Lattice QCD simulation with dynamical overlap fermions

— JLQCD Collaboration's overlap project —

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Collaboration

The JLQCD Collaboration:

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- Introduction to lattice QCD
- Chiral symmetry on the lattice
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Introduction

Strong interaction is described by
Quantum Chromodynamics (QCD)

— difficult to solve analytically

- Perturbation theory applies only at high energy
  $\leftarrow$ asymptotic freedom
- Model calculations suffer from uncontrolled systematic uncertainties

Need of general procedure from the first principle

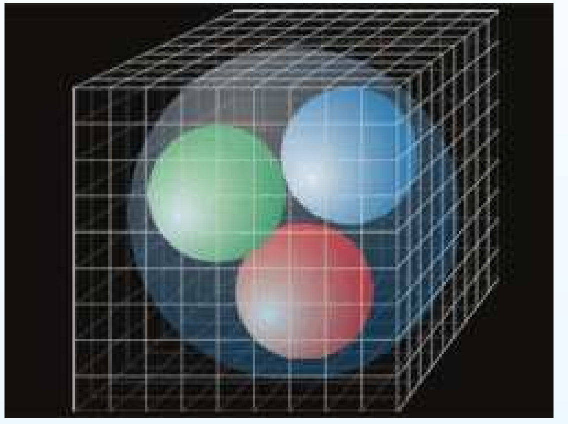
$\Rightarrow$ Lattice QCD

K.G.Wilson, Phys. Rev. D10 (1974) 2445.

Introduction

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
  $\Rightarrow$ nonperturbative calculation is possible



Powerful method for low-energy physics of QCD

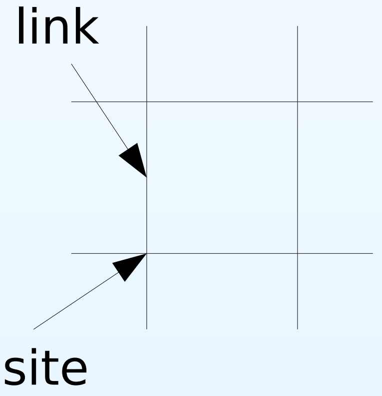
Introduction

QCD action (Euclidean space-time)

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

$\Downarrow$ discretize

Lattice QCD action



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

- 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

Lattice QCD actions:
must approache the continuum actions as $a \to 0$

Gauge field:

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

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

One can add higher order terms in a (e.g. rectangular loops)
$\longrightarrow$ improved actions (Iwasaki, DBW2, Lüscher-Weisz, etc.)

(Fermion action will be argued later)

Introduction

Path integral quantization:

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

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

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

$\Rightarrow$ Numerical simulation

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

for gauge configuration U with probability $\det D[U] \cdot \exp(-S_G)$.

Introduction

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 — dominated by quark solver
- Pseudofermion field (bosonic)

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

For positive definiteness, $\det D^2 = \det D^\dagger D$ $(N_f = 2)$
Odd flavor number algorithm is also applicable

Chiral symmetry on lattice

Lattice fermion formulation has been serious problem

Naive discretization:

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

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

16 particle modes appear (15 “doublers”)

— in momentum space,

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

E.g. for $m = 0$, poles appear at $p_\mu \sim 0$ and π

Chiral symmetry on lattice

Nielsen-Ninomiya's theorem:

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

Suppose a lattice fermion action $S_F = \psi D[U] \psi$ satisfies the following conditions.

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

Then, doublers exist.

Chiral symmetry on lattice

Wilson fermion: add Wilson term

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

$\longrightarrow$ 15 doublers disappear
This term breaks chiral symmetry explicitly

- Simple flavor structure
- Additive mass renormalization
- Complicated operator mixing

Chiral symmetry on lattice

Staggered (Kogut-Susskind) fermion

- 16 doublers $\rightarrow$ 4 spinors $\otimes$ 4 “tastes”
- Remnant of chiral symmetry
- Simulation cost is cheep
- “Fourth root trick” — nonlocal fermion action
- Taste symmetry breaking
- Staggered chiral perturbation — careful analysis needed

