Recent results from unquenched light quark simulations

Taku Izubuchi
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Introduction

- In quenched simulations ($N_F = 0$, no sea quark in QCD vacuum), Hadron spectrum found to be 5-10% different from experiments (CP-PACS, JLQCD, UKQCD)

- (RBC) $N_F = 0$, 2 DWF

$$J = \frac{dm^2}{dm_V} \bigg|_{m_V/m_{ps}=1.8}$$

- Is it only 5-10%?
More obvious quenched pathology was found in NS scalar meson

\[ a_0 \quad I^G(J)^{PC} = 1^+(0^{++}) \]

(Bardeen et al.)

\[ a_0 \rightarrow \eta'(\text{quenched}) + \pi \rightarrow a_0 \]

As \( \eta'(\text{quenched}) \) failed to get heavy having double pole, this contribution was argued to make \( a_0 \) propagator to be negative using QChPT in finite volume.

- quenched theory is not unitary nor local field theory.
Introduction...

Dynamical simulation is difficult not only it’s computationally demanding, but also gauge filed tend to be more fluctuating at short distance than quenched simulation (fixing scale at Hadronic scale).
\[ \iff \text{milder running } \alpha_S(\mu) \text{ for } N_F > 0 \text{ (asymptotic freedom)}. \]

![Graph showing \( r_0 \times [V(r) - V(r_0)] \) vs \( r/r_0 \) for DFW \( N_F = 0, 2 \).]

This makes dynamical simulation even more difficult.
Dynamical simulation for DWF (GW)

- Such short distance fluctuation has an impact on DWF (GW) fermion simulations.

- Axial Ward-Takahashi identity,

\[
\partial_\mu A_\mu^a(x) = 2m_f J_5^a(x) + 2J_{5q}^a(x) \\
\approx 2 \left( m_f + m_{res} \right) J_5^a(x)
\]

\[J_5^a(x) : \text{non-singlet pseudoscalar,} \]

\[J_{5q}^a(x) : \text{explicit breaking term} \]

\[\text{consists of field at } s = L_s/2 - 1, L_s/2.\]

A measure of the residual chiral symmetry breaking,

\[m_{res} = \frac{\sum_{x,y} \langle J_{5q}^a(y, t) J_5^a(x, 0) \rangle}{\sum_{x,y} \langle J_5^a(y, t) J_5^a(x, 0) \rangle} \sim e^{-\lambda L_s}, \lambda \sim H_W = \gamma_5 D_W\]

- Sudden growth of eigenmode size at \(\lambda = \lambda_c\).
  Roughly consistent with \(m_{res}(L_s)\) behaviors.
  DWF \(N_F = 3\) (P.Boyle, N.Christ @ chiral)
  Mobility edge (M.Goltermann, Y.Shamir)
  (S.Aoki, Y.Taniguchi)
$m_{res}$ in dynamical simulations

- In practice $L_s \ll \text{a few } 10$ is preferable. At the same time $am_{res}$ must be small, less than a few MeV, to realize the advantages of DWF.

- In $N_F = 0$ DWF QCD (RBC) tuning RG action, the negative coefficients to the rectangular plaquette, suppresses small dislocations drastically, but the parity broken phase, still exists for small enough $\beta$ (S. Aoki).

- In $N_F = 2$, $m_{res} \sim \mathcal{O}(1)$ MeV, for $L_s = 12, a^{-1} = 1.7$ GeV using DBW2 gauge action.

- In $N_F = 3$, $L_s = 8$, an order of magnitude larger $m_{res}$ than $N_F = 2, L_s = 12$. Tuning of recutangular actions (R.Mawhiney @ spectrum 11).

- Fluctuations at short distance might cause bad things (taste breaking, exceptional configuration) for other fermions as well.
Sincere apologies

I apologise sincerely to those whom I won’t cite. There are also many interesting and important works and talks I should have covered, but it was totally beyond my capability.

Let me try to understand and mention in the proceedings.

