Approaching the Chiral Limit with Dynamical Overlap Fermions

T. Kaneko for the JLQCD collaboration

[1]High Energy Accelerator Research Organization (KEK)

[2]Graduate University for Advanced Studies

"Domain Wall Fermions at Ten Years", March 15–17, 2007

1.1 introduction

- JLQCD: studying lattice QCD using computers at KEK
- w/ new supercomputer system (2006 –)

  Hitachi SR11000, IBM Blue Gene/L (∼ 60 TFLOPS)

  $\Downarrow$

  large-scale simulations w/ dynamical overlap fermions

  $\Uparrow$

  computationally expensive $\Leftarrow$ improvements of algorithm

- this talk: algorithmic aspects of production run for $N_f = 2$
  - lattice action / simulation parameters
  - our implementation of HMC
  - production run

2.1 lattice action

- quark action = overlap w/ std. Wilson kernel

$$D_{\rm ov} \;=\; \left(m_0+\frac{m}{2}\right)+\left(m_0-\frac{m}{2}\right)\gamma_5\,{\rm sgn}[H_{\rm w}(-m_0)], \quad m_0=1.6$$

  std. Wilson kernel $H_{\rm W}$ $\Rightarrow$ (near-)zero modes of $H_{\rm W}$

- gauge action = Iwasaki action $\Leftarrow$ low mode density, locality

- extra-fields $\Rightarrow$ to suppress (near-)zero modes

  Vranas, 2000; RBC, 2002 (DWF); JLQCD, 2006 (ovr)

  - Wilson fermion $\Rightarrow$ suppress zero modes
  - twisted mass ghost $\Rightarrow$ suppress effects of higher modes

  $$\text{Boltzmann weight} \;\propto\; \frac{\det[H_W(-m_0)^2]}{\det[H_W(-m_0)^2+\mu^2]}$$

  - extra-fields $\Rightarrow$ do NOT change continuum limit

2.2 simulation parameters

- $N_f = 2$ QCD
- Iwasaki gauge + overlap quark + extra-Wilson ($\mu = 0.2$)
- $\beta = 2.30 \Rightarrow a \approx 0.125$ fm
- $16^3 \times 32$ lattice $\Rightarrow L \simeq 2$ fm
- 6 sea quark masses $\in [m_{s,\text{phys}}/6, m_{s,\text{phys}}]$

  $m_{\text{sea}} = 0.015, 0.025, 0.035, 0.050, 0.070.0.100$
- focus on $Q = 0$ sector
- test runs (500 – 1000 traj.)

  $(\beta, \mu) =$ (2.30,0.2), (2.45, 0.0), (2.50,0.2), (2.60, 0.0)

3.1 algorithm

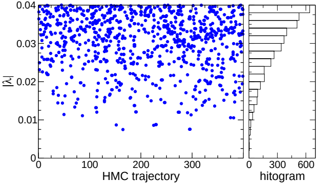
- HMC w/ dynamical overlap quarks on BG/L
  - mult D_{W} : depends on machine spec.
  - mult D_{ov} : treatment of $\mathrm{sgn}[H_{\mathrm{W}}]$
  - overlap solver : choice of algorithm, 4D or 5D
  - HMC : Hasenbusch precond., multiple time scale
- multiplication of D_{W} $\Rightarrow$ assembler code by IBM on BG/L
  - double FPU instruction of PowerPC 440D
    double pipelines enable complex number add/mult
  - use low-level communication API
    overlap computation/communication
    $\Rightarrow \sim$ 3 times faster than our Fortran code