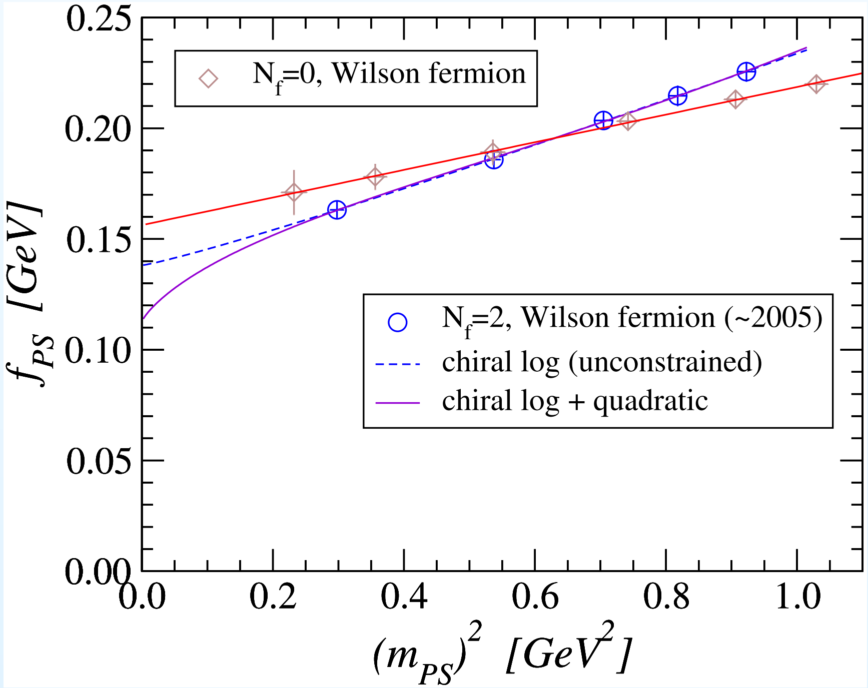
Chiral symmetry on lattice

Need of chiral symmetry

- Comparison with chiral perturbation theory
- Approaching to small quark mass region
- Controlled operator mixing
- Direct access to the chiral symmetry breaking effect

$$\frac{f}{f_0} = 1 - \frac{N_f}{2} y \log y + \alpha y$$

α: fit parameter
$y = m_\pi^2 / 4\pi f_0$
f_0: arbitrary const



Chiral symmetry on lattice

Domain-wall fermion — break through

Kaplan, Phys. Lett. B288 (1992) 342

5-dimensional formulation of fermion

- Motivated for chiral gauge theory (unsucceeded)
- Massive except for $s = 0$ ($\pm M_0$ for $s > 0/s < 0$)
- Chiral fermion mode appears at $s = 0$

For vector gauge theory (QCD)

Shamir, Nucl. Phys. B406 (1993) 90;

Furman and Shamir, Nucl. Phys. B439 (1995) 54.

- Finite 5-th dimensional extent
- Left and right modes appear at boundaries

Chiral symmetry on lattice

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.

$$D\gamma_5 + \gamma_5 D = aRD\gamma_5 D$$

Exact chiral symmetry on the lattice:

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

Lüscher, Phys. Lett. B428 (1998) 342.

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

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

Overlap fermion

Overlap fermion

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

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

H_W: Wilson Dirac operator with negative mass M_0
(M_0 is not quark mass!)

- Satisfies Ginsparg-Wilson relation
- $N_s \to \infty$, $a_5 \to 0$ limit of Domain-wall fermion
- Numerical cost is high $\leftarrow$ evaluation of $\mathrm{sign}(H_W)$
— has become possible only with recent developments of algorithms and computers

Overlap fermion

Overlap Dirac operator with quark mass m:

$$
\begin{aligned}
D(m) &= (M_0 - m)[1 + \gamma_5 \mathrm{sign}(H_W)] + m \\
&= \left(M_0 + \frac{m}{2}\right) + \left(M_0 - \frac{m}{2}\right) \gamma_5 \mathrm{sign}(H_W)
\end{aligned}
$$

H_W is hermitian Wilson-Dirac operator, $H_W = \gamma_5 D_W$,

$$
\begin{aligned}
D_W(x,y) &= (M_0 + 4)\delta_{x,y} \\
&\quad -\frac{1}{2}\sum_\mu \left[(1-\gamma_\mu)U_\mu(x)\delta_{x+\hat{\mu},y} + (1+\gamma_\mu)U_\mu^\dagger(x-\hat{\mu})\delta_{x-\hat{\mu},y}\right]
\end{aligned}
$$

Overlap fermion

Meaning of sign-function:

When applying to a vector w,

$$\begin{aligned} \mathrm{sign}(H_W)w &= \mathrm{sign}(H_W)\sum_\lambda v_\lambda(v_\lambda, w) \\ &= \sum_\lambda \mathrm{sign}(\lambda) v_\lambda (v_\lambda, w) \end{aligned}$$

where (λ, v_λ) are eigenvalue/eigenfunction of H_W.

