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

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JPS annual meeting

21 Sept. 2007, Hokkaido Univ, Sapporo

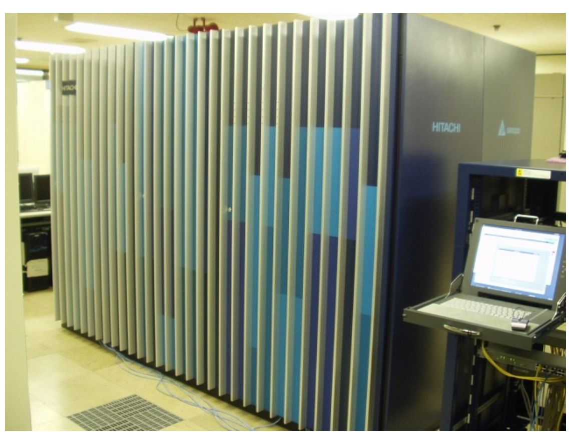
Project

Dynamical simulation with overlap fermions

- Iwasaki gauge + extra Wilson fermion (topology fixed)
- Main run: 16^3x48(32 for NF=2), larger size is planned
- Lightest ud quark mass ~m_s/6

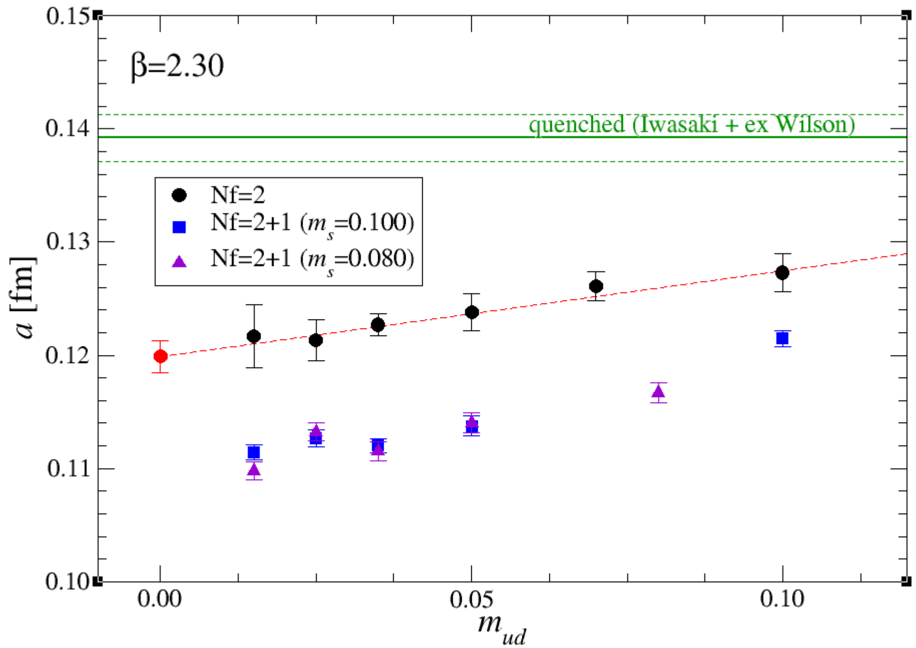
Goals:

- Exploring chiral dynamics
- Matrix elements with controlled chiral extrapolation



Status

- Nf=2: 16^3x32, a~0.12fm
  - Config generation finished, 10,000 trj
  - Physics measurements in progress (other talks)
- Nf=2+1: 16^3x48, a~0.11fm, 2 m_s values
  - Productive run in progress (now 900~1800 trj)
  - Improvement continued (this talk)



Scale set by $r_0 = 0.49\text{fm}$

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

(V: static quark potential)

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Overlap fermion

$$D = \frac{1}{Ra}\left[1 + \gamma_5 \,\mathrm{sign}(H_W(-m_0))\right]$$

H_W : hermitian Wilson-Dirac operator

(Neuberger, 1998)

- Theoretically elegant
  - Satisfies Ginsparg-Wilson relation (exact chiral symmetry)
  - *Infinite* N_s limit of Domain-wall fermion (No m_{res})
- Numerical cost is high
  - Calculation of sign function (O(5) larger cost than DW)
  - Discontinuity at zero eigenvalue of H_W
  - While has become feasible, improving algorithm is still highly desired for large lattices

