Simulation with 2+1 flavors of dynamical overlap fermions

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High Energy Accelerator Research Organization (KEK)

Collaboration

- JLQCD Collaboration
  - S.Aoki (Tsukuba), S.Hashimoto (KEK), T.Kaneko (KEK), J.Noaki (KEK), T.Onogi (YITP, Kyoto), E.Shintani (KEK), N.Yamada (KEK), H.M. (KEK)
- TWQCD Collaboration
  - T-W.Chiu (Taiwan), X, T-H.Hsieh (Academia Sinica), K. Ogawa (Taiwan)
- Other presentations:
  - Hashimoto (plenary, Wed)
  - Noaki (spectrum, Tue)
  - Chiu (topological susceptibility, Tue)
  - Kaneko (Pion form factors, Thu)
  - Ohki (Nucleon sigma term, Thu)
  - Shintani (strong coupling const, Fri)
  - Yamda (S-parameter, ps-NG boson mass, Fri)

Project

- Dynamical simulations with exact chiral symmetry
- 2-flavor runs on a 16^3x32 lattice (a=0.12fm)
  - Fixed topological charge (mainly Q=0)
  - 6 sea quark masses (m_q~(1/6–1) m_s)
  - Finished to accumulate 10,000 trj
  - many physical calculations
- 2+1-flavor runs on 16^3x48 lattice (a=0.11fm)
  - 5 m_{ud} (~(1/6–1) m_s^{phys}), 2 m_s (~m_s^{phys})
  - 2,500 trj accumulated
- epsilon regime: Nf=2 finished, 2+1 in progress
- 2+1-flavor runs on 24^3x48 lattice are being started

Action

- Neuberger's overlap Dirac operator
  - With standard Wilson kernel with negative mass $-M_0$

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

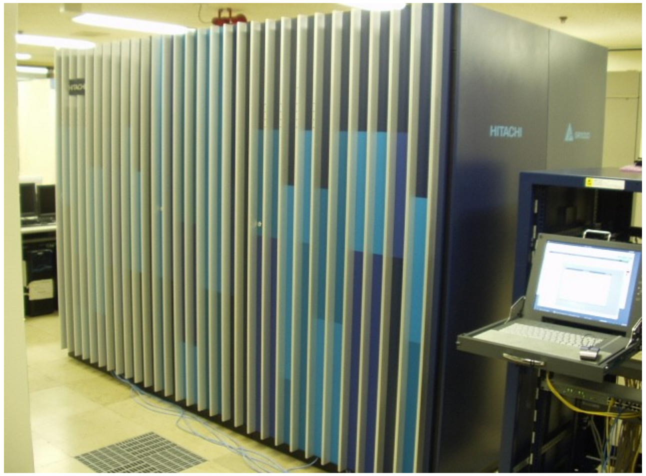
$M_0 = 1.6$

- Iwasaki gauge
- Extra (two flavors of) Wilson fermions
  - To suppress near-zero modes of H_W
  - With associated twisted mass ghost

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

Machines

- IBM Blue Gene/L at KEK
  - 57.6 Tflops peak (10 racks)
  - 0.5TB memory/rack
  - 8x8x8(16) torus network
  - ~30% performance for Wilson kernel
  - Overlap HMC: 10~15% on one rack



- Hitachi SR11000 (KEK)
  - 2.15TFlops/0.5TB memory

Overlap Operator

- Zolotarev's Rational approximation

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

  - Multi-shift solver can invert $(H_W + q_l)$ at once
  - Near-zero modes are projected out, treated exactly
  - Typically N =10 to achieve an accuracy of $10^{-(7\text{-}8)}$

- Overlap solvers
  - Nested CG with relaxation (Cundy et al., 2005)
  - 5D solver with projection

5D solver

(Borici, 2004, Edwards et al., 2006)

- Schur decomposition
  - 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.)

