Lattice QCD with light Wilson quarks

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Wilson fermions

- ⋆ Conceptually well-founded
- ⋆ Non-perturbative improvement & renormalization
- ⋆ Fully worked out in qQCD

However, $\not{q}$QCD simulations tend to be exceedingly "expensive"

SESAM & TχL '98, UKQCD '99, CP-PACS '00, JLQCD '03, ...

With Wilson quarks we need, say,

$$a = 0.1 \longrightarrow 0.04\,\mathrm{fm}$$

$$L = 2 \longrightarrow 5\,\mathrm{fm}$$

$$m_\pi = 500 \longrightarrow 200\,\mathrm{MeV}$$

$\Rightarrow$ large lattices & solver iteration numbers

$$48 \cdot 24^3,\ 64 \cdot 32^3,\ 96 \cdot 48^3,\ \ldots$$

$10^3 - 10^4$ applications of $\not{D}$ per source field

Algorithms should be designed to work well in this regime!

Domain-decomposition methods

◇ Schwarz-preconditioned solver

◇ HMC on a block-decomposed lattice

M.L. '03 [JHEP 0305 (2003) 052; CPC 156 (2004) 209; CPC 165 (2005) 199]

Del Debbio, Giusti, M.L., Petronzio & Tantalo '05 [in preparation]

Hasenbusch acceleration

◇ HMC & PHMC with polynomial preconditioner

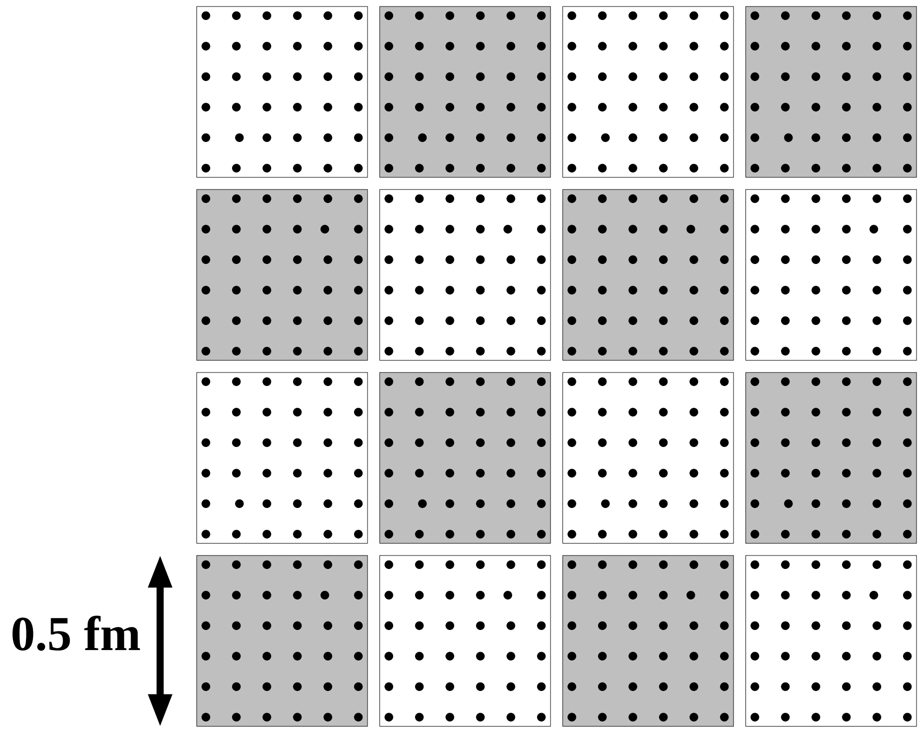
Hasenbusch '01 [PLB 519 (2001) 177]; Hasenbusch & Jansen '03 [NPB 659 (2003) 299];

Urbach, Jansen, Shindler & Wenger '05 [hep-lat/0506011] $\longrightarrow$ parallel talk by Urbach

Domain decomposition

In general the benefits are

- ⋆ *Parallel efficiency*
- ⋆ *Scale separation*
- ⋆ *Softer scaling behaviour*



The classical DD method is the *Schwarz Alternating Procedure*

Hermann Amandus Schwarz 1870:

Dirichlet problem in complicated domains

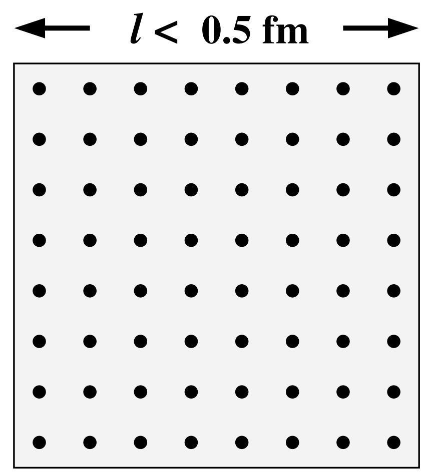
Widely used as a preconditioner in engineering (fluid dynamics etc.)

