Dynamical lattice QCD simulation with 2+1 flavors of overlap fermions

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JLQCD's overlap project

Dynamical simulation with overlap fermions

- Main run: $16^3 \times 32(48)$, $a \simeq 0.12$fm (larger size is planned)
- lightest quark mass $\simeq m_s/6$
- Fixed topology by extra Wilson fermion
  – need to examine the effect of fixing topology
- $N_f = 2$: config generation finished, 10000 trj
  $16^3 \times 32$, $a \simeq 0.12$fm
- $N_f = 2 + 1$:
  $16^3 \times 32$, test run (finished)
  $16^3 \times 48$, productive run in progress

Physical results ($N_f = 2$) $\rightarrow$ talks by other members

This talk: status of $N_f = 2 + 1$ simulation

KEK supercomputers

In service since March 2006

Hitachi SR11000

- 2.15TFlops, 512MB memory

IBM Blue Gene

- 57.3TFlops, 5TB memory
- 1024 nodes $\otimes$10 racks
- $8 \times 8 \times 8$ torus network

Wilson solver: $\sim$29% of peak performance (on cache)
Wilson kernel tuned by IBM Japan (J.Doi and H.Samukawa)

Overlap Dirac operator

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

Zolotarev's partial fractional approximation

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

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

$(H_W^2 + q_l)^{-1}$: determined by Multishift CG simultaneously

HMC time is dominated by inversion of $(D^\dagger D)$

- Nested CG with relaxation of ϵ_{in}
- 5D CG: factor 2 (4) faster at $N = 20$ (10)
  - Subtraction of low modes of H_W in progress

Hybrid Monte Carlo

$S = S_G + S_F + S_E$

- Gauge field S_G: Iwasaki (renormalization group improved)
- Extra Wilson fermion: suppresses near-zero modes of H_W

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

$\rightarrow$ no need of reflection/refraction

Ingredients of accelerating HMC:

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

$$\begin{aligned} S_{PF1} &= \phi_1^\dagger [D(m')^\dagger D(m')]^{-1} \phi_1 \quad \text{(preconditioner)} \\ S_{PF2} &= \phi_2^\dagger \left\{ D(m') [D(m)^\dagger D(m)]^{-1} D(m')^\dagger \right\} \phi_2 \end{aligned}$$

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

Performance of N_f=2 simulations

Performance on Blue Gene (512-node)

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

- HMC-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

- HMC-2: less precise 5D solver in MD + noisy Metropolis
  $\longrightarrow$ factor $\sim$2 accelerated

m_{ud}	$N_{\tau(PF2)}$	$\frac{\Delta\tau_{(PF2)}}{\Delta\tau_{(PF1)}}$	$\frac{\Delta\tau_{(PF1)}}{\Delta\tau_{(G,E)}}$	N_{PF1}	$N_{PF2}^{(MD)}$	$N_{PF2}^{(NM)}$	P_{acc}	time[min]
0.015	13	6	8	10	16	10	0.68	52
0.025	10	6	8	10	16	10	0.82	43
0.035	10	6	8	10	16	10	0.87	36

$N_f = 2 + 1$ algorithm (1)

A. Bode et al., hep-lat/9912043

T. DeGrand and S. Schaefer, JHEP 0607 (2006) 020

$H^2 = D^\dagger(m)D(m)$ commutes with γ_5

$$H^2 = P_+ H^2 P_+ + P_- H^2 P_- \equiv Q_+ + Q_-$$

$$\det H^2 = \det Q_+ \cdot \det Q_-$$

Eigenvalues of $Q+$ and Q_- are the same except for zero modes

$\Downarrow$

One of chirality sector realizes odd number of flavor
(zero modes give const. contribution)

- Topology change can be implemented
  — Not necessary in our case

$N_f = 2+1$ algorithm (2)

Pseudofermion action ($\sigma = 1$ or -1):

$$S_{PF1} = \phi_{1\sigma}^\dagger Q_\sigma^{-1}(m')\phi_{1\sigma}, \qquad S_{PF2} = \phi_{2\sigma}^\dagger \left(\frac{Q_\sigma(m')}{Q_\sigma(m)}\right)\phi_{2\sigma}$$

- Refreshing $\phi_{1\sigma}$ and $\phi_{2\sigma}$ (with Gaussian ξ_σ)

$$\phi_{1\sigma} = \sqrt{Q_\sigma(m')}\cdot\xi_{1\sigma}, \qquad \phi_{2\sigma} = \sqrt{\frac{Q_\sigma(m)}{Q_\sigma(m')}}\cdot\xi_{2\sigma}.$$

— Polynomial or partial fractional approx.

