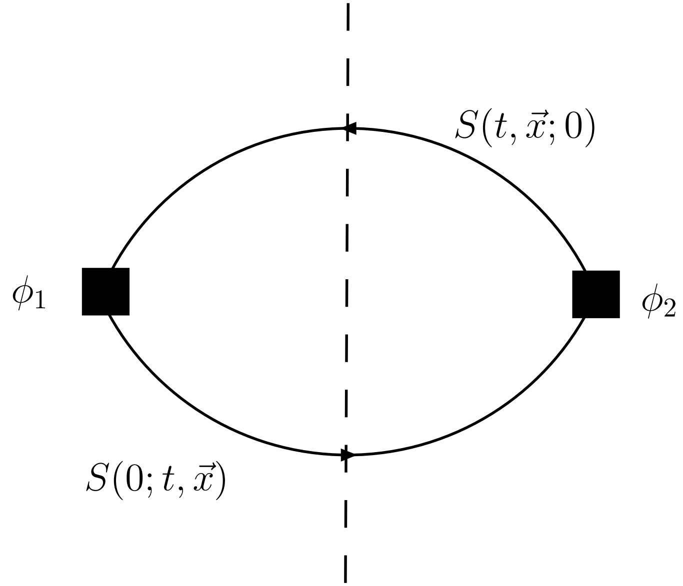

$$\mathrm{Tr}\,[\Gamma_1\, S(x,0)\, \Gamma_2\, S(0,x)]$$

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eg choose $\phi_1 = \bar{\psi}\gamma_4\gamma_5\psi$, and $\phi_2 = \bar{\psi}\gamma_5\psi$; then at large Euclidean time t:

$$C_2(t,\vec{p}) = e^{-E_{\mathrm{PS}}(\vec{p})t}\, F_{\mathrm{PS}} E_{\mathrm{PS}}(\vec{p})$$

A simple example

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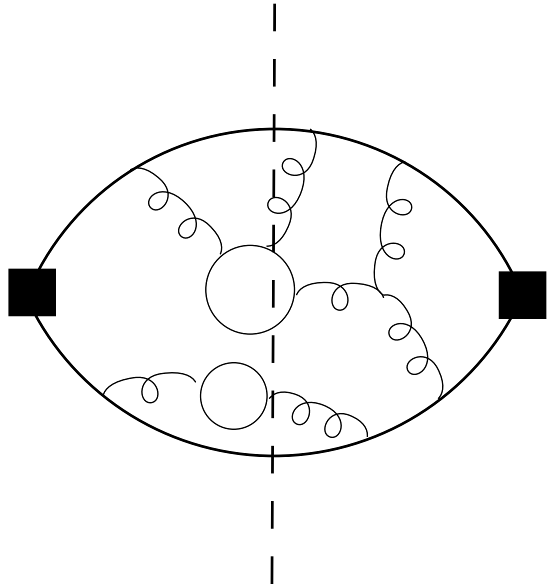

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SM phenomenology

Semi-leptonic B decays:

$$\frac{d\Gamma}{d\Phi} = [\text{kin.factor}]\,|V_{ub}|^2\,[\text{NP}]$$

$$\langle \pi | V^\mu | B \rangle = f_+(q^2)(p+p')^\mu + f_-(q^2)(p-p')^\mu$$

$K - \bar{K}$ mixing:

$$\epsilon_K = [\text{kin.factor}]\,\text{Re}\,(V_{cs}^* V_{cd})\,\text{Im}\,(V_{ts}^* V_{td})\,[\text{NP}]$$

$$\langle \bar{K} | Q(\Delta S = 2) | K \rangle = \frac{8}{3} B_K F_K^2 M_K^2$$

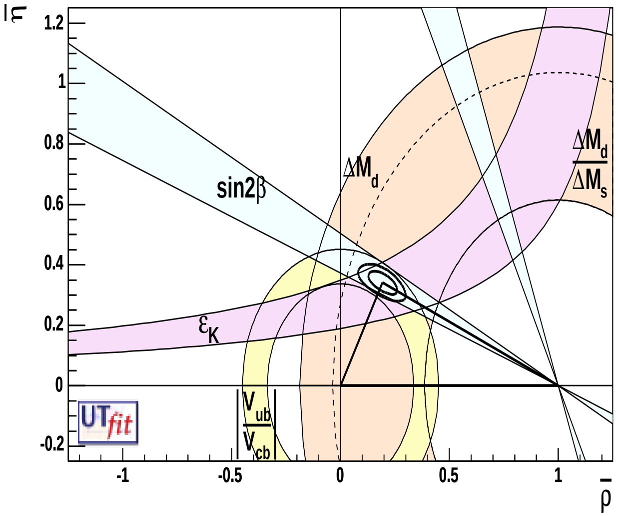
$B - \bar{B}$ mixing:

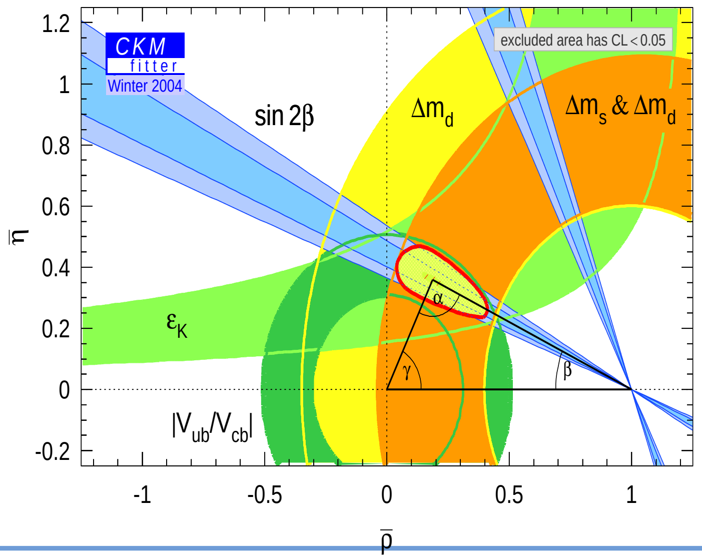
$$\Delta M_s / \Delta M_d = \left[(1-\bar{\rho})^2 + \bar{\eta}^2\right]\,[\text{NP}]$$

