Full QCD Algorithms towards the Chiral Limit

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– (clover improved) Wilson fermions with two degenerate flavours

– **Hybrid-Monte-Carlo Algorithm**
Experience from large scale simulations
Speeding up the Hybrid-Monte-Carlo

– **Finite step-size updating**
Schwarz alternating procedure
Multiboson algorithm
TDA

The Hybrid Monte Carlo Algorithm

Collective molecular dynamics evolution of all gauge-fields; Introduce yet another auxiliary field:
conjugate momenta P for the gauge-field.
The resulting Hamiltonian

$$H(U,\phi,P) = S_G(U) + |M^{-1}\phi|^2 + \frac{1}{2}\sum_{x,\mu} \mathsf{Tr} P_{x,\mu}^2$$

Evolve according to Hamilton equations:
($q \rightarrow U$), ($p \rightarrow P$)

$$\frac{\mathrm{d}q}{\mathrm{d}t} = p \qquad ; \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}$$

The evolution can not be solved exactly. Numerical solution with error. Solved in the HMC by accept/reject step (S. Duane et al. 1987)

Integration schemes:
Leap-frog: $(\delta\tau)^2$ integration error, Higher order schemes, Split time-scales (Sexton and Weingarten)

Status of dynamical Wilson fermion simulations

Examples for large scale studies:
CP-PACS, Phys.Rev. D65 (2002) 054505.
Most recent JLQCD, hep-lat/0212039:
Hitachi SR8000 model F1; 100 nodes 1.2 Tflops peak;
about 300 days of simulation.
$\beta = 5.2 \rightarrow a \approx 0.09$

$m_{PS}/m_V \gtrapprox 0.6 >> 0.18$
$\rightarrow \chi$PT can not close the gap
(panel discussion lattice 2002)

Explorative studies (lattice 2002): $m_{PS}/m_V \approx 0.4$
- A.C. Irving, UKQCD, hep-lat/0208065,
- Y. Namekawa et al., CP-PACS, hep-lat/0209073.

Machines of the near future (2004): ≈ 10 Tflops
QCDOC (Columbia university, IBM)
apeNEXT (DESY, INFN, University Paris Sud)

Numerical costs of the HMC increases as sea-quarks become lighter

- Number of iterations of the solver increases

  BiCGStab, JLQCD:
  $N_{iter} = 0.253(4)\ \ (\kappa_c - \kappa)^{-0.893(2)}$
  Same exponent found in CP-PACS simulation at $\beta = 2.2$ with improved gauge action.

  Extrapolation:
  $m_{PS}/m_V \approx 0.6 \rightarrow m_{PS}/m_V \approx 0.4$ increases number of iterations roughly by a factor 4.

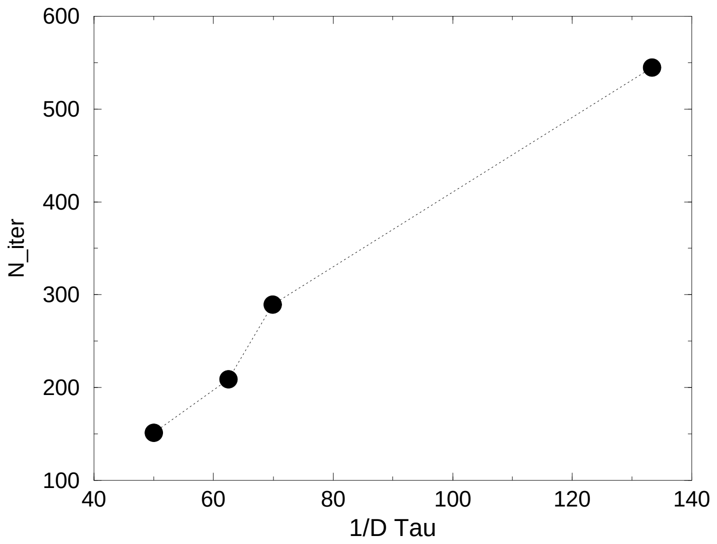
  Problems with convergence of BiCGStab:
  Y. Namekawa et al.: BiCGStab(DS-L)

  L. Gusti et al., Comp.Phys.Comm. 153 (2003) 31:
  Low mode preconditioning

- Autocorrelation times increase (?)
  No evidence from recent CP-PACS and JLQCD simulations for strong increase.
  Also studies at $m_{PS}/m_V \approx 0.4$ do not show large autocorrelation times.