If you could drop an email to taku@bnl.gov to call my attention, I will highly appreciate that.
1. Performance
Simulation for Dynamical Fermion

It is important to improve the performance of dynamical simulation to reduce the statistical error on physical output.

\[
\text{statistical error } \propto \sqrt{\frac{1}{N_{\text{conf}}}}
\]

**Hybrid Monte Carlo** (Exact algorithm)

\[
\text{Prob}(U_\mu(x)) \propto e^{-S(U_\mu)}[dU_\mu] \implies e^{-\mathcal{H}}[dU_\mu][d\Pi_\mu], \quad \mathcal{H} = \frac{1}{2}\Pi^2 + S(U)
\]

Conjugate momentum \( \Pi_\mu(x) \)

- 1. **Refresh** momentum \( \Pi \), \((\Phi, \Phi_{PV})\).
- 2. Approximately solve Hamilton’s equation (\(\mathcal{H}\) preserved, reversible, area-preserving) :1 trajectory.
- 3. correct the approximation by a Metropolis reject/accept test :acceptance.
Factors of Simulation Performance

Three factors that have impact on the performance of dynamical simulations

1. **Speed of integrator** for Hamilton’s equation (many Matrix inversions)

2. **Acceptance**

3. **Autocorrelation,\( \tau_{int} \), between consecutive trajectories**

In this conference:

- Schwartz-preconditioned HMC (domain decomposition) (M. Lüscher @ plenary)
- mass preconditioning (Hasenbusch trick) & multiple time scale integration (M. Hasenbusch, C. Urbach @ algorithm 2)
- Twisted mass (A. Shindler @ plenary, and therein)
- Ginsparg-Wilson fermions (M. Clark, P. Hasenfratz @ algorithm 2) (B. Joo, R. Edwards @ chiral 4) (A. Borici, S. Krieg @ algorithm poster)

Taku Izubuchi, Dublin, 25/July/2005
DWF (R)HMC experiences

- started by Columbia Univ. (G. Fleming, P. Vranas, et al.)
- Force term modification (P. Vranas, C. Dawson)
- Chronological inverter (Brower, Ivanenko, Levi, Orginos)
- Acceptance, autocorrelation, $\tau_{int}$, was insensitive to quark mass.
- On $N_f = 2 + 1$ DWF RHMC (double precision), acceptance is almost flat in light quark mass with multiple gauge steps ($\sim 4$ per a fermion step) in the integrator.

<table>
<thead>
<tr>
<th>$\delta t$</th>
<th>$R$ algorithm result</th>
<th>$a\delta t^2 + b$</th>
<th>$a\delta t^3 + b\delta t^2 + c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.608</td>
<td>0.60815</td>
<td>0.60835</td>
</tr>
<tr>
<td>0.002</td>
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<td>0.60815</td>
<td>0.60835</td>
</tr>
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<td>0.004</td>
<td>0.608</td>
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<tr>
<td>0.006</td>
<td>0.608</td>
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<td>0.008</td>
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</tr>
<tr>
<td>0.010</td>
<td>0.608</td>
<td>0.60815</td>
<td>0.60835</td>
</tr>
</tbody>
</table>

- $N_F = 3$ DWF, Plaquette
- R algorithm (inexact) vs RHMC (exact) (M. Clark @ algorithm 2)
  $\Rightarrow$ Use exact algorithm, unless the performance is away worse.
Cost estimation

- Panel discussion @ Berlin Lattice conference.

- Assuming \([(m_\pi/m_\rho)^2 \propto m_q)\]
  - \(\tau_{int} \propto 1/m_q\),
  - (inversion cost) \(\propto 1/m_q\),
  - \(\Delta t \propto m_q\)

- TFLOPS \(\times\) Year to generate 1,000 independent configuration
  (Thanks to K.Jansen, A.Ukawa, T.Yoshie):

\[
\text{TflopsY} = C \left[ \frac{\#\text{conf}}{1,000} \right] \left[ \frac{(m_\pi/m_\rho)}{0.6} + S \right]^{-6} \left[ \frac{L}{2.12\text{fm}} \right]^{-5} \left[ \frac{a^{-1}}{2.60\text{GeV}} \right]^{-7}
\]

\(S: \text{cost for strange quark. } C \approx 0.312 \text{ (Ukawa).}\)
MILC points are from Urbach et.al

Scaled for $a = 0.08 \text{fm}$, $24^3 \times 40$ lattice using the formula.