$$\xi^2 = F_{B_s}^2 B_{B_s} / F_{B_d}^2 B_{B_d}$$

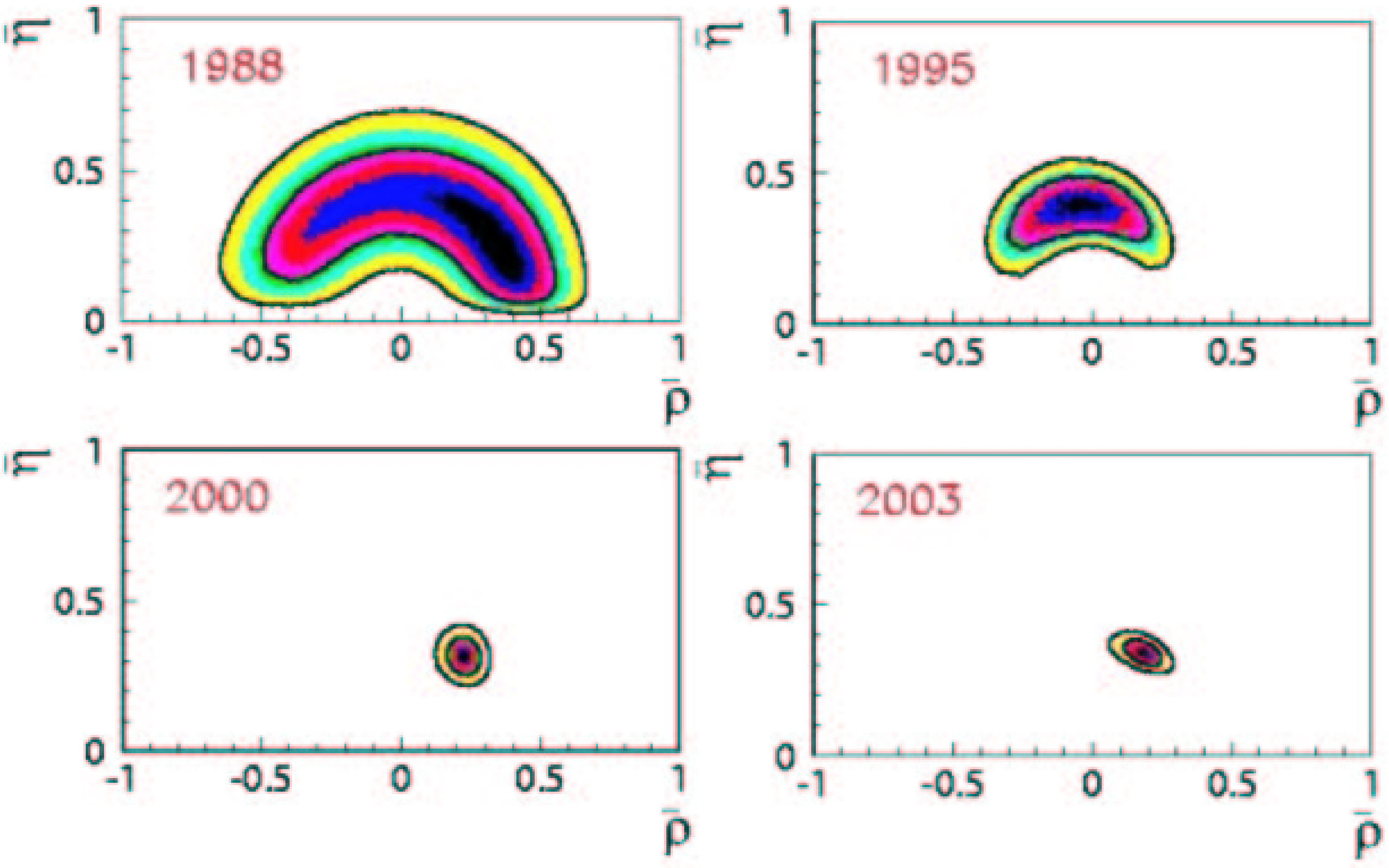
Unitarity triangle (1)

Stringent test of the SM + window on new physics





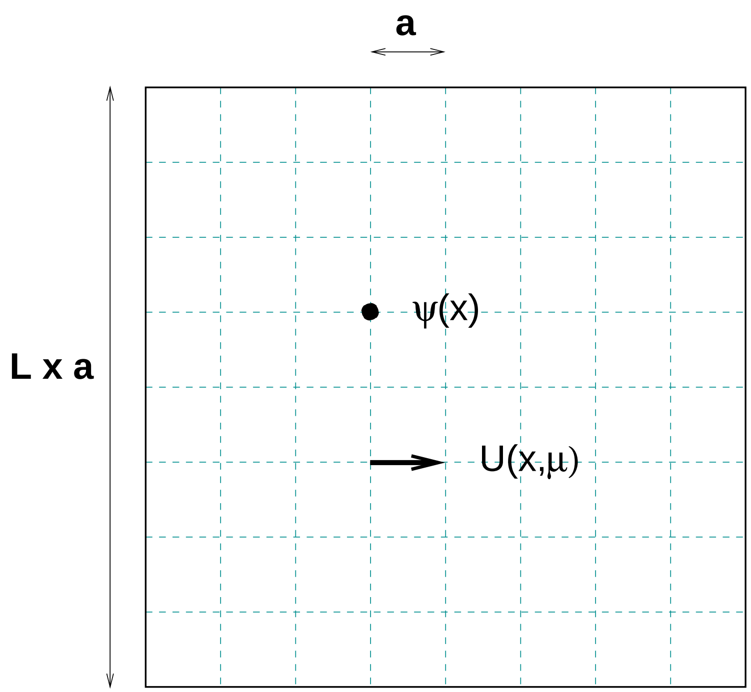
Unitarity triangle (2)



[UTFit Collaboration, http://www.utfit.org]

- **masses and CKM couplings are input values for physics BSM**

Lattice formulation



L x L sites

lattice spacing: a [fm]

Physical size: L x a [fm]

UV cutoff: a^{-1}, NP regularization

$$U(x,\mu) = \mathrm{P}\exp\left\{\int_x^{x+\mu} dx^\mu A_\mu(x)\right\} \in \mathrm{SU}(3)$$

$$Z = \int dU\, d\psi\, d\bar{\psi}\, \exp\left[-S(U,\psi,\bar{\psi})\right]$$

field correlators $\longrightarrow$ finite-dim integrals
evaluated numerically

First principles calculation

Accuracy of the numerical evaluation is limited by:

- statistical errors
- systematic errors

To have a quantitative NP tool:

(a) large computers

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(b) finite-volume effects

(c) continuum limit $a \longrightarrow 0$, at fixed La

(d) renormalization

————————————————————-

(e) quenched approximation

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(f) fermion masses ($m_q \longrightarrow 0$)

(g) symmetry breaking due to regularization

Witten-Veneziano mechanism

- The WV formula:

$$m_{\eta'}^2 = \frac{2N_f}{F_\pi^2}\chi \ ,$$

[Veneziano 79,Witten 79]

- Using GW Dirac operator:

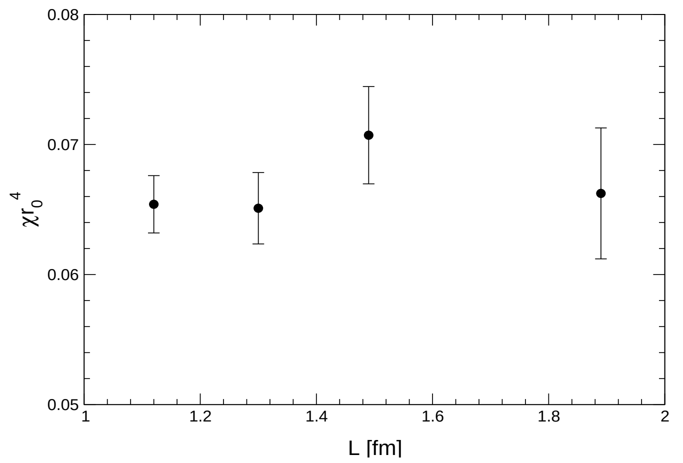
$$q(x) = -\frac{\bar{a}}{2a}\,\mathrm{Tr}\left[\gamma_5 D(x,x)\right] \ ,$$

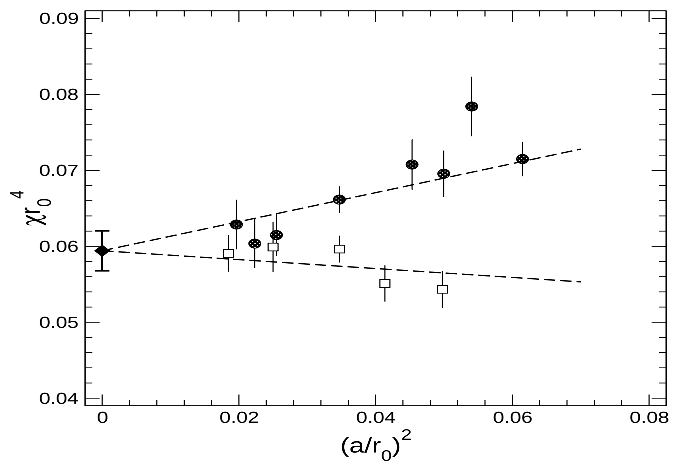
$$\chi = \frac{\langle Q^2\rangle}{V}$$

[Hasenfratz et al 98 - Giusti et al 01]

- No power divergencies if GW fermions are used

[Giusti et al 04, Luscher 04]



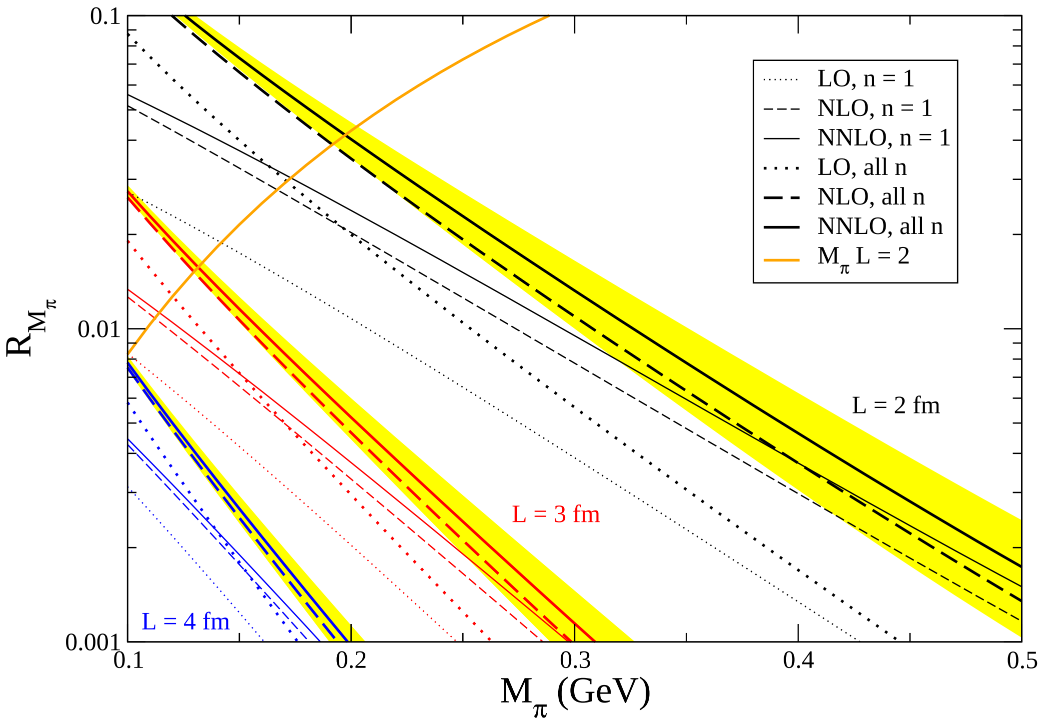


$$\chi = (191 \pm 5\mathrm{MeV})^4$$

[Del Debbio et al 04]

Finite-volume effects

Finite volume shifts can be important



[Lüscher 86 – Colangelo et al 04 – Becirevic 04]

- $R_{M_\pi} = (M_\pi(L) - M_\pi)/M_\pi$
- effect of pion loops
- computed in ChPT (no new params)
- uncertainty estimates
- few % effects

Fermionic action

dynamics is determined by the lattice action

$$S(U,\psi,\bar{\psi}) \longrightarrow -\frac{1}{4}G^2 + \bar{\psi}(D+m)\psi + O(a)$$

- gauge symmetry
- flavour symmetry
- renormalization
- chiral symmetry
- locality
- improvement

Different discretizations (gauge term + fermion term):

- Wilson fermions

$$S_F = \frac{1}{2a}\bar{\psi}(x)\left[U_\mu(x)\gamma_\mu\psi(x+\mu) - U^\dagger_\mu(x-\mu)\gamma_\mu\psi(x-\mu)\right]$$

symmetry-breaking term to eliminate doublers

Irrelevant operators can be added to improve the convergence to the continuum limit

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Different discretizations (gauge term + fermion term):

- Staggered fermions

$$S_F = \frac{1}{2a}\bar{\chi}(x)\eta_\mu(x)\left[U_\mu(x)\chi(x+\mu) - U^\dagger_\mu(x-\mu)\chi(x-\mu)\right]$$

four tastes of quarks $\rightarrow$ square-root trick

[Wingate 04]

Fermionic action

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Different discretizations (gauge term + fermion term):

- Ginsparg-Wilson fermions

$$\{\gamma_5, D\} = a\, D\gamma_5 D$$

$$D = 1 + \gamma_5 \epsilon(\gamma_5 D_{\mathrm{w}})$$

$$\text{Domain Wall fermions}$$

computationally expensive for dynamical simulations

[BNL 04 – Kennedy 04]