3.2 multiplication of D_{ov}

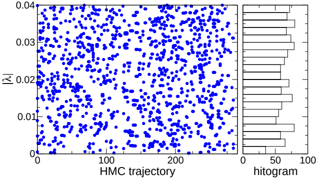
- multiplication of $D_{\mathrm{ov}} \ni \mathrm{sgn}[H_{\mathrm{W}}]$
  - $\sigma[H_W] \Rightarrow [\lambda_{\mathrm{min}}, \lambda_{\mathrm{thrs}}] \cup [\lambda_{\mathrm{thrs}}, \lambda_{\mathrm{max}}]$, $\lambda_{\mathrm{thrs}} = 0.045$
  - low mode preconditioning
    eigenmodes w/ $\lambda \in [\lambda_{\mathrm{min}}, \lambda_{\mathrm{thrs}}] \Rightarrow$ projected out
  - Zolotarev approx. of $\mathrm{sgn}[H_W]$ for $\lambda \in [\lambda_{\mathrm{thrs}}, \lambda_{\mathrm{max}}]$
    $N = 10 \Rightarrow$ accuracy of $|1 - \mathrm{sgn} H_W{}^2| \sim 10^{-7}$

example of $\lambda[H_{\mathrm{W}}]$ (test runs @ $a \sim 0.1$ fm, $m_{\mathrm{sea}} \sim m_{\mathrm{s,phys}}$)

w/ extra-Wilson



w/o extra-Wilson



3.3 4D overlap solver

inner loop:

- partial fraction form

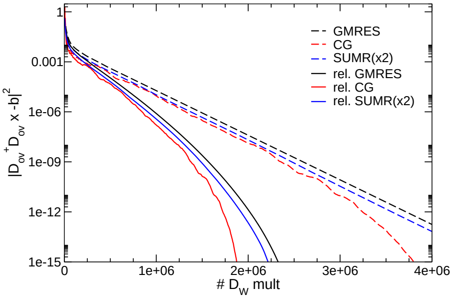
$$\mathrm{sgn}[H_W] \ni \sum_{l=1}^{N_p} \frac{b_l}{H_W^2 + c_{2l-1}}$$

- multi-shift CG *(Frommer et al., 1995)*

outer loop:

- relaxed CG *(Cundy et al., 2004)*
  - $D_{ov}^\dagger D_{ov} \Rightarrow$ CG
  - $\times$ 2 faster than unrelaxed CG

residual $|D_{ov}^\dagger D_{ov} x - b|$
vs # of D_W mult ($m_{sea} = 0.015$)



3.3 5D overlap solver

Boriçi, 2004; Edwards et al.,2005

- M_5 =(Schur decomposition)$\Rightarrow$ $\gamma_5 D_{ov} = H_{ov}$ as Schur complement

$$M_5 = \left(\begin{array}{ccccc|c} H_W & -\sqrt{q_2} & & & & 0 \\ -\sqrt{q_2} & H_W & & & & \sqrt{p_2} \\ & & \cdots & & & \cdots \\ & & & H_W & -\sqrt{q_1} & 0 \\ & & & -\sqrt{q_1} & H_W & \sqrt{p_1} \\ \hline 0 & \sqrt{p_2} & \cdots & 0 & \sqrt{p_1} & R\gamma_5 + p_0 H_W \end{array}\right)$$

$$= \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right) = \left(\begin{array}{c|c} 1 & 0 \\ \hline C A^{-1} & 1 \end{array}\right) \left(\begin{array}{c|c} A & 0 \\ \hline 0 & S \end{array}\right) \left(\begin{array}{c|c} 1 & A^{-1} B \\ \hline 0 & 1 \end{array}\right)$$

$$S = R\gamma_5 + H_W \left(p_0 + \sum_i \frac{p_i}{H_W^2 + q_i} \right) = \gamma_5 \left(R + \gamma_5 \, \mathrm{sgn}[H_W] \right) \Rightarrow H_{ov}$$

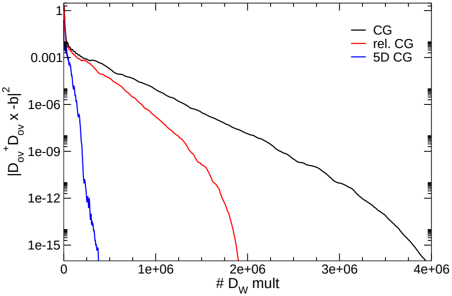
3.3 5D overlap solver

- $x = D_{\mathrm{ov}}^{-1} b$ from 5D linear equation

$$M_5 \begin{pmatrix} \chi \\ x \end{pmatrix} = \begin{pmatrix} 0 \\ b \end{pmatrix},$$

