Computational Requirements for JLab

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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

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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: $a_t^{-1} \sim 6$ 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

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Computational Methods

- Physics observables: functions of *propagators*
- Basic kernel (propagator)
  - Solve linear system of eqs Dirac * $\psi = \chi$ iteratively, e.g. Conjugate-Gradient
- Cost
  - Determined by condition number: Dirac ~ <largest ev> / <smallest ev>
  - Typically, <smallest ev> ~ <quark mass>
  - Cost increases as <quark mass> $\rightarrow$ <physical mass>
- Generating (dynamical) ensembles:
  - Construct Hamiltonian = $S_{gauge} + S_{fermion} + (1/2)\, P^2$
  - 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…)

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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

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USQCD and the World

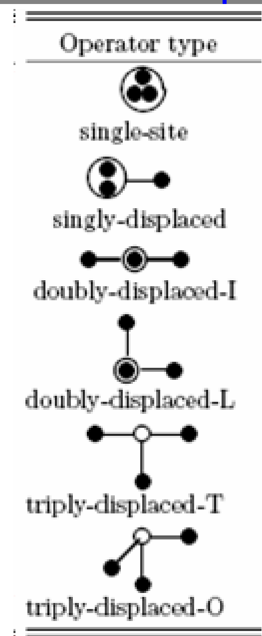
- Asqtad (Staggered) fermions:
  - Large scale generation on-going by MILC (collab).
  - Lattice spacings: a ~ 0.13fm (1.6 GeV), 0.09fm (2.2 GeV), 0.06fm (3.3 GeV)
  - Suitable for valence Domain Wall (spin-physics) via partially quenched chiral pertubation theory
  - Not suitable for baryon spectrum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

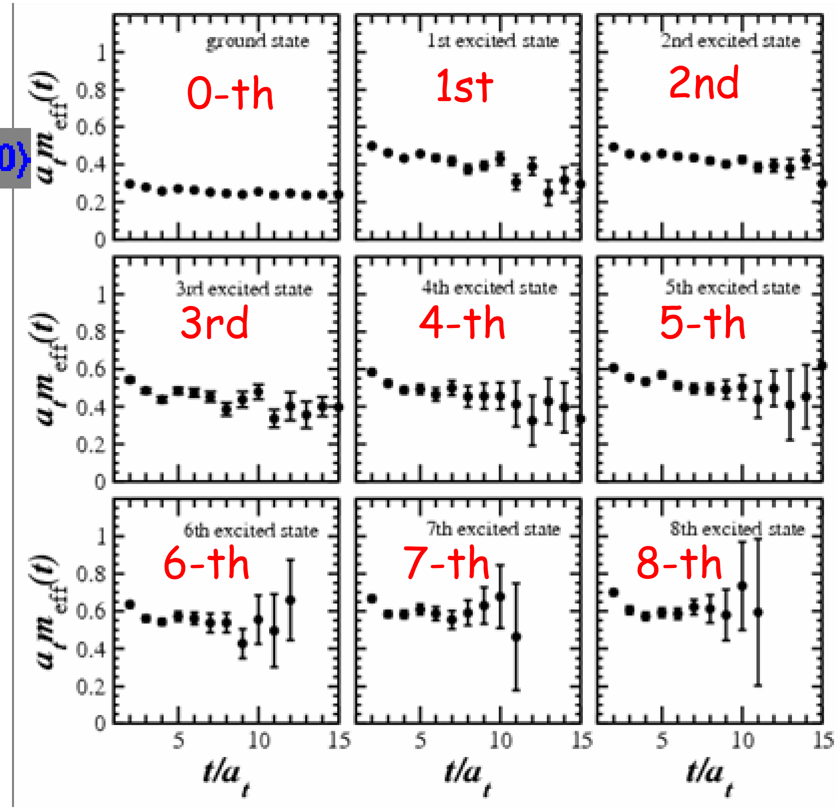
Spectrum – Need for Anisotropic Lattices

