Application of the Schwarz alternating procedure in lattice QCD

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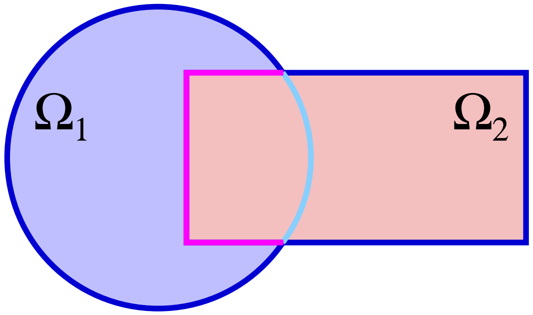
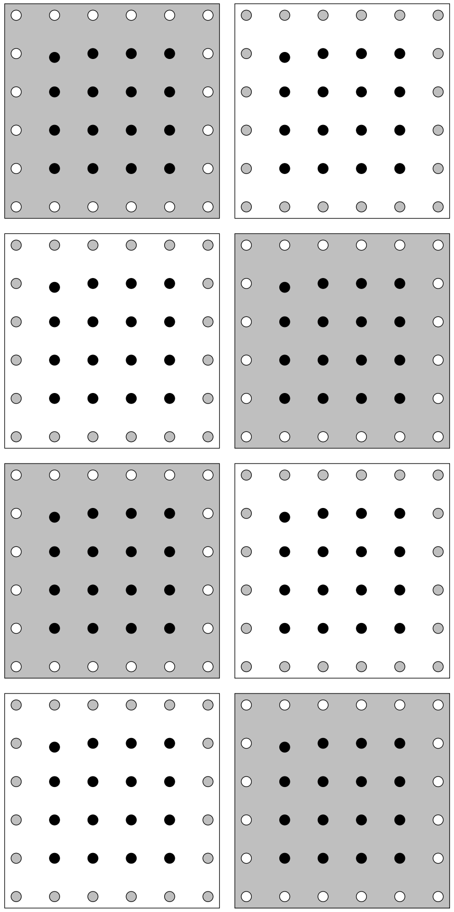
- Hermann Amandus Schwarz 1870:
  Dirichlet problem in complicated domains
- Probably first DD method
- Now very important in engineering



Center for Computational Sciences, University of Tsukuba, May 2004

Uses of the SAP in lattice QCD

12×24 lattice, periodic b.c.



1. Preconditioner for the lattice Dirac equation $D\psi = \eta$

2. Blocked HMC algorithm for two-flavour QCD

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

Which are the possible benefits?

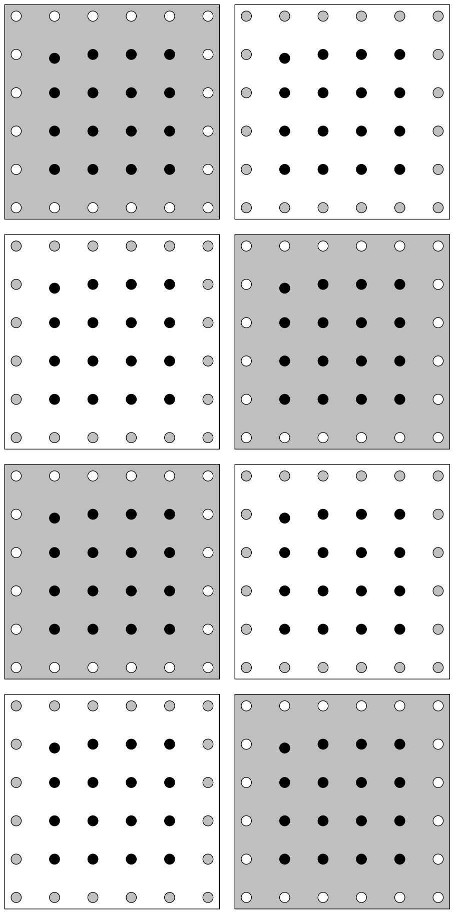
- Parallelization efficiency
  - ◇ Communication overhead
  - ◇ Data locality
- Algorithmic acceleration
  - ◇ Separation of short- & long-distance effects
  - ◇ Quark mass dependence
  - ◇ HMD stability