If one knows all (λ, v_λ), $\mathrm{sign}(H_W)w$ can be determined.
— practically impossible
(on 10^4 lattice, 120000 eigenvalues exist)

In practice:

- Determine eigenvalues/vectors only at low frequency ($\lambda \le \lambda_{thrs}$)
- Use approximate formula to $\mathrm{sign}(H_W)$ for $\lambda > \lambda_{thrs}$

Implementation of overlap fermion

Zolotarev's partial fractional approximation

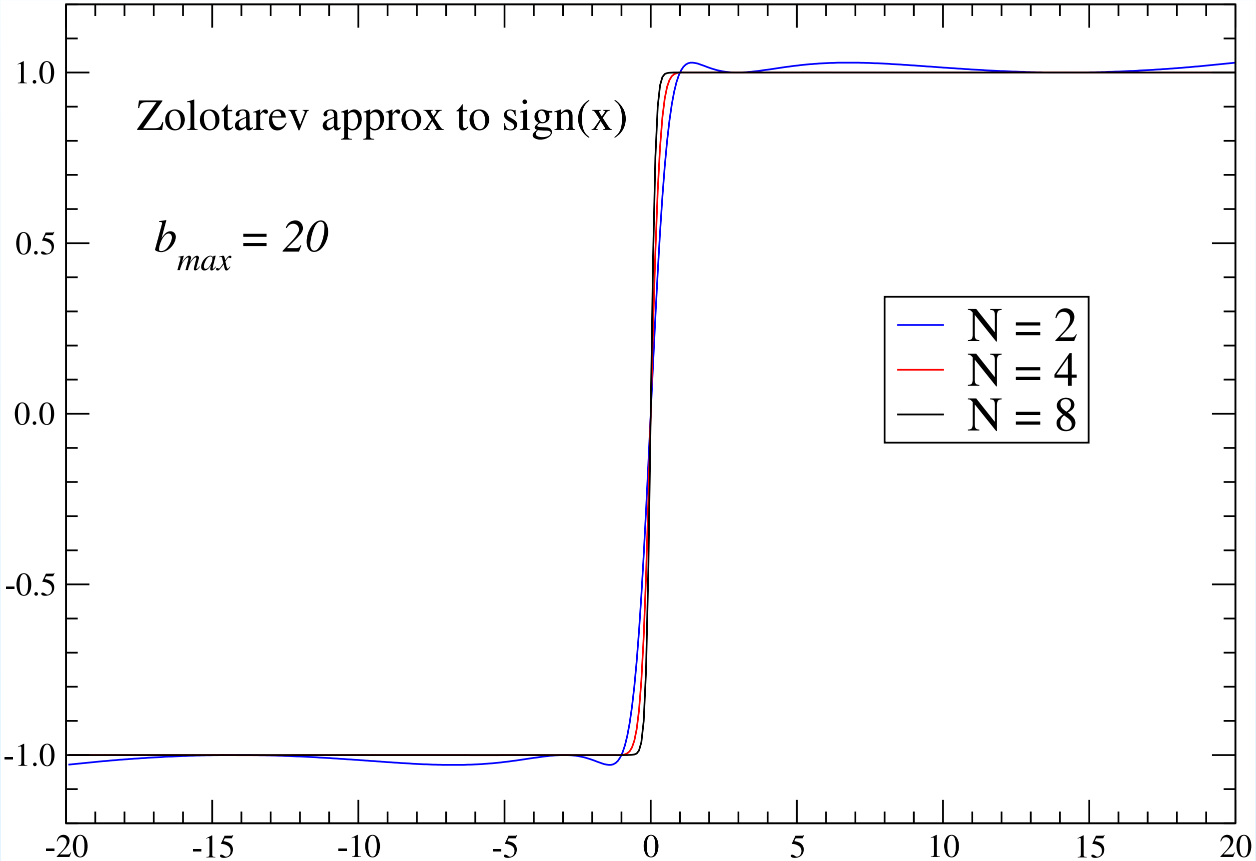
J. van den Eshof et al., Comp. Phys. Comm. 146 (2002) 203.

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

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

Zolotarev's partial fractional approximation:
approx. to $\mathrm{sign}(x)$, $1 \leq |x| \leq 20$



