Lattice QCD simulation with 2+1 flavors of dynamical overlap fermions

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Introduction (1)

Strong interaction is described by QCD
— difficult to solve analytically

- Perturbation applies only at high energy
  ← asymptotic freedom
- Model calculations suffer from systematic uncertainties

Need of general procedure from the first principle

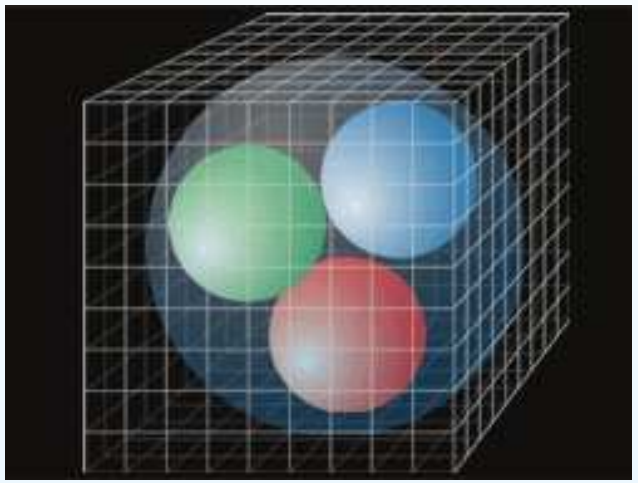
⇒ Lattice QCD

K.G.Wilson, Phys. Rev. D 10 (1974) 2445.

Introduction (2)

Lattice QCD: gauge theory on 4D Euclidean lattice

- Regularized by lattice
- Continuum limit ($a \to 0$) $\to$ QCD
- Based on gauge principle
- Path integral quantization
- Numerical simulation = nonperturbative calculation is possible



Powerful method for low-energy physics of QCD

Introduction (3)

QCD action (Euclidean space-time)

$$S_{QCD}^{cont} = \int d^4x \left[\frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \bar{\psi}(x)(\gamma_\mu D_\mu + m)\psi(x) \right]$$

$\Downarrow$ discretize

Lattice QCD

$$S_{QCD}^{latt} = S_G[U_\mu(x)] + S_F(\bar{\psi}, \psi, U)$$

(now $x = an, n \in Z^4$)

- Gauge field: $U_\mu(x) \simeq \exp(igaA_\mu(x))$
  — on links (bonds of nearest sites)
- Quark field $\bar{\psi}$, ψ: Grassmann variables on sites
  — integrated by hand (Grassmann integration)

Introduction (4)

Lattice QCD actions:

approaches to the continuum actions as $a \to 0$

Gauge field:

$$S_G = \sum_{x,\mu>\nu} \left(1 - \frac{1}{3}\mathrm{ReTr}P_{\mu\nu}(x)\right),$$

$$\begin{aligned} P_{\mu\nu}(x) &= U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu(x) \\ &\simeq \exp(ia^2 g F_{\mu\nu}) \end{aligned}$$

One can add higher order terms in a
$\to$ improved actions (e.g., Iwasaki gauge action)

(Fermion action will be argued later)

Introduction (5)

Path integral quantization:

$$\langle O \rangle = \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp(-S_{QCD})$$

- Integration over compact SU(3) group $\rightarrow$ no gauge fixing
- Fermion part: Grassmann integral

$$\int \mathcal{D}\bar{\psi} \mathcal{D}\psi \exp(-\bar{\psi} D[U] \psi) = \det D[U]$$

$\Rightarrow$ Monte Carlo simulation (important sampling)

$$\langle O \rangle \simeq \frac{1}{N} \sum_{i=1}^{N} O[U_i]$$

for gauge configuration $U_i = \{U_\mu(x)\}_i$ generated with probability $\propto \det D[U] \cdot \exp(-S_G)$.