- even-odd precond.: implemented
- low-mode precond.: not yet...
  - $\Rightarrow$ need small x_{min} and large N_{p}
  - $\Leftrightarrow$ CPU time $\propto N_{\mathrm{p}}$
- $\sim$4 times faster than 4D CG

residual vs # of D_{W} mult



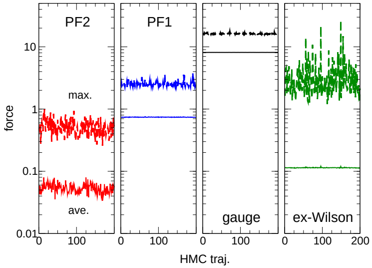
3.4 HMC w/ 4D solver

- **Hasenbusch preconditioning** *(Hasenbusch, 2001)*

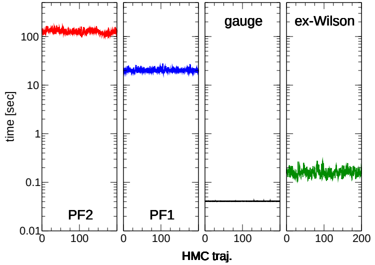
$$\det[D_{ov}(m)^2] = \det[D_{ov}(m')^2] \det\left[\frac{D_{ov}(m)^2}{D_{ov}(m')^2}\right] = \text{“PF1”} \cdot \text{“PF2”}$$

- $m' = 0.2$ ($m_{sea} = 0.015$, 0.025), 0.4 ($m_{sea} = 0.035 - 0.100$)

force (ave,max) at $m_{sea} = 0.015$



CPU time for force calc (512nodes)



PF2 ≪ PF1 ≪ gauge ≈ ex-Wilson

PF2 ≫ PF1 ≫ ex-Wilson ≫ gauge

3.4 HMC w/ 4D solver

- multiple time scale integration

  $\tau = 0.5$

  3 nested loops:

PF2 :	outer-most loop :	N_{MD} times / traj.
PF1 :	intermediate :	$N_{\mathrm{MD}}\, R_{\mathrm{PF}}$
gauge,ex-Wilson :	inner-most :	$N_{\mathrm{MD}}\, R_{\mathrm{PF}}\, R_{\mathrm{G}}$

m_{sea}	N_{MD}	R_{PF}	R_{G}	m'	P_{HMC}
0.015	9	4	5	0.2	0.89
0.025	8	4	5	0.2	0.90
0.035	6	5	6	0.4	0.74
0.050	6	5	6	0.4	0.79
0.070	5	5	6	0.4	0.81
0.100	5	5	6	0.4	0.85

3.5 HMC w/ 5D solver

- Hasenbusch precond. + multiple time scale

$$\det[D_{\mathrm{ov}}(m)^2] = \det[D_{\mathrm{ov,5D}}(m')^2] \det\left[\frac{D_{\mathrm{ov,5D}}(m)^2}{D_{\mathrm{ov,5D}}(m')^2}\right] \det\left[\frac{D_{\mathrm{ov}}(m)^2}{D_{\mathrm{ov,5D}}(m)^2}\right]$$

$$= \text{“PF1”} \cdot \text{“PF2”} \cdot \text{“noisy Metropolis test”}$$

  - sufficiently high “N_s” to achieve reasonable P_{HMC}
  - factor of 2 – 3 faster than HMC w/ 4D solver

m_{sea}	N_{MD}	R_{PF}	R_{G}	m'	P_{HMC}
0.015	13	6	8	0.2	0.68
0.025	10	6	8	0.2	0.82
0.035	10	6	8	0.4	0.87
0.050	9	6	8	0.4	0.87
0.070	8	6	8	0.4	0.90
0.100	7	6	8	0.4	0.91

3.6 reflection / refraction

- extra-Wilson fermion

  $\Rightarrow$ suppress zero-modes of H_W

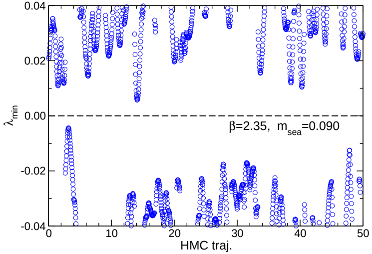
  $\Rightarrow$ switch off reflection/refraction step

  - reflection/refraction is not rare event!