Simulating lattice QCD

Expectation values are computed as:

$$\langle O \rangle = Z^{-1} \int \mathcal{D}\phi \, e^{-S(\phi)} \, O(\phi) = \frac{1}{N_{\mathrm{conf}}} \sum_k O(\phi_k)$$

$$p(\phi) \propto e^{-S(\phi)}$$

by generating an ergodic Markov chain, detailed balance:

$$p(\phi) \, P(\phi \to \phi') = p(\phi') P(\phi' \to \phi)$$

Integrating out the Grassman variables:

$$\langle O \rangle = \int \mathcal{D}U \, e^{-S_G} \, (\det D)^{N_f} \, \langle O \rangle_F$$

Gluonic background is generated with an effective action:

$$S_{\mathrm{eff}} = S_G - \frac{N_f}{2} \log \det Q, \qquad Q = D^\dagger D$$

Simulating lattice QCD

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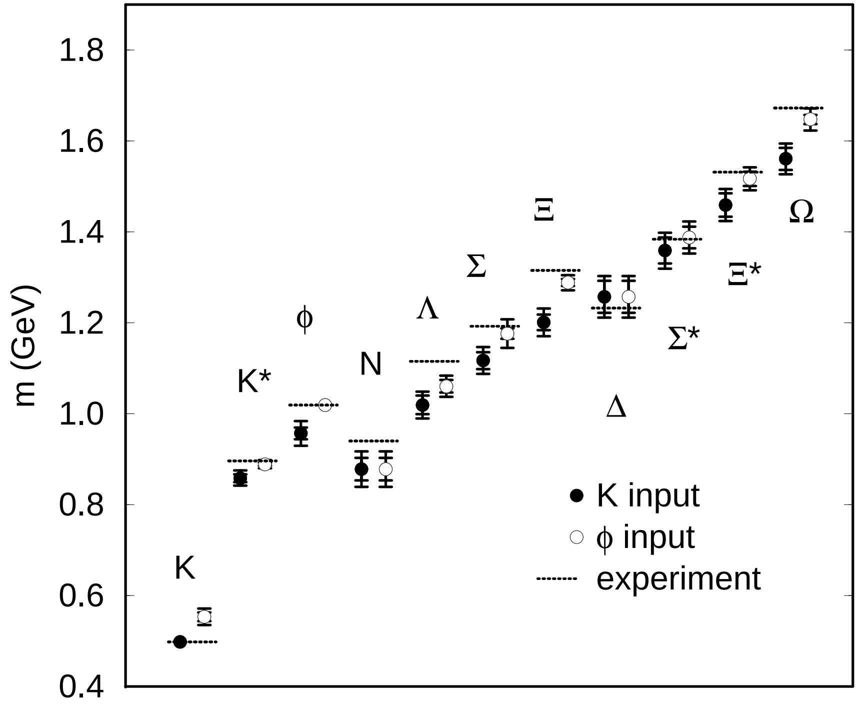
Introducing pseudofermion fields for $N_f = 2$:

$$\langle O \rangle = \int \mathcal{D}U \mathcal{D}\phi \mathcal{D}\phi^* \exp[-S_G - (D^{-1}\phi, D^{-1}\phi)] \, \langle O \rangle_F$$

Quenched approximation

$$\det D = 1$$

- the theory is not unitary
- chiral limit is pathological (quenched chiral log)
- spectrum: 10% error [CP-PACS 03]
- B_K: 16 % error [Lellouch 02]
- F_B: 10 % error [Lellouch 02]
- form factors: 10-15% error [CKM WS 03]



[CP-PACS Collaboration]

Hybrid Monte Carlo (1)

Including the fermionic determinant:

$$
\begin{aligned}
Z &= \int \mathcal{D}U\mathcal{D}\phi\mathcal{D}\phi^* \exp[-S_G - \phi^* Q^{-1}\phi] \\
&= \int \mathcal{D}\Pi\mathcal{D}U\mathcal{D}\phi\mathcal{D}\phi^* \exp[-\frac{1}{2}(\Pi,\Pi) - S_G - (D^{-1}\phi, D^{-1}\phi)]
\end{aligned}
$$

Molecular dynamics evolution:

$$
\begin{aligned}
\frac{d}{dt}\Pi(x,\mu) &= -\frac{\delta\mathcal{H}}{\delta U(x,\mu)} = \sum_k F_k(x,\mu) \\
\frac{d}{dt}U(x,\mu) &= \Pi(x,\mu)U(x,\mu)
\end{aligned}
$$

Performed numerically through discrete leapfrog integration

Metropolis acceptance test at the end of the evolution

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\end{aligned}
$$

Preconditioned molecular dynamics:

$$\det D = \det R_1 \ldots \det R_n$$

yields:

$$
\begin{aligned}
(\omega, F_0) &= \delta_\omega S_G, \\
(\omega, F_k) &= 2\mathrm{Re}\left(R_k^{-1}\phi_k, \delta_\omega R_k^{-1}\phi_k\right), \qquad k = 1, \ldots, n
\end{aligned}
$$

for all infinitesimal variations of the gauge field:

$$\delta_\omega U(x,\mu) = \omega(x,\mu)U(x,\mu)$$

HMC (2)

- cost of the inversion dictated by the small eigenvalues
  $\Rightarrow$ more expensive as $m_q \to 0, V \to \infty$
- time-step in the classical evolution dictated by the magnitude of the forces

