Approaching the Chiral Limit with Dynamical Overlap Fermions

T. Kaneko for the JLQCD collaboration

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“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)

- large-scale simulations w/ dynamical overlap fermions

- computationally expensive ⇐ 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

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

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

- Gauge action = Iwasaki action \( \Leftarrow \) low mode density, locality

- Extra-fields \( \Rightarrow \) to suppress (near-)zero modes

  - 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

\[ \text{T. Kaneko} \quad \text{Approaching the chiral limit with dynamical overlap fermions} \]
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 \( \Rightarrow L \approx 2 \) 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 $\text{sgn}[H_W]$
  - overlap solver: choice of algorithm, 4D or 5D
  - HMC: Hasenbusch precond., multiple time scale

- multiplication of $D_W$ ⇒ 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
  ⇒ $\sim 3$ times faster than our Fortran code
3.2 multiplication of $D_{ov}$

- Multiplication of $D_{ov} \ni \text{sgn}[H_W]$
  - $\sigma[H_W] \Rightarrow [\lambda_{\text{min}}, \lambda_{\text{thrs}}] \cup [\lambda_{\text{thrs}}, \lambda_{\text{max}}], \quad \lambda_{\text{thrs}} = 0.045$
  
- Low mode preconditioning
  - Eigenmodes w/ $\lambda \in [\lambda_{\text{min}}, \lambda_{\text{thrs}}] \Rightarrow$ projected out

- Zolotarev approx. of $\text{sgn}[H_W]$ for $\lambda \in [\lambda_{\text{thrs}}, \lambda_{\text{max}}]$
  - $N = 10 \Rightarrow$ accuracy of $|1 - \text{sgn}H_W^2| \sim 10^{-7}$

- Example of $\lambda[H_W]$ (test runs @ $a \sim 0.1$ fm, $m_{\text{sea}} \sim m_{\text{s,phys}}$)

W/ extra-Wilson

W/o extra-Wilson
3.3 4D overlap solver

inner loop:
- partial fraction form

\[
\text{sgn}[H_W] \ni \sum_{l=1}^{N_p} \frac{b_l}{H_W^2 + c_{2l-1}}
\]
- multi-shift CG (Frommer et al., 1995)

outer loop:
- relaxed CG (Cundy et al., 2004)
  - \(D_{ov}^\dagger D_{ov} \Rightarrow \text{CG}\)
  - \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

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

\[
M_5 = \begin{pmatrix}
H_W & -\sqrt{q_2} \\
-\sqrt{q_2} & H_W \\
& \ddots & \ddots & \ddots \\
& & H_W & -\sqrt{q_1} \\
& & -\sqrt{q_1} & H_W \\
0 & \sqrt{p_2} & \cdots & 0 & \sqrt{p_1} \\
0 & \sqrt{p_1} & & & R \gamma_5 + p_0 H_W
\end{pmatrix}
\]

\[
= \begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
= \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
A & 0 \\
0 & S
\end{pmatrix}
\begin{pmatrix}
1 & A^{-1} B \\
0 & 1
\end{pmatrix}
\]

\[
S = R \gamma_5 + H_W \left( p_0 + \sum_i \frac{p_i}{H_{W}^2 + q_i} \right) = \gamma_5 \left( R + \gamma_5 \text{sgn}[H_W] \right) \Rightarrow H_{ov}
\]
### 3.3 5D overlap solver

- \( x = D^{-1}_{ov} b \) 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 \( x_{\text{min}} \) and large \( N_p \)
  - \( \Leftrightarrow \) CPU time \( \propto N_p \)
- \(~4\) times faster than 4D CG

![Graph showing residual vs # of \( D_W \) mult]
3.4 HMC w/ 4D solver

- Hasenbusch preconditioning \((\text{Hasenbusch, 2001})\)

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

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

**force (ave,max) at \(m_{\text{sea}} = 0.015\)**

PF2 \(\ll\) PF1 \(\ll\) gauge \(\approx\) ex-Wilson

**CPU time for force calc (512nodes)**

PF2 \(\gg\) PF1 \(\gg\) ex-Wilson \(\gg\) gauge
3.4 HMC w/ 4D solver

- multiple time scale integration

\[ \tau = 0.5 \]

3 nested loops:

PF2 : outer-most loop : \( N_{\text{MD}} \) times / traj.

PF1 : intermediate : \( N_{\text{MD}} R_{\text{PF}} \)

gauge, ex-Wilson : inner-most : \( N_{\text{MD}} R_{\text{PF}} R_{\text{G}} \)

<table>
<thead>
<tr>
<th>( m_{\text{sea}} )</th>
<th>( N_{\text{MD}} )</th>
<th>( R_{\text{PF}} )</th>
<th>( R_{\text{G}} )</th>
<th>( m' )</th>
<th>( P_{\text{HMC}} )</th>
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<tr>
<td>0.015</td>
<td>9</td>
<td>4</td>
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<td>0.89</td>
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<tr>
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<td>0.2</td>
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<tr>
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<tr>
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<td>6</td>
<td>0.4</td>
<td>0.85</td>
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</table>
3.5 HMC w/ 5D solver

- Hasenbusch precond. + multiple time scale

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

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

- sufficiently high “\(N_s\)” to achieve reasonable \(P_{\text{HMC}}\)

