Simulations with $N_f=2+1$ Flavors of Anisotropic Clover Fermions

Huey-Wen Lin

Perspectives and Challenges for Full-QCD Lattice Calculations
ECT, Trento, Italy
May 07, 2008
Physics Research Directions

Wanted:

**Spectrum:**

- Excited-state baryon resonances (Hall B)
- Conventional and exotic (hybrid) mesons (Hall D)

Example: $N, P_{11}, S_{11}$ spectrum

Huey-Wen Lin — ECT Workshop, May 08
Physics Research Directions

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- **Spectrum:**
  - Excited-state baryon resonances (Hall B)
  - Conventional and exotic (hybrid) mesons (Hall D)

- **Form factors:** ground-state and excited-state form factors and transition form factors

Experiments at Jefferson Laboratory (CLAS), MIT-Bates, LEGS, Mainz, Bonn, GRAAL, and Spring-8

Many models disagree (a selection are shown here)

Example: $N-P_{11}$ transition FF
Physics Research Directions

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- **Spectrum:**
  - Excited-state baryon resonances (Hall B)
  - Conventional and exotic (hybrid) mesons (Hall D)

- Form factors: ground-state and excited-state form factors and transition form factors

Solution: increase resolution
- Anisotropic lattices \( a_t < a_{x,y,z} \)
Going to larger $t$ does not always work well with three-point correlators

Example:

Quark helicity distribution
LHPC & SESAM


50% increase in error budget at $t_{\text{sep}} = 14$

Confronting the excited states might be a better solution than avoiding them.
Actions

- Anisotropic Symanzik gauge action with bare anisotropy $\gamma_g$

$$S_G = \frac{\beta}{N_c \gamma_g} \left\{ \sum_{x, s > s'} \left[ \frac{5}{3} P_{ss'} - \frac{1}{12} R_{ss'} \right] + \sum_{x, s} \left[ \frac{4}{3} P_{st} - \frac{1}{12} R_{st} \right] \right\}$$

*(Morningstar, Peardon ’99)*

- Anisotropic clover fermion action with 3d stout-link smeared $U$'s (spatially smeared only)

$$S_{FW}^S = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \bar{\psi} \left[ c_t \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

- Tree-level values for $c_t$ and $c_s$

$$c_s = \frac{\gamma_g}{\gamma_f}, \quad c_t = \frac{1}{2} \left( \frac{\gamma_g}{\gamma_f} + \frac{1}{\xi} \right)$$

*(P. Chen 2001)*

- Tadpole improvement factors $u_s$ (gauge) and $u'_s$ (fermion)

- Coefficients to tune: $\gamma_g$, $\gamma_f$, $m_0$, $\beta$
Actions

- Anisotropic Symanzik gauge action with bare anisotropy $\gamma_g$
  
  \[ S_G = \frac{\beta}{N_c \gamma_g} \left\{ \sum_{x,s,s'} \left[ \frac{5}{3} P_{ss'} - \frac{1}{12} R_{ss'} \right] + \sum_{x,s} \left[ \frac{4}{3} P_{st} - \frac{1}{12} R_{st} \right] \right\} \]

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- Anisotropic clover fermion action with 3d stout-link smeared $U'$s (spatially smeared only)
  
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- Tadpole improvement factors $u_s$ (gauge) and $u'_s$ (fermion)

- Coefficients to tune: $\gamma_g$, $\gamma_f$, $m_0$, $\beta$

- “SLAC” = Stout Link Anisotropic Clover
3D Stout-Link Smearing

Morningstar, Peardon ’04

- Smoothes out dislocations; impressive glueball results
- Updating **spatial** links only
- Differentiable!
  Direct implementation for dynamical simulation

Why 3d Stout-link smearing?