... and now also in lattice QCD**!**

see Y. Saad: Methods for Sparse Linear Systems, SIAM 2003, for example

The properties of QCD we shall exploit are

(a) *Asymptotic freedom*



Dirichlet b.c. on the blocks imply

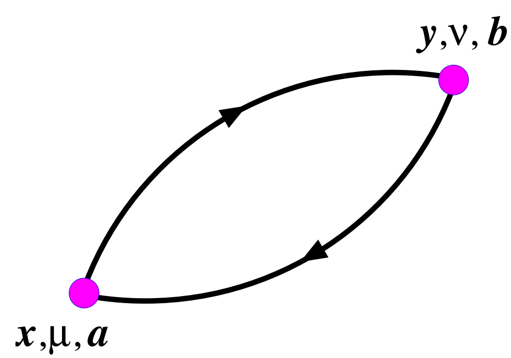
$$q \geq \pi/l > 1\,\mathrm{GeV}$$

$\Rightarrow$ easy to simulate at all quark masses

(b) *Ellipticity of the Dirac operator*

$$\frac{\delta^2 S_{\mathrm{eff}}}{\delta A_\mu^a(x)\delta A_\nu^b(y)} = 2\,\mathrm{tr}\{T^a\gamma_\mu S(x,y)T^b\gamma_\nu S(y,x)\}$$

$$\sim |x-y|^{-6}$$



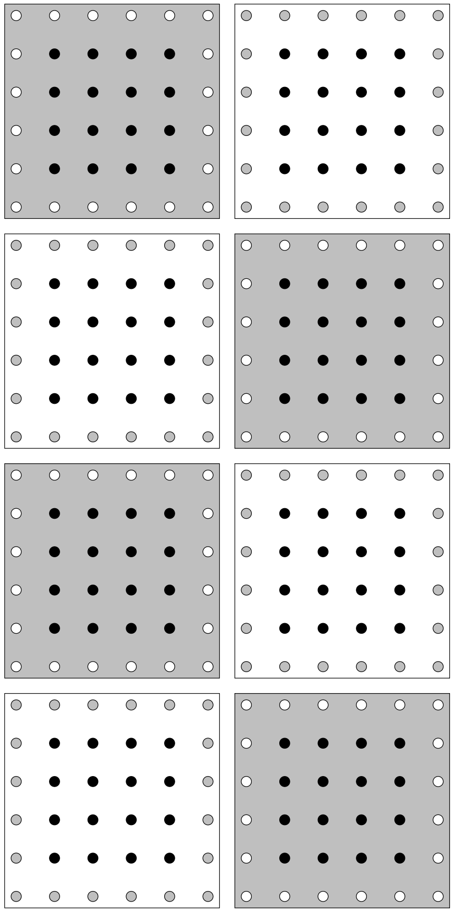
$\Rightarrow$ blocks are approximately decoupled

Block decomposition of the Dirac operator

black blocks: Ω

white blocks: Ω^*

exterior boundaries: $\partial\Omega$, $\partial\Omega^*$



$$D = \tfrac{1}{2}\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^*\nabla_\mu\} + m_0$$