  - Even-odd preconditioning
  - Low-mode projection of H_W in lower-right corner

Even-odd preconditioning

- Acceleration by solving $\left(1 - M_{ee}^{-1} M_{eo} M_{oo}^{-1} M_{oe}\right) x_e = b_e'$
  - Need fast inversion of the "ee" and "oo" block; easy if there is no projection operator
  - $M_{ee(oo)}^{-1}$ mixes in the 5th direction, while $M_{eo(oe)}$ is confined in the 4D blocks
- Low-mode projection
  - Lower-right corner must be replaced by

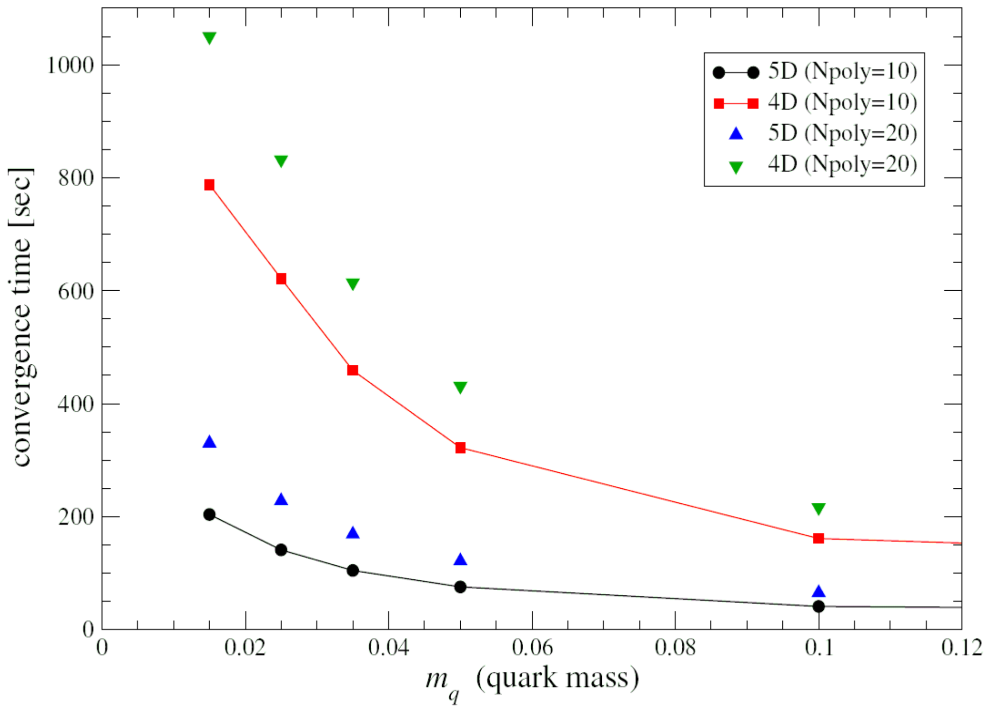
$$R(1-P_H)\gamma_5(1-P_H) + p_0 H_W + \left(m_0 + \frac{m}{2}\right)\sum_{j=1}^{N_{ev}} \mathrm{sgn}(\lambda_j) v_j \otimes v_j^+, \quad P_H = 1 - \sum_{j=1}^{N_{ev}} v_j \otimes v_j^+$$

  - Inversion of $M_{ee(oo)}$ becomes non-trivial, but can be calculated cheaply because the rank of the operator is only 2(N +1).

$$\left\{ x_e, \gamma_5 x_e, \{ v_{je}, \gamma_5 v_{je} \} \right\}$$

Solver performance

- Comparison on 16^3x48 lattice



On BG/L 1024-node

(N_{sbt}=8)

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

  - 5D solver is 3-4 times faster than 4D solver

Odd number of flavors

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

- $H^2 = D^\dagger(m)D(m)$ commutes with γ_5
  - Decomposition to chiral sectors is possible