Block decomposition of the Dirac operator

black blocks: Ω

white blocks: Ω^*

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



Wilson–Dirac operator

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

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

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

Classical SAP

Generates approximate solutions $\psi_0, \psi_1, \ldots$ of $D\psi = \eta$ through

$$\psi_{n+1} = \psi_n + D_{\Omega}^{-1}(\eta - D\psi_n) \qquad \text{(if } n \text{ is even)}$$

$$= \psi_n + D_{\Omega^*}^{-1}(\eta - D\psi_n) \qquad \text{(if } n \text{ is odd)}$$

* $\psi_{n+1} = \psi_n$ in the complementary domain
* Amounts to alternatingly solving the Dirichlet problem on Ω and Ω^*

After $2n$ steps, starting from $\psi_0 = 0$, the procedure yields

$$\psi_{2n} = K \sum_{\nu=0}^{n-1} (1 - KD)^{\nu} \eta$$

$$K \equiv D_{\Omega}^{-1} + D_{\Omega^*}^{-1} - D_{\Omega^*}^{-1} D_{\partial\Omega^*} D_{\Omega}^{-1}$$

$\Rightarrow$ ψ_{2n} converges to the exact solution if $\|1 - KD\| < 1$

Appears to be so in practice, but the convergence is slow

Schwarz preconditioner

Solve the preconditioned system

$$DM_{\text{sap}}\phi = \eta, \qquad M_{\text{sap}} \equiv \text{a few Schwarz cycles},$$

using a Krylov space solver, and set $\psi = M_{\text{sap}}\phi$

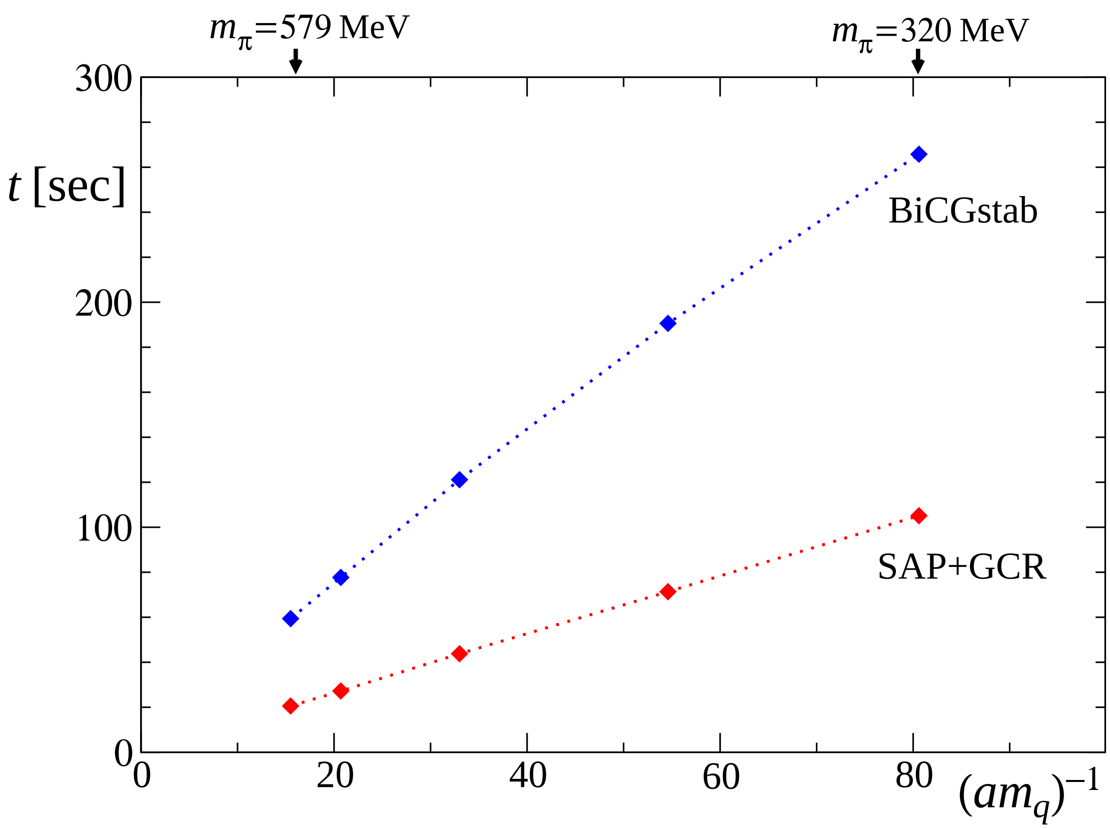
- GCR or FGMRES can be used here
- Accurate block solves are not required
- Ex.: 4 block MR steps, 5 Schwarz cycles