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

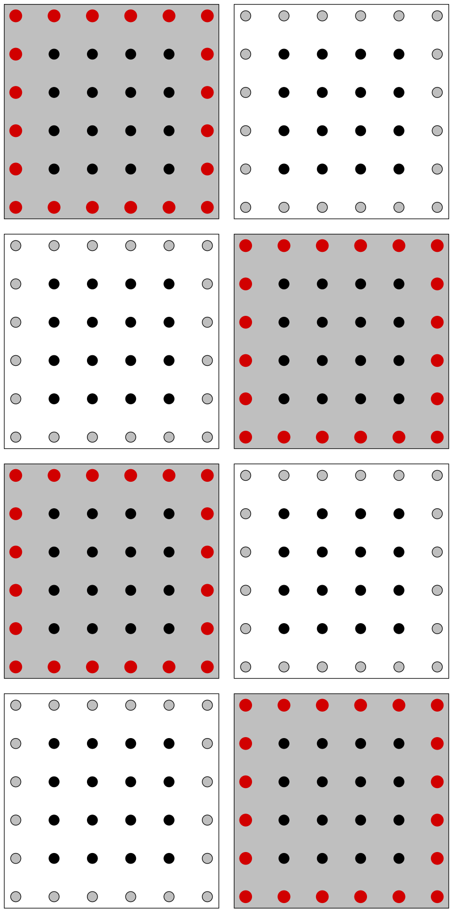
$$D_\Omega = \sum_{\text{black}\,\Lambda} D_\Lambda, \qquad D_{\Omega^*} = \sum_{\text{white}\,\Lambda} D_\Lambda$$

The quark determinant factorizes into

$$\det D = \prod_{\text{blocks}\,\Lambda} \det \hat{D}_\Lambda \times \det R$$

$\uparrow$ eo preconditioned, Dirichlet b.c.

$\mathcal{H}_{\partial\Omega^*}$: quark fields on $\partial\Omega^*$



where the block interaction is given by

$$R : \mathcal{H}_{\partial\Omega^*} \to \mathcal{H}_{\partial\Omega^*}$$

$$R = 1 - P_{\partial\Omega^*} D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}$$

Note that

$$R^{-1} = 1 - P_{\partial\Omega^*} D^{-1} D_{\partial\Omega^*}$$

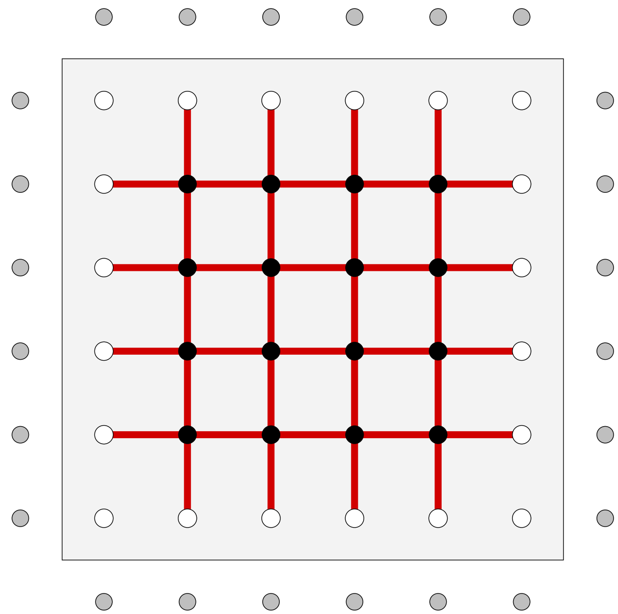
For $N_{\mathrm{f}} = 2$ flavours

$$S_{\mathrm{pf}} = \sum_{\mathrm{blocks}\,\Lambda} \|\hat{D}_{\Lambda}^{-1}\phi_{\Lambda}\|^2 + \|R^{-1}\chi\|^2$$

where χ is defined on $\partial\Omega^*$ and ϕ_Λ on the even sites in Λ

We now

- *evolve only the active link variables in the blocks and*
- *translate the gauge field after each trajectory by a random vector*