- Step-size of the integration-scheme decreases for a constant acceptance rate
  Higher order schemes worse than leap-frog

  $\beta = 2.1$ Iwasaki gauge action, $24^3 \times 48$ lattice. Taken from table II of CP-PACS, hep-lat/0105015, Phys.Rev. D65 (2002) 054505. m_{PS}/m_V from 0.806(1) down to 0.576(3). Acceptance rate $P_{acc} \approx 0.78$ for all four points.



Modified Pseudo-Fermion Actions

Motivation:
Using the even-odd preconditioned Fermion matrix instead of the original fermion matrix allows for a larger step-size in the HMC at constant acceptance rate.

Split the Fermion matrix in two (or more) factors with reduced condition number each.

$$\bar{M} \ := \ W^{-1} M \ ,$$

Original choice: shift in the hopping parameter

$$W = M + \rho$$

Second choice (ALPHA-collaboration) inspired by twisted mass QCD:

$$W = M + i\rho\gamma_5$$

We introduce pseudo-fermions for both W and $\bar{M}$:

$$\det M M^{\dagger} \quad \propto$$

$$\int \mathcal{D}\phi_1^{\dagger} \int \mathcal{D}\phi_1 \int \mathcal{D}\phi_2^{\dagger} \int \mathcal{D}\phi_2 \; \exp(-|W^{-1}\phi_1|^2 - |\bar{M}^{-1}\phi_2|^2)$$

$$S_F = S_{F1} + S_{F2} = |W^{-1}\phi_1|^2 \; + |\bar{M}^{-1}\phi_2|^2$$

Variation of S_{F2} :

$$\delta S_{F2} = -X^{\dagger}\delta M Y - Y^{\dagger}\delta M^{\dagger} X + X^{\dagger}\delta W \phi_2 + \phi_2^{\dagger}\delta W^{\dagger} X$$

where

$$X = M^{\dagger -1} M^{-1} W \phi_2 \quad , \quad Y = M^{-1} W \phi_2$$

Even-odd preconditioning

K. Jansen and C. Liu, Comp.Phys.Com.99 (1997) 221

– Asymmetric even-odd preconditioning:

$$\det \begin{pmatrix} 1_{ee}+T_{ee} & H_{eo} \\ H_{oe} & 1_{oo}+T_{oo} \end{pmatrix} \propto \det(1_{ee}+T_{ee}) \det \hat{M}$$

where

$$\hat{M} = 1_{oo} + T_{oo} - H_{oe}(1_{ee}+T_{ee})^{-1}H_{eo}$$

– Symmetric even-odd preconditioning:

$$\det \begin{pmatrix} 1_{ee}+T_{ee} & H_{eo} \\ H_{oe} & 1_{oo}+T_{oo} \end{pmatrix}$$

$$\propto \det(1_{ee}+T_{ee}) \det(1_{oo}+T_{oo}) \det \hat{M}$$

where now

$$\hat{M} = 1_{oo} - (1_{oo}+T_{oo})^{-1}H_{oe}(1_{ee}+T_{ee})^{-1}H_{eo}$$

ll-SSOR, W. Bietenholz et al. Comput. Phys. Commun. 119, (?!).

Numerical Results for clover-improved Wilson-Fermions with even-odd preconditioning, Wilson gauge action

– Hasenbusch and Jansen, hep-lat/0211042, Nucl.Phys.B 659 (2003) 299.
$\beta = 5.2$, $c_{sw} = 1.76$ (preliminary value),
$m_{PS}/m_V \approx 0.856, 0.792, 0.715$ and 0.686
$16^3 \times 24$ lattice.