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

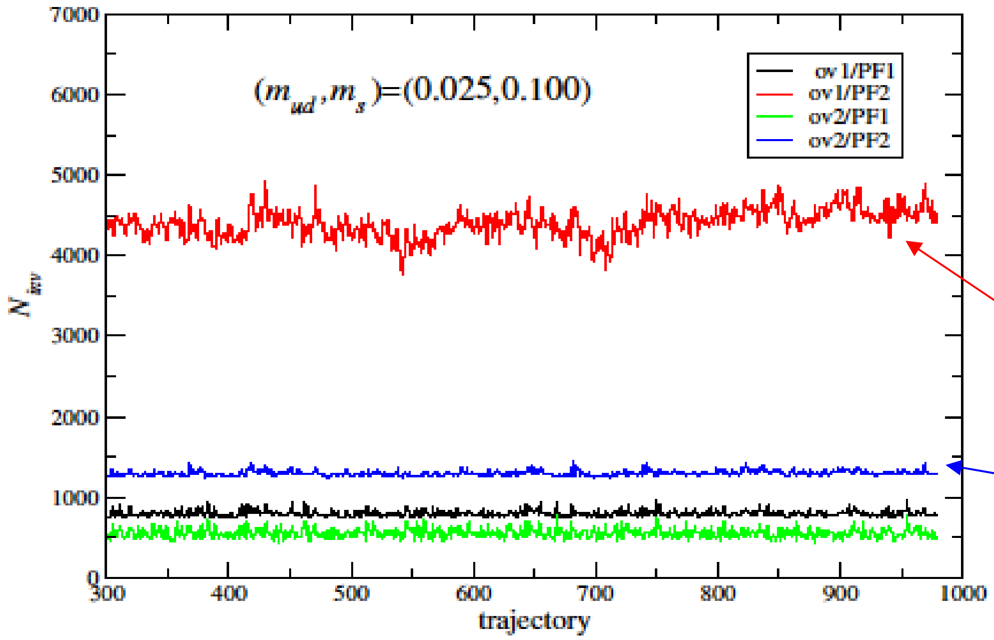
  - $P_+H^2P_+$ and $P_-H^2P_-$ share eigenvalues except for zero-modes
  - 1-flavor: one chirality sector
  - Zero-mode contribution is constant throughout MC, thus neglected
- Pseudo-fermion: $S_{PF} = \sum_x \phi^\dagger_\sigma(x) Q_\sigma^{-1}\phi_\sigma(x), \quad Q_\sigma = P_\sigma H^2 P_\sigma$

  σ is either + or -
  - Refreshing ϕ from Gaussian distributed ξ as $\phi_\sigma(x) = Q_\sigma^{1/2}\xi(x)$
  - sqrt is performed using a rational approximation
  - Other parts are straightforward

Algorithm

- HMC
  - Hasenbusch preconditioning with heavier mass m'
  - Multi-time step for PF2(m), PF1(m'), Gauge/ExWilson

$$F_G \sim F_E \gg F_{PF1} \gg F_{PF2}. \Longrightarrow \Delta\tau_{(PF2)} \gg \Delta\tau_{(PF1)} \gg \Delta\tau_{(G)} = \Delta\tau_{(E)}.$$