Fermion forces

$$\frac{\mathrm{d}}{\mathrm{d}t} U(x,\mu) = \Pi(x,\mu) U(x,\mu)$$

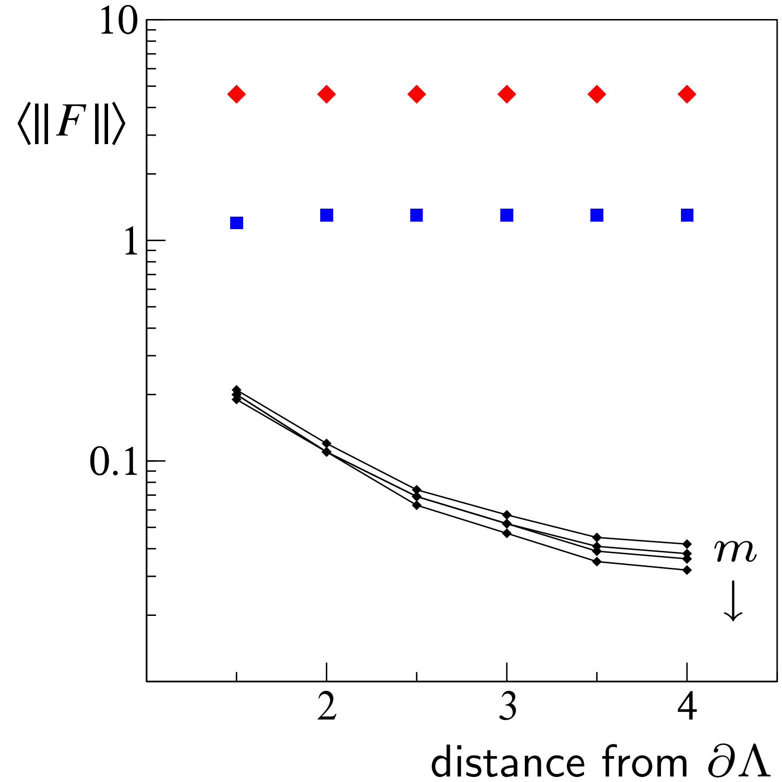
$$\frac{\mathrm{d}}{\mathrm{d}t} \Pi(x,\mu) = -F_{\mathrm{G}}(x,\mu) - F_{\Lambda}(x,\mu) - F_{R}(x,\mu)$$

Example

$32 \cdot 16^3$ lattice, 8^4 blocks

$\beta = 5.3$, $c_{\mathrm{sw}} = 1.9095$

$a \sim 0.1\,\mathrm{fm}$, $m \sim 14 - 70\,\mathrm{MeV}$



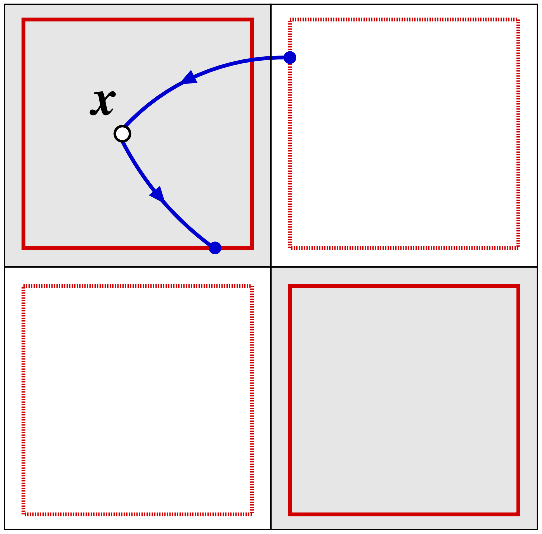
This behaviour is not unexpected since

(a) F_Λ is protected by the b.c. (*asymptotic freedom*)

(b) F_R is suppressed by propagators (*ellipticity*)

$$F_R(x,\mu) =$$

$$2\mathrm{Re}\left(R^{-1}\chi, D^{-1}\delta^U_{x,\mu} D D^{-1} D_{\partial\Omega^*}\chi\right)$$



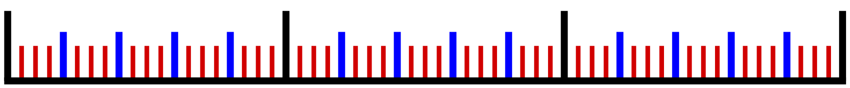
Leap-frog integration

Sexton & Weingarten '92; Peardon & Sexton '02

Choose integration step-sizes $\varepsilon_0, \varepsilon_1, \varepsilon_2$ such that

$$\varepsilon_0 \| F_{\mathrm{G}} \| \simeq \varepsilon_1 \| F_{\Lambda} \| \simeq \varepsilon_2 \| F_R \|$$

For example



$$\varepsilon_1 = 4\,\varepsilon_0, \quad \varepsilon_2 = 5\,\varepsilon_1$$

$\Rightarrow$ F_R is the most "expensive" but least-often computed force

Simulations

Del Debbio, Giusti, M.L., Petronzio, Tantalo [CERN – Tor Vergata]

$N_{\mathrm{f}} = 2$, Wilson action

Trajectory length $\tau = 0.5$ $\Rightarrow$ $\langle$link path length$\rangle = 0.53$

Schwarz-preconditioned solver

Residues $10^{-7} \ldots 10^{-11}$ $\Rightarrow$ reversibility $|(U' - U)_{ij}| < 10^{-9}$

lattice	β	κ	$\sim m/m_{\mathrm{s}}$	block size	τ/ε_2	N_{traj}	P_{acc}
$32 \cdot 24^3$	5.6	0.15750	0.93	$8 \cdot 6^2 \cdot 12$	5	6400	0.80
		0.15800	0.48		6	9500	0.80
		0.15825	0.30		10	9400	0.86
		0.15835	0.17		16	5000	0.91