Simulation algorithm (1)

Numerical simulation:

– Quenched approximation: $\det D \to 1$

- Neglect all quark loop effect
- Low-lying hadron spectrum: consistent within 10%

– Dynamical simulations

- Costs more than 100 times of quenched approx.
- Hybrid Monte Carlo algorithm — currently standard
- Pseudofermion field (bosonic field)

$$\det D = \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \exp(-\bar{\phi}D^{-1}\phi)$$

For positive definiteness, $\det D^2 = \det D^\dagger D$ $(N_f = 2)$

Simulation algorithm (2)

Hybrid Monte Carlo algorithm

- Generate gauge configurations as 4D microcanonical ensemble
- Conjugate momenta $H_\mu(x)$ to gauge field $U_\mu(x)$
- Hamiltonian:

$$\mathcal{H} = \frac{1}{2}\sum_{x,\mu} \mathrm{tr} H_\mu^2(x) + S_G[U] + S_{PF}[U]$$

- Molecular dynamics — evolution with Hamilton equation

$$\begin{aligned} \frac{d}{d\tau} U_\mu(\tau) &= H_\mu(\tau) \\ \frac{d}{d\tau} H_\mu(\tau) &= -\frac{\partial}{\partial U_\mu}(S_G + S_F) \end{aligned}$$

In practice, leapfrog evolution is applied

Simulation algorithm (3)

Hybrid Monte Carlo algorithm (cont.)

- Initial momenta: given by Gaussian distribution
- Fermion field: treated as external field

$$P[\phi] \quad \propto \quad \exp(-\phi^\dagger [D^\dagger D]^{-1} \phi) \qquad (N_f = 2),$$
$$\leftarrow \quad P[\xi] \propto \exp(-\xi^\dagger \xi), \quad \phi = D^\dagger \xi$$

— ϕ is constant during evolution of U and H

- Metropolis test at the end of evolution:
  corrects finite step size error $\rightarrow$ Detailed balance

  Accepted new configuration with probability

$$P_{acc} = \min\{1, e^{-\mathcal{H}[U_{new}]+\mathcal{H}[U_{old}]}\}$$

Simulation algorithm (4)

Recipe of Hybrid Monte Carlo:

- Refresh conjugate momenta and fermion fields with Gaussian distribution
- Molecular dynamical evolution for certain trajectory length
- Metropolis test

Repeat these steps for enough number of trajectories

Measure observables on these configurations

Overlap fermion (1)

Lattice fermion formulation has been serious problem

Naive discretization:

$$S_F = \sum_x \bar{\psi} \left[\frac{1}{2} \sum_\mu [U_\mu(x)\psi(x) - U_\mu(x-\hat{\mu})\psi(x-\hat{\mu})] + m\psi(x) \right]$$

$a = 1,\ U_\mu \simeq 1 + igA_\mu,\ \hat{\mu}$: unit vector in μ-th direction

16 particle modes appear (15 “doublers”)

— in momentum space, poles at $p_\mu \sim 0, \pi$

$$S_q(p)|_{free} = \frac{1}{\sum_\mu \gamma_\mu \sin(p_\mu a) + ma}$$

Wilson fermion: add Wilson term

$$\frac{r}{2} \sum_{x,\mu} \bar{\psi} \left[U_\mu(x)\psi(x) + U_\mu(x-\hat{\mu})\psi(x-\hat{\mu})2\psi(x) \right]$$

This term breaks chiral symmetry explicitly

Overlap fermion (2)

Nielsen-Ninomiya' theorem:

Nielsen and Ninomiya, Nucl. Phys. B185 (1981) 20.

Suppose a lattice fermion action $S_F = \bar{\psi} D[U] \psi$ satisfies the following condition.

- Translational invariance
- Chiral symmetry: $D\gamma_5 + \gamma_5 D = 0$
- Hermiticity
- Bilinear in fermion field
- Locality

Then, doublers exist.