i. Still have positive-definite transfer matrix in time (good for spectroscopy with multiple excited states)

ii. Light quark action (more) stable

iii. Tadpole $c_{s,t}$ is closer to nonperturbative one
3D Stout-Link Smearing

*Morningstar, Peardon ‘04*

- Smoothes out dislocations; impressive glueball results
- Updating \textit{spatial} links only
- Differentiable!
  - Direct implementation for dynamical simulation

**Scaling Study:**

with $n_\rho = 2$ and $\rho = 0.22$

- Quenched Wilson gauge comparison

- Clover: small scaling violations

\begin{equation}
\mathbf{U} = \mathbf{U} + \frac{1}{2} \sum_{\nu \neq \mu} \rho_{\mu \nu} \{ \mathbf{U} + \mathbf{U} + \mathbf{U} + \mathbf{U} \}
\end{equation}
Computational Facilities

Two major resources:

**USQCD**

7n cluster (13 TF) @ JLab

**INCITE**

Jaguar cluster (119 TF) @ ORNL
Algorithm

- Rational Hybrid Monte Carlo (RHMC)
- Multi-scale anisotropic molecular dynamics update
- Even-odd preconditioning for the clover term
- Stout-link smearing in fermion actions

\[
\frac{d\tilde{Q}}{dU_{\text{thin}}} = \frac{d\tilde{Q}}{dU_{\text{stout}}} \frac{dU_{\text{stout}}}{dU_{\text{thin}}}
\]

- Split gauge term
- Three time scales
  - \(\delta t_1\): Omelyan integrator for tr \(\log A_{ee}\) and \(\phi^+ r^{-\frac{1}{2}} (\tilde{Q}) \phi\)
  - \(\delta t_2\): Leapfrog integrator \(S_{G,(S)}\)
  - \(\delta t_3\): Leapfrog integrator \(S_{G,(T)}\)
  - Choice: \((\delta t_1, \delta t_2, \delta t_3) = (1/4, 1/4, 1/3)\) for \(12^3 \times 96\)
    \((1/5, 1/3, 1/2)\) for \(12^3 \times 32\)
- Acceptance rate: 60–70%
Dynamical Generation Costs

- Cost in terms of cost of producing one MD trajectory

\[ \text{Cost}_{\text{traj}} = \xi^{1.25} \left( \frac{\text{fm}}{a_s} \right)^6 \left[ \left( \frac{L_s}{\text{fm}} \right)^3 \left( \frac{L_t}{\text{fm}} \right) \right]^{5/4} \cdot [C_1 + C_2/m_l]. \]

- Extra cost – a dimension taken to (near) continuum limit!
- Improvement: Temporal preconditions of clover Dirac operator (Edwards, Joo, Peardon, work in progress)
- Gain factor of 2.5 in quenched study
- Ready to implement on next anisotropic runs
Tadpole Factors and Stout Smearing

**Stout parameter study:**

one-loop (Foley et al.)

Conservative choices: $n_\rho = 2$ and $\rho = 0.14$ ($< 1/2d$)

Padé approximation for $u_s$ over a wide range of $g^2 = 6/\beta$

\[ \langle P_s \rangle = 1 - e^{14} g^2 \]
$N_f=3$ Nonperturbative Tuning

Nonperturbatively determine $\gamma_g, \gamma_f, m_0$ on anisotropic lattice

$$S_{SW}^{SW} = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi \bar{\psi} \left[ c_t \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

Three calculations:
- Background field in time: PCAC gives $M_t$
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Three calculations:
- Background field in time: PCAC gives $M_t$
- Background field in space: sideways potential gives $\gamma_{g,R}$

Klassen Method: ratio of Wilson loops

Wanted: $V_s(ya_s) = V_s(ta_s / \xi_R)$

$\Rightarrow$ Condition: $R_{ss}(x,y) = R_{st}(x,t)$

$$L(\xi_g) = \sum_{x,y} \frac{(R_{ss}(x,y) - R_{st}(x,\xi_g y))^2}{(\Delta R_s)^2 + (\Delta R_t)^2}$$