Simulations performed on 8 nodes (16 Xeon processors) at the ITP Bern

Large-lattice runs

lattice	β	κ	$\sim m/m_{\mathrm{s}}$	block size	τ/ε_2	N_{traj}	P_{acc}
$64 \cdot 32^3$	5.8	0.15410	0.75	$16 \cdot 8^3$	8	5000	0.86
		0.15440	0.38		10	5050	0.89

Simulations performed on $32+32$ nodes at the Fermi Institute

The lattice spacing is

$$\left.\begin{array}{lll} a \sim 0.080\,\mathrm{fm} & \text{at} & \beta = 5.6 \\ a \sim 0.064\,\mathrm{fm} & \text{at} & \beta = 5.8 \end{array}\right\} L \simeq 2\,\mathrm{fm}$$

(Setting $r_0 = 0.5\,\mathrm{fm}$ at the point where $r_0 m_\pi = 1.26$)

Chiral behaviour of m_π and F_π

SU(2) ChPT predicts

$$m_\pi^2 = M^2 R_\pi, \quad M^2 = 2Bm$$

$$R_\pi = 1 + \frac{M^2}{32\pi^2 F^2} \ln(M^2/\Lambda_\pi^2) + \ldots$$

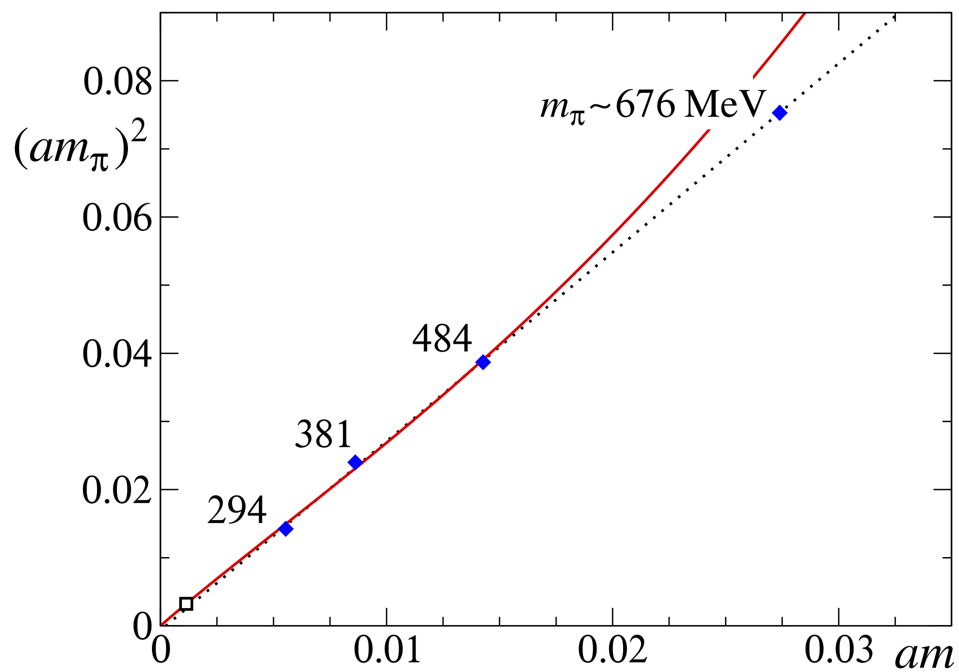
where, in real-world QCD,

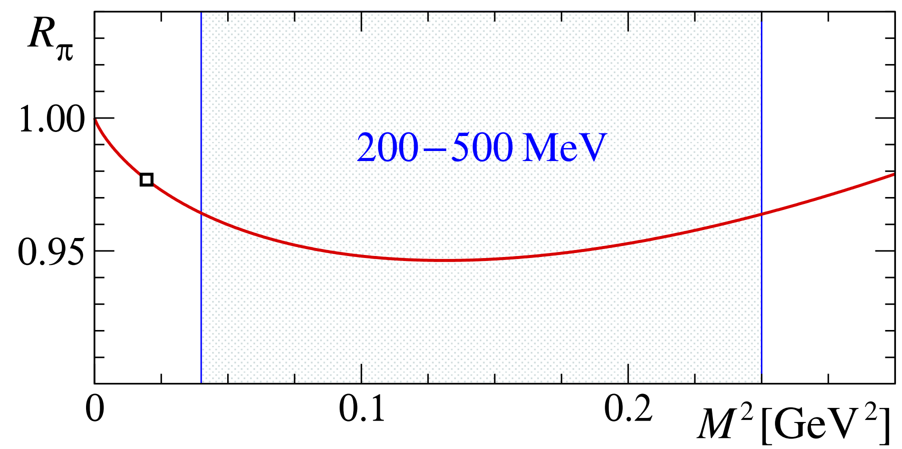
$$\ln(\Lambda_\pi^2/M^2)\big|_{M=140\,\mathrm{MeV}} \simeq 2.9 \pm 2.4$$

