Computational Requirements for JLab

Robert Edwards
Theory Group
Jefferson Lab

Outline:
- Physics requirements
- Computational requirements
- Formulations
- Production strategies
- Resource requirements
- Milestones
Physics Research Directions

In broad terms - 2 main physics directions in support of experimental program

- **Spectrum**
  - Excited state baryon resonances
  - Strong, weak and electromagnetic decays
  - Form-factors and transition form-factors

- **Hadron Structure (Spin Physics)**
  - Moments of structure functions
  - Generalized form-factors
  - Moments of GPD’s
Physics Requirements (N_f=2+1 QCD)

Spectrum

- Pion masses < 200MeV; small scaling violations
- Precise isospin, parity and charge conj. (mesons)
- High lying excited states: $a_f^{-1} \sim 6$ GeV !!!
- Stochastic estimation
  - Multi-hadron state ID
  - Disconnected contributions
- Fully consistent valence and sea quarks
- Several lattice spacings for continuum extrap.
- Multiple volumes - finite-V analysis of strong decays
- Non-local group theoretical based operators
  - Mainly 2-pt correlator diagonalization
  - (Initially) positive definite transfer matrix
  - Simple 3-pt correlators (vector/axial vector current)
Physics Requirements ($N_f=2+1$ QCD)

**Hadron Structure**

- Pion masses < 250MeV, small scaling violations
- Precise valence isospin, parity and charge conj. (mesons)
- Good valence chiral symmetry
- Mostly ground state baryons
- Prefer same valence/sea - can be partially quenched
- Several lattice spacings for continuum extrap.
- Complicated operator/derivative matrix elements
  - 3-pt and 4-pt correlators
-Disconnected contributions - stochastic estimation
Computational Methods

- Physics observables: functions of *propagators*

- Basic kernel (propagator)
  - Solve linear system of eqs \( \text{Dirac} \ast \psi = \chi \) iteratively, e.g. Conjugate-Gradient

- Cost
  - Determined by condition number: \( \text{Dirac} \sim \langle \text{largest ev} \rangle / \langle \text{smallest ev} \rangle \)
  - Typically, \( \langle \text{smallest ev} \rangle \sim \langle \text{quark mass} \rangle \)
  - Cost increases as \( \langle \text{quark mass} \rangle \rightarrow \langle \text{physical mass} \rangle \)

- Generating (dynamical) ensembles:
  - Construct Hamiltonian = \( S_{\text{gauge}} + S_{\text{fermion}} + (1/2) P^2 \)
  - Integrate Hamilton’s eqs (partial diff. eq.), have linear system solvers at each integration step

- Upshot: lowest quark mass most expensive (good news here: more later...)
Formulations

- **(Improved) Staggered fermions (Asqtad):**
  - Relatively cheap for dynamical fermions (good)
  - Mixing among parities and flavors or *tastes*
  - Baryonic operators a nightmare - not suitable

- **Clover (anisotropic):**
  - Relatively cheap (now):
  - Good flavor, parity and isospin control, small scaling violations
  - Positive definite transfer matrix
  - Requires (non-perturbative) field improvement - prohibitive for spin physics

- **Chiral fermions (e.g., Domain-Wall/Overlap):**
  - Automatically $O(a)$ improved, suitable for spin physics and weak-matrix elements
  - No transfer matrix - problematic for spectrum (at large lattice spacings)
  - Expensive
USQCD and the World

- **Asqtad (Staggered) fermions:**
  - Large scale generation on-going by MILC (collab).
  - Lattice spacings: $a \sim 0.13\,\text{fm} \ (1.6 \,\text{GeV}), \ 0.09\,\text{fm} \ (2.2 \,\text{GeV}), \ 0.06\,\text{fm} \ (3.3 \,\text{GeV})$
  - Suitable for valence Domain Wall (spin-physics) via partially quenched chiral pertubation theory
  - Not suitable for baryon spectrum program

- **Clover (anisotropic):**
  - Suitable for spectrum and simple form-factors
  - Anisotropy requires new calculation (no existing configs)

- **Chiral fermions (e.g., Domain-Wall/Overlap):**
  - Algorithm investigations on-going at JLab
  - Large scale production by UKQCD and RBC
  - Too coarse lattice for JLab spectra
  - Configs not released
Why anisotropic? 
COST!!

Lower cost with only one fine lattice spacing instead of all 4.

Group theoretical construction of baryon interpolating fields

Find 8 excited states!!

