Improvement of algorithms for dynamical overlap fermions

Hideo Matsufuru for JLQCD Collaboration

(with H.Fukaya, S.Hashimoto, K.Kanaya, T.Kaneko,

M.Okamoto, K.Ogawa, T.Onogi, and N.Yamada)

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Project

Dynamical simulation with overlap fermions

- New project of JLQCD Collaboration
- Main run: $16^3 \times 32$, $a \simeq 0.12$fm (larger size is planned)
- lightest quark mass $\simeq m_s/6$
- $N_f = 2 \to$ extended to $N_f = 2 + 1$
- Fixed topology by extra Wilson fermion
  - need to examine the effect of fixing topology

Other talks at Lattice 2006

- *T.Kaneko, overview of project*
- *S.Hashimoto, extra-Wilson fermion to fix topology*
- *N.Yamada, locality and choice of gauge action*
- *H.Fukaya, ϵ regime*
- *M.Okamoto, spectrum and chiral log (canceled)*

New machines at KEK

Working since March 2006

Hitachi SR11000

- 2.15TFlops, 512MB memory
- 16 Power5+ $\otimes$16 nodes

IBM System Blue Gene Solution

- 57.3TFlops, 5TB memory
- 1024 nodes $\otimes$10 racks
- $8 \times 8 \times 8$ torus network
- 2 PowerPC440 shares 4MB cache

Wilson kernel for BG:
Tuned by IBM Japan (J.Doi and H.Samukawa)

- double FPU instructions for complex arithmetics
- low level communication API

Wilson solver: $\sim$24% of peak performance (on cache)

Action

$$S = S_G + S_F + S_E$$

- Gauge field S_G: Iwasaki (renormalization group improved)
- Overlap fermion ($N_f = 2$): $S_F = \phi^\dagger [D(m)^\dagger D(m)]^{-1} \phi$

  overlap Dirac operator

$$D(m) = \left(M_0 + \frac{m}{2} \right) + \left(M_0 - \frac{m}{2} \right) \gamma_5 \mathsf{sign}(H_W)$$

  $H_W = \gamma_5 D_W$, D_W is Wilson-Dirac operator with $-M_0$
- Extra Wilson fermion:

$$\det \left(\frac{H_W^2}{H_W^2 + \mu^2} \right) = \int \mathcal{D}\chi^\dagger \mathcal{D}\chi \exp[-S_E]$$

  — suppresses near-zero modes of H_W

  Vranas (2000), Fukaya (2006) $\longrightarrow$ S.Hashimoto's talk for details

HMC algorithm

Building blocks of accelerating HMC:

- Hasenbusch preconditioning: $S_F = S_{PF1} + S_{PF2}$

  M.Hasenbusch, Phys. Lett. B 519 (2001) 177.

$$S_{PF1} = \phi_1^\dagger [D(m')^\dagger D(m')]^{-1} \phi_1 \quad \text{(preconditioner)}$$

$$S_{PF2} = \phi_2^\dagger \left\{ D(m')[D(m)^\dagger D(m)]^{-1} D(m')^\dagger \right\} \phi_2$$

- Multi-time step: $\Delta\tau_{(PF2)} > \Delta\tau_{(PF1)} > \Delta\tau_{(G)} = \Delta\tau_{(E)}$

  J.C.Sexton and D.H.Weingarten, Nucl. Phys. B 380 (1992) 665.

- Overlap solver: 5D CG/relaxed CG
- Reflection/refraction at $\lambda_{min} = 0$

  Z.Fodor, S.D.Katz and K.K.Szabo, JHEP0408 (2004) 003.

  – Needs monitoring of λ_{min} and inverting $D^\dagger D$

  $\Rightarrow$ skipped: $\lambda_{min} = 0$ is avoided by S_E

Noisy Metropolis

Most time consuming part: solvers in molecular dynamics
Cost in MD is reduced by

- assuming no near-zero mode
- fixed λ_{thrs}, $N \simeq 10 \to$ adopting 5D solver
- no eigenvalue determination

Error in MD is corrected by Noisy Metropolis:

A.D.Kennedy and J.Kuti, Phys. Rev. Lett. 54 (1985) 2473.

