2+1 flavor lattice QCD simulation with $O(a)$-improved Wilson quarks

Naoya Ukita (CCS, University of Tsukuba)
for PACS-CS Collaboration

Lattice 2008

July 14, 2008

PACS-CS Collaboration Member

S. Aoki, N. Ishii, N. Ishizuka, D. Kadoh, K. Kanaya,
Y. Kuramashi, Y. Namekawa, Y. Taniguchi,
A. Ukawa, N. Ukita, T. Yoshie (University of Tsukuba)

K.-I. Ishikawa, M. Okawa (Hiroshima Univ.)

T. Izubuchi (Kanazawa Univ.)

Introduction

PACS-CS Project:

$N_f = 2+1$Simulations at the Physical Point on large enough lattices

(→ plenary talk by Kuramashi)

u-d quarks : Domain-Decomposed HMC (DDHMC) algorithm (Lüscher, 2003)

+ Hasenbusch trick (Hasenbusch, 2001; Hasenbusch, Jansen, 2003) $+\cdots$

s quark : UV-filterd Polynomial HMC (UVPHMC) algorithm

(JLQCD Collaborations, 2002)

- $O(a)$ improved Wilson quark action with nonperturbative $c_{\rm SW}$

  (CP-PACS and JLQCD Collaborations, 2006)

- Iwasaki gauge action (Iwasaki, 1983)
- $\beta = 1.90$ ($a = 0.0907(13)$fm)
- $32^3 \times 64$ lattice
- $m_{\rm ud} = 3.5 \sim 67$ MeV

on the PACS-CS computer ($2560 \rm nodes, 14.3 TFLOPS$) at University of Tsukuba.

Introduction

Plan to this talk :

- Introduction
- Algorithm for $N_f = 2$ part : DDHMC, Hasenbusch trick, Solver
  (→ plenary talk by Ishikawa)
- Simulation Parameters and Data Set
- Run Status
- Conclusion

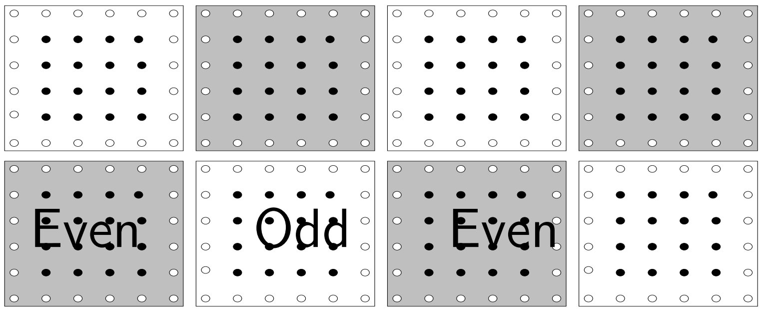
DDHMC Algorithm (Lüscher, 2003)

Here we consider preconditioning for $N_f = 2$ O(a)-improved Wilson-Dirac op.

- Jacobi preconditioning : $|\det(1+T)|^2\ |\det D|^2$

  $D = 1 + (1+T)^{-1}M$, T : clover term, M : hopping term

- Domain decomposition splitting lattice sites into even & odd domains



domain size we use is 8^4

$$D = \begin{pmatrix} D_{EE} & D_{EO} \\ D_{OE} & D_{OO} \end{pmatrix} = \begin{pmatrix} D_{EE} & 0 \\ 0 & D_{OO} \end{pmatrix} \begin{pmatrix} 1 & D_{EE}^{-1} D_{EO} \\ D_{OO}^{-1} D_{OE} & 1 \end{pmatrix}$$

$$\Rightarrow\ |\det(1+T)|^2 \underbrace{|\det D_{EE}|^2\ |\det D_{OO}|^2}_{\text{UV part}}\ |\det(\underbrace{1 - D_{EE}^{-1} D_{EO} D_{OO}^{-1} D_{OE}}_{\equiv \hat{D}_{IR}\ :\ \text{IR part}})|^2$$

- Even-Odd site preconditioning for $D_{EE(OO)}$: $|\det D_{EE}|^2 \Rightarrow |\det \bar{D}_{EE}|^2$

- Further preconditioning by spin & hopping structure : $|\det \hat{D}_{IR}|^2 \Rightarrow |\det D_{IR}|^2$

After all these preconditioning, we have partition function,

$$Z = \int DU \underbrace{e^{-S_G} \, |\det(1+T)|^2}_{\text{Gauge part}} \underbrace{|\det \bar{D}_{EE}|^2 \, |\det \bar{D}_{OO}|^2}_{\text{UV part}} \underbrace{|\det D_{IR}}_{\text{IR part}})|^2.$$

To reduce the HMC simulation cost, Multi time step integrator is employed for Gauge, UV and IR parts. (Sexton and Weingarten, 1992)

In our simulations, the relative magnitudes of force terms, F_G, F_{IR}, F_{UV}, are

$$||F_G|| : ||F_{UV}|| : ||F_{IR}|| \approx 16 : 4 : 1.$$

We choose the associated step sizes, $\delta\tau_G, \delta\tau_{UV}, \delta\tau_{IR}$ such that

$$\delta\tau_G||F_G|| \approx \delta\tau_{UV}||F_{UV}|| \approx \delta\tau_{IR}||F_{IR}||,$$

$$\delta\tau_G = \tau/N_0N_1N_2, \quad \delta\tau_{UV} = \tau/N_1N_2, \quad \delta\tau_{IR} = \tau/N_2, \quad N_0 = N_1 = 4.$$

For strange quark, we employ UVPHMC algorithm (CP-PACS and JLQCD Collaborations, 2006) where the domain decomposition is not used.

$$\|F_{\rm s}\| \approx \|F_{IR}\| \Rightarrow \delta\tau_{\rm s} = \delta\tau_{IR}.$$

For $m_{\rm ud} \geq 12$MeV, this DDHMC + UVPHMC algorithm works stable, while 3.5MeV run has large fluctuation of $\|F_{IR}\|$ and is slow to keep simulation stable.