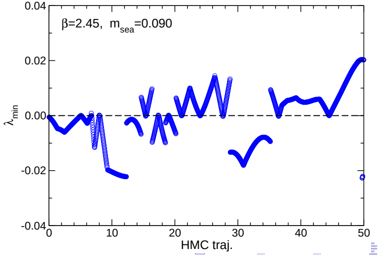
    (at $a = 0.11$ fm w/o extra-Wilson)

  $\Rightarrow$ factor of ~ 3 faster

w/ extra-Wilson



w/o extra-Wilson



4.1 production run

10,000 traj. ($\times \tau = 0.5$) have been accumulated

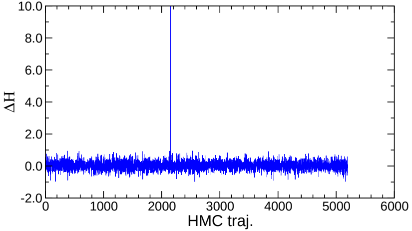
$m_{\rm sea}$	$N_{\rm MD}$	$R_{\rm PF}$	$R_{\rm G}$	m'	traj.	$P_{\rm HMC}$	$M_{\rm PS}/M_{\rm V}$
0.015	9	4	5	0.2	2800	0.89	0.34
0.025	8	4	5	0.2	5200	0.90	0.40
0.035	6	5	6	0.4	4600	0.74	0.46
0.050	6	5	6	0.4	4800	0.79	0.54
0.070	5	5	6	0.4	4500	0.81	0.60
0.100	5	5	6	0.4	4600	0.85	0.67

$m_{\rm sea}$	$N_{\rm MD}$	$R_{\rm PF}$	$R_{\rm G}$	m'	traj	$P_{\rm HMC}$	$M_{\rm PS}/M_{\rm V}$
0.015	13	6	8	0.2	7200	0.68	0.34
0.025	10	6	8	0.2	4800	0.82	0.40
0.035	10	6	8	0.4	5400	0.87	0.46
0.050	9	6	8	0.4	5200	0.87	0.54
0.070	8	6	8	0.4	5500	0.90	0.60
0.100	7	6	8	0.4	5400	0.91	0.67

4.2 basic properties of HMC

area preserving

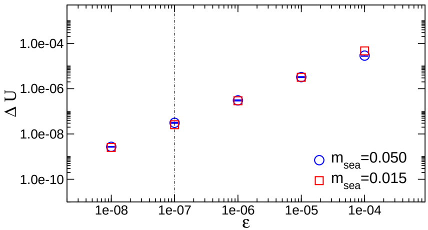
ΔH at $m_{\rm sea}=0.025$



- a few spikes per $O(10,000)$ trajectories: $P_{\rm spike} \lesssim 0.03$ %
- $\langle \exp[-\Delta H] \rangle = 1$ in all runs
- does not need “replay” trick

reversibility

ΔU vs ϵ



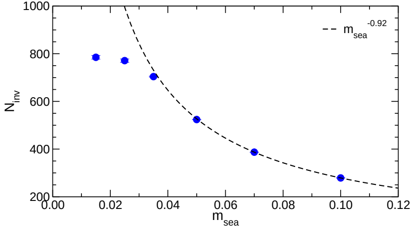
$\Delta U = \sqrt{\sum |U(\tau+1-1) - U(\tau)|^2 / N_{\rm dof}}$

ϵ : stop. cond. for MS/overlap solver

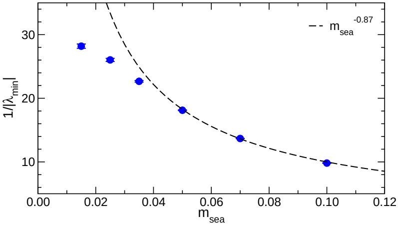
- $\Delta U \lesssim 10^{-8}$: comparable to previous simulations

4.3 effects of low modes of D_{ov}

$N_{\text{inv,H}}$ vs m_{sea}



$|\lambda_{\text{ov,min}}|$ vs m_{sea}



- as approaching to ϵ-regime

  cost is governed by $\lambda_{\text{ov,min}}$ rather than m_{sea}

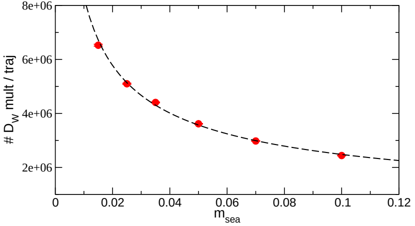
- too small volume?