Overlap fermion (3)

Recent progress: realization of chiral symmetry on the lattice

Ginsparg-Wilson relation: least broken chiral symmetry

Ginsparg and Wilson, Phys. Rev. D 25 (1982) 2649.

$$D\gamma_5 + \gamma_5 D = aRaD\gamma_5 D$$

Chiral symmetry on the lattice:

Hasenfratz, Laliena and Niedermayer, Phys. Lett. B427 (1998) 342;

Lüscher, Phys. Lett. B428 (1998) 342.

$$\begin{aligned} \psi &\rightarrow \psi + \gamma_5(1 - a\frac{R}{2}D)\psi \\ \bar{\psi} &\rightarrow \bar{\psi} + \bar{\psi}(1 - a\frac{R}{2}D)\gamma_5 \end{aligned}$$

Fermion formulation which satisfies Ginsparg-Wilson relation realizes this lattice chiral symmetry

Overlap fermion (4)

Overlap fermion

Neuberger, Phys. Lett. B417 (1998) 141; B427 (1998) 353.

$$D = \frac{1}{Ra}\left[1 + \frac{\gamma_5 H_5}{\sqrt{H_W^2}}\right] = \frac{1}{Ra}\left[1 + \gamma_5 \mathrm{sign}(H_5)\right]$$

H_W: Wilson fermion kernel with negative mass M_0
(M_0 is not quark mass!)

- Satisfies the Ginsparg-Wilson relation
- $N_s \to \infty$ limit of Domain-wall fermion
  (5D formulation for chirally symmetric fermions)
- Numerical cost is high: evaluation of $\mathrm{sign}(H_W)$
  — has become possible only with recent developments of algorithms and computers

JLQCD's overlap project (1)

Dynamical simulation with overlap fermions

- Main run: $16^3 \times 32$, $a \simeq 0.12$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
- $N_f = 2$ is now in productive run
- $N_f = 2 + 1$ is in progress

JLQCD's overlap project (2)

New supercomputer at KEK (March 2006$\sim$)

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)
Wilson solver: $\sim$29% of peak performance
(on cache)

JLQCD's overlap project (3)

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

$$D(m) = \left(m_0 + \frac{m}{2}\right) + \left(m_0 - \frac{m}{2}\right) \gamma_5 \mathrm{sign}(H_W)$$

  $H_W = \gamma_5 D_W$, 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); S.Hashimoto et al., hep-lat/0610011

Implementation of overlap fermion (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

Implementation of overlap fermion (2)

☐ Nested CG algorithm

- Outer CG for $D(m)$, inner CG for $(H_W^2 + q_l)^{-1}$ (multishift)
  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 (safe from $\lambda_{min} \sim 0$)
- Cost is almost unchanged as N

☐ 5-dimensional CG

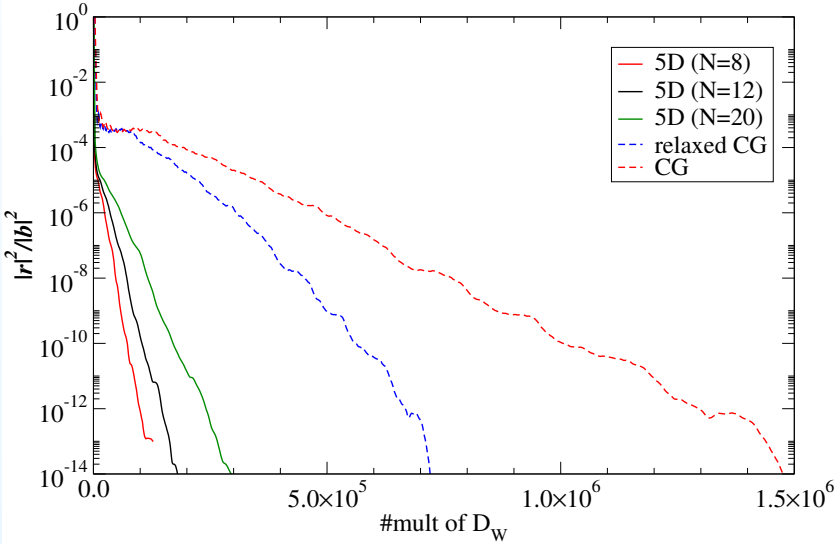
A. Borici, hep-lat/0402035; R.G.Edwards et al., PoS LAT2005 (2006) 146.