We combine DDHMC with Hasenbusch's mass precondition for IR part (MPDDHMC).

+ Hasenbusch trick (Hasenbusch, 2001; Hasenbusch, Jansen, 2003)

$D'_{IR} = D_{IR}(\kappa \rightarrow \kappa' = \rho\kappa)$, eg. $\rho = 0.9995$ to shift to the heavier mass

$$|\det D_{IR}|^2 = |\det D'_{IR}| \left|\det\left(\frac{D_{IR}}{D'_{IR}}\right)\right|^2$$

Step sizes, $\delta\tau_G,\ \delta\tau_{UV},\ \delta\tau_{IR'},\ \delta_{IR/IR'}$, are controlled by (N_0, N_1, N_2, N_3).

$N_0 = N_1 = 4$, N_2 and N_3 are chosen to reduce the fluctuation of $\|F_{IR'}\|$, $\|F_{IR/IR'}\|$.

Solver : $Dx = b$

For DDHMC algorithm $(12\mathrm{MeV} \leq m_{\mathrm{ud}} \leq 67\mathrm{MeV})$,

- IR solver : SAP(single prec.) preconditioned GCR(double prec.) (Lüscher, 2004)
- UV solver : SSOR(single prec.) preconditioned GCR(double prec.)
- Stopping condition : $|\mathrm{Dx} - \mathrm{b}|/|\mathrm{b}| \leq 10^{-14}$ for H, 10^{-9} for F

  $\rightarrow$ Reversibility : $|\Delta U| \leq 10^{-12}$, $|\Delta H| \leq 10^{-8}$

Solver : $Dx = b$

For MPDDHMC algorithm ($m_{\rm ud}$ =3.5 MeV),

⋆ Chronological guess for IR part (Brower, Ivanenko, Levi, Orginos, 1997)

⋆ nested BiCGStab solver for IR and UV part :

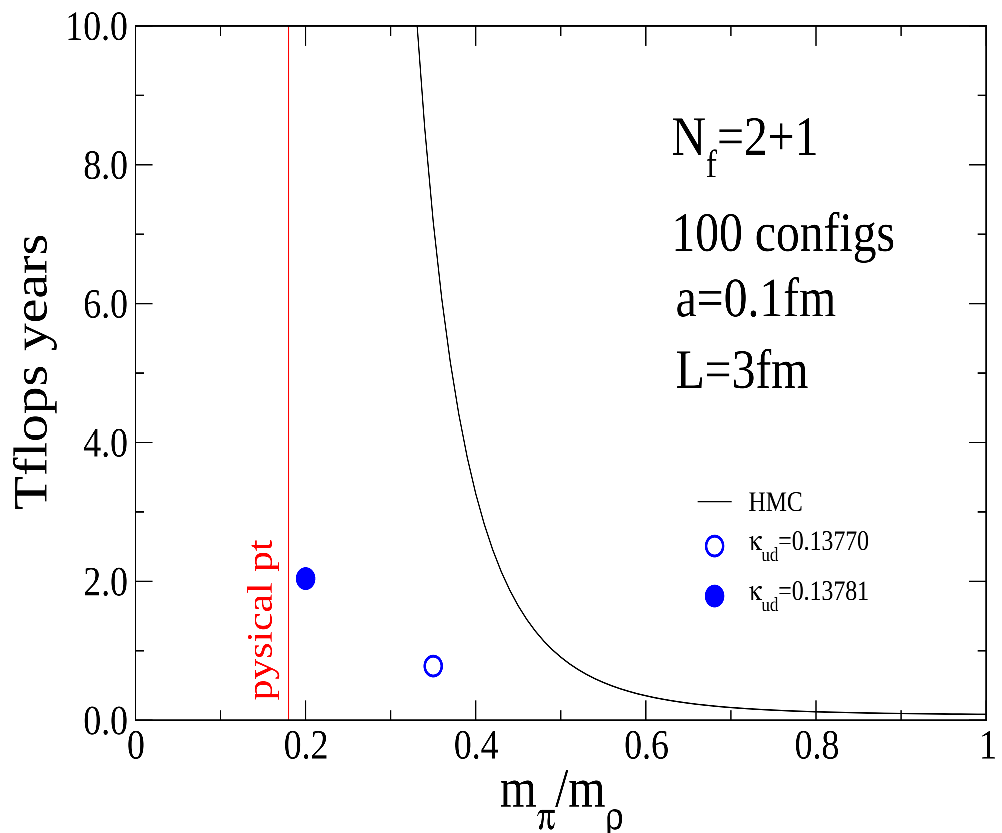
- Outer solver(double prec.) : Solve $Dx = b$ with preconditioner $M \approx D^{-1}$ with strict stopping condition 10^{-14} for F

- Inner solver(single prec.) : Solve $M \approx D^{-1}$ with appropriate precoditioner with automatic tolerance control $tol_{inner} = \min\left(\max\left(\frac{err_{outer}}{tol_{outer}}, 10^{-6}\right), 10^{-3}\right)$

⋆ Deflation technique (Morgan, Wilcox, 2002; Lüscher, 2007)

- inner BiCGStab stagnant $\longrightarrow$ GCRO-DR (Parks et al, 2006)

(Generalized Conjugate Residual with implicit inner Orthogonalization and Deflated Restarting)



(Ukawa, 2002; PACS-CS Collaboration, 2007)

Physical Point simulations require

HMC : $O(100)$ Tflops computer ,

MPDDHMC : $O(10)$ Tflops computer.