  $M_{\text{PS}}\,L \gtrsim 2.7$, $\exp[-M_{\text{PS}}\,L] \Rightarrow \lesssim 1-2\%$ effects on M_{PS}

  larger L for $m_{\text{sea}} \ll 0.015$

4.3 timing

D_W mult vs m_{sea}



CPU time [min] on BG/L×10 racks

	HMC-4D		HMC-5D	
m_{sea}	traj.	time	traj.	time
0.015	2800	6.1	7200	2.6
0.025	5200	4.7	4800	2.2
0.035	4600	3.0	5400	1.5
0.050	4800	2.6	5200	1.3
0.070	4500	2.1	5500	1.1
0.100	4600	2.0	5400	1.0

- mild m_{sea} dep. of $N_{inv,H}$ and N_{MD}

  $\Downarrow$

  CPU time $\propto 1/m_{sea}^{-\alpha}$, w/ $\alpha \sim 0.53$

  $\Updownarrow$

  naive expectation: $N_{inv} \propto 1/m_{sea}$,

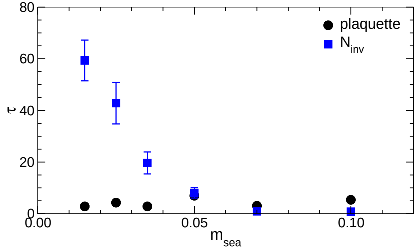
  $N_{MD} \propto 1/m_{sea}$

- BG/L × 10 racks × 1 month

  $\Rightarrow$ 4000 traj. at all m_{sea}

4.4 autocorrelation

τ_{int} vs m_{sea}



- plaquette: local

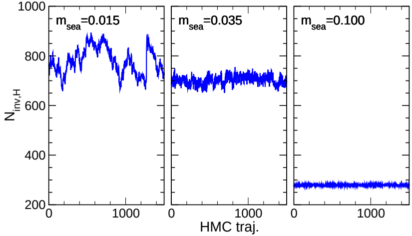
  $\Rightarrow$ small m_q dependence

- $N_{\mathrm{inv,H}}$: long range

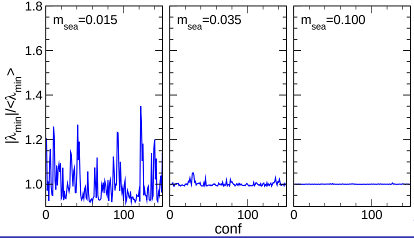
  $\Rightarrow$ rapid increase as $m_q \to 0$

  $\Rightarrow$ may need large statistics

history of $N_{\mathrm{inv,H}}$



history of $\lambda_{\mathrm{ov,min}}/\langle\lambda_{\mathrm{ov,min}}\rangle$



5. summary

- algorithm for JLQCD's dynamical overlap simulations
  - Hasenbusch precond. + multiple time scale MD + $\cdots$
  - 5D solver
  - extra-Wilson fermion to suppress (near-)zero modes

    $\Rightarrow$ cheap approx. for $\mathrm{sgn}[H_{\mathrm{W}}]$, $\Rightarrow$ turn off reflection/refraction
- effects due to fixed (global) topology *(R.Brower et al., 2003)*
  - topological properties (χ_t,...) $\Rightarrow$ *talks by T-W.Chiu, T.Onogi*
  - Q-dependence of observables $\Leftarrow$ simulations w/ $Q \neq 0$
  - suitable for ϵ-regime $\Rightarrow$ *talk by S.Hashimoto*
- on-going/future plans
  - spectrum/matix elements $\Rightarrow$ *talks by J.Noaki, N.Yamada*
  - simulations of $N_f = 3$ QCD
  - extend to larger volumes