Gasser & Leutwyler '84

$\Rightarrow$ $R_\pi \simeq$ constant $= 0.956(8)$ in the range $M = 200 - 500\,\mathrm{MeV}$

$32 \cdot 24^3$ lattice





For F_π we expect

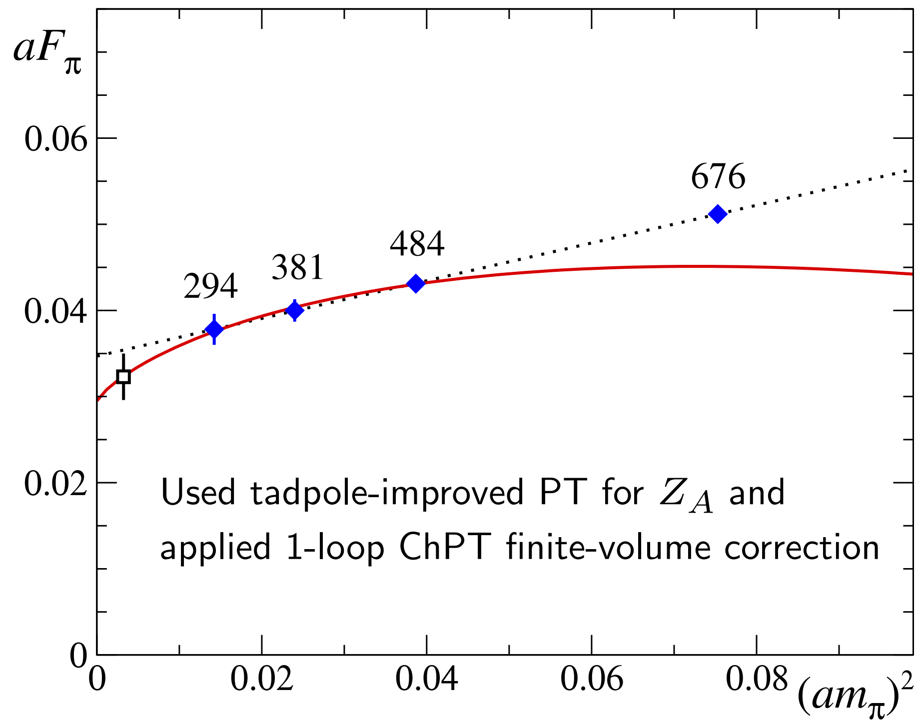
$$F_\pi = F - \frac{M^2}{16\pi^2 F}\ln(M^2/\Lambda_F^2) + \ldots$$