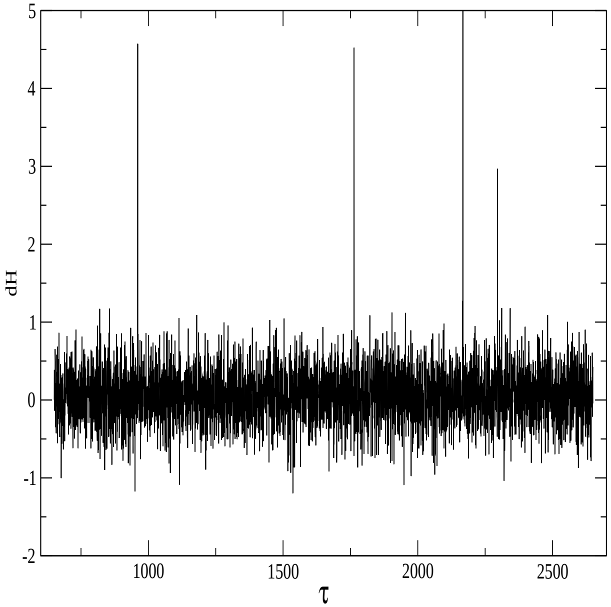
Simulation Parameters and Data Set

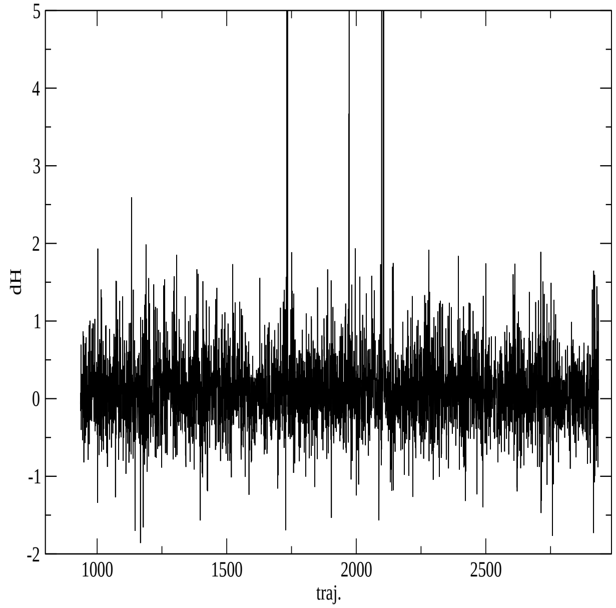
$\kappa_{\rm ud}$	0.13700	0.13727	0.13754	0.13754	0.13770	0.13781	0.137785
$\kappa_{\rm s}$	0.13640	0.13640	0.13640	0.13660	0.13640	0.13640	0.13660
Algorithm	DDHMC	DDHMC	DDHMC	DDHMC	DDHMC	MPDDHMC	MPDDHMC
τ	0.5	0.5	0.5	0.5	0.25	0.25	0.25
(N_0,N_1,N_2,N_3,N_4)	(4,4,10)	(4,4,14)	(4,4,20)	(4,4,28)	(4,4,16)	(4,4,4,6) (4,4,6,6)	(4,4,2,4,4)
ρ_1	—	—	—	—	—	0.9995	0.9995
ρ_2	—	—	—	—	—	—	0.9990
$N_{\rm poly}$	180	180	180	220	180	200	220
Replay	on	on	on	on	on	off	off
MD time	2000	2000	2250	2000	2000	1400	850
$m_{ud}[MeV]$	67	45	24	21	12	3.5	3.5
$m_\pi[MeV]$	702	570	411	385	296	156	162
CPU time [h]$/\tau$	0.29	0.44	1.3	1.1	2.7	7.1	6.0

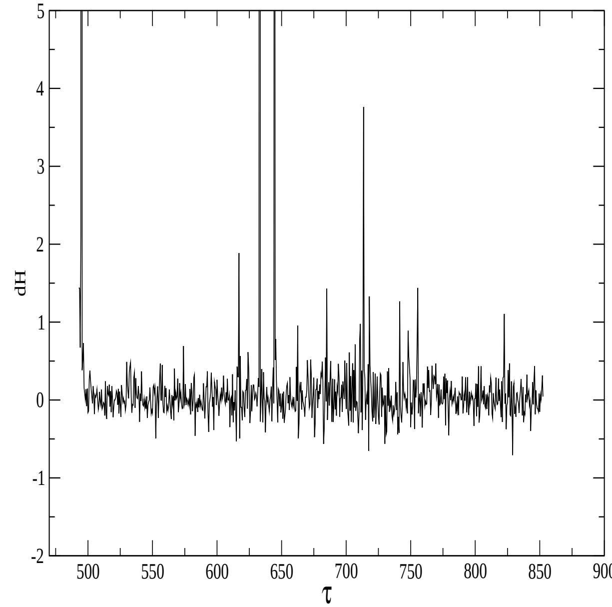
shifted hopping parameter $\kappa'_{\rm ud} = \rho_1\kappa_{\rm ud} \sim 0.1377$