CP-PACS JLQCD $N_F = 3$ clover on Earth simulator $\tau_{int} = 0.6 / (a m_q)$

Urbach et.al multiple time scale $\tau_{int}(\text{plaq})$ (Sexton, Weingarten) + Hasenbusch accel.

Note the formula’s assumptions are not totally confirmed: try lighter quark mass to see if $\tau_{int}, C \Delta H$ change.

fixing $a^{-1}$ has no absolute meaning.

c.f. $O(a)$ vs $O(a^2)$ discretization.
2. Dynamical Simulations
Dynamical simulations

Dynamical Wilson fermions  (M. Lüscher @ plenary)

Dynamical twisted mass Wilson  (R. Frezzotti and G.C. Rossi)  (A. Shindler @ plenary)

parameters of dynamical simulations

- Gauge action
- Fermion action
- $N_F$ : number of dynamical light quarks
- $a^{-1}$
- $m_{sea} (m_\pi/m_\rho)$
- renormalization
MILC collaboration

RG(Symanzik) + Improved staggered (Asqtad) $N_F = 2 + 1$

R algorithm

300-700 configurations, $(2.4 \text{ fm})^3$
$( (2.9 \text{ fm})^3 / (3.4 \text{ fm})^3$ for coarse/fine lightest mass)

- coarse lattice $a^{-1} = 1.6 \text{ GeV}$ $m_q = 10 - 50 \text{ MeV}$ 5 points ($m_\pi/m_\rho = 0.3 - 0.6$)
  Added second (40% lighter) strange quark points (2 mass points).
- fine lattice $a^{-1} = 2.3 \text{ GeV}$ $m_q = 10 - 30 \text{ MeV}$ 3 points $m_\pi/m_\rho = 0.3 - 0.5$)
  Added lightest quark mass points (now 170 confs)
- Also quenched simulations on similar lattice spacing/size to study quenched staggered chiral perturbation theory.

perturbative renormalization
(C. Bernard @ spectrum poster, also thanks to D. Toussaint)
The new lightest quark points doesn’t change mass results much, so doesn’t quark masses.

Including new data, decay constants shifted by a significant amount.

new (preliminary) results of decay constants.
MILC collaboration

- only analytic terms in NNLO, (and NNNLO) are included in the fits.
- R algorithm.
- Electromagnetic effects is the biggest error on $m_u/m_d$.
  (N.Yamada, Y.Namekawa @ spectrum 10)
- Quenched $f_\pi$ is larger than experimental value by 28%.
  (Setting scale by $r_0, \sigma$, 21%, 14% larger respectively).
  consistent with other quenched simulations?

(A.Mason @ plenary )
(C. McNeile @ spectrum 1)
(J. Bailey @ spectrum 2)
(C.Aubin @ spectrum 10 )
• $B_q : b$ (NRQCD) + light quark (staggered) meson

• $\Phi_q = f_{B_q} \sqrt{M_{Bq}}$
staggered $a_0$ on staggered sea

(A.Irving @ spectrum poster)

- flavour nonsinglet scalar
- Spin $\times$ Taste $= 1 \otimes 1$
- excited state is compatible to $a_0(980)$
- ground state: partially quenched effect?
- (S.Dürr @ plenary)

\[ C(t) = \sum_n A^{(n)} e^{-m^{(n)} t} + A^{(n)} e^{+m^{(n)} t} \]

\[ m_* : \gamma_4 \gamma_5 \otimes \gamma_4 \gamma_5 \quad \text{(taste-split pion)} \]
**DWF $a_0$ on staggered sea**

(S. Prelovsek @ spectrum 8)

- **Partially quenched ChPT.**
- **For DWF-valence + DWF-sea, $C(t) < 0$ for $m_\pi(\text{sea}) > m_\pi(\text{val})$, vice versa.** *(S. Prelovsek, et.al.)*
- **DWF $a_0$ could be a ‘‘detector’’ of $m_\pi(\text{sea}).$**

- For GW-valence pion on staggered sea: $m_\pi(\text{val})=m_\pi,1(\text{sea})$ leads ‘‘continuum like’’ NLO pion mass formula *(O. Baer, et.al.)*.

- For DWF-valence + staggered-sea mixed action, $a_0$’s $C(t)$ is still **negative** for $m_{\pi,5}(\text{sea}) = m_\pi(\text{val})$ for a range of unknown parameter $\Delta_{mix}$.