Implementation of overlap fermion

Quark propagator $S_q(x,y)$: solution of

$$\sum_z D(m;x,z)S_q(z,y) = \delta_{x,y}$$

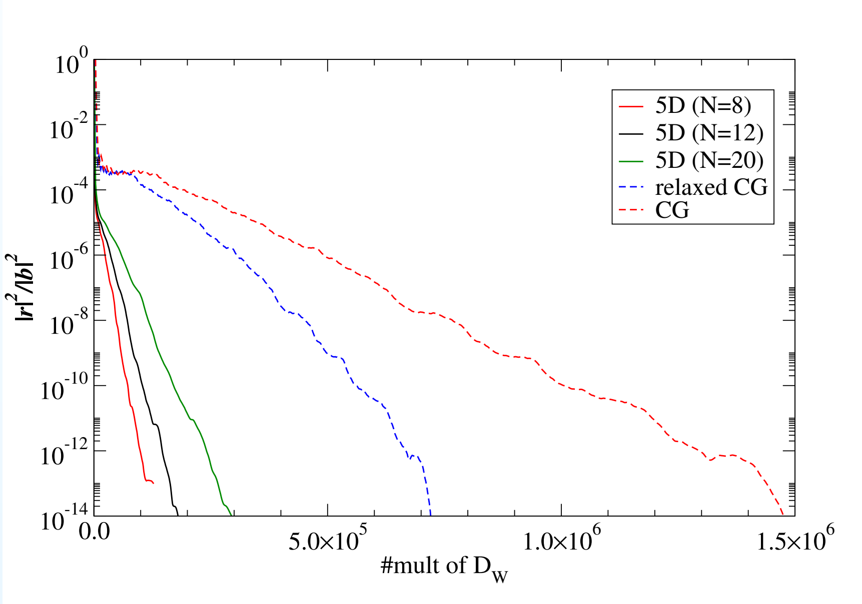
Numerical cost is most sensitive to solver algorithm

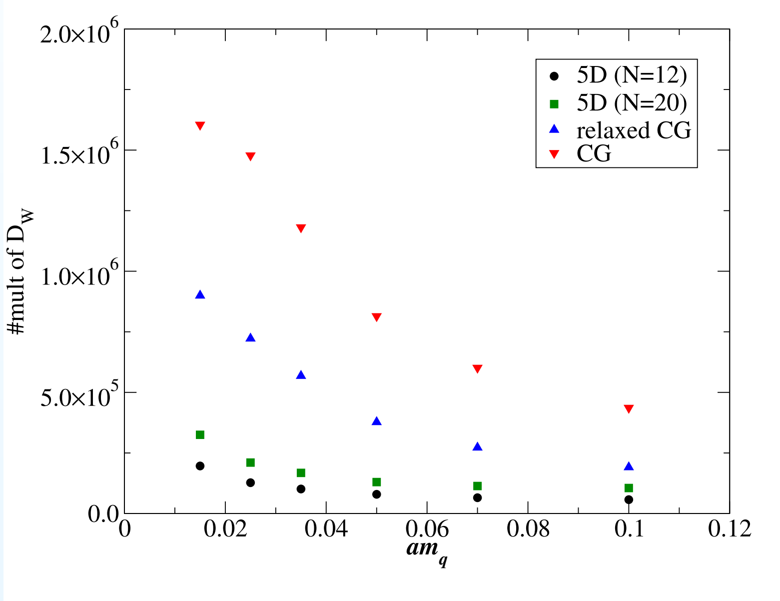
- Nested CG algorithm
  - Outer CG for $D(m)$, inner CG for $(H_W^2 + q_l)^{-1}$ (multishift)
    A.Frommer et al., Int. J. Mod. Phys. C 6 (1995) 627.
  - Improvement: CG with relaxation of inner loop convergence
    N.Cundy et al., Comp. Phys. Comm. 165 (2004) 221.
- 5-dimensional CG
  A. Borici, hep-lat/0402035; R.G.Edwards et al., PoS LAT2005 (2006) 146.
  - Subtraction of low-modes of H_W is not applicable
    $\rightarrow$ difficulty at $\lambda_{min} \sim 0$

Implementation of overlap fermion

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

JLQCD's overlap project

Dynamical simulation with $N_f = 2$ 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
- At $Q = 0$, generation of config. is almost over

$N_f = 2 + 1$ simulation

- Test run at $16^3 \times 32$, $a \simeq 0.12$fm
- Productive run soon starts at $16^3 \times 48$, $a \simeq 0.12$fm

JLQCD's overlap project

Measured quantities (in progress)

- Static quark potential (setting scales)
- Light meson spectrum, decay constants
- B_K parameter with nonperturbative renormalization
- Chiral condensate, low energy constants in ϵ-regime
- Topological susceptibility
- Heavy-light matrix elements

as well as

- Improvement of algorithms and code
- Check of locality
- Q-dependence of observables

JLQCD's overlap project

New machines at KEK (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$29% 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

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

  $H_W = \gamma_5 D_W$, 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

Results

Productive run: $16^3 \times 32$ lattice at $\beta = 2.30$ ($a \sim 0.12$fm)

- $\mu = 0.2$, $Q = 0$ *(fixed topology)*
- *Trajectory length* $l_\tau = 0.5$, *10,000 trjs at each* m_{ud}

Performance on Blue Gene (512-node):

— Less precise 5D solver in MD + noisy Metropolis

(fully improved HMC algorithm)