dH History

$m_\pi = 570\mathrm{MeV}$ $m_\pi = 296\mathrm{MeV}$ $m_\pi = 156\mathrm{MeV}$





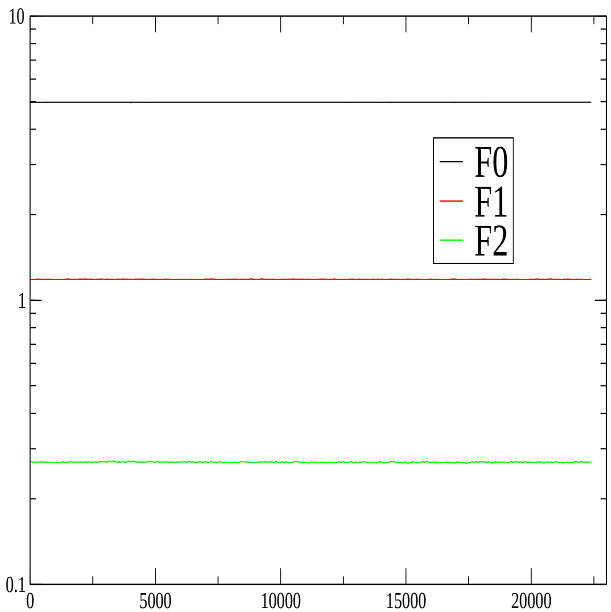


acc(HMC)=0.87 acc(HMC)=0.84 acc(HMC)=0.88

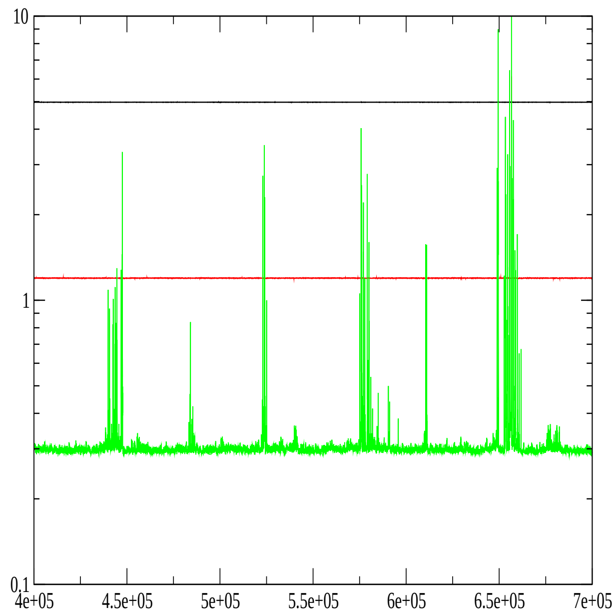
replay trick$\sim 0.1\%$ replay trick$\sim 3\%$