- **DWF $a_0$ feels staggered $m_\pi(\text{sea})$ is heavier than NG pion $m_{\pi,5}$?**
CP-PACS and JLQCD collaboration

- RG improved gauge action + nonperturbatively $O(a)$ improved Wilson $N_F = 2 + 1$,

- 3k-10k trajectories, $(2\text{fm})^3$ box.

- $a^{-1} = 1.6, 2.0, 2.6$ GeV ($m_\pi/m_\rho = 0.60 - 0.78$)

- measure on dynamical (unitary, $m_{\text{sea}} = m_{\text{val}}$) points.

- Exact $N_F=2+1$, PHMC (K.Ishikawa)

- perturbative renormalization

- AWI quark masses
  \[
  m_{q}^{AWI} = \frac{\Delta_4 A_4(t) J_5(0)}{2(J_5(t) J_5(0))}
  \]

- $r_0 = 0.5\text{fm}$ is consistent with $m_\rho$ input.

(T. Ishikawa’s talk @ spectrum 3, S.Takeda @ spectrum 2)
The plots show the \( m_s^{\overline{MS}}(\mu=2\text{GeV}) \) results for different flavors and inputs. Key points:

- Polynomial chiral extrapolations.
- Perturbative renormalization.

Legend:

- \( N_f=0, VWI \)
- \( N_f=0, AWI \)
- \( N_f=2, VWI \)
- \( N_f=2, AWI \)
- \( N_f=2+1, VWI \)
- \( N_f=2+1, AWI \)
$NF = 2$ Dynamical Wilson simulations

- **ALPHA**
  Wilson + nonperturbatively $O(a)$ improved Wilson $NF = 2$,
  $a^{-1} = 2.1, 2.4, 2.8$ GeV ($m_{ps} = 495$ MeV)
  nonperturbative renormalization (Schrodinger functional)
  (M.D.Morte’s talk @ improvement 1, also thanks to F.Knechtli)

- **QCDSF-UKQCD**
  Wilson + nonperturbatively $O(a)$ improved Wilson $NF = 2$,
  $a^{-1} = 2.1, 2.4, 2.8$ GeV ($m_\pi/m_\rho \geq 0.6$)
  NLO
  nonperturbative renormalization (RI-MOM)
  (R.Horsley’s talk @ spectrum 8, D.Pleiter @ spectrum 4,
  also thanks to G.Schierholz)

- **SPQcdR**
  Wilson + Wilson $NF = 2$,
  $a^{-1} = 3.2$ GeV ($m_\pi/m_\rho = 0.63 - 0.75$)
  nonperturbative renormalization (RI-MOM)
  Also quenched simulation at similar at $a$
  (C.Tarantino’s talk @ spectrum 8)
• $m_\pi / m_\rho \geq 0.6$, too heavy?

• Chiral extrapolation, Wilson ChPTs (O. Baer et al., S. Aoki).

• Perturbative renormalizations tend to underestimate quark mass?
RBC collaboration

- RG(DBW2) + Domain Wall Fermions, $N_F = 2$
- $a^{-1} = 1.7$ GeV ($m_\pi/m_\rho = 0.54 - 0.65$), $(1.9\text{fm})^3$ box. 6k trajectories, 94 confs.
- non-perturbative renormalization (RI-MOM)
- LO and NLO ChPT fit.
- $L_s = 12$, $m_{res} = 0.001372(44) \sim 0.1m_{sea} \sim$ a few MeV.

( C.Dawson, T.Blum’s talk @ plenary)
( S.Prelovsek @ spectrum 8, N.Yamada @ spectrum 10)
• NLO fits are also examined.

• $m_{val}, m_{sea} \in [0.01, 0.03]$  

• 30% smaller $f$ than linear fit.

• Larger mass points are missed badly.  
  $\Rightarrow$ LO (linear) extrapolation.

Taku Izubuchi, Dublin, 25/July/2005
Pseudoscalar Meson mass

Fit using $m_{\text{sea,val}} \leq 0.03$ only

- NLO fit using $m_{\text{sea,val}} \leq 0.03$
  - not inconsistent.