After usual Metropolis, accept U_{new} with $P = \min\{1, e^{-dS}\}$,

$$dS = \left| W^{-1}[U_{new}] W[U_{old}]\, \xi \right|^2 - |\xi|^2$$

where $W = D(m)/D'(m)$, ξ Gaussian noise vector,

- D': relaxed overlap operator used in MD
- D: accurate overlap operator

Solver algorithm (1)

Overlap Dirac operator

$$D(m) = \left(M_0 + \frac{m}{2}\right) + \left(M_0 - \frac{m}{2}\right)\gamma_5 \mathrm{sign}(H_W)$$

Zolotarev's partial fractional approximation

J. van den Eshof et al., Comp. Phys. Comm. 146 (2002) 203.

$$\mathrm{sign}(H_W) = \frac{H_W}{\sqrt{H_W^2}} = H_W \left(p_0 + \sum_{l=1}^{N} \frac{p_l}{H_W^2 + q_l}\right)$$

- $(H_W^2 + q_l)^{-1}$: determined by Multishift CG simultaneously
- For smaller λ_{min}, larger N is needed for accuracy
  e.g. for N=10, $O(10^{-7})$ accuracy for λ_{min}=0.05 and $O(10^{-5})$ for 0.01.
- Subtraction of low modes of H_W
  $\rightarrow$ sign(λ) ($\lambda < \lambda_{thrs}$) is explicitly determined

Solver algorithm (2)

Overlap solver algorithms

- Nested CG
- 5-dimensional CG

□ Nested CG algorithm

- Outer CG for overlap operator
- Inner CG for $(H_W^2 + q_l)^{-1}$ $(l = 1, ..., N)$: multishift CG

  A.Frommer et al., Int. J. Mod. Phys. C 6 (1995) 627.

  – Relaxed CG: ϵ_{in} is relaxed as outer iteration proceeds

  N.Cundy et al., Comp. Phys. Comm. 165 (2004) 221.

- Subtraction of low-modes of H_W applicable.

  $\longrightarrow$ stable against $\lambda_{min} \sim 0$
- Cost is almost unchanged as N

Solver algorithm (3)

- 5-dimensional CG solver
  R.G.Edwards et al., PoS LAT2005 (2006) 146.

$$M_5 = \left(\begin{array}{cccc|c} H & -\sqrt{q_2} & & & 0 \\ -\sqrt{q_2} & -H & & & \sqrt{p_2} \\ & & H & -\sqrt{q_1} & 0 \\ & & -\sqrt{q_1} & -H & \sqrt{p_1} \\ \hline 0 & \sqrt{p_2} & 0 & \sqrt{p_1} & R\gamma_5 + p_0 H \end{array}\right) = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right)$$

Schur decomposition:

$$M_5 = \tilde{L}\tilde{D}\tilde{U} = \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix}$$

where

$$S = D - CA^{-1}B = R\gamma_5 + p_0 H + H \sum_i \frac{p_i}{H^2 + q_i}$$

Solver algorithm (4)

By solving

$$M_5 \begin{pmatrix} \phi \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix},$$

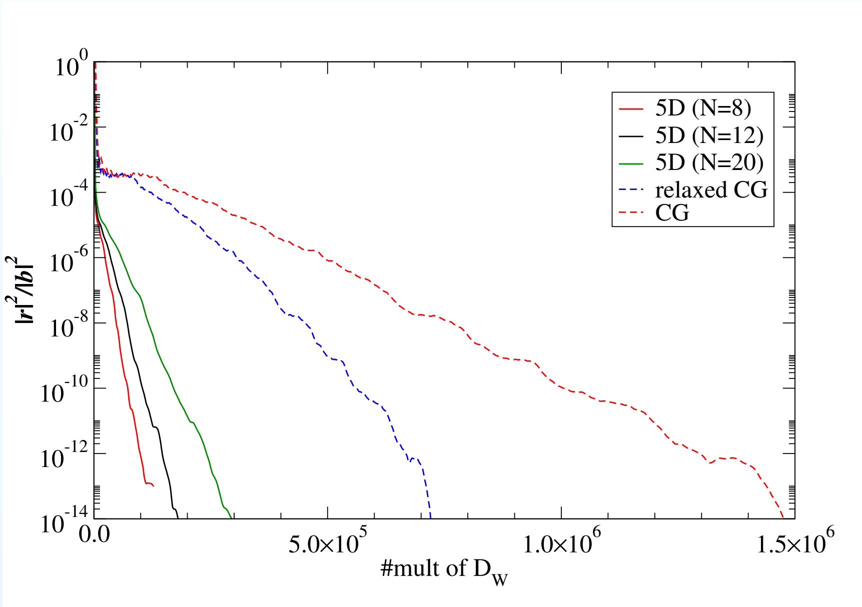
$\psi_4 = S^{-1}\chi_4$ is determined.