- 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. $(1/2)^+$

$$C_{\alpha\beta}(t) = \langle 0|\phi_\alpha(t)\phi^\dagger_\beta(0)|0\rangle$$



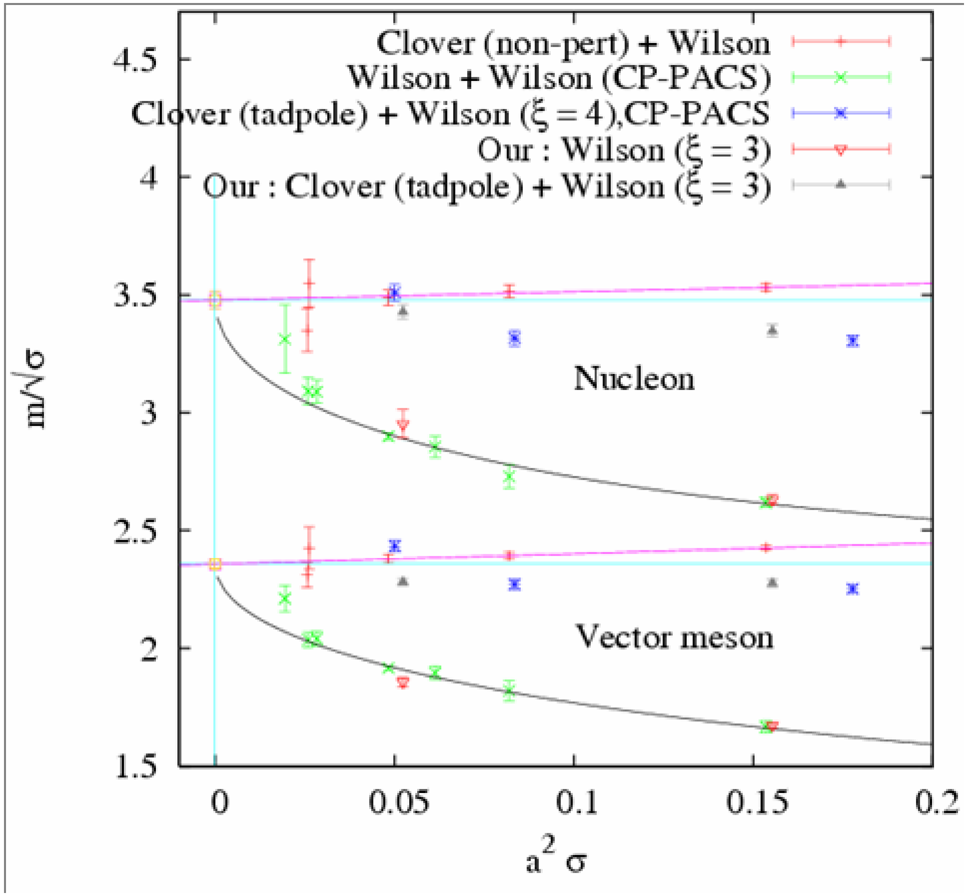


Small volume quenched Wilson fermion test case

LHPC, PRD 72: 094506, 074501 (2005)