- Autocorrelation times for fixed acceptance rate does not depend on the type of pseudo-fermion action
- Reversibility violations are similar for standard and modified pseudo-fermion action
- $W = M + \rho$ a little better than $W = M + i\rho\gamma_5$
- At the smallest m_{PS}/m_V partially improved integration scheme of Sexton and Weingarten profits more than leap-frog:

scheme	ρ	$\delta\tau$	P_{acc}	N^{total}
L	0.0	0.01	0.77(3)	17000
L	0.5	0.02	0.78(2)	9500
S	0.0	0.0166...	0.82(2)	21200
S	0.2	0.066...	0.74(3)	6900

– QCDSF Collaboration, hep-lat/0303026
See Poster by H. Stüben for details

- $W = M + \rho$
- leap-frog integration scheme
- S_{F1} on smaller time scale as S_{F2}
  (Following Peardon and Sexton)

$\beta = 5.29$, $c_{sw} = 1.9192$, $\kappa = 0.1355$, $m_{PS}/m_V \approx 0.7$, $16^3 \times 32$ lattice.
Speedup of 2.82 for method B and 3.42 for method C.
A factor 1.5 reduction in N_{iter} . (?)

– ALPHA Collaboration, hep-lat/0307008,
See talk by F. Knechlti

- $W = M + i\rho\gamma_5$
- partially improved scheme of Sexton and Weingarten
- Schrödinger functional boundary conditions ; small physical Volume

Very careful study of reversibility and autocorrelation times

Speedup of about 2

Preliminary results for 3 pseudo-fermion fields

Repeating a run of A. Irving reported at the lattice 2002 conference:
2300 trajectories. $16^3 \times 32$ Lattice, $\beta = 5.2$, $c_{sw} = 2.0171$, $\kappa = 0.1358$, $m_{PS}/m_V = 0.43(2)$, $m_\pi L = 3.3(1)$.
<Plaq>=0.53770(4), $\tau \approx 7$
Step-size for the leapfrog: 1/400

50 trajectories, 2 pseudo-fermion fields, $\rho = 0.05$ Step-size: $1/33$ for the Sexton-Weingarten improved scheme. Acceptance rate: $0.81(4)$.

1500 trajectories, 3 pseudo-fermion fields, $\rho_1 = 0.4$, $\rho_2 = 0.03$, Step-size: $1/25$ for the Sexton-Weingarten improved scheme. Acceptance rate: $0.809(6)$. <Plaq>=0.53773(5) , $\tau = 7.5 \pm 3.0$.

Variants of the method

M. Peardon, hep-lat/0201003, Nucl.Phys.Proc.Suppl. 106 (2002) 3.
M. Peardon and J. Sexton, hep-lat/0209037.

$$W^{-1} = P_0(M)$$

where $P_0(M)$ is a low order polynomial approximation of M^{-1}.
Put $S_{F1} = |P_0(M)\phi_1|^2$ and $S_{F2} = |(P_0(M)M)^{-1}\phi_2|^2$ on different time scales

Tests only in the 2D Schwinger model yet.
For application to QCD see talk by M. Peardon

Simple Modification: Polynomial HMC with

$$M^{-1} \approx P_0(M)P_1(M)$$

Pseudo-fermion field for each of the two polynomials.

Remark on Reversibility

P. de Forcrand and Takaishi, Nucl.Phys.Proc.Suppl. 53 (1997) 968:
Relaxed stopping criterion for the solver (with fixed start vector) does not destroy reversibility of the integration scheme. (Assuming exact arithmetics)

In practice: Reversibility violations become large as the stopping criterion is relaxed.

Therefore start vector from educated guess (Brower et al.) in combination with high accuracy solution seems more favourable.