$$\epsilon_k ||F_k|| \simeq \mathrm{const}$$

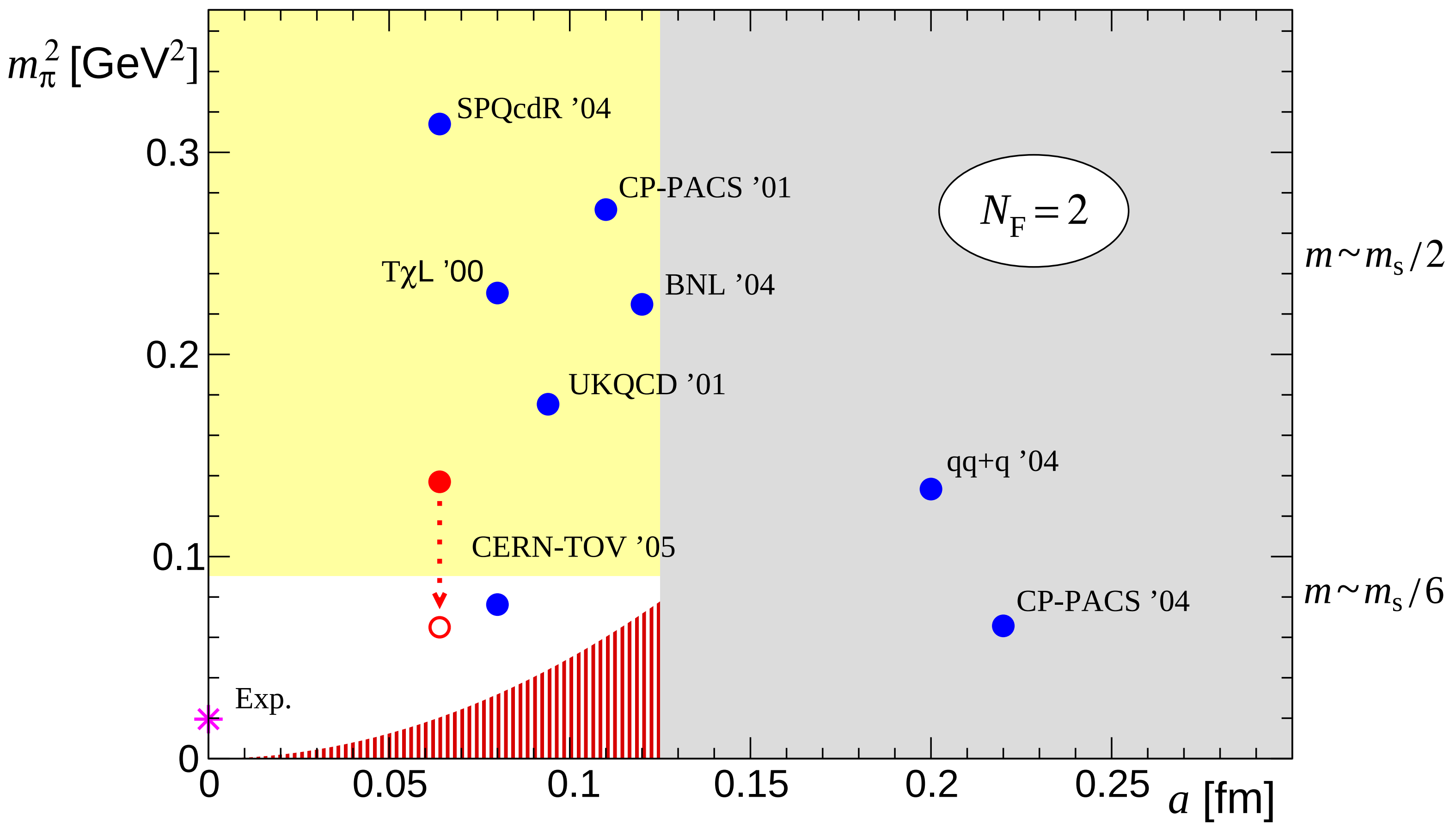
- chiral limit requires small a: $O(a/m_\pi^2)$ lattice artefacts appear
- total cost with Wilson/stag fermions:

$$\mathrm{TFlop} \times \mathrm{yrs} \quad = \quad 0.7 \left(\frac{N_{\mathrm{conf}}}{1000}\right) \left(\frac{L_s \times a}{3\mathrm{fm}}\right)^5 \left(\frac{L_t}{2L_s}\right) \left(\frac{0.6}{m_\pi/m_\rho}\right)^6 \left(\frac{0.1\mathrm{fm}}{a}\right)^7$$

$$\mathrm{TFlop} \times \mathrm{yrs} \quad = \quad 1.31 \left(\frac{N_{\mathrm{conf}}}{1000}\right) \left(\frac{L_s \times a}{3\mathrm{fm}}\right)^4 \left(\frac{L_t}{2L_s}\right) \left(\frac{0.2}{m/m_s}\right)^{2.5} \left(\frac{0.1\mathrm{fm}}{a}\right)^7$$

[Ukawa 02 - Gottlieb 02]

Current simulations



Schwarz preconditioning

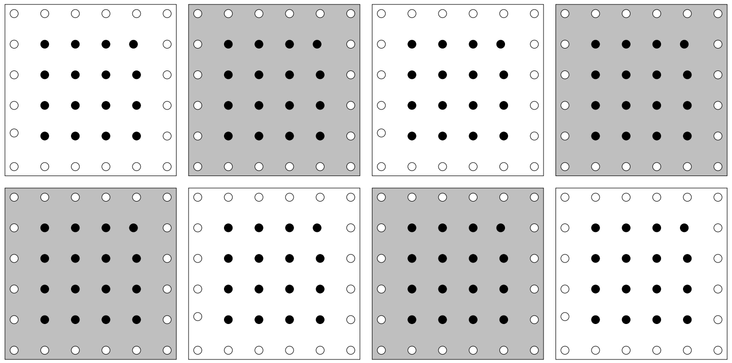
Design the algorithm using knowledge of the physical system

- Domain decomposition

$$D = D_\Omega + D_{\Omega^*} + D_{\partial\Omega} + D_{\partial\Omega^*}$$

yields:

$$\det D = \prod \hat{D}_\Lambda \det\left\{1 - D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}\right\}$$



- Schur complement only acts on $\partial\Omega^*$
- Block decoupling via active links; inner integration can be performed in parallel
- Hierarchical integration with different time-steps
- Block size $\sim$ $1\mathrm{fm}$, avoid small blocks in units of a

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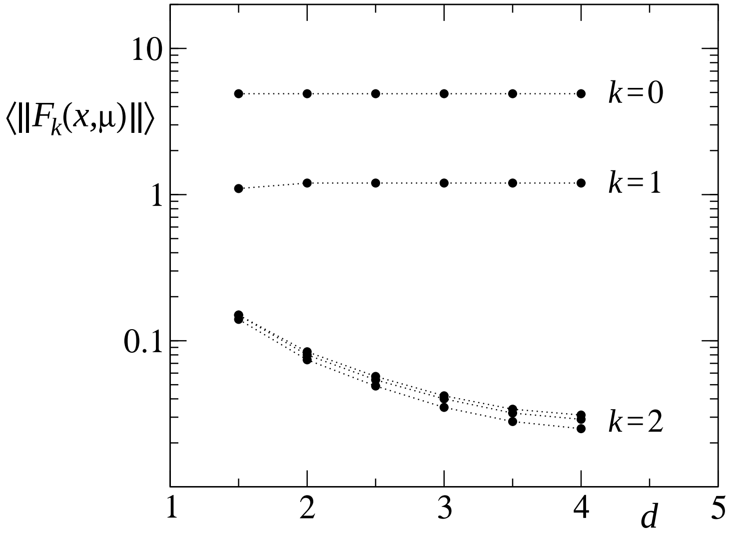