Clover Scaling Studies

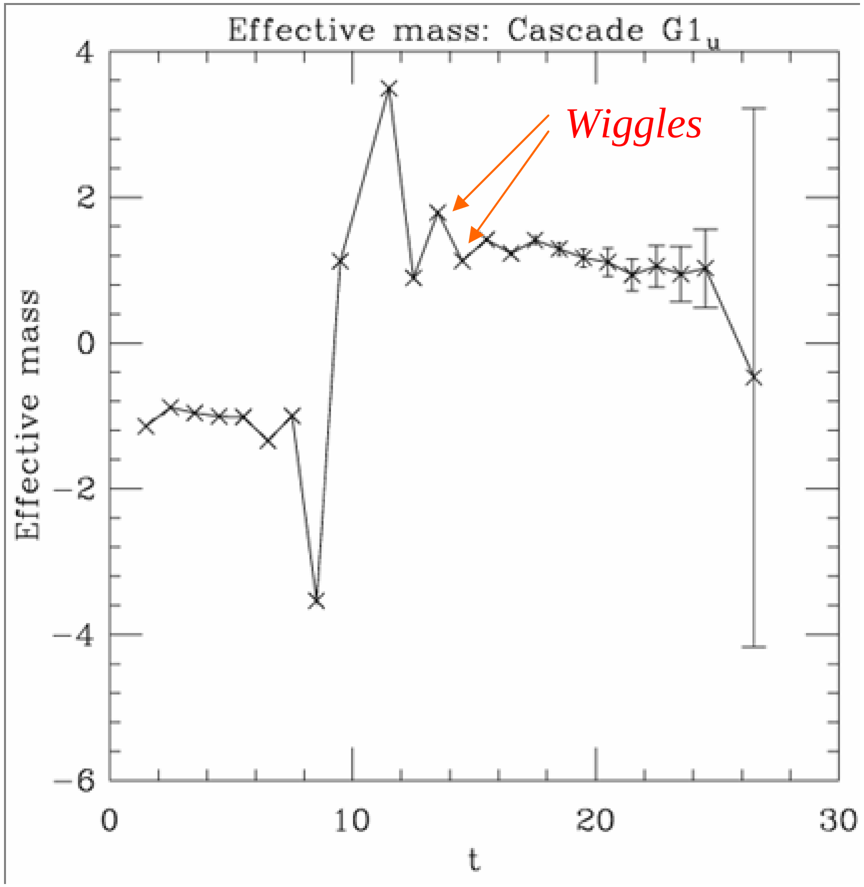
- Clover has very small scaling violations and a positive def. transfer matrix
- Shown is a plot of clover scaling compared to various actions
- Scaling holds for anisotropic lattices
- Non-perturbative improvement also done at JLab
- Cost savings over chiral fermions is large



Edwards, Heller, Klassen, PRL 80 (1998)

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 ~ 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



Source at t=10

Production Strategy

- Hadron Structure (Hybrid approach):
  - Domain Wall valence fermions on MILC supplied Asqtad lattices
  - Lattice spacings: a ~ 0.13fm (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~ 0.125fm, 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

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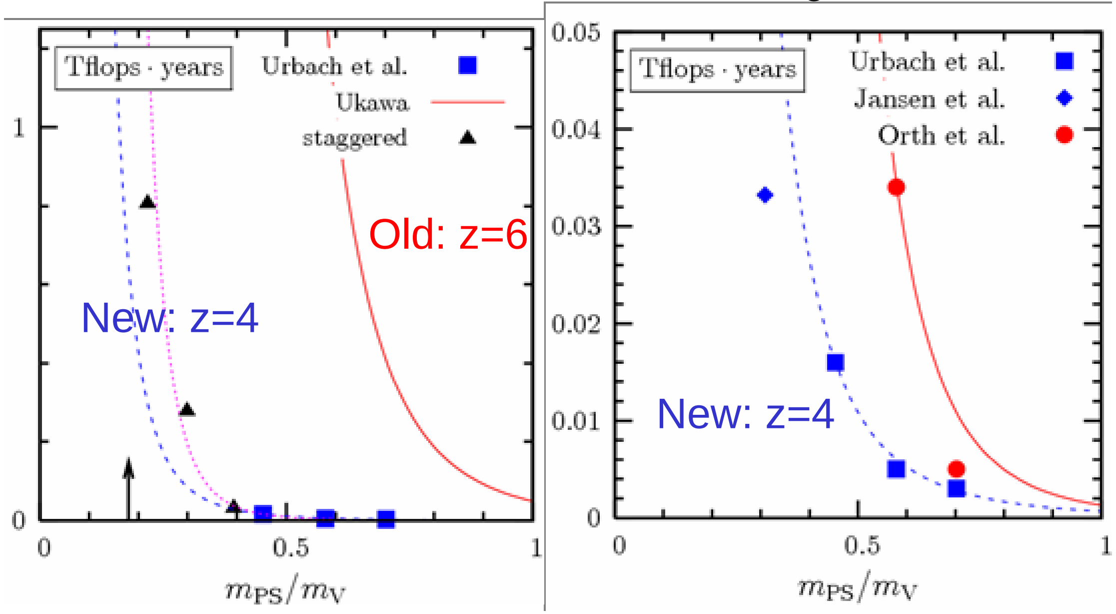
Scaling of Full QCD Gauge Generation