Comparison with PBC result

Example:
$(\gamma_g = 4.4, \gamma_f = 3.4, m_0 = -0.0570, \beta = 1.5)$
Nonperturbatively determine $\gamma_g, \gamma_f, m_0$ on anisotropic lattice

$$S^{SW}_{F} = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \bar{\psi} \left[ c_l \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

Three calculations:
- Background field in time: PCAC gives $M_t$
- Background field in space: sideways potential gives $\gamma_{g,R}$
- Antiperiodic in time: dispersion relation gives $\gamma_{f,R}$, $(m_0, r_0, \text{etc.})$
\( N_f=3 \) Nonperturbative Tuning

Nonperturbatively determine \( \gamma_g, \gamma_f, m_0 \) on anisotropic lattice

\[
S_{SW}^{SW} = \overline{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \overline{\psi} \left[ c_t \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi
\]

Three calculations:

- Background field in time: PCAC gives \( M_t \)
- Background field in space: sideways potential gives \( \gamma_g, R \)
- Antiperiodic in time: dispersion relation gives \( \gamma_f, R \), \( (m_0, r_0, etc.) \)

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$N_f=3$ Nonperturbative Tuning

Nonperturbatively determine $\gamma_g$, $\gamma_f$, $m_0$ on anisotropic lattice

$$S_{SW}^F = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \bar{\psi} \left[ c_t \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

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Parametrize anisotropies and PCAC mass linearly:

$$\xi_g(\gamma_g, \gamma_f, m_0) = a_0 + a_1 \gamma_g + a_2 \gamma_f + a_3 m_0$$
$$\xi_f(\gamma_g, \gamma_f, m_0) = b_0 + b_1 \gamma_g + b_2 \gamma_f + b_3 m_0$$
$$M_t(\gamma_g, \gamma_f, m_0) = c_0 + c_1 \gamma_g + c_2 \gamma_f + c_3 m_0.$$

Use space & time BC simulations to fit $a$’s, $b$’s, $c$’s separately

Improvement condition: solve $3 \times 3$ linear system for each $m_q$ with $\xi = a_s/a_t = 3.5$

$$\xi_g(\gamma_g^*, \gamma_f^*, m_0^*) \equiv \xi$$
$$\xi_f(\gamma_g^*, \gamma_f^*, m_0^*) \equiv \xi$$
$$M_t(\gamma_g^*, \gamma_f^*, m_0^*) \equiv m_q$$
Nonperturbatively determine $\gamma_g$, $\gamma_f$, $m_0$ on anisotropic lattice

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$N_f = 3$, $\xi = 3.5$, $\beta = 1.5$  

Plot of $\gamma_g$ and $\gamma_f$ versus input current quark mass

Mild dependence on quark mass; fix $\gamma_g$ and $\gamma_f$
Nonperturbatively determine $\gamma_g$, $\gamma_f$, $m_0$ on anisotropic lattice

$$S_F^SW = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \bar{\psi} \left[ c_l \sum_s \sigma_{ls} F_{ls}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

$N_f = 3$, $\xi = 3.5$, $\beta = 1.5$ \texttt{arxiv:0803.3960}

- Plot of $\gamma_g$ and $\gamma_f$ versus input current quark mass
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PCAC mass measured in SF scheme: $m_{cr} = -0.0854(5)$
Nonperturbatively determine $\gamma_g$, $\gamma_f$, $m_0$ on anisotropic lattice

$$S_{SW}^c = \bar{\psi} \left[ m_0 + D_t(U') + \frac{1}{\gamma_f} D_s(U') \right] \psi - \bar{\psi} \left[ c_t \sum_s \sigma_{ts} F_{ts}(U') + \frac{c_s}{\gamma_g} \sum_{rs} \sigma_{rs} F_{rs}(U') \right] \psi$$

$N_f = 3$, $\xi = 3.5$, $\beta = 1.5$ [arxiv:0803.3960]