Overlap operator

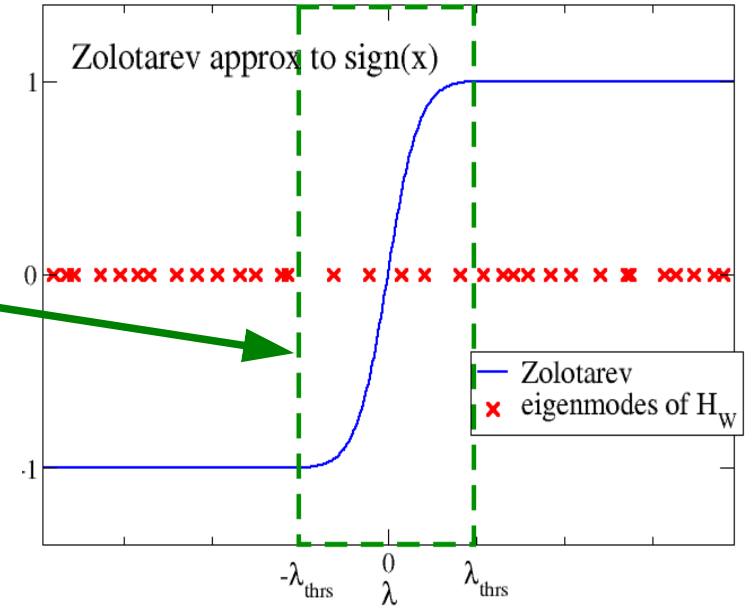
$$D(m) = \left(M_0 + \frac{m}{2}\right) + \left(M_0 - \frac{m}{2}\right)\gamma_5 \mathrm{sign}(H_W)$$

Zolotarev's Rational approximation

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

- Valid for $|\lambda|$ (eigenmode of H_W) $\in [\lambda_{thrs}, \lambda_{max}]$
- Smaller λ_{thrs}, larger N is needed for accuracy: $\sim \exp(-\lambda_{thrs} N)$
- Projecting out low-modes of H_W below λ_{thrs}

$\rightarrow$ $\mathrm{sign}(\lambda)$ $(\lambda < \lambda_{thrs})$ explicitly determined keeping modest value of λ_{thrs}