- Cost of gauge generation (*Berlin Wall*):
  - Cost: $Cost(TF-yr) = const \left(\frac{m_{PS}}{m_V}\right)^{-z} V^{5/4} a^{-7}$
  - 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)

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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 $$m_\pi L \geq 11\sqrt{a(fm)}$$
- Smallest obtainable pion masses

Lattice Spacing	Bound	2.4fm	3.2fm	4.0fm
$a = 0.08$ fm	3.0	250	188	150
$a = 0.10$ fm	3.5	290	220	175
$a = 0.125$ fm	4.0	333	250	200
$a = 0.15$ fm	4.5	375	282	225

- 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

Lattice Spacing	ξ	2.4fm	3.2fm	4.0fm
$a = 0.08$ fm	2.5	$28^3 \times 128$	$40^3 \times 128$	$48^3 \times 128$
$a = 0.10$ fm	3	$24^3 \times 128$	$32^3 \times 128$	$40^3 \times 128$
$a = 0.125$ fm	4	$20^3 \times 128$	$24^3 \times 128$	$32^3 \times 128$

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-yrs) using z_π=4

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

- 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=0.08fm
  - Light pion mass and continuum limit
  - cost = 23 TF-yr + 50% analysis

Lattice Spacing	m_π (MeV)	2.4fm	3.2fm	4.0fm	Total (TFlop-yr)
$a = 0.08$ fm	181			7.9	7.9
	200		2.7	5.4	8.1
	254	0.4	1.1	2.3	3.8
	380	0.2	0.6	1.3	2.1
	485	0.05	0.1	0.3	0.5
				Total=	23 TF-yr
$a = 0.10$ fm	181			2.0	2.0
	220		0.4	1.0	1.4
	254		0.3	0.6	0.8
	300	0.05	0.1	0.3	0.5
	380	0.02	0.07	0.15	0.24
	485	0.01	0.03	0.07	0.12
		Sub-total=	1.0 TF-yr	Total=	5.1 TF-yr
$a = 0.125$ fm	200			0.3	0.3
	220			0.2	0.2
	254		0.04	0.1	0.15
	300		0.02	0.1	0.08
	380	0.005	0.01	0.06	0.04
	485	0.002	0.005	0.01	0.02
		Sub-total=	0.1 TF-yr	Total=	0.76 TF-yr