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PCAC mass measured in SF scheme: $m_{cr} = -0.0854(5)$

Check NP $c_{s,t}$ condition in SF scheme

![Graph showing $\Delta M_t$ vs. $m_0$ with data points and lines indicating different scenarios]
2+1-Flavor Runs

- Mass-independent scheme (fixed $\beta = 1.5$ approach)
- Scale and masses are defined in chiral limit

(Edwards, Joo, Lin, Peardon, work in progress)

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<th>$L_t$</th>
<th>$m_\ell$</th>
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Algorithm

- Rational Hybrid Monte Carlo (RHMC)
- Multi-scale anisotropic molecular dynamics update
- Even-odd preconditioning for the clover term
- Stout-link smearing in fermion actions

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\frac{d\tilde{Q}}{dU_{\text{thin}}} = \frac{d\tilde{Q}}{dU_{\text{stout}}} \frac{dU_{\text{stout}}}{dU_{\text{thin}}}
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  - \( \delta t_2 \): Omelyan integrator \( S_{G,(S)} \)
  - \( \delta t_3 \): Omelyan integrator \( S_{G,(T)} \)
  - Choice: \( \delta t_1 = \delta t_2 \)
- Acceptance rate: 75%
Autocorrelation

- Example: $24^3 \times 128$ volume, with pion mass 315 MeV
- Plaquette history

Graphs showing spatial and temporal autocorrelation.
Lowest Eigenvalue

- Example: $24^3 \times 128$ volume, with pion mass 315 MeV
- Histogram distributions
2+1-Flavor Runs

- Preliminary spectroscopic measurements
  - 3 Gaussian smearing parameters + Point/Smeared sink
  - Average over 4 time sources
    (w/ eigcg solver 0707.0131 [hep-lat])
    \{0,0,0,0\}, \{8,8,8,32\}, \{0,0,64\}, \{8,8,8,128\}
  - Ground states obtained from 2-state fits
  - For example: 12 pion correlators
2+1-Flavor Runs

- Preliminary spectroscopic measurements
  - 3 Gaussian smearing parameters + Point/Smeared sink
  - Average over 4 time sources
    (w/ eigcg solver 0707.0131 [hep-lat])
    \{0,0,0,0\}, \{8,8,8,32\}, \{0,0,64\}, \{8,8,8,128\}
  - Ground states obtained from 2-state fits
  - For example: 6 Lambda correlators

More spectroscopy results by Saul Cohen
2+1-Flavor Runs

Meson strange-sea dependence

\[
\begin{align*}
\rho & & m_{1} = -0.0743 & & m_{2} = -0.0540 & & m_{3} = -0.0618 \\
\phi & & m_{1} = -0.0743 & & m_{2} = -0.0540 & & m_{3} = -0.0618 \\
\alpha & & m_{1} = -0.0743 & & m_{2} = -0.0540 & & m_{3} = -0.0618 \\
\beta & & m_{1} = -0.0743 & & m_{2} = -0.0540 & & m_{3} = -0.0618 \\
\end{align*}
\]
2+1-Flavor Runs

Meson strange-sea dependence

\[ K, \eta_s, \rho, K^*, \phi, a_0, a_1, b_1 \]

\[ m_s = -0.0743, m_s = -0.0618, m_s = -0.0540 \]
Baryon strange-sea dependence

2+1-Flavor Runs
Baryon strange-sea dependence

2+1-Flavor Runs

\[ N \]
\[ \Sigma \]
\[ \Lambda \]
\[ \Delta \]
\[ \Sigma^* \]
\[ \Xi^* \]
\[ \Omega \]
Strange-Quark Mass

Difficult: Chiral extrapolation to obtain \( m_s \) and \( r_0/a_s \)

Strange-quark tuning

Candidates: kaon, \( \phi \), \( \Omega \) mass, etc.