Force History

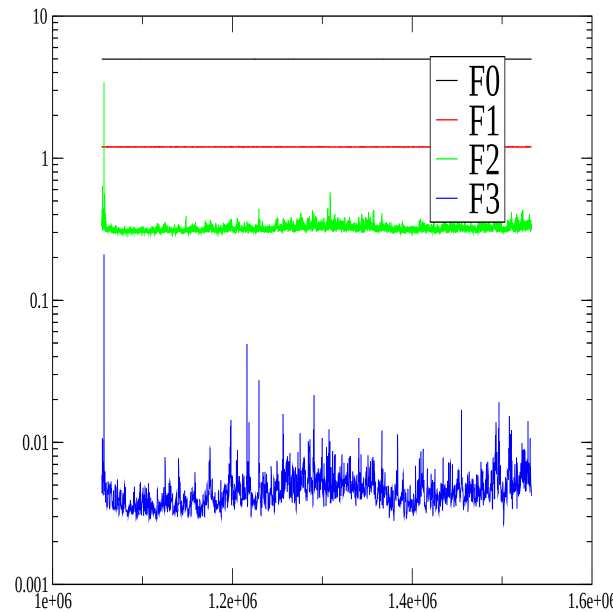
$m_\pi = 570\text{MeV}$



$m_\pi = 296\text{MeV}$



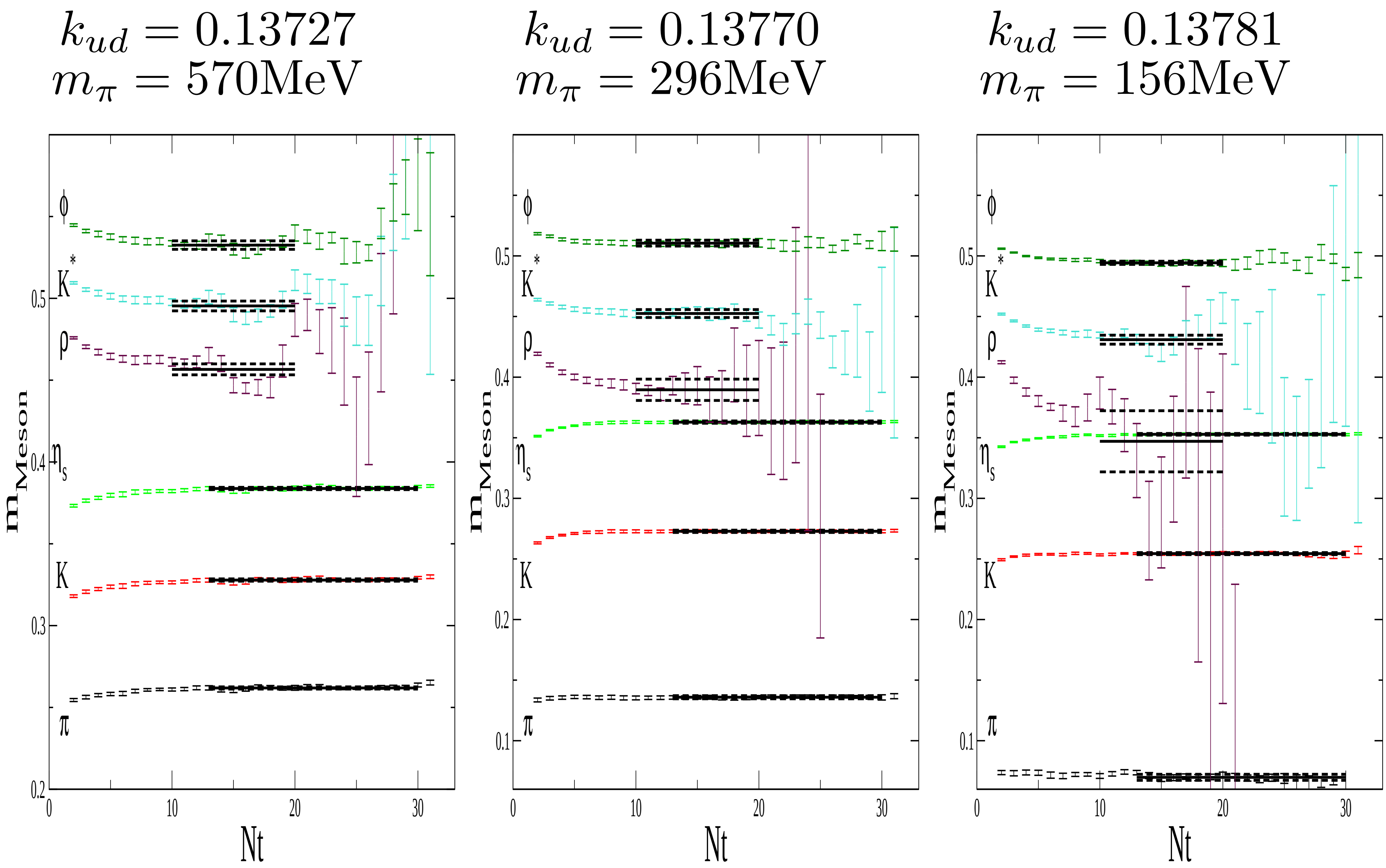
$m_\pi = 156\text{MeV}$



F_0 : Gauge + clv
F_1 : UV
F_2 : IR + s

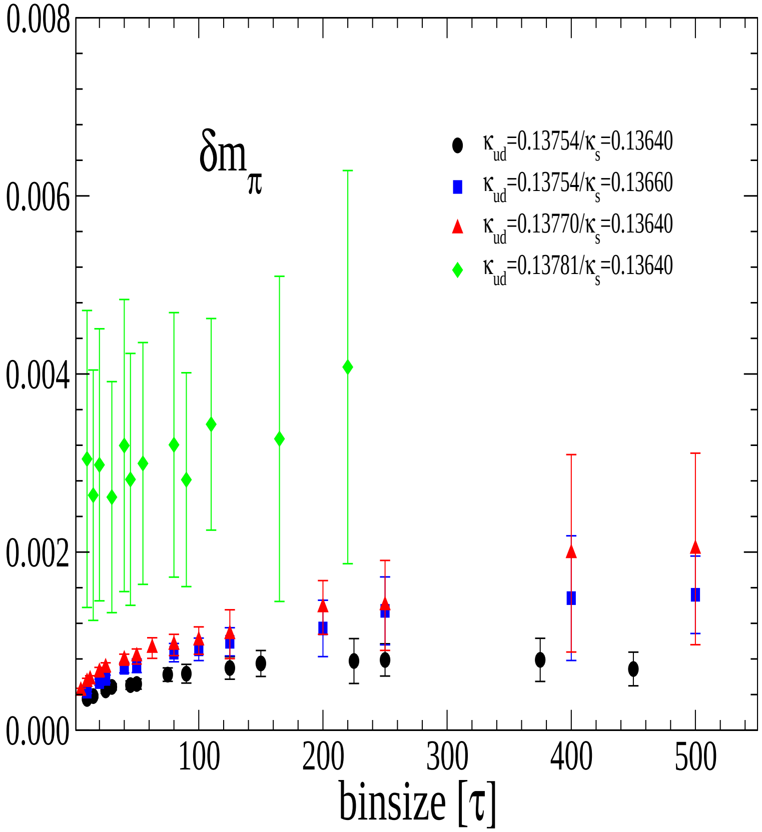
F_0 : Gauge + clv
F_1 : UV
F_2 : IR$'$ + s
F_3 : IR/IR$'$