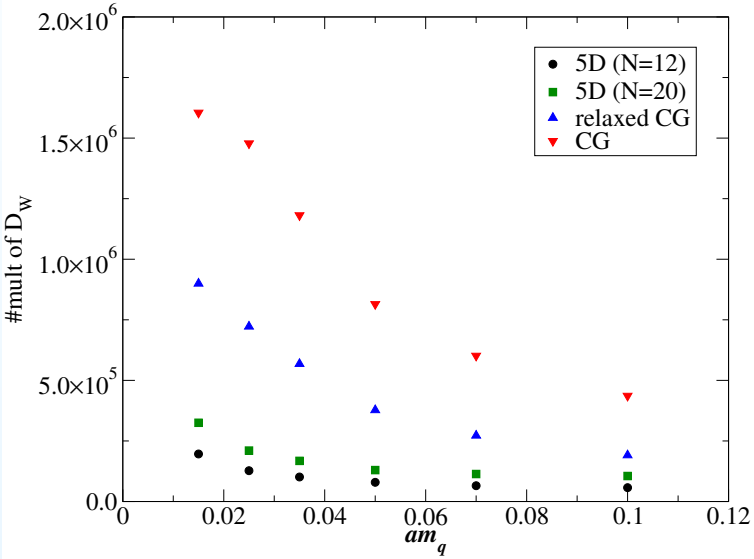
- Making use of Schur decomposition
- Even-odd preconditioning
- Cost increases linearly in N
- Subtraction of low-modes of H_W is not applicable
  $\rightarrow$ difficulty at $\lambda_{min} \sim 0$

Implementation of overlap fermion (3)

Comparison:

($a \simeq 0.12\mathrm{fm}$, $m \simeq 0.4 m_s$, single conf.)





- 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

$N_f = 2$ algorithm (1)

Building blocks of accelerating HMC:

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

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

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

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

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

- Overlap solver: relaxed CG/5D 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 $D^\dagger D$ twice

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

$N_f = 2$ algorithm (2)

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

- assuming no near-zero mode
- fixed λ_{thrs}, $N \simeq 10 \rightarrow$ 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 $W = D(m)/D'(m)$,

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

$N_f = 2$ algorithm (3)

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.

$N_f = 2 + 1$ algorithm (3)

Check: N_f=2 vs N_f=1+1

$16^3 \times 32$ lattice, $\beta = 2.5$, $m_q = 0.09$

- Two positive chirality PS-fermions
- HMC-1 (4D solver, w/o noisy Metropolis)
  — compared with $N_f = 2$, HMC-1
- Initial: $N_f = 2$ thermalized config.
- $M_{MD}^{(pf2)} = 4$, $R_{MD}^{(pf1)} = 5$, $R_{MD}^{(GE)} = 6$, $l_{trj} = 0.5$, $m' = 0.4$

	trj	plaq	P_{acc}	min/trj(BG 512 node)
Nf=1+1	1500	0.651219(16)	$\sim$0.8	23
Nf=2	1000	0.651173(21)	0.81	13

- Consistent with $N_f = 2$.
- Increased cost: largely due to refreshment of ϕ's
  (Now Zolotarev approx. is used)

$N_f = 2 + 1$ algorithm (4)

Test run:

$\beta = 2.30$, $m_{ud} = 0.10$, $m_s = 0.10$, $Q = 0$

- $N_f = 2 \oplus$ positive chirality sector
- Other parameters are same as $N_f = 2$
- HMC-1 (4D solver, w/o noisy Metropolis)
- $M_{MD}^{(pf2)} = 5$, $R_{MD}^{(pf1)} = 5$, $R_{MD}^{(GE)} = 6$, $l_{trj} = 0.5$, $m' = 0.4$
- Thermalization: 300 trjs (very preliminary)

	trj	plaq	P_{acc}	time/trj(BG 512 node)
Nf=2+1	150	0.609724(50)	$\sim$0.76	70 min
Nf=2	4600	0.614685(12)	0.85	40 min