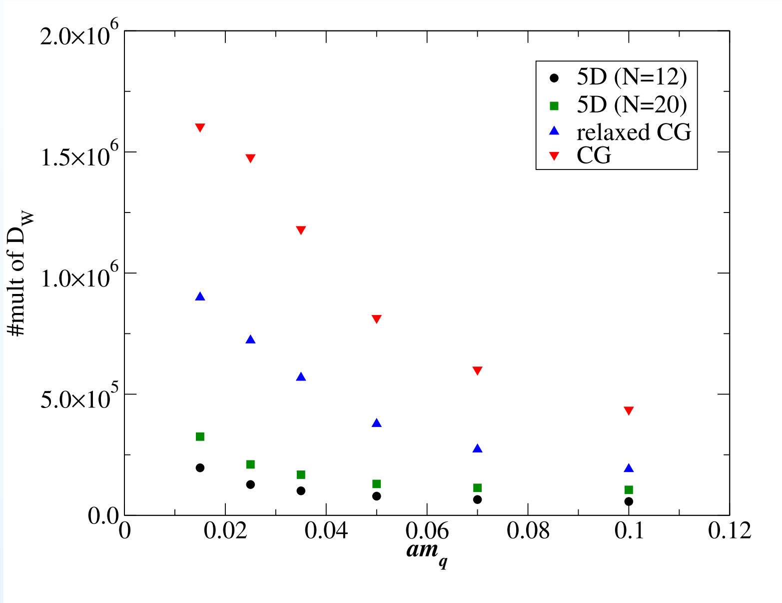
- Preconditioning: $M_5^{(0)} = M_5[U = 0]$ easily inverted
- Even-odd preconditioning (*best solution*).
- Cost increases linearly in N
- Subtraction of low-modes of H_W is not applicable.
  $\longrightarrow$ difficulty at $\lambda_{min} \sim 0$

Solver algorithm (5)

Comparison:

($a \simeq 0.12\mathrm{fm}$, $m \simeq m_s/4$, single conf.: $\lambda_{min} \simeq$0.006)



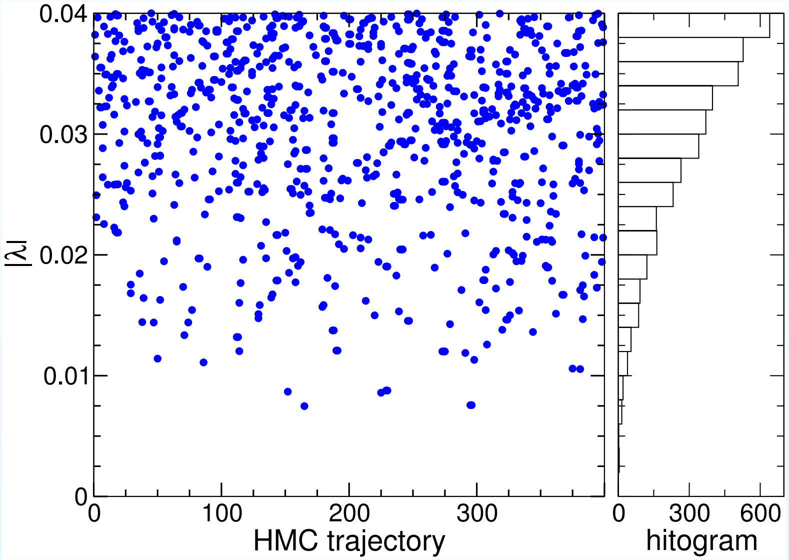


- Relaxed CG is factor 2 faster than standard CG
- 5D solver is 2-3 times faster than relaxed CG for $N = 20$
- If $\lambda \simeq 0$ does not appear, 5D solver has advantage

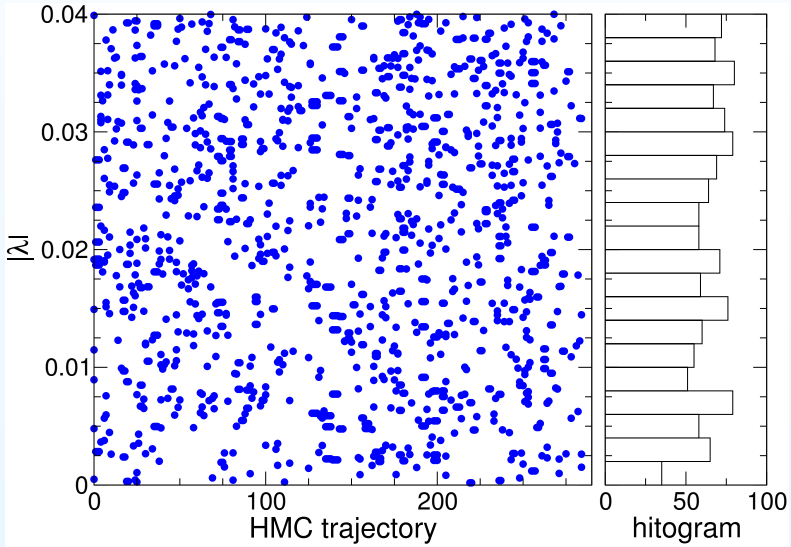
Effect of extra Wilson term (1)