Need long plateau for cross-correlator diag. and high energies

Effective mass: Nucleon \( G_{1g} \) rep. \((1/2)^+\)

Small volume quenched Wilson fermion test case

LHPC, PRD 72: 094506, 074501 (2005)
Clover has very small scaling violations and a positive def. transfer matrix

Shown is a plot of clover scaling compared to various actions

Scaling holds for anisotropic lattices

Non-perturbative improvement also done at JLab

Cost savings over chiral fermions is large

Unsuitability of Chiral Fermions for Spectrum

- Chiral fermions lack a positive definite transfer matrix
- Results in unphysical excited states. Obscures true excited states
- Unphysical masses $\sim 1/a$, so separate in continuum limit
- Shown is the Cascade effective mass of DWF over Asqtad

- Upshot: chiral fermions not suited for high lying excited state program at currently achievable lattice spacings
Production Strategy

- **Hadron Structure (Hybrid approach):**
  - Domain Wall valence fermions on MILC supplied Asqtad lattices
  - Lattice spacings: $a \sim 0.13\text{fm}$ (1.6 GeV), 0.09fm (2.2 GeV), 0.06fm (3.3 GeV)
  - Expect roughly 2-3 years of work

- **Spectrum:**
  - Anisotropic clover at $a \sim 0.125\text{fm}$, 0.10fm and 0.08fm.
  - Expect 2-3 years of work

- **Chiral valence over chiral sea**
  - On-going algorithm investigations
  - Initial joint USQCD production on ANL BG/P in 2007
Scaling of Full QCD Gauge Generation

- **Cost of gauge generation (Berlin Wall):**
  - Cost: $\text{Cost}(TF - yr) = \text{const} \left( \frac{m_{PS}}{m_V} \right)^{-z} V^{5/4} a^{-7}$
  - Old methods, $z = 6$
  - Improvements in dyn. fermion technology: $z = 4$ instead of 6
    - Multi-time scale integrators & determinant preconditioners

- Wilson fermion comparisons: **old** ($z=6$) vs **new** ($z=4$)

- New Wilson scaling similar to Staggered

- Upshot: no computational advantage for Staggered over Wilson!

Magnified

Jansen, et.al., CPC (2006)
Anisotropic Clover: dynamical generation

- **Problem:** lack of full chiral symmetry:
  - Unprotected fluctuations of smallest Dirac eigenvalue
  - Large fluctuations in fermionic force & propagators
- **Solution:** recent study of large volumes (Luescher):
  - Empirical bound on smallest eigenvalue implies stability of integration when
    \[ m_{\pi} L \geq 11 \sqrt{a \text{ (fm)}} \]
- **Smallest obtainable pion masses**

<table>
<thead>
<tr>
<th>Lattice Spacing</th>
<th>Bound</th>
<th>2.4fm</th>
<th>3.2fm</th>
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- **Upshot:** physics requires large \( m_{\pi} L \), smallest mass not an issue

Luescher, et.al., JHEP (2006)
Anisotropic Clover: dynamical generation

Expected lattice sizes and anisotropies

<table>
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<th>Lattice Spacing</th>
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<th>3.2fm</th>
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<td>$20^3 \times 128$</td>
<td>$24^3 \times 128$</td>
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Lattice sizes for each physical size and lattice spacing.

The temporal lattice spacing and extent are held to $a_t \sim 0.033$fm and $L_t \sim 4.0$fm, resp.
Anisotropic Clover: dynamical generation

Estimated cost of $N_f=2+1$ production (in TFlop-yr) using $z_\pi=4$

$$\text{Cost(TFlop - yr)} = \text{const} \left( \frac{m_{PS}}{m_V} \right)^{-4} V(\text{fm})^{5/4} a(\text{fm})^{-7}$$

- **Phase I - initial production + 10% analysis overhead**
  - Hybrid photo-couplings
  - cost = 1.1 TF-yr + 10% analysis

- **Phase II - all of 0.10fm and 0.125fm lattices**
  - Baryon spectra
  - cost = 4.8 TF-yr + 50% analysis

- **Phase III - $a=0.08$fm**
  - Light pion mass and continuum limit
  - cost = 23 TF-yr + 50% analysis
## Hadron Structure (DWF/Asqtad)

- Estimated cost of (Hybrid) Domain wall valence/Asqtad sea using existing or new MILC configs
- **Phase I** - finish \( a=0.125 \text{ fm} \), cost = 1.6 TF-yr
- **Phase II** - finish \( a=0.09\text{fm} \) and \( 0.06\text{fm} \), cost = 5.6 TF-yr
- **Total to finish only isovector work** = 7.2 TFlop-yr

### Table

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| \( a=0.125\text{fm}, L_t=64, L_5=16 \) | \( a=0.09\text{fm}, L_t=96, L_5=12 \) | \( a=0.06\text{fm}, L_t=144, L_5=8 \)
Algorithm Improvements - Chiral fermions

- Cost of dynamical chiral fermions influenced by residual chiral symmetry breaking
- Collaboration of JLab, Edinburgh and BU
- Recent method/algorithm improvements lower residual mass by > 10X!!