- factor of 2–3 faster than HMC w/ 4D solver

<table>
<thead>
<tr>
<th>(m_{\text{sea}})</th>
<th>(N_{\text{MD}})</th>
<th>(R_{\text{PF}})</th>
<th>(R_G)</th>
<th>(m')</th>
<th>(P_{\text{HMC}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.015</td>
<td>13</td>
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<tr>
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<tr>
<td>0.035</td>
<td>10</td>
<td>6</td>
<td>8</td>
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<td>6</td>
<td>8</td>
<td>0.4</td>
<td>0.90</td>
</tr>
<tr>
<td>0.100</td>
<td>7</td>
<td>6</td>
<td>8</td>
<td>0.4</td>
<td>0.91</td>
</tr>
</tbody>
</table>
3.6 reflection / refraction

- extra-Wilson fermion
  \[ \Rightarrow \text{suppress zero-modes of } H_W \]
  \[ \Rightarrow \text{switch off reflection/refraction step} \]
  - reflection/refraction is not rare event!
    (at \( a = 0.11 \text{ fm w/o extra-Wilson} \))
  \[ \Rightarrow \text{factor of } \sim 3 \text{ faster} \]

\[ \beta=2.35, \ m_{\text{sea}}=0.090 \]

\[ \beta=2.45, \ m_{\text{sea}}=0.090 \]
4.1 production run

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

<table>
<thead>
<tr>
<th>$m_{\text{sea}}$</th>
<th>$N_{\text{MD}}$</th>
<th>$R_{\text{PF}}$</th>
<th>$R_{\text{G}}$</th>
<th>$m'$</th>
<th>traj.</th>
<th>$P_{\text{HMC}}$</th>
<th>$M_{\text{PS}}/M_{\text{V}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.015</td>
<td>9</td>
<td>4</td>
<td>5</td>
<td>0.2</td>
<td>2800</td>
<td>0.89</td>
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<tr>
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<td>8</td>
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<td>0.46</td>
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<td>0.79</td>
<td>0.54</td>
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</tbody>
</table>
4.2 basic properties of HMC

area preserving

\[ \Delta H \text{ at } m_{\text{sea}} = 0.025 \]

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

reversibility

\[ \Delta U \text{ vs } \epsilon \]

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

\( \epsilon \): stop. cond. for MS/overlap solver

\( \Delta U \lesssim 10^{-8} \): comparable to previous simulations
4.3 effects of low modes of $D_{ov}$

- as approaching to $\epsilon$-regime
  cost is governed by $\lambda_{ov, min}$ rather than $m_{sea}$

- too small volume?
  $$M_{PS} L \gtrsim 2.7, \quad \exp[-M_{PS} L] \Rightarrow \lesssim 1-2\% \text{ effects on } M_{PS}$$
  larger $L$ for $m_{sea} \ll 0.015$
4.3 timing

**# $D_W$ mult vs $m_{\text{sea}}$**

- **CPU time [min] on BG/L x 10 racks**

<table>
<thead>
<tr>
<th>$m_{\text{sea}}$</th>
<th>CPU time traj. time</th>
<th>CPU time traj. time</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.015</td>
<td>2800 6.1</td>
<td>7200 2.6</td>
</tr>
<tr>
<td>0.025</td>
<td>5200 4.7</td>
<td>4800 2.2</td>
</tr>
<tr>
<td>0.035</td>
<td>4600 3.0</td>
<td>5400 1.5</td>
</tr>
<tr>
<td>0.050</td>
<td>4800 2.6</td>
<td>5200 1.3</td>
</tr>
<tr>
<td>0.070</td>
<td>4500 2.1</td>
<td>5500 1.1</td>
</tr>
<tr>
<td>0.100</td>
<td>4600 2.0</td>
<td>5400 1.0</td>
</tr>
</tbody>
</table>

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

**naive expectation:**

- $N_{\text{inv}} \propto 1/m_{\text{sea}}$
- $N_{\text{MD}} \propto 1/m_{\text{sea}}$

**BG/L x 10 racks x 1 month $\Rightarrow$ 4000 traj. at all $m_{\text{sea}}$**
4.4 autocorrelation

- plaquette: local
  \[ \Rightarrow \text{small } m_q \text{ dependence} \]
- \( \mathcal{N}_{\text{inv}, H} \): long range
  \[ \Rightarrow \text{rapid increase as } m_q \rightarrow 0 \]
  \[ \Rightarrow \text{may need large statistics} \]

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5. summary

- algorithm for JLQCD's dynamical overlap simulations
  - Hasenbusch precond. + multiple time scale MD + · · ·
  - 5D solver
  - extra-Wilson fermion to suppress (near-)zero modes
    ⇒ cheap approx. for $\text{sgn}[H_W]$, ⇒ turn off reflection/refraction
- effects due to fixed (global) topology \(^{(R.Brower \text{ et al.}, 2003)}\)
  - topological properties ($\chi_t, \ldots$) ⇒ talks by T-W.Chiu, T.Onogi
  - $Q$-dependence of observables ⇐ simulations w/ $Q \neq 0$
  - suitable for $\epsilon$-regime ⇒ talk by S.Hashimoto
- on-going/future plans
  - spectrum/matix elements ⇒ talks by J.Noaki, N.Yamada
  - simulations of $N_f = 3$ QCD
  - extend to larger volumes

(R.Brower et al., 2003)