Consider the linear equations

$$Q^2[U]\psi = \phi \quad \text{and} \quad Q^2[U']\psi' = \phi$$

where $|U_{x,\mu} - U'_{x,\mu}| \sim \epsilon$

Denote the approximate solution of the CG-solver after i iterations by $\psi^{(i)}$ and $\psi^{(i)'}$. We start the iteration with the same vector in both cases.

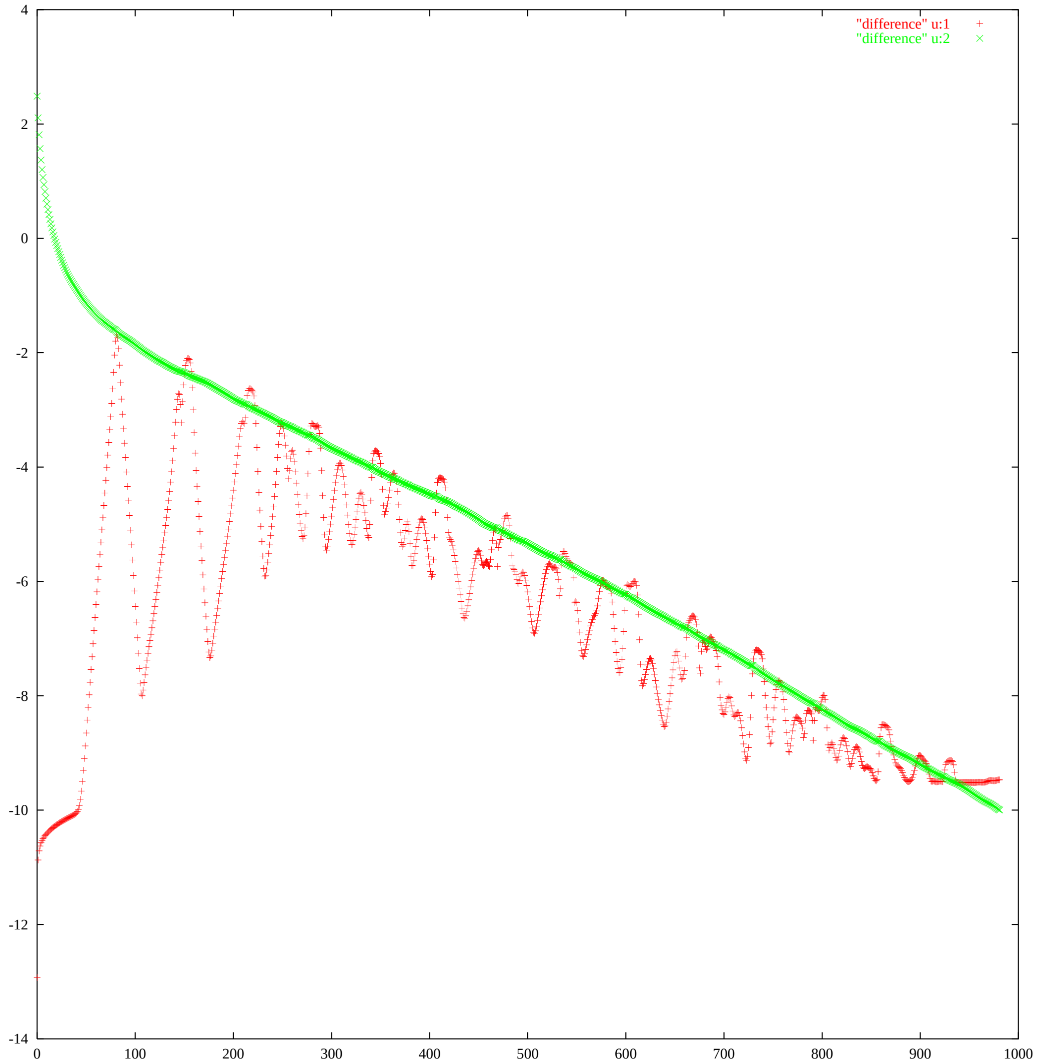
Study

$$\Delta^{(i)} := ||\psi^{(i)} - \psi^{(i)'}||$$

The Residue

$$r^{(i)} := ||Q^2[U]\psi^{(i)} - \phi||$$

Gauge-field U from $16^3 \times 24$ lattice, $\beta = 5.2$, $m_{PS}/m_V \approx 0.686$, $\epsilon = 10^{-14}$