Cost versus residual mass and 5th-dim extent

\[ \frac{m_{\text{res}}}{m_q} \rightarrow \text{“badness”} \]
**Hadron Structure (fully Chiral)**

- **Estimated cost of fully consistent DWF valence/DWF sea**
  \[
  \text{Cost(TFlop – yr)} = \left( 0.9 + 0.1 \left[ \frac{0.023}{m_l} \right]^{1.5} \right) V(\text{fm})^{5/4} a(\text{fm})^{-7}
  \]

- **Phase I** – initial joint USQCD production on ANL BGL/P 100TF-peak machine
  - Cost of production = 9.2 TF-yr

- **Phase II**
  - Cost of production = 23 TF-yr

- **Phase III**
  - Cost of production = 91 TF-yr

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\[ a=0.094\text{fm}, L_t=64, L_5=16 \]

Christ, Negele (USQCD), ANL proposal
Project Milestones - Spectrum

Spectrum project (anisotropic Clover)

- Phase I - $a=0.1\text{fm}$ lattice spacing, 2.4fm to 3.2fm boxes
  - Smallest pion mass is 220 MeV
  - Result: first full QCD calculation of $\pi_1 (1^{-+})$ hybrid photo-coupling and exotic meson masses
  - Cost of production = 1.1 TF-yr + 10% analysis
- Phase II - finish $a=0.1\text{fm}$ and 0.12fm lattices on 2.4fm, 3.2fm, and 4.0fm boxes
  - Smallest pion mass is 181 to 200 MeV
  - Result: several (more than 2 or 3) low-lying excited baryon resonance masses with decay widths, nucleon form-factors, strange FF in nucleon
  - Cost of production = 0.66 + 4.1 = 4.8 TF-yr + 50% analysis
- Phase III - finish $a=0.08\text{fm}$ lattice on 2.4fm, 3.2fm and 4.0fm boxes
  - Smallest pion mass is 181 MeV
  - Result: continuum limit of resonance masses, nucleon form-factors $Q^2 > 10 \text{ GeV}^2$, $N-\Delta$ and Roper transition FF, strange FF in nucleon
  - Cost of production = 23 TF-yr + 50% analysis
Project Milestones - Hadron Structure

Hadron Structure (DWF/Asqtad):

- Quantifies error bars of spin quantities
- Phase I - finish a=0.125fm lattice
  - Smallest pion mass is 254 MeV
  - Result: full QCD
    - Moments of non-singlet nucleon structure funcs and GPD's
    - Non-singlet Nucleon FF's, N-Δ transition FF
    - Nucleon polarizabilities
  - Cost = 1.6 TF-yr
- Phase II - finish a=0.09fm and 0.06fm lattices
  - Smallest pion mass is 254 MeV
  - Result:
    - Continuum limit of structure funcs, GPD's, polarizabilites
    - Nucleon FF's at $Q^2 > 10 \text{ GeV}^2$
  - Cost = 5.6 TF-yr
Project Milestones - Hadron Structure

Hadron Structure (fully consistent DWF/DWF)

- Error bars in chiral extrapolation fully quantifiable
- Phase I - $a=0.094$ fm lattice
  - Smallest pion mass is 295 MeV
  - Result: full QCD
    - Moments of non-singlet nucleon structure funcs and GPD’s
    - Non-singlet Nucleon FF’s, N-$\Delta$ transition FF
    - Nucleon polarizabilities
  - Cost of production = 9 TF-yr + 10% analysis
- Phase II
  - Smallest pion mass is 254 MeV
  - Result: full QCD
    - Error bar control to < 10% (e.g., momentum fraction)
  - Cost of production = 23 TF-yr + 10% analysis
- Phase III
  - Smallest pion mass is 181 MeV
  - Result: full QCD
    - Error bar control to 5% on some moments
  - Cost of production = 91 TF-yr + 10% analysis
USQCD Computing Allocations (2006)

- **QCDOC**: requested 6.3 TFlop, allocated 3.4 TFlop
- **Clusters**: requested 6.0 TFlop, allocated 2.0 TFlop
- Scheduled by USQCD allocations committee
- Upshot: resources heavily oversubscribed
- Below: major projects allocated

<table>
<thead>
<tr>
<th>JLab impact</th>
<th>Project</th>
<th>Requested (TF-yr)</th>
<th>Allocated TF-yr</th>
<th>Systems</th>
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**Total near-term JLab impact**: 20% of total allocations
Summary

- JLab Lattice research program is aligned with experimental program
- JLab has world leadership position in investigations of hadron structure, spectrum and algorithm techniques
- Different project requirements result in different lattice formulations
  - Following a tiered approach to satisfy Jlab’s mission
  - Different approaches optimize science output – most science per dollar of computing infrastructure
- Current USQCD systems way oversubscribed
- Without additional computing resources, risk losing leadership position from world competition and not delivering on support of experimental program