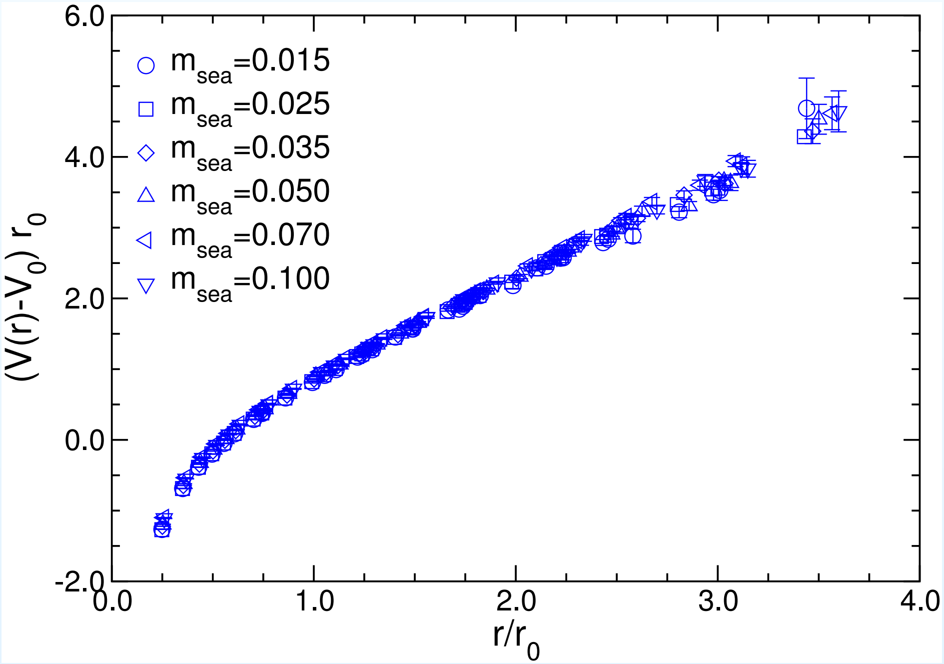
m_{ud}	P_{acc}	Plaquette	time/trj [min]
0.015	0.68	0.614795(12)	52
0.025	0.82	0.614779(11)	43
0.035	0.87	0.614779(8)	36
0.050	0.89	0.614717(10)	33
0.070	0.92	0.614709(12)	25
0.100	0.93	0.614652(8)	21

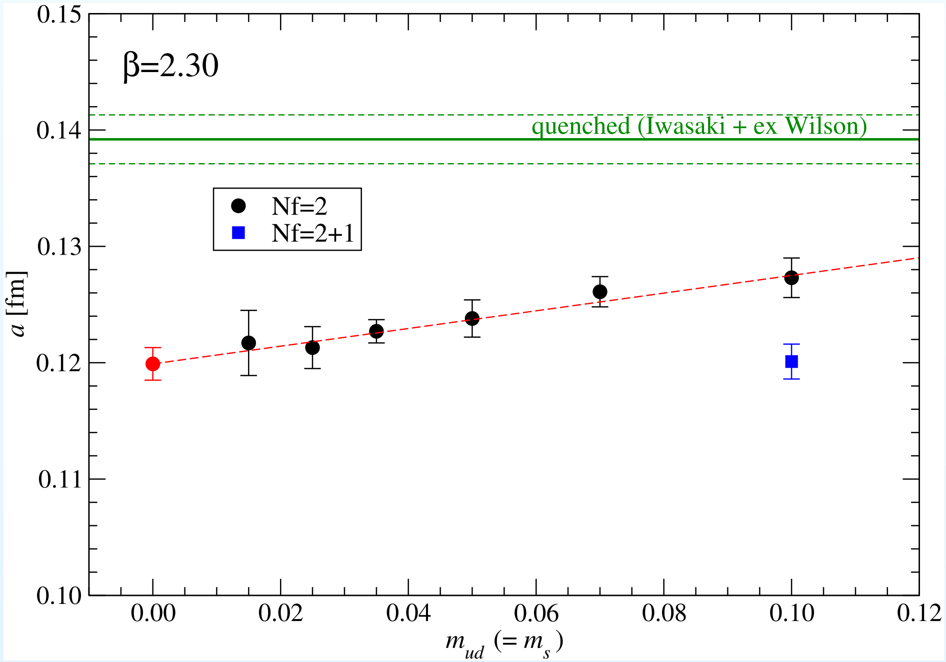
Results: Static potential

Static quark potential $\Leftarrow$ Wilson loop

Lattice scale is set by $r_0 = 0.5$ fm:

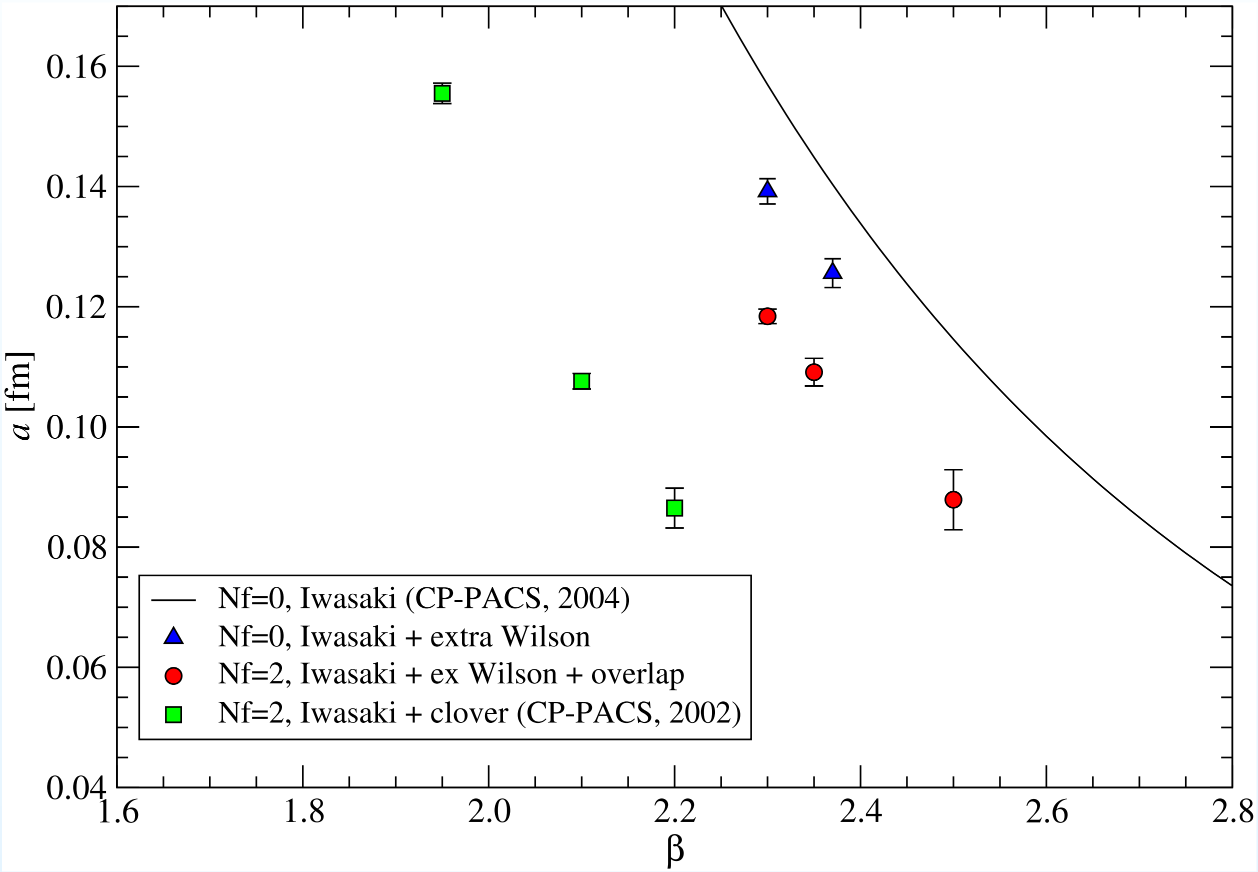
$$r^2 \frac{\partial V(r)}{\partial r}\bigg|_{r=r_0} = 1.65$$





($N_f = 2+1$: very preliminary)

Results: β-shift



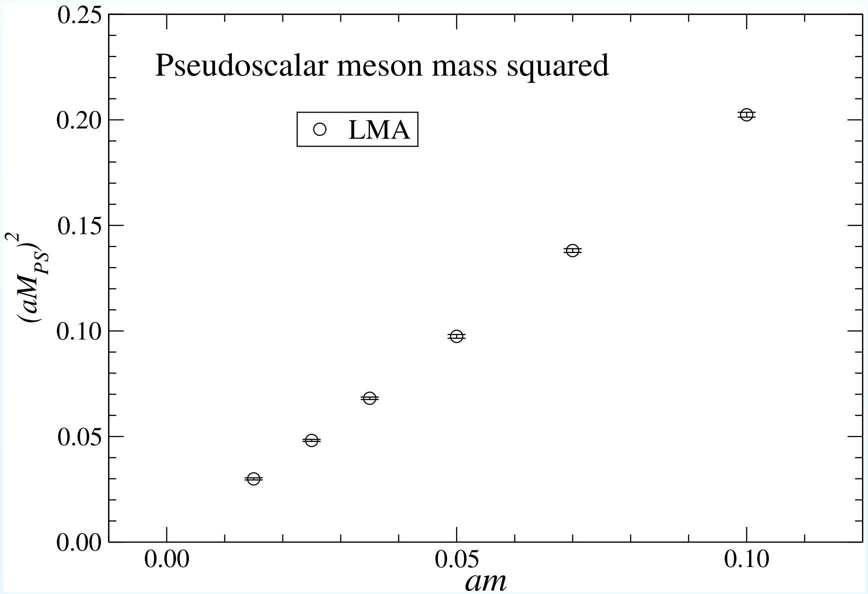
Milder β-shift than Wilson-type fermions