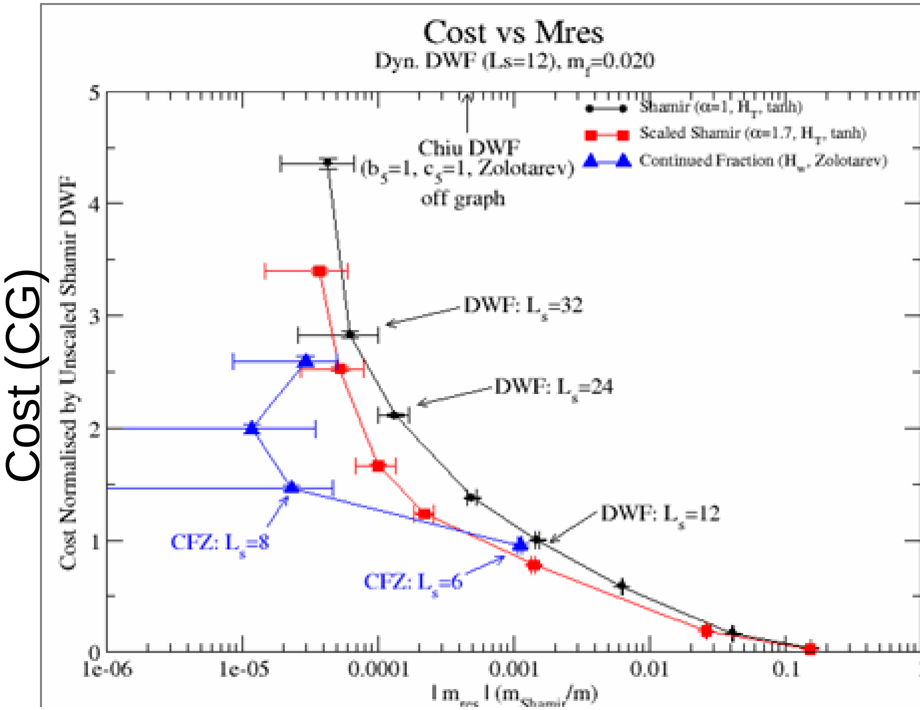
Hadron Structure (DWF/Asqtad)

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

		a=0.125fm, L_t=64, L_5=16			a=0.09fm, L_t=96, L_5=12			a=0.06fm, L_t=144, L_5=8		
m_l/m_s	m_π(MeV)	L	cfgs	TF-yr	L	cfgs	TF-yr	L	cfgs	TF-yr
1.0	775				28	500	0.07			
0.6	605	20	200	0.008						
0.4	498	20	200	0.01	28	514	0.15	48	530	1.04
0.2	359	20	695	0.14						
0.2	359	28	275	0.19	28	512	0.27	48	300	1.12
0.14	300	20	650	0.18						
0.1	254	24	529	1.07	40	200	0.77	48	300	2.18
				1.6 TF-yr			1.3 TF-yr			4.3 TF-yr

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 !!



$m_{res}/ m_q \rightarrow$ "badness"

Cost versus residual mass and 5th-dim extent

Hadron Structure (fully Chiral)

- Estimated cost of fully consistent DWF valence/DWF sea

$$\text{Cost(TFlop}-\text{yr)} = \left(0.9 + 0.1\left[\frac{0.023}{m_l}\right]^{1.5}\right) V(\text{fm})^{5/4} a(\text{fm})^{-7}$$

- 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

m_l/m_s	m_π(MeV)	L	#traj	TF-yrs
0.54	498	24	3200	0.3
0.27	352	32	3200	1.0
0.19	295	48	5000	7.9
0.11	254	48	10000	23
0.05	181	56	10000	91

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

Christ, Negele (USQCD), ANL proposal

Project Milestones - Spectrum

Spectrum project (anisotropic Clover)

- Phase I – a=0.1fm lattice spacing, 2.4fm to 3.2fm boxes
  - Smallest pion mass is 220 MeV
  - Result: first full QCD calculation of π_1 (1^{-+}) hybrid photo-coupling and exotic meson masses
  - Cost of production = 1.1 TF-yr + 10% analysis
- Phase II – finish a=0.1fm 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=0.08fm 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 GeV^2, N-Δ 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 $Q^2 > 10$ GeV^2
  - Cost = 5.6 TF-yr

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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-Δ 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

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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

JLab impact	Project	Requested (TF-yr)	Allocated TF-yr	Systems
YES	HASTE	0.94	0.40	Clusters
	RBC	2.4	1.02	QCDOC
YES	Spectrum	0.56 + 0.3	0.45 + 0.1	QCDOC/Clusters
	MILC	2.11 + 0.4	1.3 + 0.2	QCDOC/Clusters
YES	NPLQCD	1.1	0.2	Clusters
	Thermo	1.1	0.55	QCDOC

- Total **near-term** JLab impact: 20% of total allocations

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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