Number of two 5D CG iterations in the calculation of Hamiltonian

PF2 for ud

PF2 for s

2+1-flavor run status

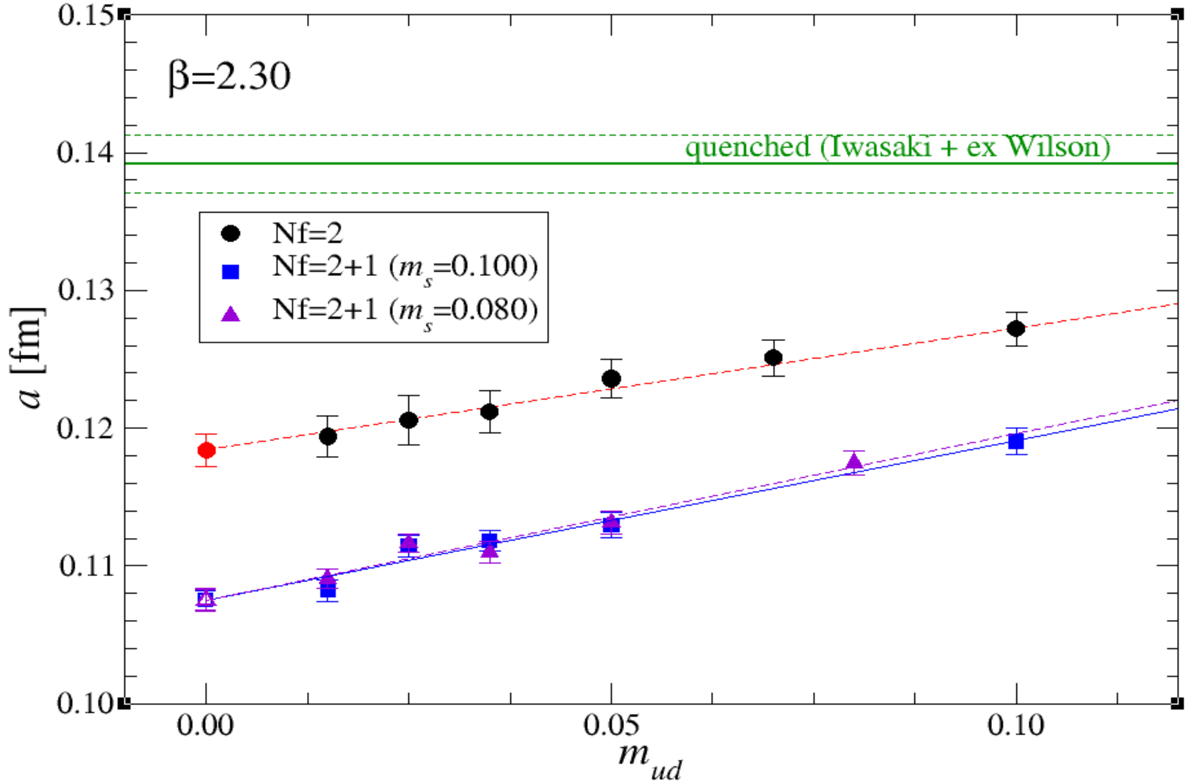
- 16^3x48 lattice, a~0.11 fm
  - β =2.3, topological charge Q=0
  - 2 strange quark masses around physical m_s

    $m_s = 0.10, 0.08$
  - 5 ud quark masses covering (1/6~1)m_s

    $m_{ud} = 0.015, 0,025, 0,035, 0.050, m_s$
  - 2,500 trajectories of length 1 for each (m_{ud}, m_s)
  - About 2 hours/traj on BG/L 1024 nodes

Lattice scale

- Scale: set by $r_0 = 0.49$fm



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

Nf=2 result includes systematic error.

  - Strange quark effect is invisible
  - Slightly smaller lattice spacing than Nf=2
  - Milder β-shift than Wilson-type fermions