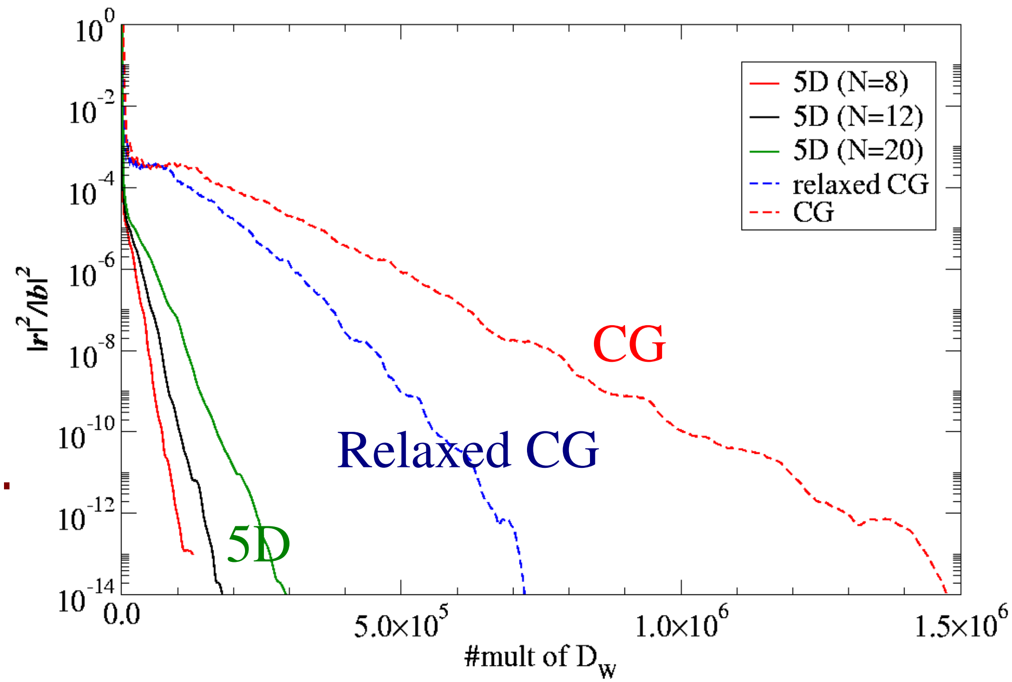


Overlap solver

--- Most time-consuming part of HMC

- Two algorithms used: Nested (4D) CG and 5D CG

- Nested CG (Fromer et al., 1995, Cundy et al., 2004)
  - Outer CG for $D(m)$, inner CG for $(H_W^2 + q_l)^{-1}$ (multishift)
  - Relaxed CG: ε_{in} is relaxed as outer loop iteration proceeds
  - Cost mildly depends on N



Nf=2, a=0.12fm, on single config.
Without low-mode projection

5D solver

- 5-dimensional CG (Borici, 2004, Edwards et al., 2006)
  - One can solve $S\psi_4 = \chi_4$ by solving (example: N=2 case)

$$M_5 \begin{pmatrix} \phi \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix}, \quad M_5 = \left(\begin{array}{cccc|c} H_W & -\sqrt{q_2} & & & 0 \\ -\sqrt{q_2} & -H_W & & & \sqrt{p_2} \\ & & H_W & -\sqrt{q_1} & 0 \\ & & -\sqrt{q_1} & -H_W & \sqrt{p_1} \\ \hline 0 & \sqrt{p_2} & 0 & \sqrt{p_1} & R\gamma_5 + p_0 H \end{array}\right) = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right)$$

$$S = D - CA^{-1}B$$: overlap operator (rational approx.)

  - Low-mode projection (New)

$$D = R\gamma_5 + p_0 H_W \quad \longrightarrow \quad D = R\gamma_5 + p_0 H_W + (M_0 - \frac{m}{2}) \sum_{j=1}^{N_{ev}} \mathrm{sign}(\lambda_j) v_j \otimes v_j^\dagger$$

$$\sqrt{p_i} \quad \longrightarrow \quad \sqrt{p_i} P_H \quad (P_H = 1 - \sum_{j=1}^{N_{ev}} v_j \otimes v_j^\dagger)$$

5D solver

- Even-odd preconditioning
  - Acceleration by solving $[1 - M_{ee}^{-1} M_{eo} M_{oo}^{-1} M_{oe}] x_e = b'_e$

    where $$M_5 x = \begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix} \begin{pmatrix} x_e \\ x_o \end{pmatrix} = \begin{pmatrix} b_e \\ b_o \end{pmatrix}$$
  - Inversion of M_{ee} and M_{oo} is necessary
    - Easy in the case without projection
    - With projection, inversion becomes nontrivial, but can be done cheaply because rank of operator is only $2(N_{ev}+1)$.