Effective mass : Meson



Fit Range $[t_{\min}, t_{\max}]$: Pseudoscalar $[13 - 30]$, Vector $[10 - 20]$

Bin Size Dependence of Jacknife Error for m_π



$156\text{MeV} \leq m_\pi \leq 411\text{MeV}$

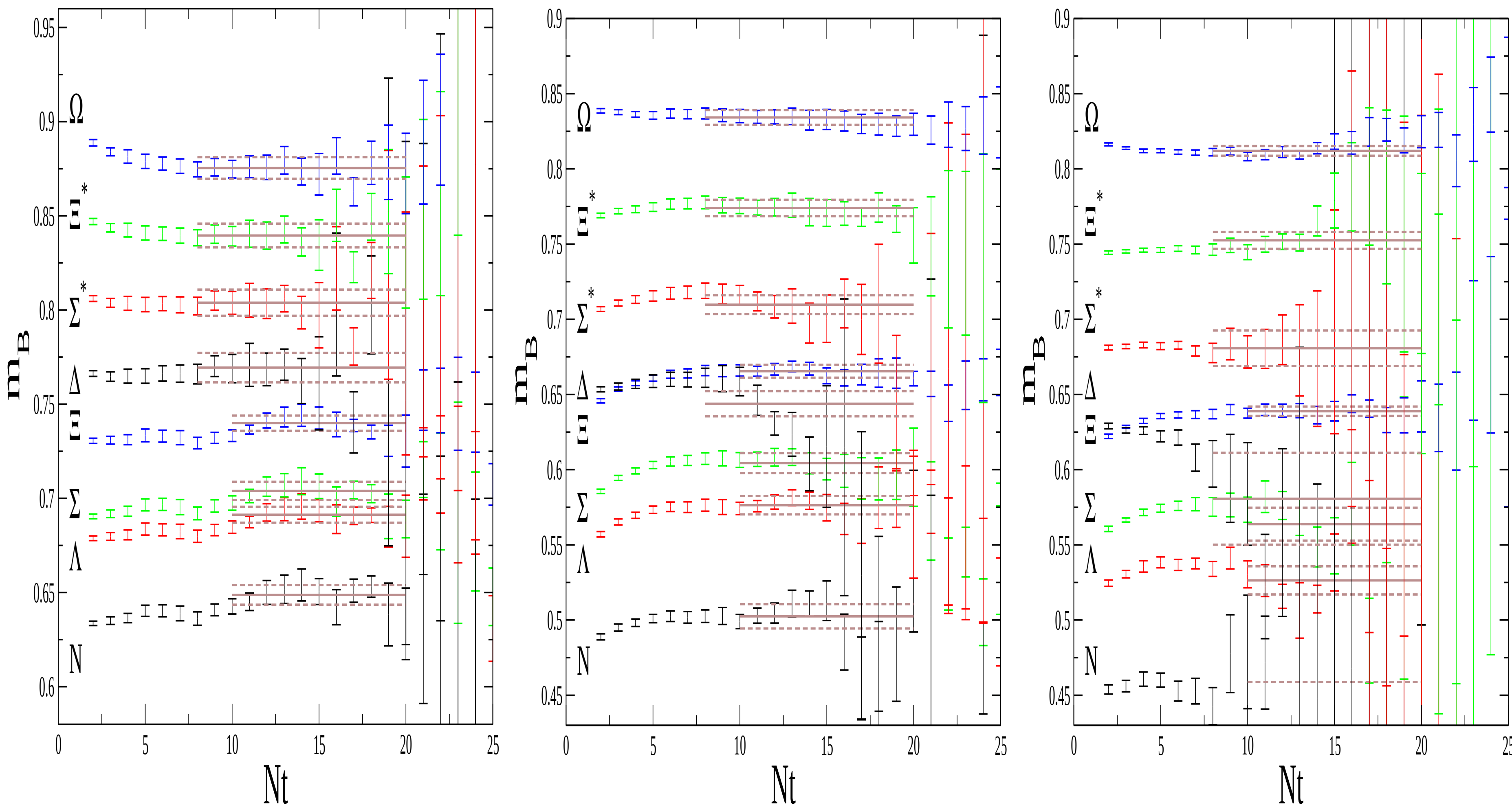
plateau : after 100-200τ

same behavior for other masses

jackknife analysis : 250τ (110τ)

Effective mass : Baryon

$k_{ud} = 0.13727$ $m_\pi = 570\text{MeV}$ | $k_{ud} = 0.13770$ $m_\pi = 296\text{MeV}$ | $k_{ud} = 0.13781$ $m_\pi = 156\text{MeV}$