Example: at a fixed \( m_s \), see 30% variation in phi mass

Need multiple 2+1 runs to obtain reasonable \( m_s \)
Better description for $s$-quark tuning
- Use ratio of hadron masses to eliminate lattice spacing
- **Leading-order XPT**
  \[ l_\Omega = (9/4) \frac{m_\pi^2}{m_\Omega^2} \text{ and } \]
  \[ s_\Omega = (9/4) \frac{2m_K^2 - m_\pi^2}{m_\Omega^2} \]
Better description for $s$-quark tuning

- Use ratio of hadron masses to eliminate lattice spacing

**Leading-order XPT**

\[ l_\Omega = \left( \frac{9}{4} \right) \frac{m_\pi^2}{m_\Omega^2} \text{ and } s_\Omega = \left( \frac{9}{4} \right) \frac{(2m_K^2 - m_\pi^2)}{m_\Omega^2} \]

- Tune $N_f = 3$ quark mass until physical $s_\Omega$ achieved
Better description for $s$-quark tuning

- Use ratio of hadron masses to eliminate lattice spacing

**Leading-order XPT**

\[ l_\Omega = \left( \frac{9}{4} \right) \frac{m_\pi^2}{m_\Omega^2} \text{ and} \]

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- Tune $N_f = 3$ quark mass until physical $s_\Omega$ achieved

- 2+1f comparison plot

  - Aniso-clover, $a_s = 0.13$ fm
  - DWF on asqtad, $a = 0.125$ fm (LHPC)
  - DWF on DWF, $a = 0.116$ fm (RBC+UKQCD)
Better description for $s$-quark tuning

- Use ratio of hadron masses to eliminate lattice spacing

**Leading-order XPT**

\[ l_\Omega = \frac{(9/4) m_\pi^2}{m_\Omega^2} \quad \text{and} \quad s_\Omega = \frac{(9/4) (2m_K^2 - m_\pi^2)}{m_\Omega^2} \]

- Tune $N_f = 3$ quark mass until physical $s_\Omega$ achieved

- 2+1f comparison plot

  - Aniso-clover, $a_s \sim 0.13$ fm
  - DWF on asqtad, $a = 0.125$ fm (LHPC)
  - DWF on DWF, $a = 0.116$ fm (RBC+UKQCD)

**LO Extrapolation**

- Strange is off by 4–6%

**NLO correction?**

<table>
<thead>
<tr>
<th>Inputs</th>
<th>$a_\pi^{-1}$ (GeV)</th>
<th>$m_i^{\text{phys}}$</th>
<th>$m_s^{\text{phys}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_\pi^2$, $m_K^2$, $m_\Omega$</td>
<td>5.39(8)</td>
<td>-0.08668(11)</td>
<td>-0.0705(4)</td>
</tr>
<tr>
<td>$m_\pi^2$, $m_K^2$, $m_\phi$</td>
<td>5.47(5)</td>
<td>-0.08651(8)</td>
<td>-0.0710(2)</td>
</tr>
</tbody>
</table>
Where we stand now:

- Scaling based on actual $(24^3)$ runs down to ~170 MeV

  \[ \text{Cost}_{\text{traj}} = \xi^{1.25} \left( \frac{\text{fm}}{a_s} \right)^6 \left[ \left( \frac{L_s}{\text{fm}} \right)^3 \left( \frac{L_t}{\text{fm}} \right) \right]^{5/4} \cdot [C_1 + C_2/m] \]

- Currently, ~5k traj @ 875, 580, ~3k @ 456 MeV ($16^3$): ~6k by July 1
- 315 MeV ($24^3$), currently 3k traj, get ~1k traj/week
- $24^3$ 315 MeV ORNL runs underway now
- $24^3$ and $32^3$ 250 MeV for the near future

Future plans:

- < 200 MeV generation possible within next year or two
- Excited single-particle state vs. multi-particle ones
- Multiple lattice spacings