Numerical tests

48×24^3 lattice, $a = 0.10\,\text{fm}$, $m_q = 0.2 \ldots 0.7 \times m_s$ (pts of CP-PACS '03)

Using 8 nodes (16 processors) of a recent PC cluster

Schwarz block size $6^2 \times 4^2$, residue $\|\eta - D\psi\| \leq 10^{-8}\|\eta\|$



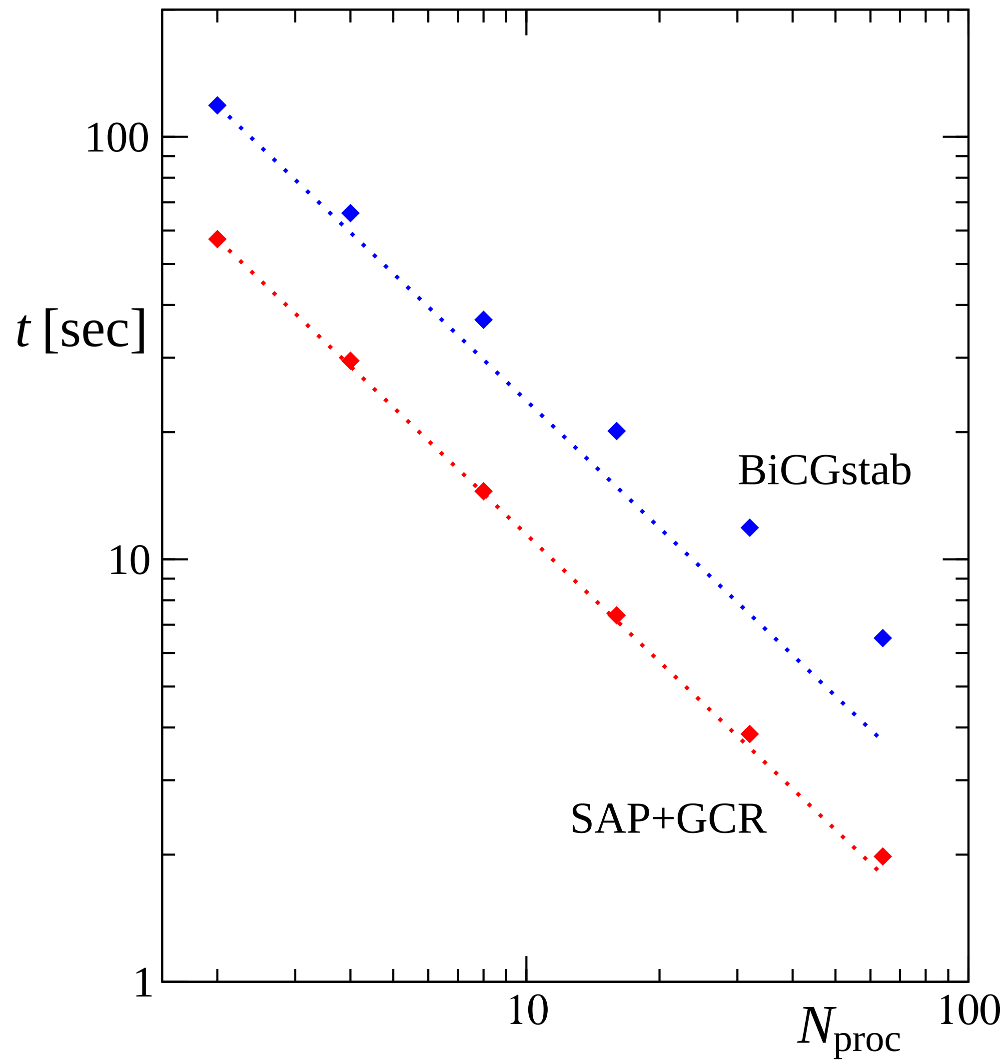
Parallel efficiency

32×16^3 lattice, $a = 0.10\,\mathrm{fm}$

$m_q \simeq 0.2 \times m_s$, residue 10^{-8}

Schwarz block size 8×4^3

Using up to 32 nodes (64 processors)