Low-lying modes in HMC run ($a \simeq 0.125$ fm, $m \simeq m_s$)

With S_E ($\mu = 0.2$)



Without S_E

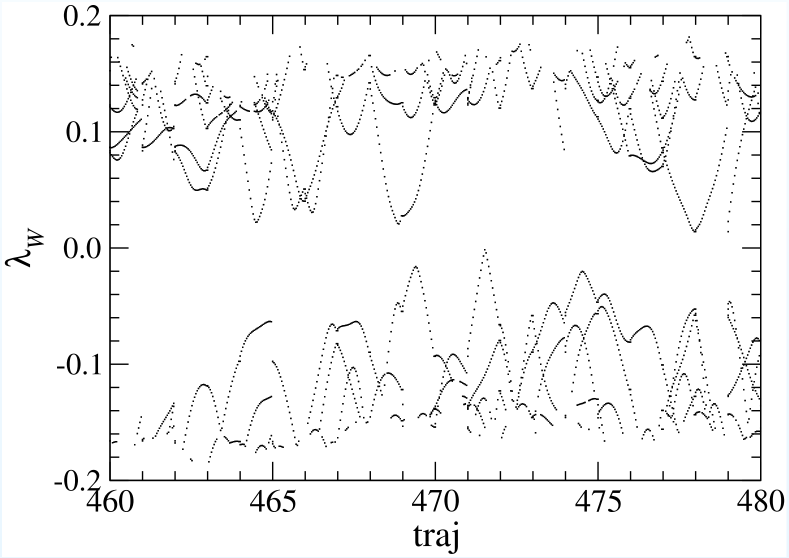


- Extra Wilson fermion works well
- $\lambda_{thrs} \simeq 0.01$ for $D(m)$ is reasonable choice
  (error is corrected by noisy Metropolis)

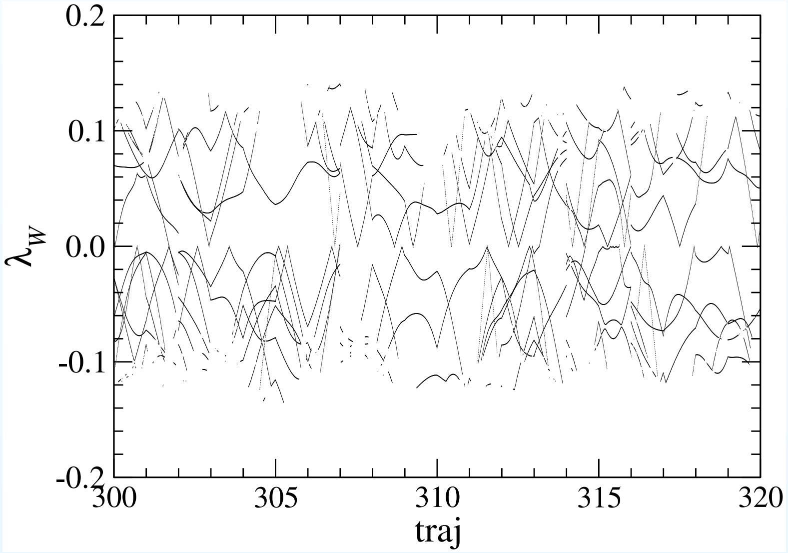
Effect of extra Wilson term (2)

Evolution of λ_{min} in MD ($a \simeq 0.12$fm, $m \simeq m_s$)