- constraints:
  - $m^2_{ps} = 0$ at $m_{\text{val,sea}} = -m_{\text{res}}$,
  - $f = 0.0781$ from linear fit of $f_{ps}$.
Physical Results

- NLO fits results using $m_{ps}^2$ at $m_f = m_{sea,val} \leq m_f^{(max)}$. Pseudo-scalar wall-point (upper two column), and axial-vector wall point. uncorrelated $\chi^2$. Gasser-Leutwyler low energy constants $L_i$ multiplied by $10^4$ at $\Lambda_\chi = 1$ GeV.

<table>
<thead>
<tr>
<th>$m_f^{(max)}$</th>
<th>$\chi^2$/dof</th>
<th>$2 B_0$</th>
<th>$L_4 - 2L_6$</th>
<th>$L_5 - 2L_8$</th>
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<tbody>
<tr>
<td>0.03</td>
<td>0.1(1)</td>
<td>4.0(3)</td>
<td>-1.5(7)</td>
<td>-2(1)</td>
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<tr>
<td>0.04</td>
<td>2(1)</td>
<td>4.2(1)</td>
<td>-0.2(4)</td>
<td>-1.1(4)</td>
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<tr>
<td>0.03</td>
<td>0.3(2)</td>
<td>4.0(3)</td>
<td>-1.9(8)</td>
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<tr>
<td>0.04</td>
<td>1.9(9)</td>
<td>4.2(1)</td>
<td>-0.4(4)</td>
<td>-0.8(3)</td>
</tr>
</tbody>
</table>

- By linear extrapolations/interpolations for $f_{ps}$ to $\bar{m}$ and $m_s$,

<table>
<thead>
<tr>
<th>$N_F = 2$</th>
<th>experiment</th>
<th>$N_F = 0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_\pi$</td>
<td>134(4)</td>
<td>130.7</td>
</tr>
<tr>
<td>$f_K$</td>
<td>157(4)</td>
<td>160</td>
</tr>
<tr>
<td>$f_K/f_\pi$</td>
<td>1.18(1)</td>
<td>1.224</td>
</tr>
</tbody>
</table>

better agreement with experiment than quenched DWF simulations.
RBC and UKQCD collaboration

- RG(Iwasaki, DBW2) + Domain Wall Fermions $N_F = 2 + 1$

- $L_s = 8$ parameter search runs. $am_{res} \ll \mathcal{O}(0.01)$

- $a^{-1} = 1.7$-2.0 GeV

- QCDOC, QCDOC collaboration (T. Wettig @ plenary)

- R algorithm and Exact RHMC algorithm (M. Clark @ algorithm 2) in CPS++ (maintainer: C. Jung)

- 1.5-6 k trajectories.

- $24^3 \times 64, L_s = 16$ started.

preliminary investigations
- Static quark potential (preliminary)
- \( r_0 = 0.5 \text{ fm} \)
- \[
\begin{array}{ccc}
\beta & a^{-1} \\
DBW2 & 0.764 & 2.0 \text{ GeV} \\
& 0.72 & 1.7 \text{ GeV} \\
Iwasaki & 2.2 & 2.1 \text{ GeV} \\
& 2.13 & 1.8 \text{ GeV} \\
\end{array}
\]
- consistent with \( f_\pi, m_\rho \) inputs within \( \sim 10\% \).
Spectrum
(C.Maynard @ spectrum 11)  (S. Cohen @ weak 2)

roughly consistent with experimental value
topology, \( \langle \bar{q}q \rangle \), ...

Scaling study of decay constants, ....

evolution details, decay constants....
GW/overlap/chirally improved dynamical simulations

(P. Majumdar @ chiral 2) (W. Ortner @ chiral poster)

(D. Kadoh @ chiral 2) (Y. Kikukawa @ chiral poster)

(T. DeGrand @ chiral 3) (S. Schaefer @ chiral 3)

(B. Joo @ chiral 4) (R. Edwards @ chiral 4)

(W. Kamleh @ algorithms poster) (S. Kreig @ algorithms poster)
3. quark masses
Light quark masses

Quark mass is a fundamental parameter of the standard model Lagrangian, which is not directly accessible from experiments due to confinement.