Blocked HMC algorithm for two-flavour QCD

Factorization of the quark determinant

$$D = \begin{pmatrix} D_{\Omega} & D_{\partial\Omega} \\ D_{\partial\Omega^*} & D_{\Omega^*} \end{pmatrix} \begin{matrix} \}\,\Omega \\ \}\,\Omega^* \end{matrix}$$

$$\det D = \det D_{\Omega} \, \det D_{\Omega^*} \, \det\{1 - D_{\Omega}^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}\}$$

May use even-odd preconditioning on the blocks

$$\det D_{\Omega} \, \det D_{\Omega^*} = \prod_{\text{blocks}\,\Lambda} \det \hat{D}_{\Lambda}$$

↑ Dirichlet b.c., even-odd preconditioned

The quark determinant thus becomes

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

where the block interaction operator R is

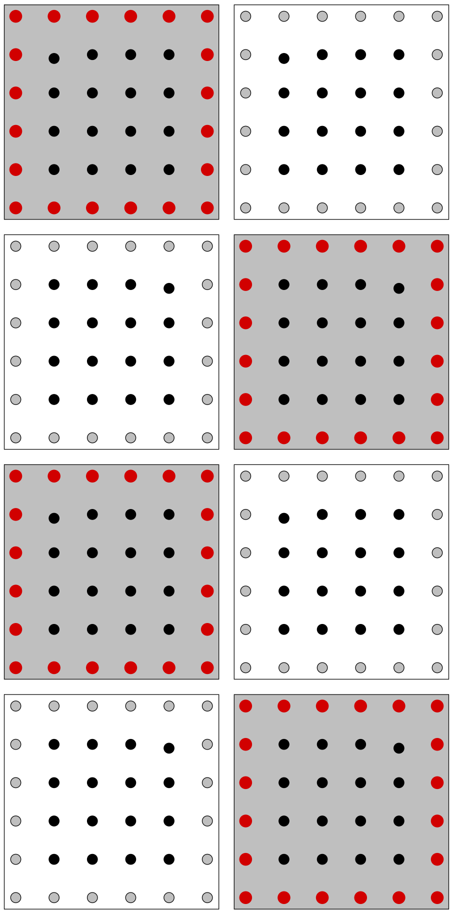
$$R : \mathcal{H}_{\partial\Omega^*} \longrightarrow \mathcal{H}_{\partial\Omega^*}$$

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

Its inverse is simply given by

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

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



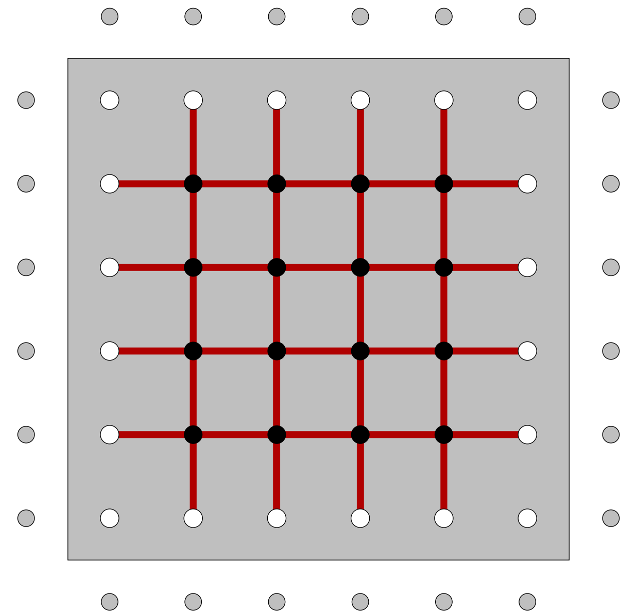
The associated pseudo-fermion action reads