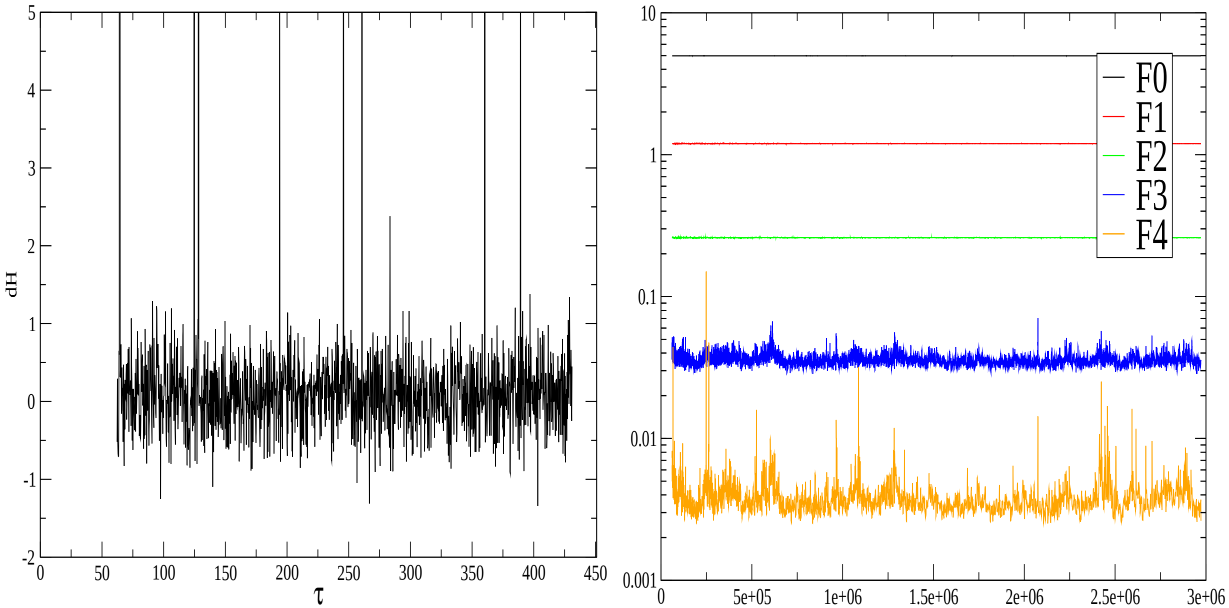


Fit Range $[t_{\min}, t_{\max}]$: Decuplet $[13 - 30]$, Octet $[10 - 20]$

$\kappa_{\rm ud} = 0.137785, \kappa_{\rm s} = 0.13660 : Preliminary$

$\kappa_{\rm ud} = 0.137785, \kappa_{\rm s} = 0.13660$ is estimated as the physical point from our ChPT analysis. (ChPT $\rightarrow$ talk by Kadoh)

$$\text{IR part in MPDDHMC} : |\det D_{IR}|^2 = |\det D''_{IR}|^2 \left|\det \frac{D'_{IR}}{D''_{IR}}\right|^2 \left|\det \frac{D_{IR}}{D'_{IR}}\right|^2$$