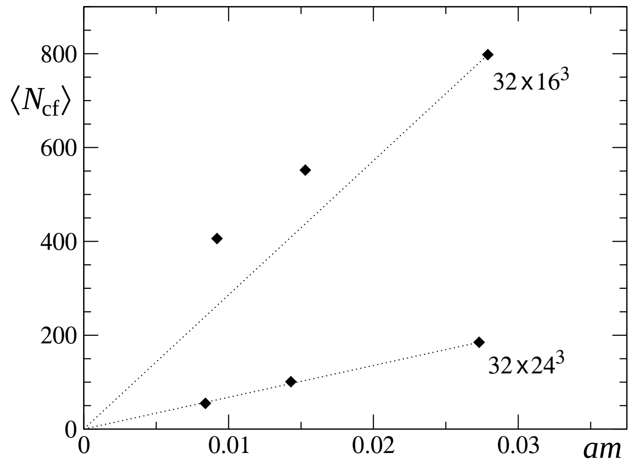
Schwarz simulations

Lattice	κ	am	am_π
32×16^3	0.15750	0.0279(4)	0.298(5)
	0.15800	0.0154(4)	0.242(4)
	0.15825	0.0092(4)	0.209(7)
32×24^3	0.15750	0.0273(4)	0.280(3)
	0.15800	0.0143(3)	0.188(5)
	0.15825	0.0084(4)	0.153(4)

scale set by the sommer radius r_0: $a = 0.08\text{fm}$

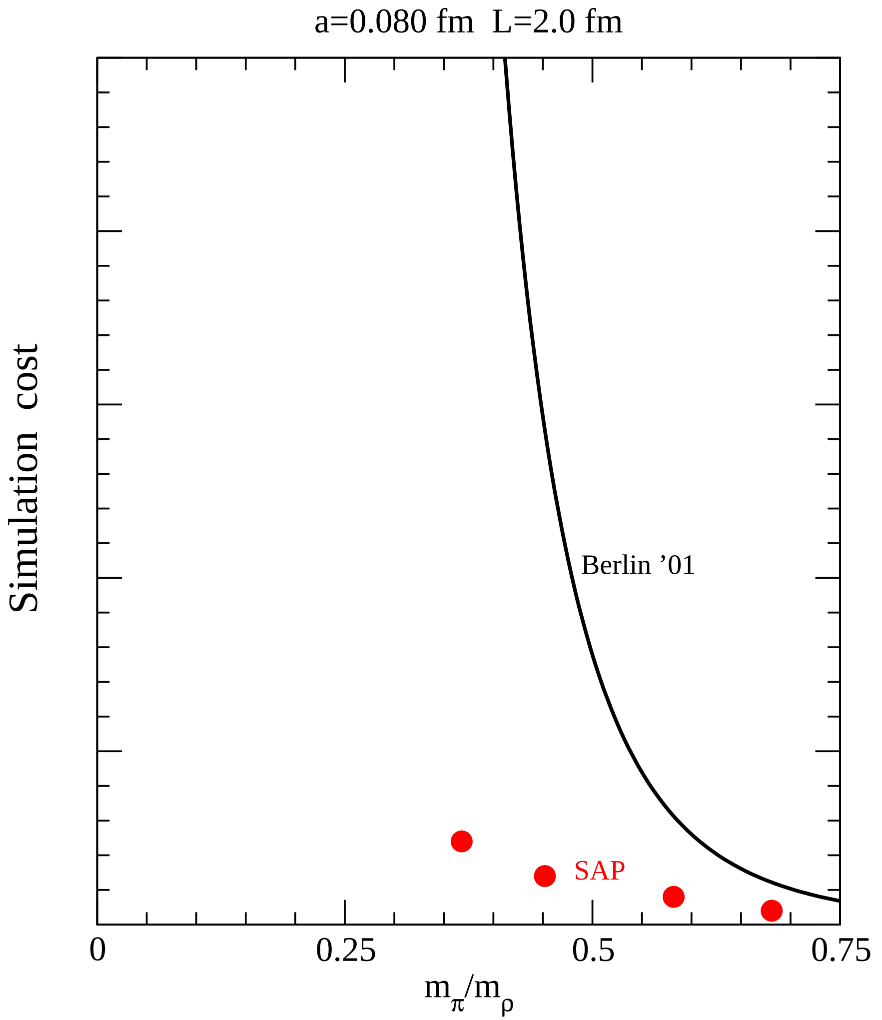
Lattice	κ	m(MeV)	m_π (MeV)
64×32^3	0.15410	0.01936(9)	0.1965(8)
	0.15440	***	***
	0.15470	***	***