- Other parts are straightforward

  e.g., force:

$$\frac{dS_{PF1}}{d\tau} = \phi_{1\sigma}^\dagger P_\sigma \left(\frac{dH^2(m')^{-1}}{d\tau}\right) P_\sigma \phi_{1\sigma}$$

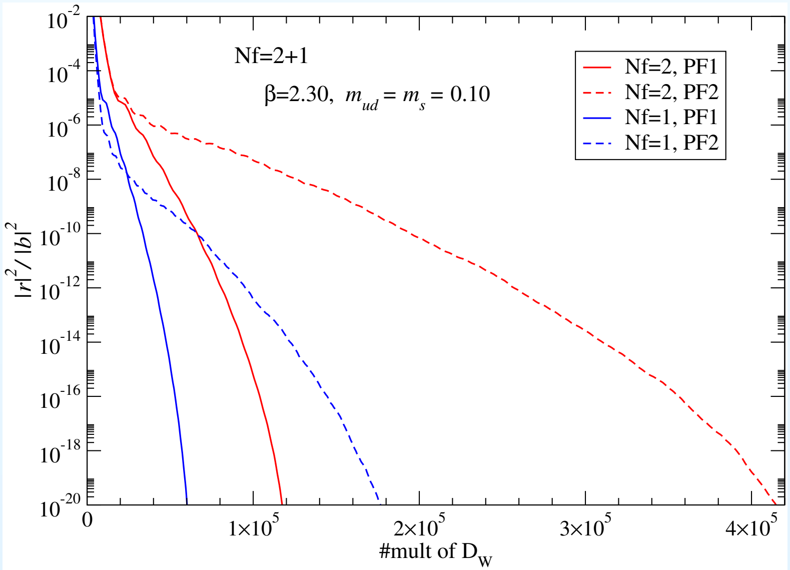
  etc.

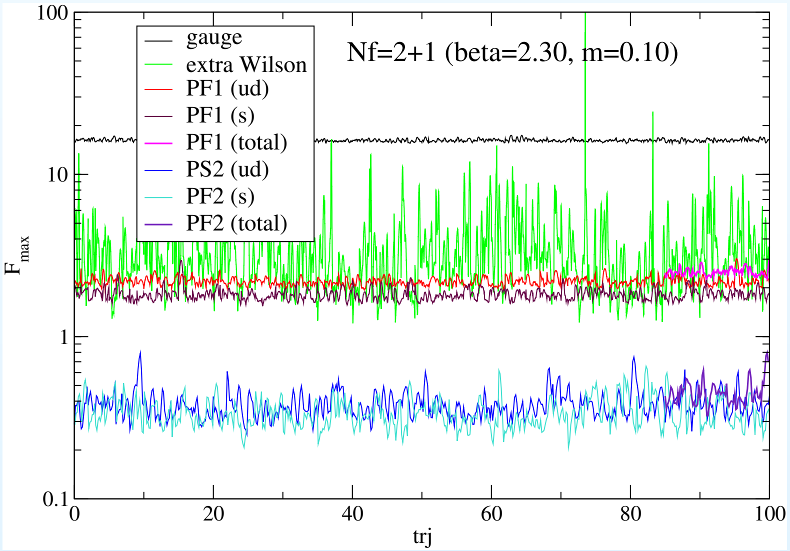
N_f=2+1: solver/force

Solver: one flavor part is twice faster than $N_f = 2$
For Q_σ, number of H_W mult is effectively half of H^2.

$$P_\sigma H^2 P_\sigma = P_\sigma \left[a + \frac{b}{2} \{ \gamma_5, \mathrm{sign}(H_W) \} \right] P_\sigma = P_\sigma \left[a + \sigma b \cdot \mathrm{sign}(H_W) \right] P_\sigma$$