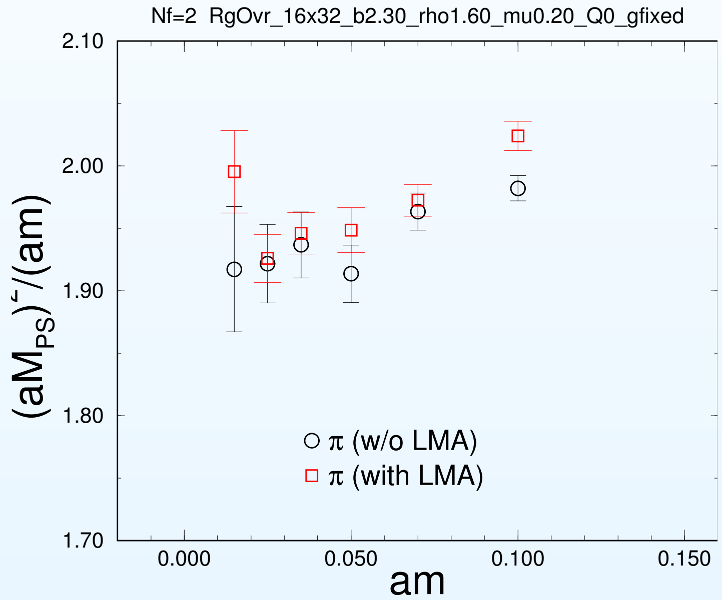
Results: Light meson spectrum (1)

Light meson spectroscopy (preliminary)

— still not all configs are analyzed

Pseudoscalar meson mass



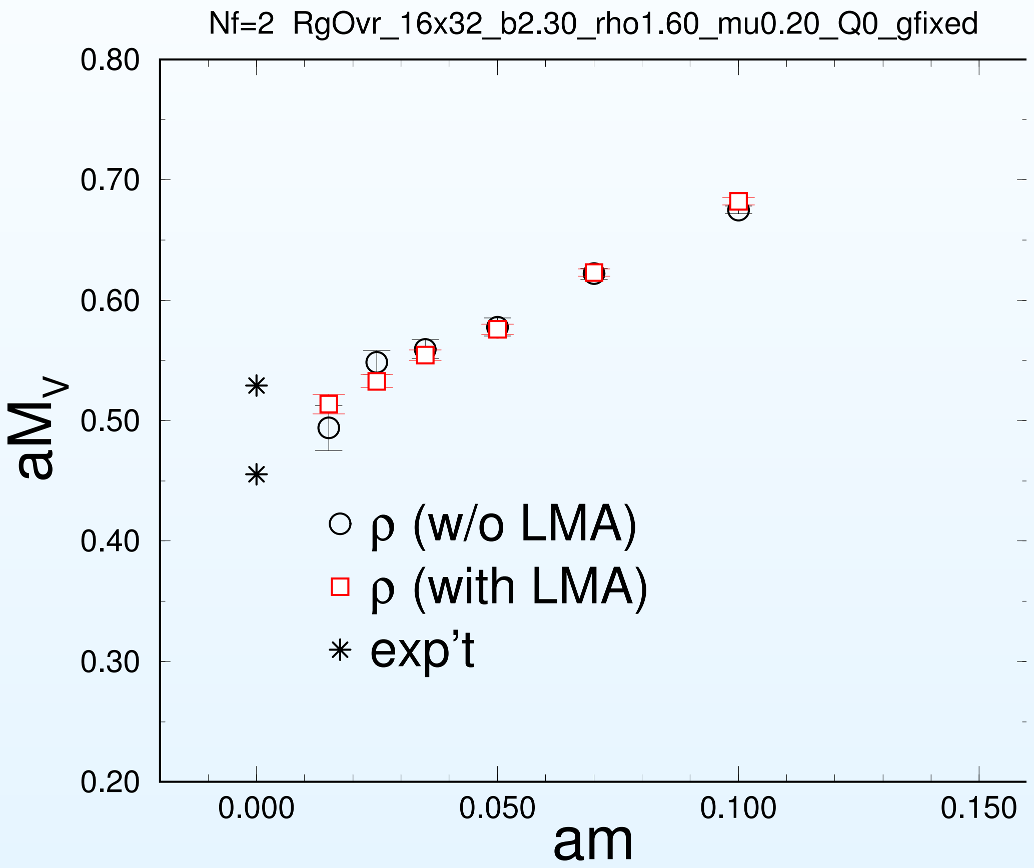


At small quark mass, consistent with linear behavior

LMA (low-mode averaging): technique to reduce fluctuation of low-mode contributions