With $S_E(\mu = 0.2)$



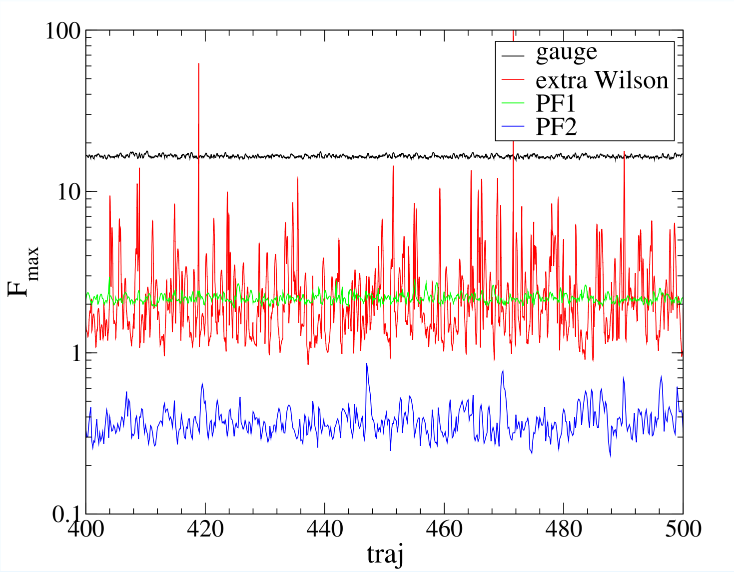
Without S_E

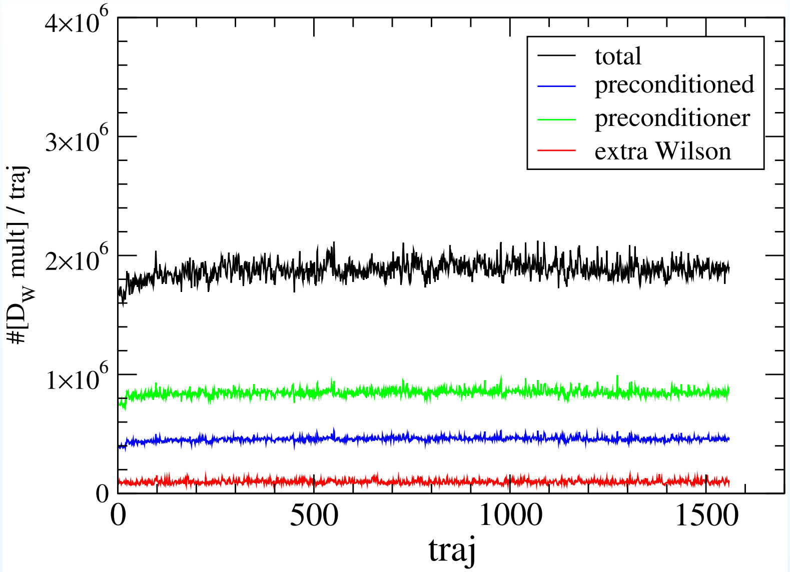


- Without S_E, reflection/refraction frequently occurs
- With S_E almost no near-zero mode
  $\longrightarrow$ monitoring of λ can be switched off
  If it occurs, signaled by large ΔH and rejected in Metropolis

Multi-time step

Maximum values of forces/costs of forces ($a \simeq 0.12$fm, $m \simeq m_s$)





- Inner-most: gauge + extra Wilson
- Cost of PF2(dynamical overlap) $>$ PF1(preconditioner)
- Example: $$\frac{\Delta\tau_{(PF2)}}{\Delta\tau_{(PF1)}} = 5 \qquad \frac{\Delta\tau_{(PF1)}}{\Delta\tau_{(G,E)}} = 6$$

Performance

Performance on Blue Gene (512-node)

$a \sim 0.12$*fm*, $\mu = 0.2$, *trajectory length:* $\tau = 0.5$

- Step-1: With 4D (relaxed CG) solver

m_{ud}	$N_{\tau(PF2)}$	$\frac{\Delta\tau_{(PF2)}}{\Delta\tau_{(PF1)}}$	$\frac{\Delta\tau_{(PF1)}}{\Delta\tau_{(G,E)}}$	$N_{PF1,2}$	P_{acc}	time[min]
0.015	9	4	5	10	0.87	112
0.025	8	4	5	10	0.90	94
0.035	6	5	6	10	0.74	63

- Step-2: less precise 5D solver in MD + noisy Metropolis $\longrightarrow$ factor $\sim$3 accelerated *(preliminary)*

m_{ud}	$N_{\tau(PF2)}$	N_{PF1}	N_{PF2}	P_{acc}	time[min]
0.035	7	10	10	0.68	22
0.035	8	10	10	0.80	26
0.035	8	6	10	0.78	23

Summary

Large scale dynamical simulation with $N_f = 2$ overlap fermions at $16^3 \times 32$, $a \simeq 0.12$fm, $\simeq m_s/6$, with fixed topology

- topology fixing extra Wilson term works well
- 5D CG solver is faster than 4D CG, particularly for small N
- Multi-time step with Hasenbusch preconditioner
- Our present best solution:
  less precise 5D solver in MD + noisy Metropolis test