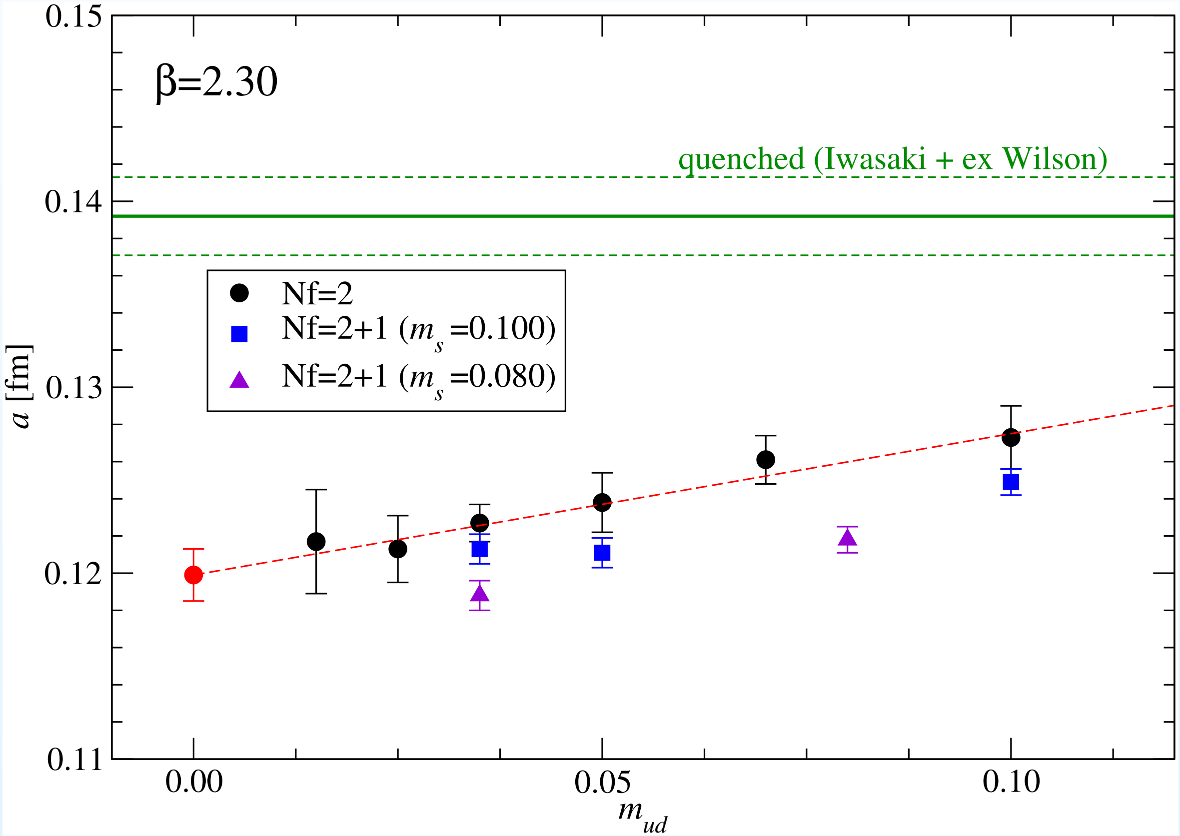
Total forces of 2+1 flavors are similar to $N_f = 2$





N_f=2+1: a vs m_q

- $\beta = 2.30$, $16^3 \times 32$ (test run), 1000 trjs, $l_{trj} = 0.5$
- a is determined by hadronic radius (Sommer scale)



Performance of N_f=2+1 simulations

Performance of productive run on Blue Gene 1024-node

- $16^3 \times 48$, $a \sim 0.12$fm, $l_{trj} = 1$, just started
- Now HMC-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	18	4	5	10	0.87	265(112)
0.025	16	4	5	10	0.90	210(94)
0.035	16	5	6	10	0.74	195(63)

(corresponding $N_f = 2$ at $l_{trj} = 1$, N_t=32)

- Implementation of 5D solver is in progress
  $\longrightarrow$ factor $\sim$2 acceleration expected

Summary/Outlook

JLQCD's dynamical overlap project

- $N_f = 2$: production of configs finished
  - $16^3 \times 32$, $a \simeq 0.12$fm, $\simeq m_s/6$
  - Measuring observables in progress
  - Global Q dependence
- $N_f = 2 + 1$: production run in progress
  - $16^3 \times 48$, $a \simeq 0.12$fm, $\simeq m_s/6$
  - Still factor $\geq$2 acceleration expected
- Outlook
  - Physics results
  - Larger lattices ($24^3\times$ something)