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

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

We now

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



Test runs

$\beta = 5.6$, $a \sim 0.085\,\mathrm{fm}$ SESAM & TχL '03

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

SAP+GCR solver for $D\psi = \eta$

Residues $10^{-6} \ldots 10^{-11}$ $\Rightarrow$ reversibility $|(U' - U)_{ij}| < 10^{-8}$

lattice	κ	$\sim m_q/m_s$	block size	HMD steps	N_{traj}	P_{acc}
32×16^3	0.15750	0.84	8^4	$4, 5, 4$	12000	0.81
	0.15800	0.44	8^4	$5, 5, 4$	13100	0.86
	0.15825	0.26	8^4	$6, 5, 4$	9800	0.90
32×24^3	0.15750	0.84	$8 \times 6^2 \times 12$	$5, 5, 4$	8000	0.82

HMD driving force

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

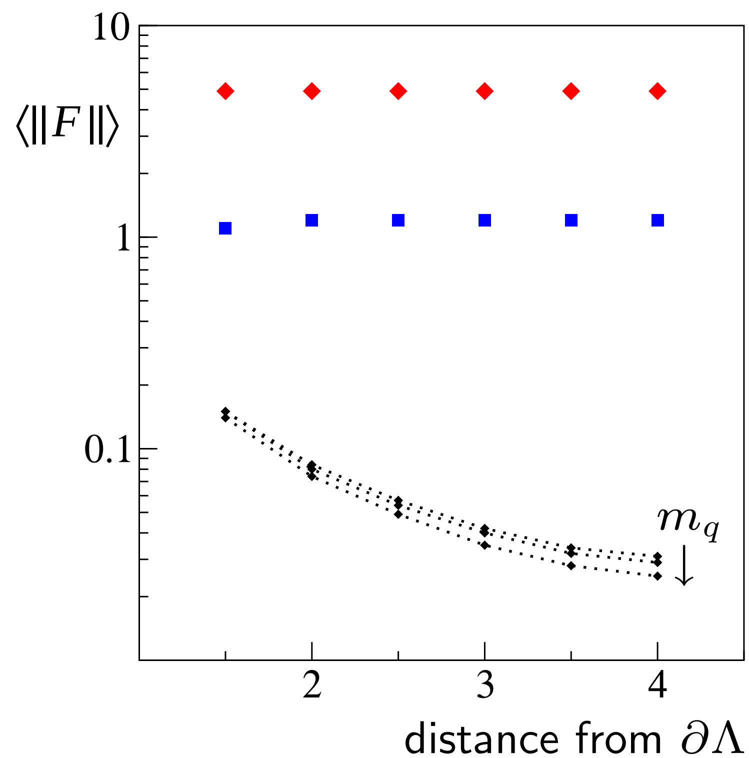
$$\frac{\mathrm{d}}{\mathrm{d}t} \Pi(x,\mu) = -F_{\mathrm{G}}(x,\mu) - F_{\Lambda}(x,\mu) - F_{R}(x,\mu)$$

★ The magnitudes are roughly
$28 : 7 : 1$

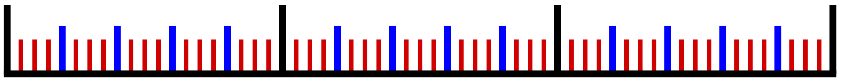
★ Short- and long-distance effects are separated