$$\ln(\Lambda_F^2/M^2)\big|_{M=140\,\mathrm{MeV}} \simeq 4.6 \pm 0.9$$

This fits the last three points

$$\Rightarrow F_\pi\big|_{M=140\,\mathrm{MeV}} = 80(7)\,\mathrm{MeV}$$

$32 \cdot 24^3$ lattice

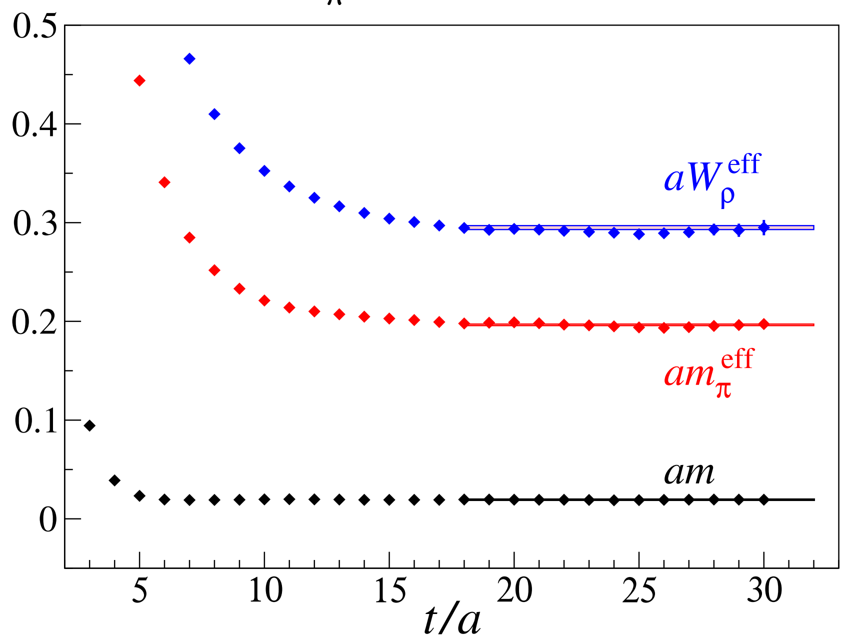


Within errors and up to $m_\pi \sim 500\,\mathrm{MeV}$,
the data are compatible with 1-loop ChPT

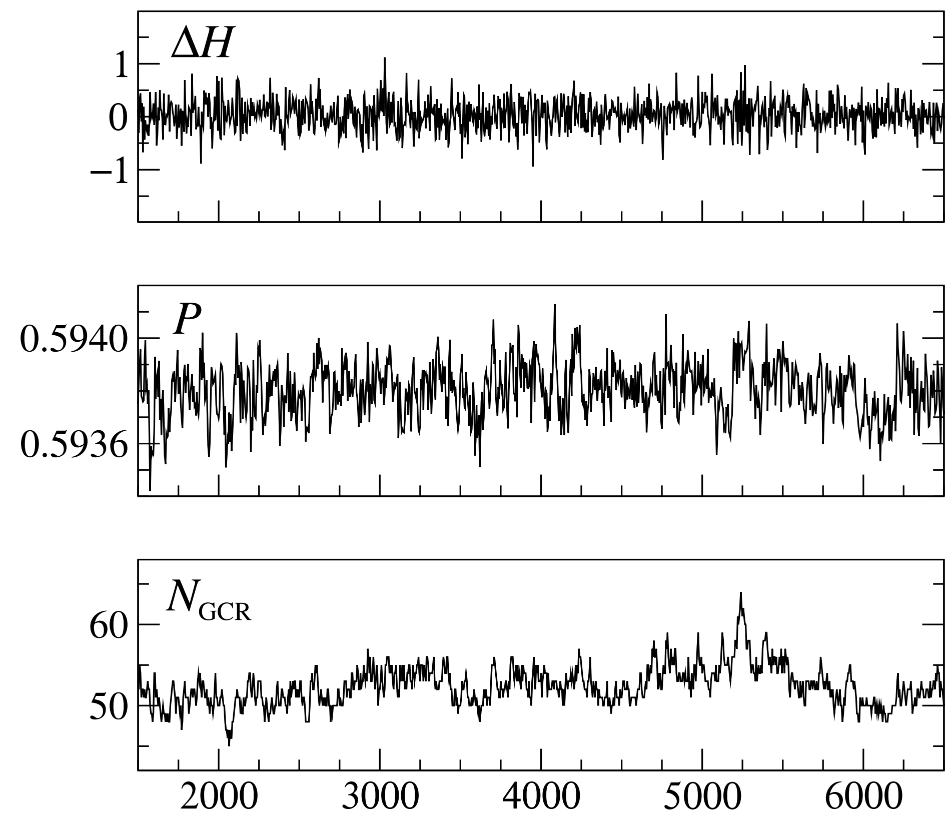
Large-lattice experiences

- ⋆ Similar step numbers as on the small lattices
- ⋆ Runs are very stable
- ⋆ Long effective-mass plateaus

$m_\pi \simeq 606\,\mathrm{MeV}$



$64 \cdot 32^3$ lattice, $m_\pi \simeq 429\,\mathrm{MeV}$



Performance figures & timings

A comparison of algorithms is non-trivial since

- *their efficiency depends on the lattice parameters, the program and the computer*
- *there are many tunable parameters*
- *it is generally difficult to determine the relevant auto-correlation times reliably*