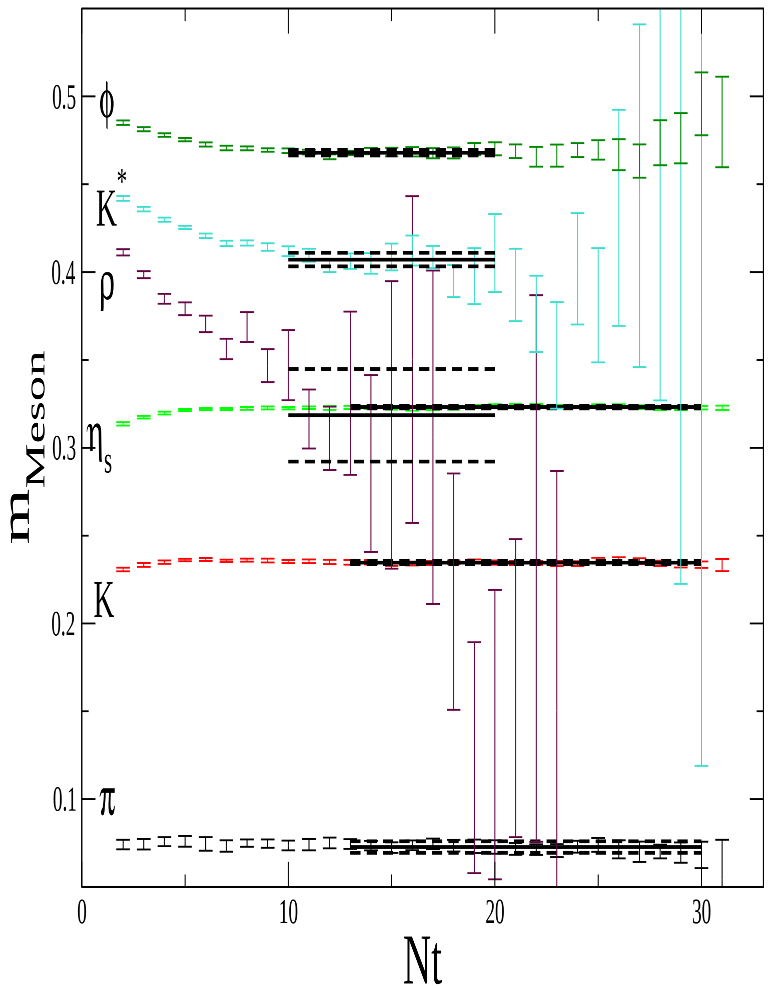


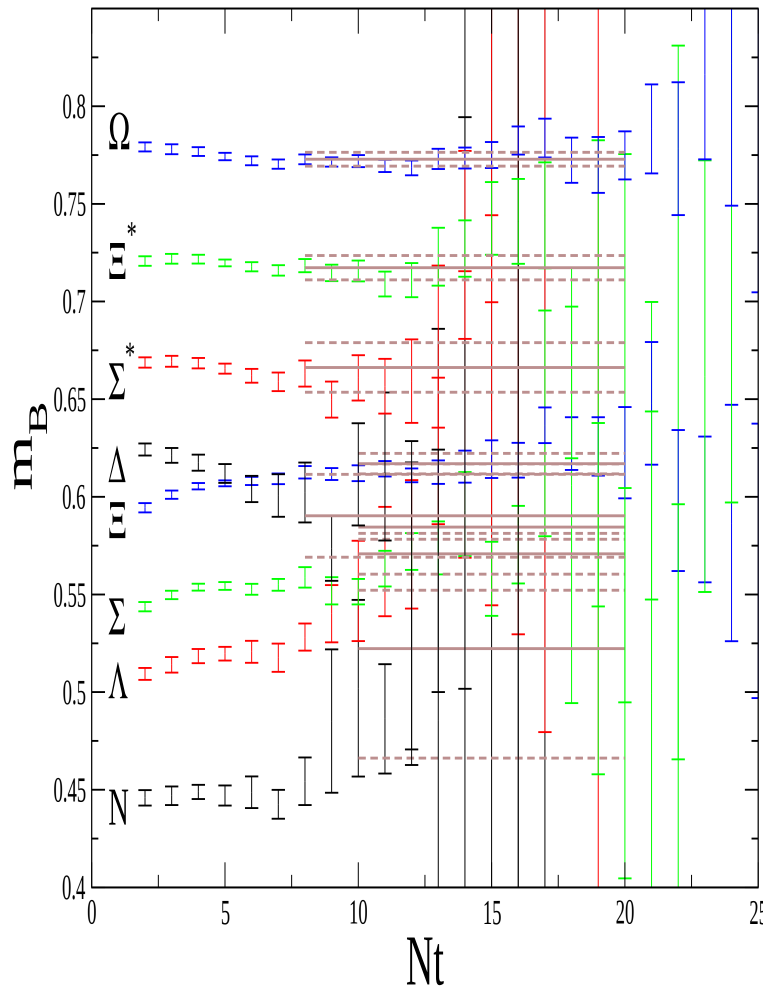
F_0 : Gauge + clv
F_1 : UV
F_2 : IR$''$ + s
F_3 : IR$'$/IR$''$
F_4 : IR/IR$'$

acc(HMC)=0.83, CPU time = 6.0 [h]/τ

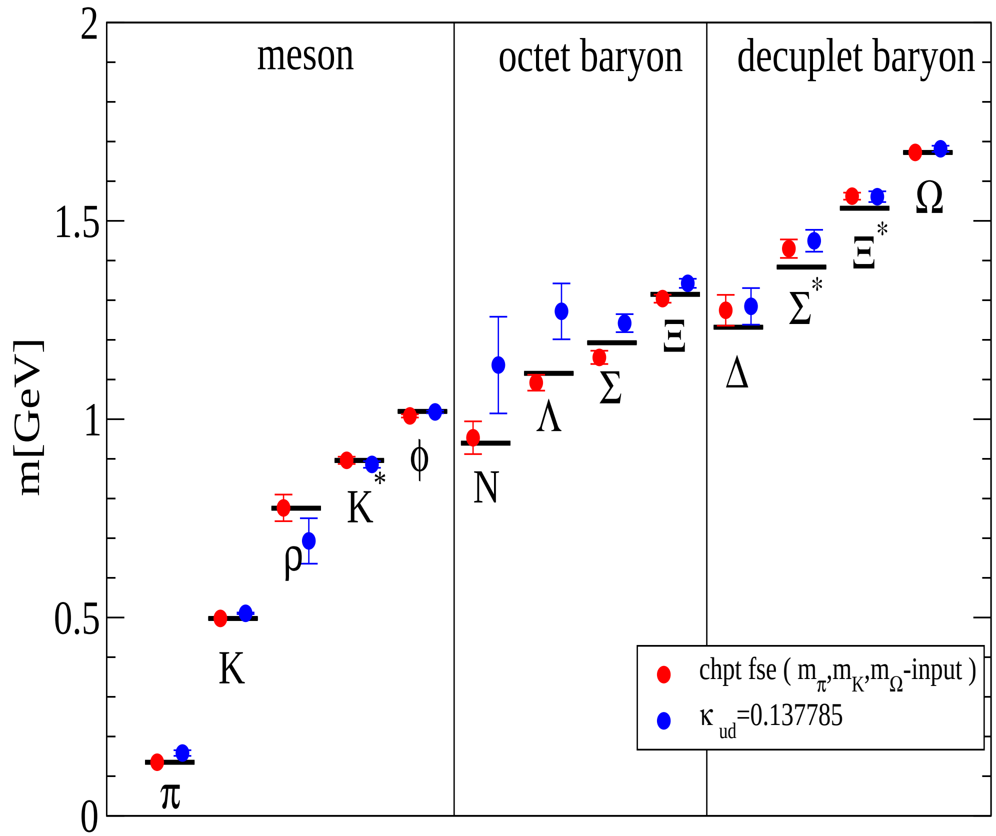
Effective mass

$m_\pi = 162\text{MeV}$





Comparison with Chpt and Experiment



Preliminary

jackknife analysis $= 50\tau$

at $\kappa_{\rm ud} = 0.137785$

	ChPT	experiment	$\kappa_{\rm ud} = 0.137785$
$m_{\rm ud}^{\overline{MS}}$ [MeV]	2.53(5)	—	3.5(3)
$m_{\rm s}^{\overline{MS}}$ [MeV]	72.7(8)	—	73.4(2)
f_π [MeV]	134.0(4.2)	$130.7 \pm 0.1 \pm 0.36$	129.0(5.4)
f_K [MeV]	159.4(3.1)	$159.8 \pm 1.4 \pm 0.44$	160.6(1.4)

Conclusion

- $N_f = 2 + 1$ full QCD with $O(a)$ improved Wilson quarks on $(2.9\mathrm{fm})^3$
- domain-decomposed HMC + Hasenbusch trick
- $m_{ud} = 3.5 \sim 67$[MeV]
- $m_\pi = 156 \sim 702$[MeV]
- $a = 0.0907(13)$ fm
- Physical Point simulation in progress