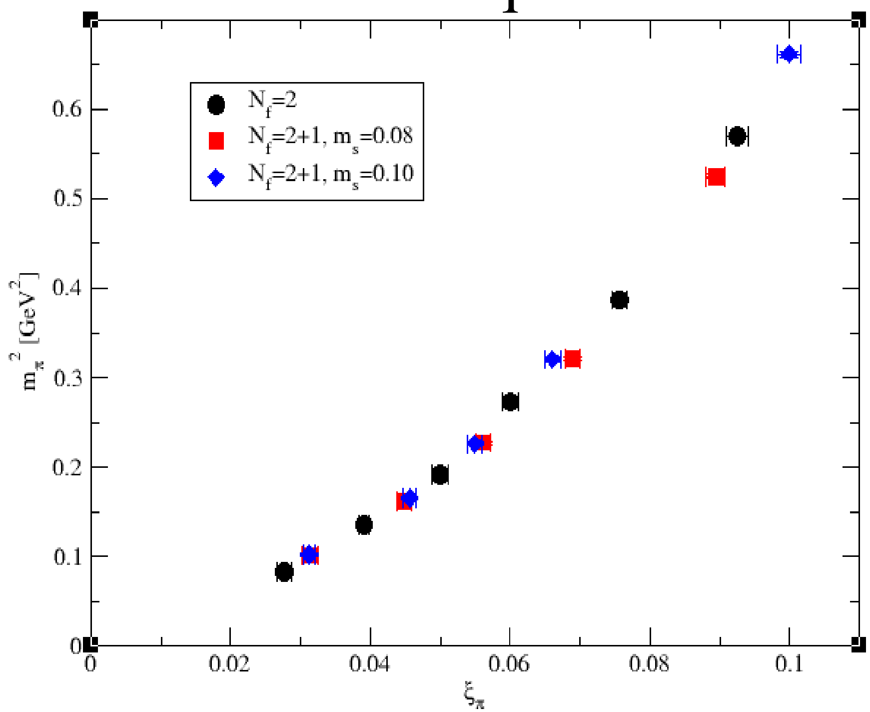
Spectrum

- Pion mass and decay const

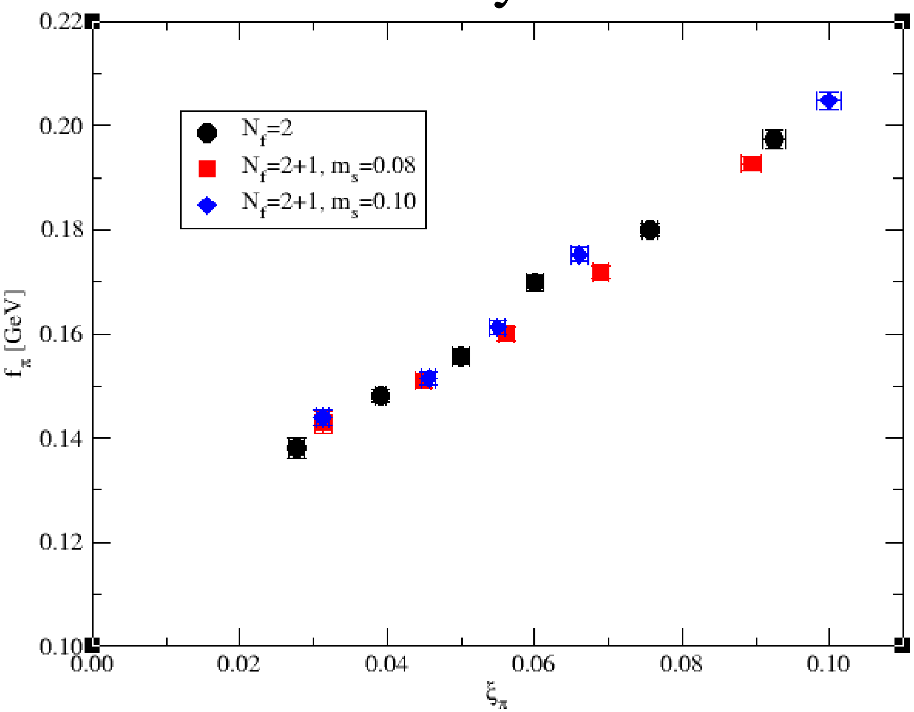
Talk by J.Noaki (Tue)

  - Comparison with ChPT is in progress
  - Fit parameter: $\xi \equiv \left(\frac{m_\pi}{4\pi f_\pi}\right)^2$ (f_π is mass dependent)

Pion mass squared



Pion decay constant



Further improvement

- Chronological estimator (Brower et al., 1997)
  - Approx. solution for CG solver from previous solutions
  - From 4D estimate ψ, estimate of 5D solver is constructed:

$$M_5 = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix} \equiv L\Gamma U$$

$$M_5 \begin{pmatrix} \phi \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix} \Longrightarrow \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} \phi + A^{-1}B\psi_4 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} 0 \\ \chi_4 \end{pmatrix}$$