Results: Light meson spectrum (2)

Vector meson mass



Consistent with linear behavior

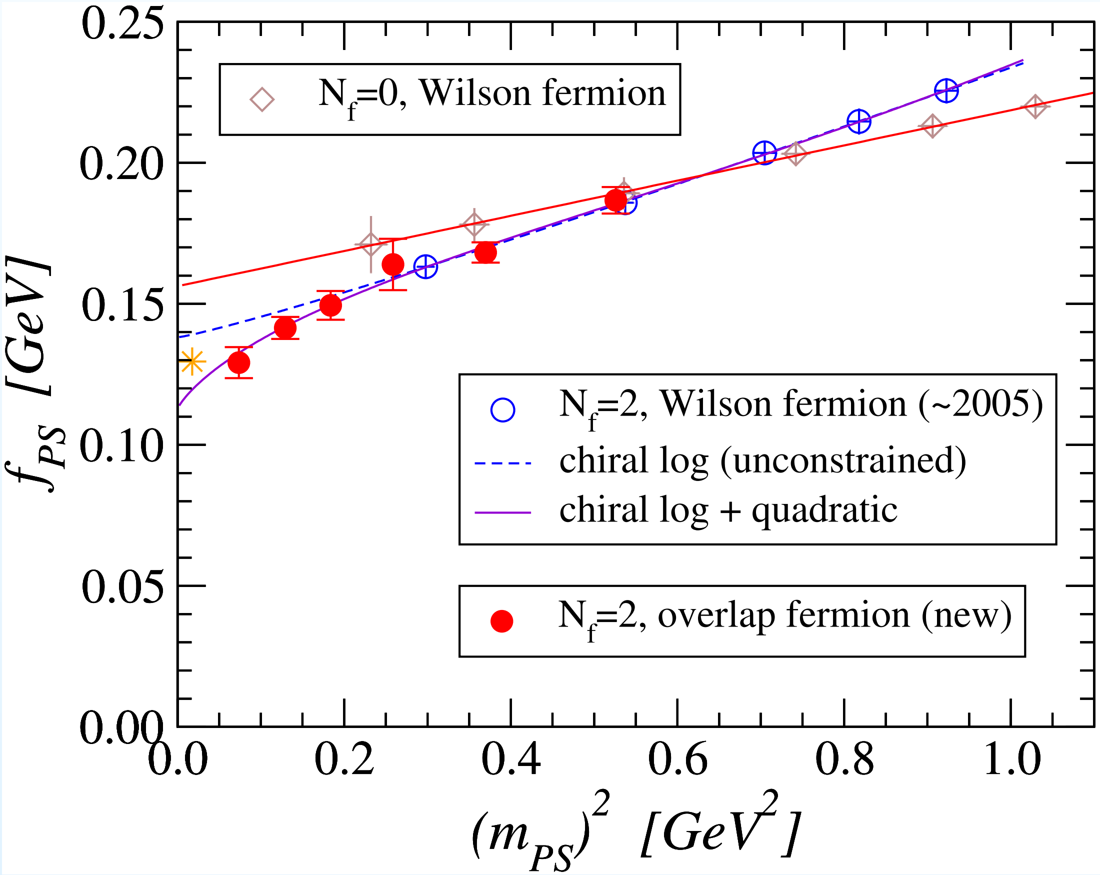
Results: Pseudoscalar meson decay constant

Chiral log visible ?

$$\frac{f}{f_0} = 1 - \frac{N_f}{2} y \log y + \alpha y$$

α: fit parameter
$y = m_\pi^2 / 4\pi f_0$
f_0: arbitrary const

Chiral log behavior is reproduced.



Summary/outlook

Lattice QCD has entered new generation:

- Understanding of chiral symmetry on the lattice
- Simulation with fermion having exact lattice chiral symmetry
- Exploring light quark mass region

JLQCD Collaboration is performing dynamical overlap project.

- $N_f = 2$ simulation on $16^3 \times 32$ lattice, $a \simeq 1.2$ fm
- Fixed topology
- Various observables are being measured
- Results so far are encouraging
- $N_f = 2 + 1$ simulation is in progress