★ Quark mass dependence is weak

32×16^3 lattice



Integration step sizes



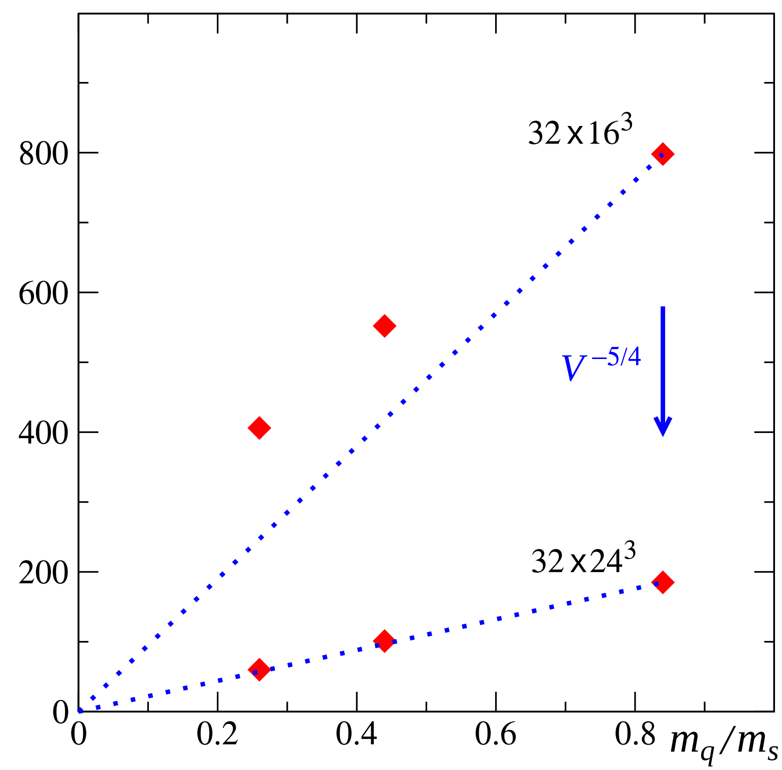
$$\delta\tau_R = 5\delta\tau_\Lambda\,, \qquad \delta\tau_\Lambda = 4\delta\tau_G$$

$\Rightarrow$ only few evaluations of F_R are required

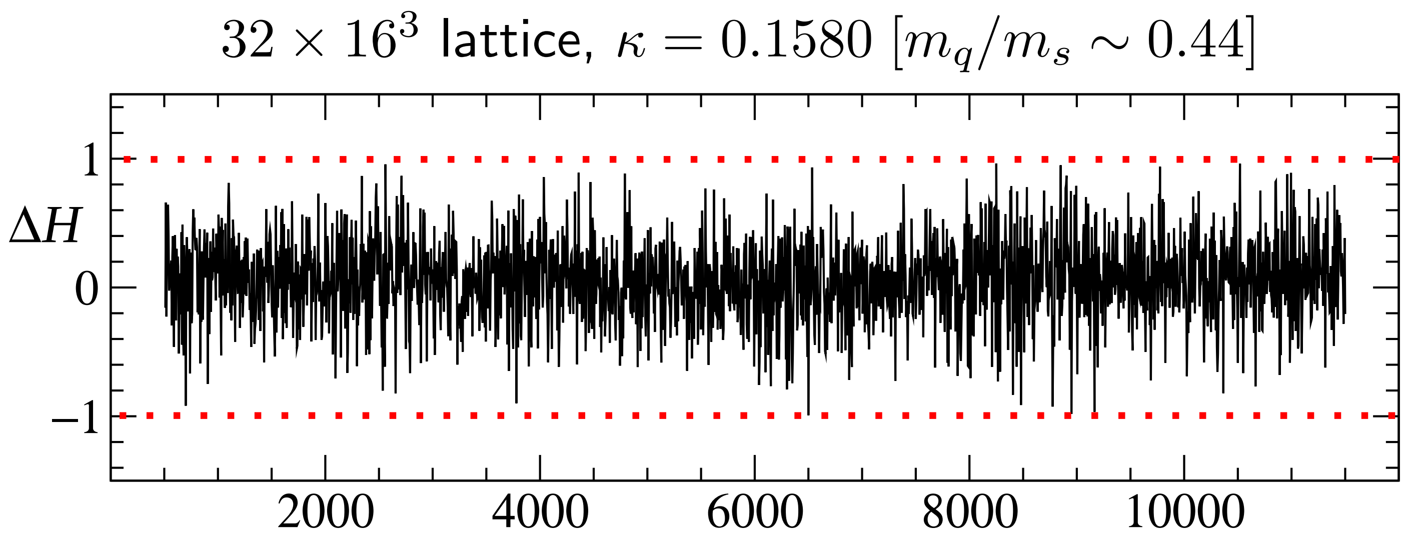
Sexton & Weingarten '92; Peardon & Sexton '02

Timings

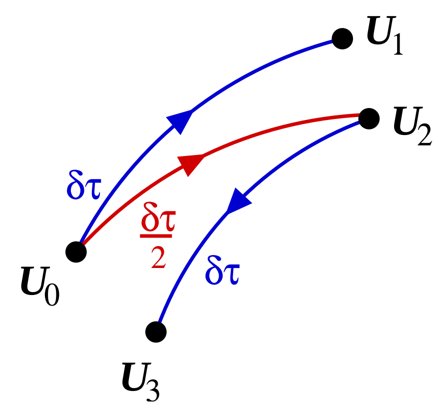
Accepted trajectories per day
using 8 nodes (16 processors)