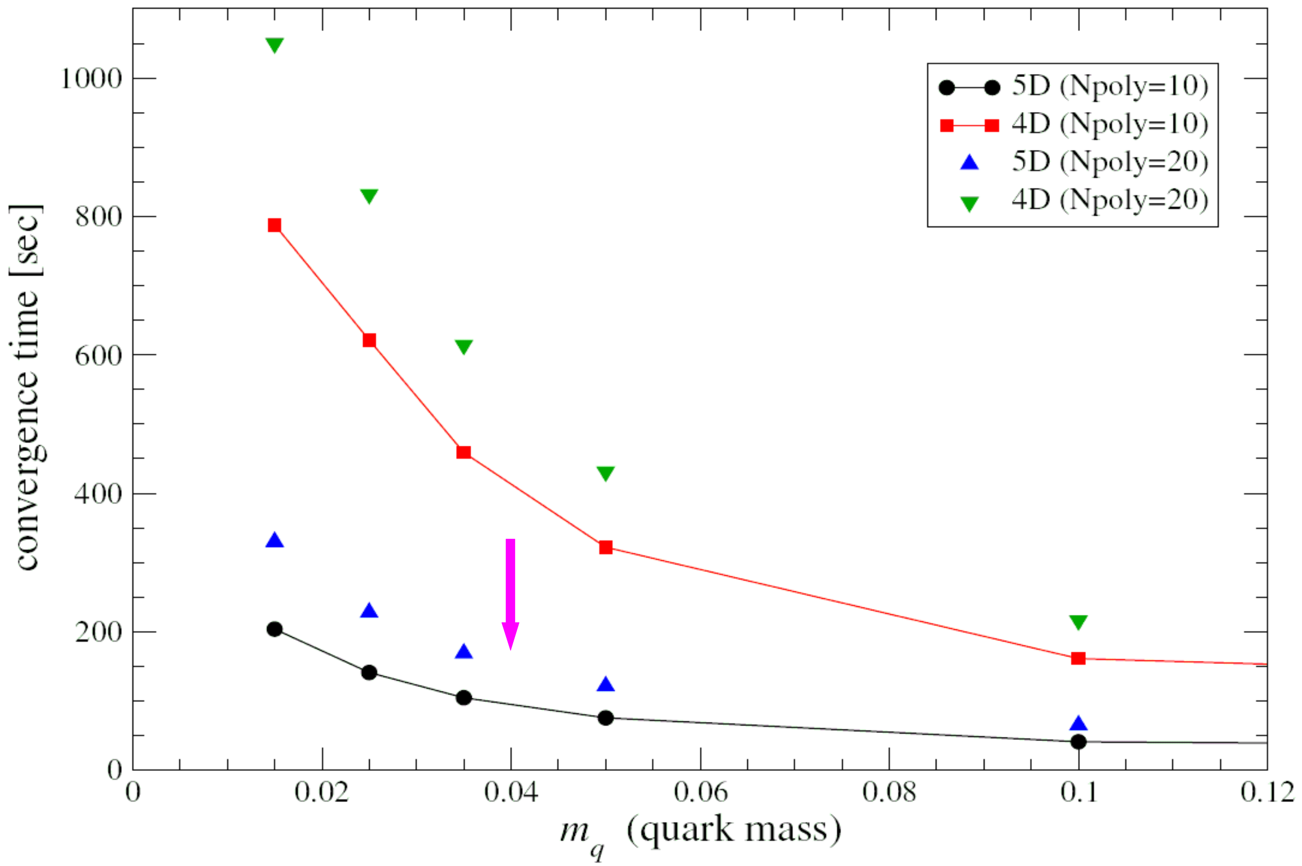
      ⇒ $M_{ee}^{-1} x_e$ is spanned by $\{x_e, \gamma_5 x_e, v_j, \gamma_5 v_j\}$
  - To solve even equation, CGNE is used:

    Improvement of inversion algorithm still desired

5D solver

- Solver performance
  - 5D solver is O(3-4) times faster than 4DCG

Nf=2+1 HMC on BG/L 1024-node (16^3x48)



$$|r|/|b| < 10^{-10}$$

(N_{sbt}=8)

HMC algorithm

<u>Nf=2+1 algorithm</u>

- Nf=1 part: one chirality sector

  (Bode et al., 1999, DeGrand and Schaefer, 2006)

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

$$H^2 = P_+H^2P_+ + P_-H^2P_- \Rightarrow \det H^2 = \det(P_+H^2P_+)\cdot\det(P_-H^2P_-)$$

$$S_{PF} = \phi_\sigma^\dagger[P_\sigma H^2 P_\sigma]\phi_\sigma \quad (\sigma = +, -)$$