scale set by the sommer radius r_0: $a = 0.06\text{fm}$

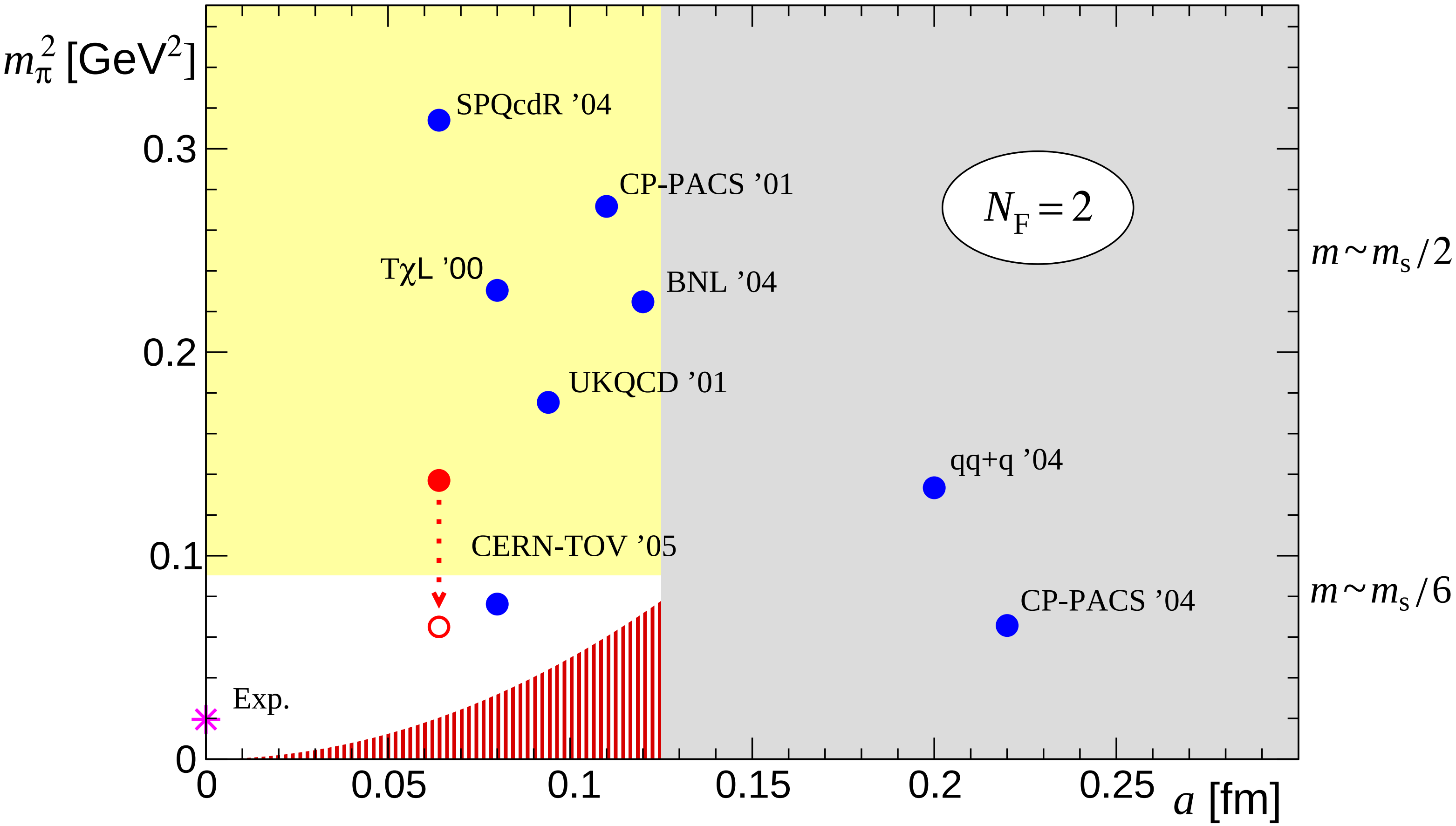


Lattice	κ	$\tau_{\text{int}}[P]$	$\tau_{\text{int}}[N_{\text{GCR}}]$
32×16^3	0.15750	68(25)	168(42)
	0.15800	32(7)	162(56)
	0.15825	57(18)	135(39)
32×24^3	0.15750	53(22)	144(51)
	0.15800	33(11)	122(36)
	0.15825	12(4)	22(6)

Simulation cost



Current simulations



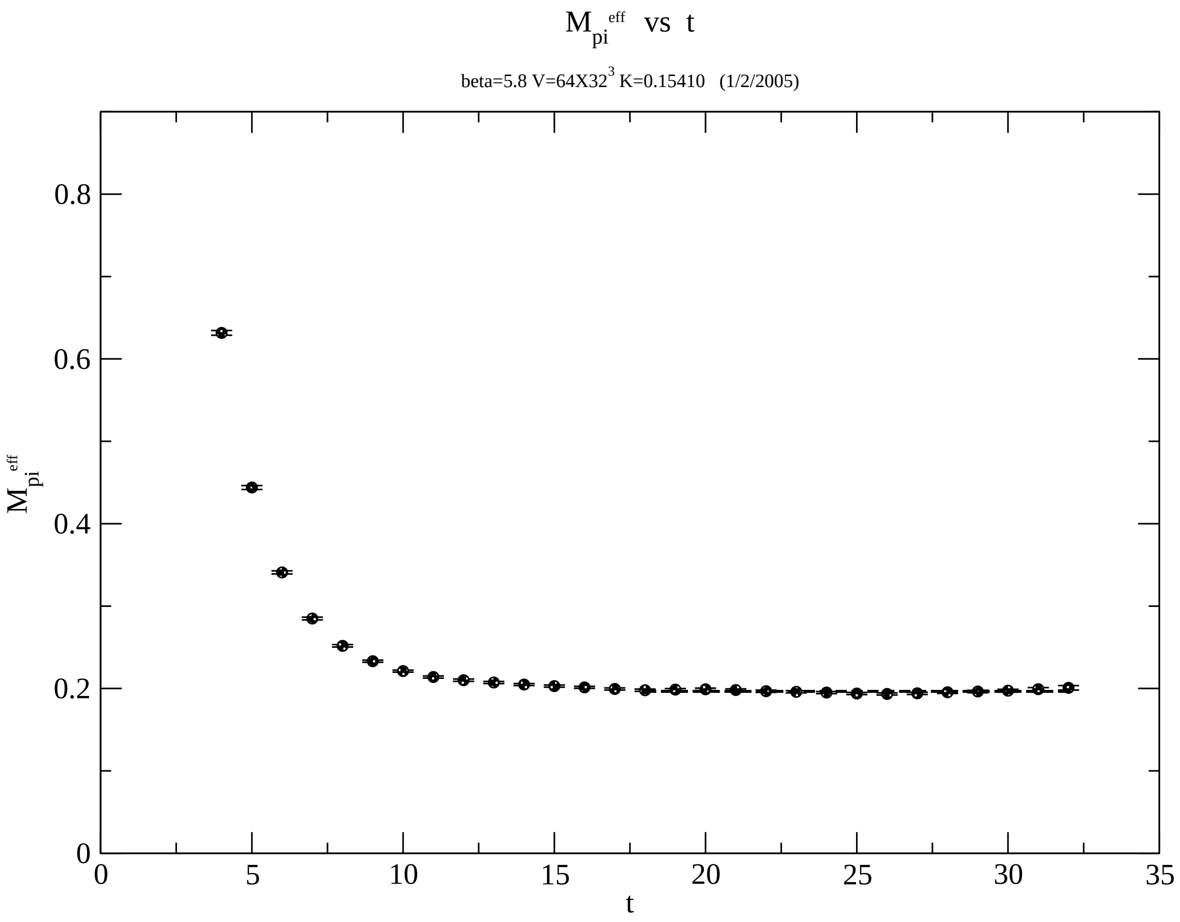
PC Cluster

[Fermi Institute, Rome 04]