HMD stability



Large spikes in ΔH are avoided by applying the rule



if $|\Delta H_{0\to1}| > 1.0$ replay trajectory with $\delta\tau \to \frac{1}{2}\delta\tau$

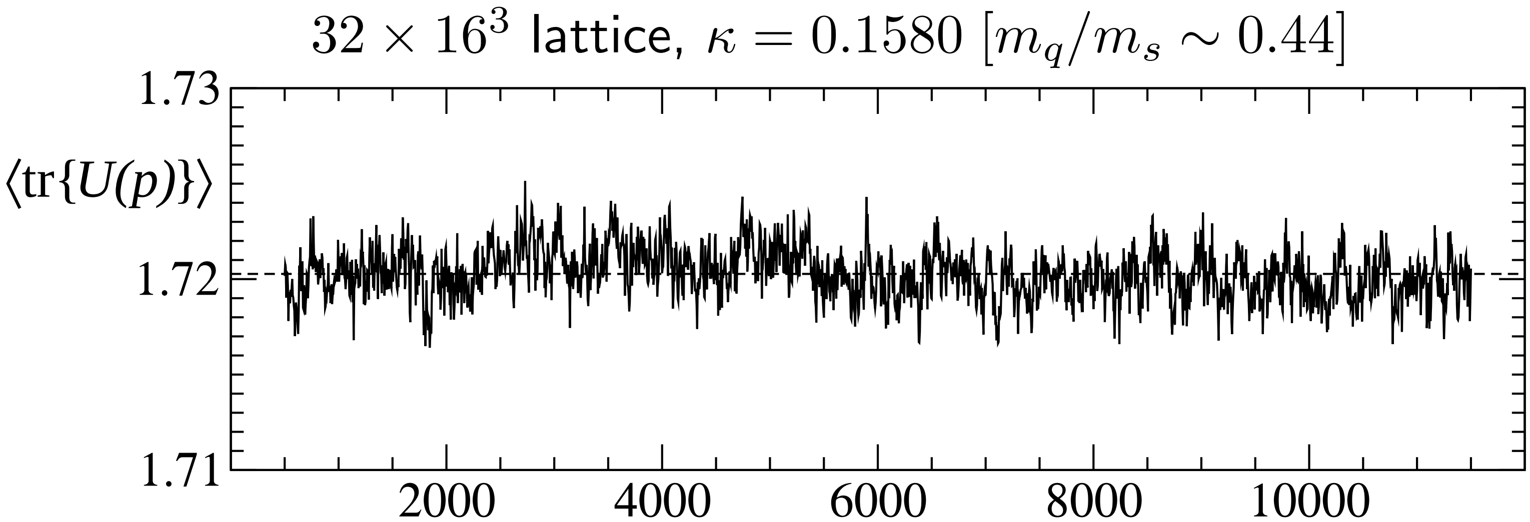
and accept with $P_{\rm acc} = \min\{1, e^{-\Delta H_{0\to2}}\}$ if $|\Delta H_{2\to3}| > 1.0$

Preserves detailed balance

M.L. & R. Sommer '04 (to be published)

Autocorrelation times

Still working on this . . .



* τ_{int}(plaquette) $= \mathrm{O}(50)$ trajectories

* Fields separated by ~ 100 trajectories are practically decorrelated

  Verified for $\sum_{\vec{x}} \langle P(x)P(0)\rangle$, $\sum_{\vec{x}} \langle A_0(x)P(0)\rangle$, . . .

Conclusion

The application of the Schwarz procedure in QCD leads to a

- ⋆ fast solver for the Dirac equation and an
- ⋆ efficient simulation algorithm for "QCD light"

Ex.: 64×32^3 lattice, $a \sim 0.1\,\mathrm{fm}$, $m_q \sim \frac{1}{4} m_s$ looks feasible on a PC cluster with 128 nodes

Todo list

- ⋆ Improved actions (SW, Iwasaki, LW, . . .)
- ⋆ QCD with $2 + 1$ flavours of quarks
- ⋆ Low-mode deflation