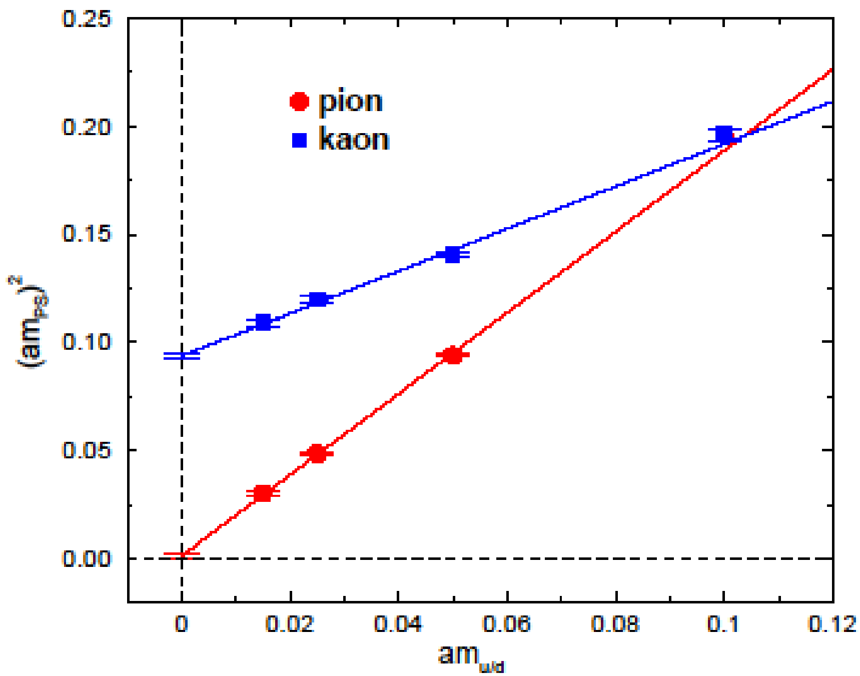
- Improved HMC algorithms: same as Nf=2
  - Hasenbusch mass preconditioning
  - Multi-time step
  - For Nf=2, noisy Metropolis + 5D solver (w/o projection) was used. Now no need of noisy Metropolis.
  - Present performance: 1-2 hours/trj (unit length)

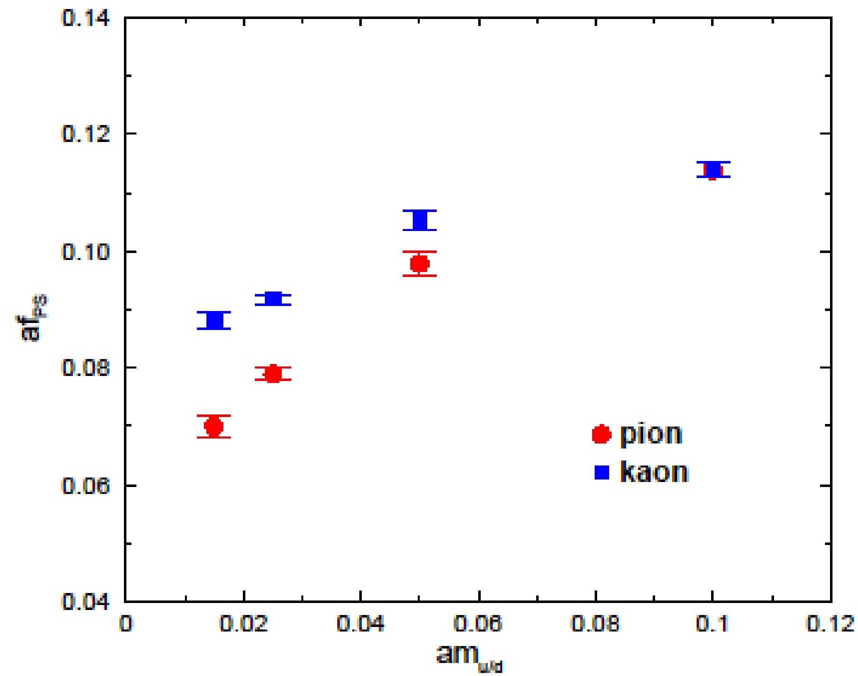
    Still improvement is necessary!

Measurement

- Now mainly at m_s=0.100, m_s=0.080 in preparation
- measurements at every 5 trj
- 160 eigenvalues/eigenvectors are calculated
  - low-mode preconditioning/averaging

PS meson mass and decay constant





Summary/Outlook

Nf=2+1 dynamical overlap simulation

- On 16^3x48, a~0.11fm, 5 ud x 2 strange quark masses
- Production run in progress
- 5D solver with low-mode projection has become possible
- Further improvement of algorithm is needed
- Larger lattice size (24^3x64) is planned