$N_f = 2 + 1$ algorithm (5)

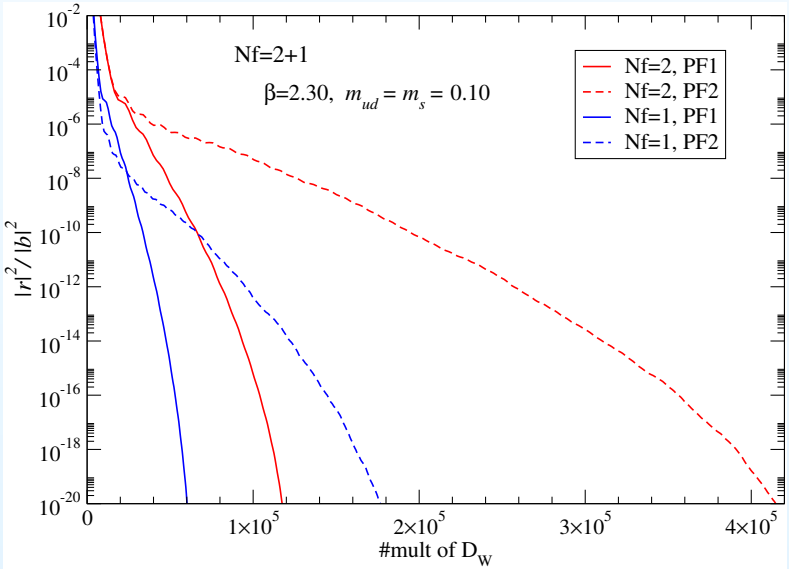
Solver convergence:

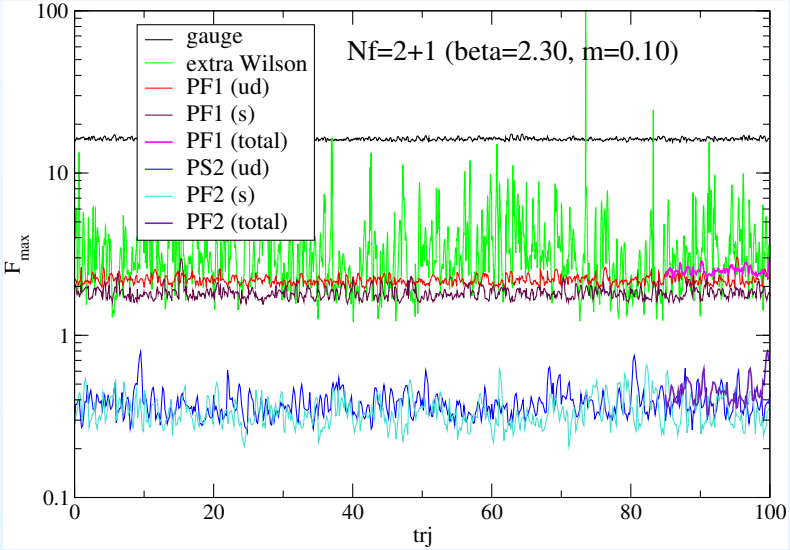
One flavor part is twice faster than $N_f = 2$

$\rightarrow$ total cost is $\sim$ 1.5 times

Force hierarchy:

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





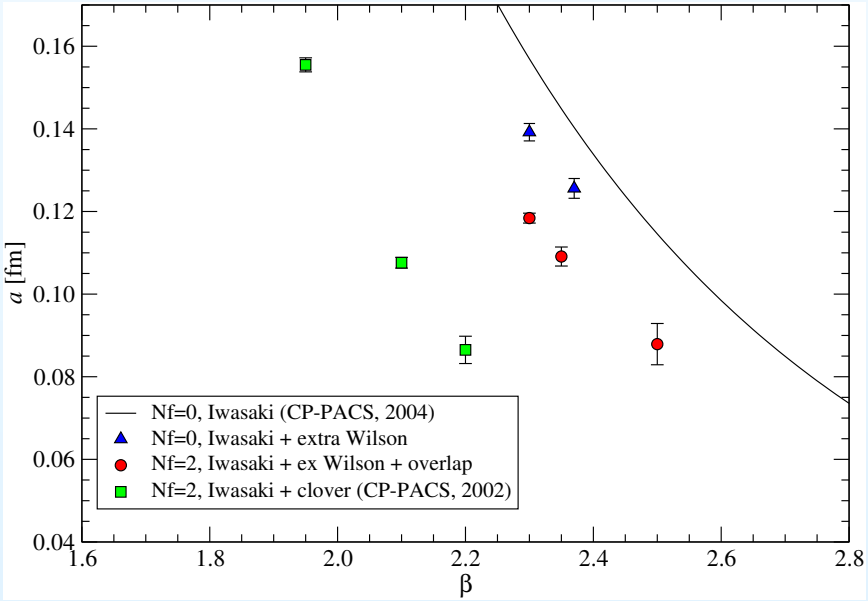
$N_f = 2 + 1$ algorithm (6)

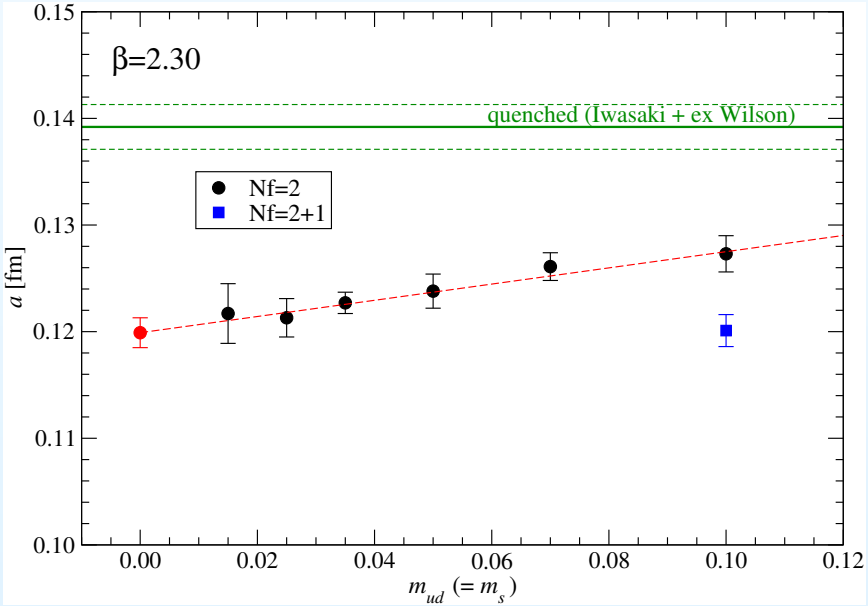
Very preliminary result

$\beta = 2.30$, $m_{ud} = m_s = 0.10$, $Q = 0$

- 300 thermalization trjs.
- 30 configs (5 trj separated)

a is determined by hadronic radius (Sommer scale)
— tendency consistent with $N_f = 2$





Summary/Outlook

JLQCD's dynamical overlap project

$N_f = 2$ is now in productive run at $16^3 \times 32$, $a \simeq 0.12$fm, $\simeq m_s/6$

- Best solution: less precise 5D solver $\oplus$ Noisy Metropolis
- Various observables are being measured
- Effect of fixed topology (simulations at various Q)

We are preparing for $N_f = 2 + 1$ simulations

- Improvement and parameter tuning are in progress
- Main target of the next year
- Larger lattice ($24^3 \times 48$) is planned