A purely algorithmic cost figure is

$$\nu = 10^{-3}\,(2N_2 + 3)\,\tau_{\rm int}[P], \quad N_2 = \tau/\varepsilon_2$$

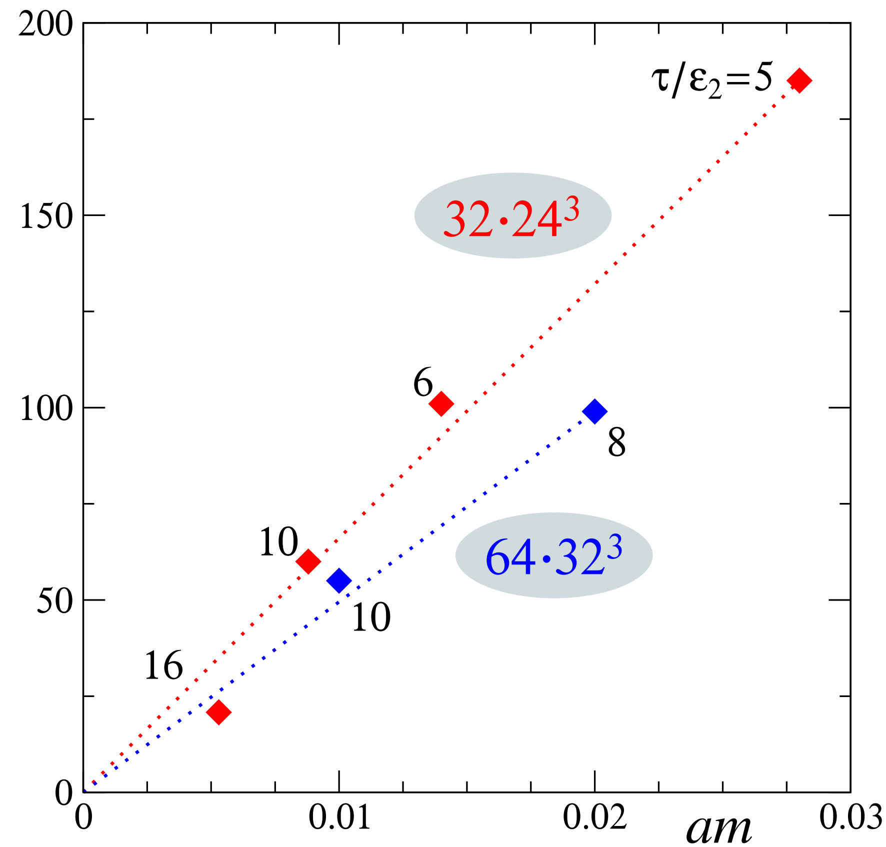
$\nu \simeq 5 - 29$ in previous HMC simulations [SESAM, UKQCD, CP-PACS, ...]

lattice	β	$c_{\rm sw}$	am	$\tau_{\rm int}[P]$	ν	
$32 \cdot 16^3$	5.3	1.9095	0.035	56(26)	0.84(39)	preliminary
			0.021	14(4)	0.27(8)	
			0.011	21(6)	0.40(11)	
			0.007	17(5)	0.39(12)	
$32 \cdot 24^3$	5.6	0.0	0.027	53(22)	0.69(29)	
			0.014	33(11)	0.50(17)	
			0.009	27(10)	0.62(23)	
			0.006	21(5)	0.74(18)	
$64 \cdot 32^3$	5.8	0.0	0.019	16(3)	0.30(6)	
			0.011	13(2)	0.30(5)	

Timings

Accepted trajectories per day using 8 and 32 nodes

Note that $\dfrac{64 \cdot 32^3}{32 \cdot 24^3} = 4.74$



Conclusions

Numerical simulations of LQCD with light Wilson quarks are much less "expensive" than previously estimated!

$\Rightarrow$ it is now possible to reach the chiral regime on large lattices

Example

$96 \cdot 48^3$ lattice, $12^2 \cdot 8^2$ blocks

$a = 0.06\,\mathrm{fm}$, $am = 0.0035$, $m_\pi = 270\,\mathrm{MeV}$

To simulate this lattice, a (current) PC cluster with 288 nodes should be sufficient

The Schwarz-preconditioned HMC algorithm

- ⋆ works out at $a \leq 0.1\,\mathrm{fm}$ and on large lattices, now also with $\mathrm{O}(a)$ improvement
- ⋆ scales favourably & is highly parallel
- ⋆ easily extends to gauge actions with 6-link terms (Iwasaki, Symanzik)

A wide range of physics questions may now be addressed, in a conceptually solid framework