64 nodes: 200 GFlops sustained

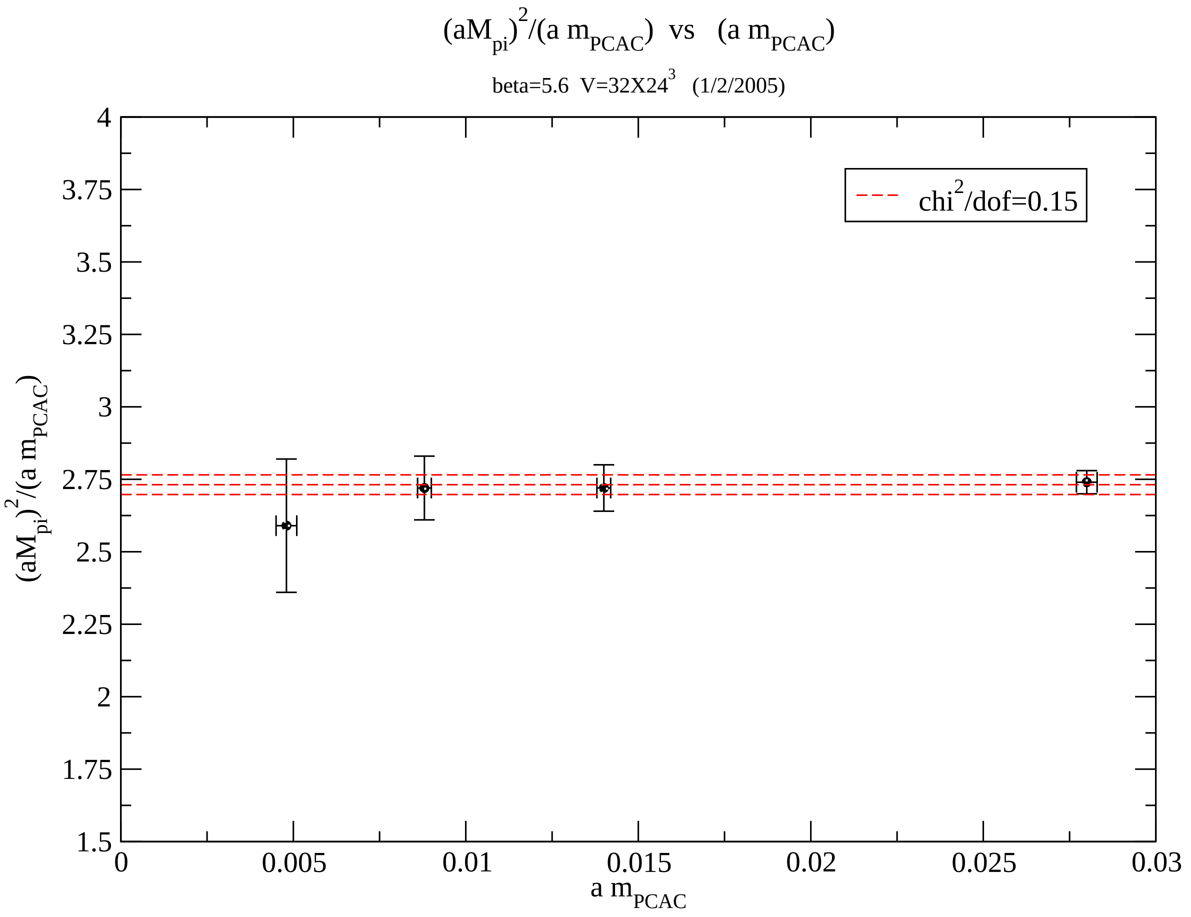
2 lattice spacings, 2 fm lattices, 4 masses $\approx$ 1 year

Preliminary results



[Del Debbio, Giusti, Lüscher, Petronzio, Tantalo]

Preliminary results



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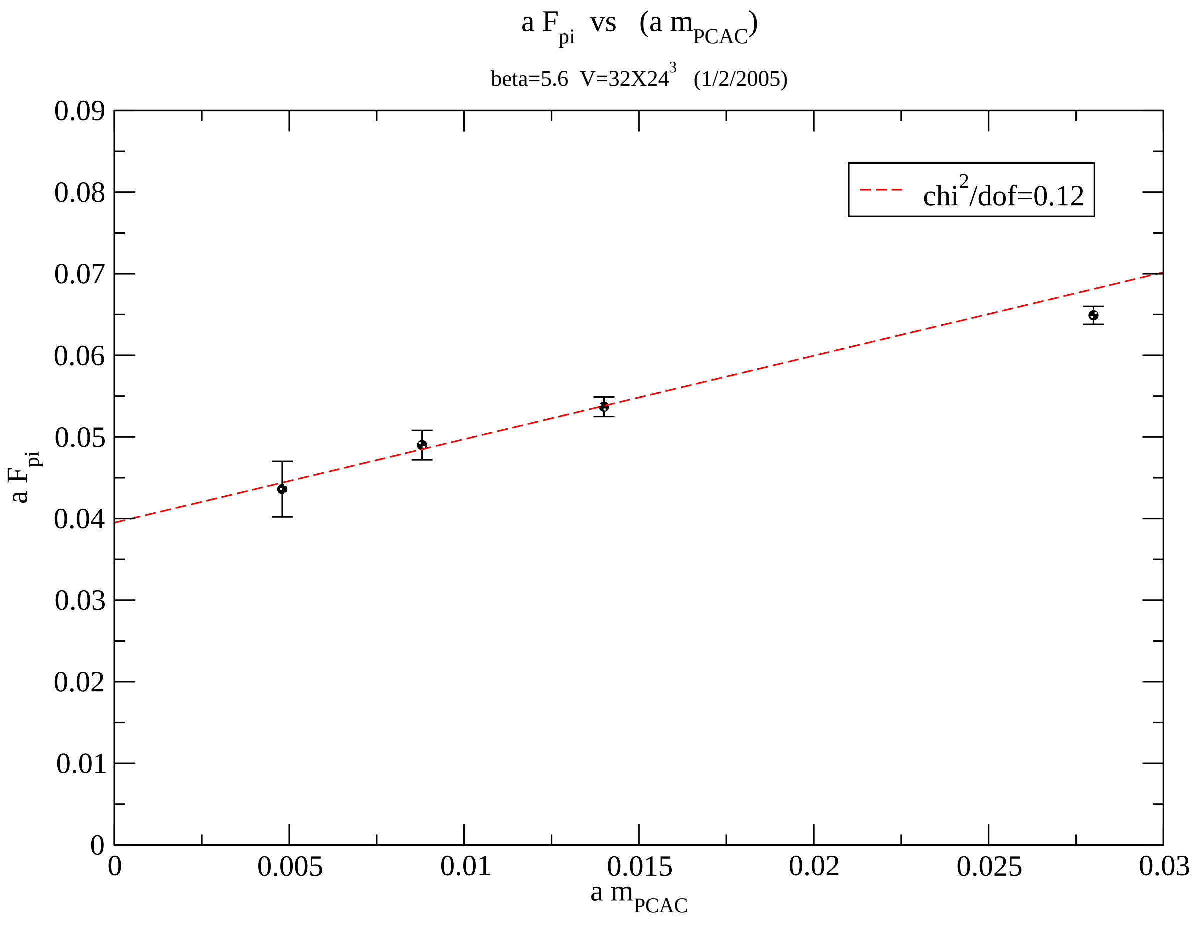

[Del Debbio, Giusti, Lüscher, Petronzio, Tantalo]

Perspectives

"Convincing precision" for CKM studies

$$a = 0.06 \div 0.09\text{fm} \qquad m_\pi = 300\text{MeV} \qquad L > 2.5\text{fm}$$

Quantity	precision
F_π	1.8%
F_K/F_π	<1 %
$K \to \pi$	<1 %
B_K	5%
$F_B\sqrt{B_B}$	5%
ξ	3%
$B \to \pi$	7%
$B \to D$	2%

[Sharpe 04]

Perspectives

- unquenching is fundamental to eliminate systematic errors
- lattice QCD: quantitative tool for NP physics

- dedicated algorithms + machines
- entering the age of “precision” full QCD simulations

- establish QCD as the theory of strong interactions
- precise determination of the SM parameters $[N_f = 3]$
- light dynamical quarks are the gateway to new strong dynamics