- Lattice QCD: map between hadronic observables (hadron mass, decay constant) and quark mass,

\[ M_{\text{had}}(m_q) = M_{\text{had}}^{(\text{exp})} \]

- fix lattice scale, \( a^{-1} \) (Sommer scale \( r_0, m_\rho, f_\pi \))

- Extrapolate to chiral regime \( (m_{u,d} \sim \mathcal{O}(1) \text{ MeV}) \).

- mass renormalization, \( Z \) factors, for non-lattice community.

- Extrapolate to continuum \( (a \rightarrow 0) \).
map between hadronic mass and quark mass on lattice

- Set lattice scale, $a^{-1}$, from $m_\rho$, $r_0$, or $f_\pi$.

- Quark mass at physical Kaon mass (horizontal line)

- By using non-degenerate ChPT formula (red dots), $am_{\text{strange}} = 0.0446(29)$ is extracted.

- If one uses dynamical, $m_{\text{sea}} = m_{\text{val}}$, points instead of $N_F = 2$ sea quarks, one finds $am_{\text{strange}} = 0.04177(64)$, 7% smaller than partially quenched analysis.
Operator Renormalization on lattice

Lattice perturbative calculation (improved)

RI-MOM (Rome/Southhampton)

Schrodinger Functional (ALPHA)

Real-space NPR (Giménez et.al.) (V.Porretti @ spectrum 8)
NPR(RI-MOM) on dynamical lattice

- measure quark propagator, $S_F(q)$, on Landau gauge fixed gauge configuration.
- calculate amputated green function of bilinear operators, $\Gamma = 1, \gamma_5, \gamma_5\gamma_\mu, \ldots$

\[
\Pi_\Gamma = \bigl\langle u(-p)[\bar{u}\Gamma d]\bar{d}(q)\bigr\rangle_{\text{AMP}}
\]
\[
\Lambda_\Gamma = \frac{\text{Tr}(\Gamma \Pi_\Gamma)}{\text{Tr}(\Gamma \Gamma)} \bigg|_{p^2, q^2 = \mu^2}
\]
on lattice ensemble.

- Subtract mass pole to avoid non-perturbative effects ($\langle \bar{q}q \rangle$) by fitting

\[
\Lambda_{\gamma_5} = \frac{c_1}{m_q} + \frac{Z_q}{Z_P} + c_3m_q + \cdots
\]

at $\Lambda_{QCD} \ll |p| \ll a^{-1}$ on each sea quark ensemble.
($Z_q$ quark field normalization, $Z_{P,S,A}$ pseudoscalar, scalar, axial current)
NPR(RI-MOM) on dynamical lattice...

- $\Lambda_P \approx \Lambda_S \approx \partial S^{-1}/\partial m \rightarrow \frac{Z_q}{Z_P}$

- convert from RI to $\overline{MS}$ with $c(pa)^2$ subtraction.

- constant fit all $m_{sea}$ (mild dependency).

- $Z_P = 0.62(5)$
  $(250 \text{ MeV} \leq \Lambda_{QCD} \leq 300 \text{ MeV})$
recent dynamical strange quark masses
based on ALPHA’s compilation (Thanks to F.Knechtli) + new results.

Preliminary

Taku Izubuchi, Dublin, 25/July/2005
\( N_F = 2, 3 \) (difference is small in CP-PACS/JLQCD)

scale is \( r_0 = 0.5 \) fm. (MILC corresponds to \( r_0 = 0.467 \) fm, not corrected)

chiral extrapolation ?

perturbation tends to give smaller \( Z_m \) ?

(QCDSF–UKQCD, SPQcdR, ALPHA)

<table>
<thead>
<tr>
<th></th>
<th>NPR</th>
<th>Pert ((K_c))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Z_{V,A} )</td>
<td>0.7574(1)</td>
<td>0.770</td>
</tr>
<tr>
<td>( Z_{S,P} )</td>
<td>0.62(5)</td>
<td>0.847</td>
</tr>
</tbody>
</table>
Conclusions

• Performance of Dynamical simulation is updated.
• We need ‘‘fair’’ way to compare different simulations other than fixing $a$.
• Seemingly promising {new,improved} algorithms.
• Now three $N_F = 2 + 1$ dynamical simulations.
• New dynamical Wilson fermion simulations with NPR.
• New strange quark mass results (4 Wilson, 1 DWF).
• Systematic error (chiral extrapolation, perturbative $Z$)