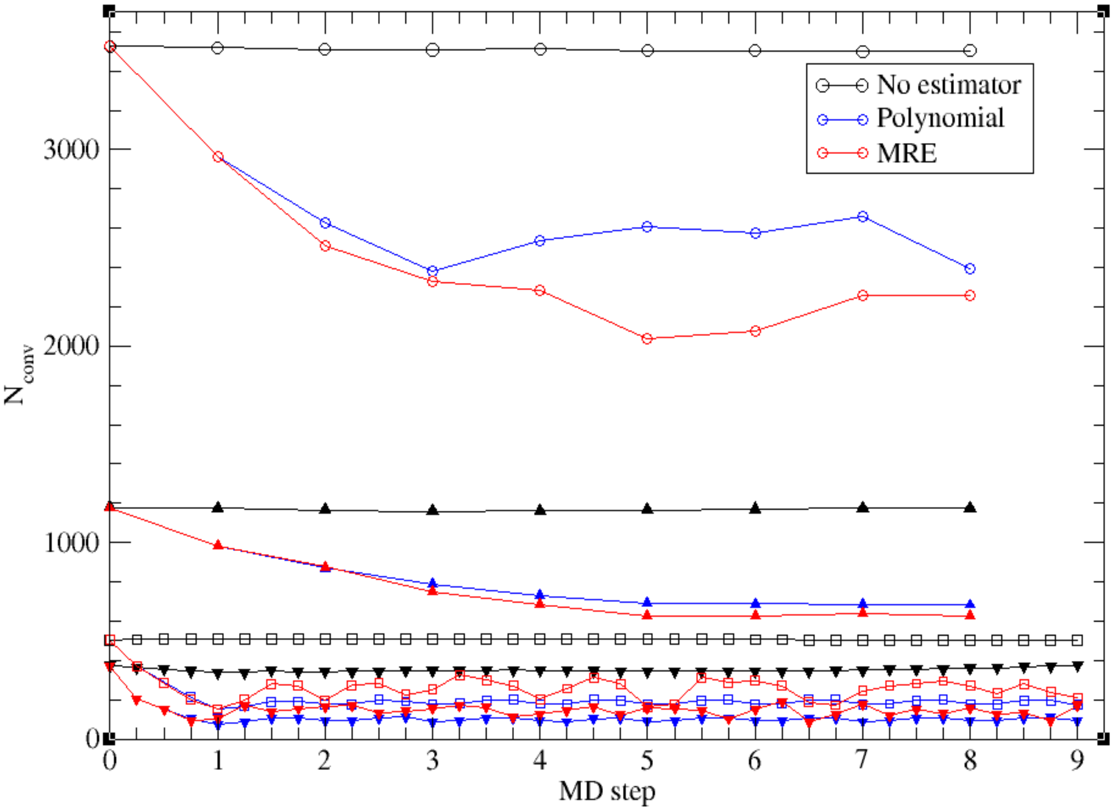
ϕ is given by solving $A\phi = -B\psi_4$ (by multi-shift solver)

  - Keeping 4D solution vectors: less memory consuming

- Also applicable to ''adaptive 5D solver''
  - Change N (number of poles) during iteration

Test of chronological estimator

- Convergence of 5D solver
  - 16^3x48, 2+1 flavor
  - m=0.015, m'=0.2
  - m=0.080, m'=0.4
- Estimate with 5 previous solution vectors
  - Polynomial extrap.
  - MRE (minimum residual extrap.)



- For preconditioner, polynomial extrap. works well
- To keep reversibility, higher precision is required
  - not efficient without other improvement

Summary/Outlook

We are performing dynamical overlap project at fixed topological charge

- Nf=2 on 16^3x32, a~0.12fm: producing rich physics results
- Nf=2+1 on 16^3x48, a~0.11fm: generation finished, physics measurements in progress
- Nf=2+1 on 24^3x48 being started

- Further improvements of algorithm are essential
  - Solver with deflation
  - Improved stimator (Omelyan, etc.)
- Supply of configs to ILDG is in preparation
  - Nf=2 will be soon
  - Cf. T.Yoshie's talk