Possible solution of the Problem: Use Polynomial approximation of M^{-1} instead of solver

Finite Step-Size Algorithms

Multiboson and variants of it

qq+q collaboration, TSMB algorithm,
I. Montvay, hep-lat/0301013

$\frac{1}{6}m_s < m_q < 2m_s$ on coarse lattices

Costs of the simulation increase as m_{PS}^z with $3 < z < 4$
- Order of the polynomials increases
- Autocorrelation times increase

Clover term difficult to implement

Low modes with Lanczos

A. Duncan, E. Eichten, J. Yoo, hep-lat/0209123:

- The extraction of low eigenvalues by Kylov subspace methods such as the Lanczos algorithm does not deteriorate as a consequence of very small eigenvalues.

TDA approximation:

$$\text{det}Q^2 \approx \prod_{i=1}^{N_{eig}} \lambda_i^2$$

Test at $a \approx 0.17$ fm, $10^3 \times 20$ lattice, $N_{eig} = 520$, $m_{PS} \approx 200$ MeV

Combination with MB algorithm or PHMC algorithm: Correction with

$$\prod_i \lambda_i^2 P(\lambda_i)^2$$

Lattice QCD and the Schwarz alternating procedure

Split the lattice into a block Λ and its complement Λ^*.

```
o o o o o o o o o o
o o o o o o o o o o
o o o x x x x o o o
o o o x x x x o o o
o o o x x x x o o o
o o o x x x x o o o
o o o o o o o o o o
o o o o o o o o o o
```

Perform updates (HMC restricted to the block, local updates ...) inside the block Λ that generate the gauge fields with a probability

$$P(U) \propto \exp(-S_G(U))\, \mathrm{det}(Q_\Lambda + Q_{\Lambda^*})^2$$

where Q_Λ and Q_{Λ^*} is the (Hermitian) fermion matrix restricted to Λ and Λ^* respectively.
Note that Q_Λ has a much smaller condtion number than Q for sufficiently small Λ.

Then a Metropolis accept/reject step is needed

$$A = \min\left[1, \quad \frac{\frac{\mathrm{det} Q'^2}{\mathrm{det}(Q'_\Lambda + Q_{\Lambda^*})^2}}{\frac{\mathrm{det} Q^2}{\mathrm{det}(Q_\Lambda + Q_{\Lambda^*})^2}}\right]$$

Since it is too expensive to compute the determinants of Q, $Q_\Lambda + Q_{\Lambda^*}$ we need stochastic estimates:

Naively: introduce standard Pseudo-fermions for the ratio

$$\frac{\mathrm{det} Q^2}{\mathrm{det}(Q_\Lambda + Q_{\Lambda^*})^2}$$

Important result:
Elimination of boundary terms
Only noise vector with support on the boundary of Λ needed.

Implementation as full algorithm still missing.
M. Lüscher is working on it.

Conclusion and Outlook

- Modified pseudo-fermion actions allow for larger step-size in the HMC and PHMC algorithm.
  Speedup increases as the mass of the quarks decreases.
  Higher order intergration schemes seem to profit more from a modified pseudo-fermion action than the leap-frog

- Improvement of the iterative solvers highly desireable;
  new idea: low mode preconditioning

- HMC or PHMC simulation of dynamical clover-improved Wilson fermions at $a \approx 0.1$ fm down to $m_{PS}/m_V \approx 0.4$ on the next generation of computers seems feasable

- HMC and PHMC still seem to be the first choice
  But keep on working on alternative methods!