Jefferson Lab – MIT
Lattice Hadron Physics Initiative

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for the
Lattice Hadron Physics Collaboration
Brookhaven National Laboratory October 12, 2000

Outline

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Physics Goals
Lattice Hadron Physics Collaboration
Prototype Alpha Clusters
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  Performance
  Physics Results
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Phase II Alpha Clusters
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Motivation

• Lattice QCD is only known way to calculate the structure of hadrons

• Lattice calculations essential to extract physics from major experimental studies of hadron structure

  Bates, CEBAF, HERMES, EMC, SMC, NMC, Fermilab, RHIC Spin

• Fundamental problems can be solved now with adequate human and computer resources

• Algorithm development is creating new opportunities

• Prior to this initiative:

  No large-scale computer resources available to national hadronic physics community

  No collaboration established to carry out calculations on appropriate scale

Goal

To build the physics collaboration and computer resources to understand the structure of hadrons from first principles
Physics Goals

Nucleon structure

- Form factors

  Electromagnetic \( G_E(q^2) \quad G_M(q^2) \)

  Pion cloud essential – demanding lattice calculation
  large volume \( L^3 \)
  small \( m_q \)

Axial \( G_A \)

Strange form factor

  Parity-violating electron scattering at Bates and JLab
  measures strange quark content of nucleon
  \( \langle r^2 \rangle^{1/2}_{\text{strange}} \quad \langle \mu \rangle_{\text{strange}} \)

Sea quark physics – disconnected diagrams

\[
\begin{align*}
G_M^s &+ 0.39 G_M^s \\
G_E^s &+ 0.1 \\
0 &
\end{align*}
\]
Nucleon structure (cont.)

Parton distributions at $Q = 5$ GeV

- Moments of quark and gluon distributions

  **Leading twist**

  \[
  \langle p | \bar{\psi} \gamma_\mu D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) + q_\downarrow(x))
  \]

  \[
  \langle p | \bar{\psi} \gamma_5 \gamma_\mu D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) - q_\downarrow(x))
  \]

  \[
  \langle p | \bar{\psi} \gamma_5 \sigma_{\mu \nu} D \cdots D \psi | p \rangle \rightarrow \int dx \, x^n (q_\uparrow(x) + q_\downarrow(x))
  \]

  **Higher twist**

  \[
  \langle p | \bar{\psi} F^{\mu \nu} \gamma_5 \gamma_\mu \psi | p \rangle, \ldots
  \]

  **Off forward**

  \[
  \langle p' | \bar{\psi} \mathcal{O} D \cdots D | p \rangle
  \]
Physics Goals \textit{(cont.)}

Spectroscopy

\begin{itemize}
  \item $N^*$ spectrum
    \begin{itemize}
      \item Number and structure of states
      \item Flux tube confinement
      \item Fine and hyperfine structure
      \item Transition form factors
      \item Experimental focus at JLab – CLAS spectrometer
    \end{itemize}
  \item Glueballs
  \item Exotics, $H$
\end{itemize}
Physics Goals (cont.)

Hadron-hadron interactions

- Heavy-light mesons and baryon interactions
  - Light quark exchange
  - Gluon contributions
  
  ![Graph showing binding energy vs. R/R°]

  Adiabatic potential for $I = S = 0$ heavy-light mesons

- Fundamental aspects of QCD
  - Chiral symmetry breaking
    - Role of instantons, zero modes
  - Confinement
    - Role of center vortices, monopoles
  - Dense hadronic matter
    - Phases and equation of state
  - Effective Chiral Lagrangian
Physics Goals (cont.)

Lattice field theory

- Improved actions
- Chiral fermions
- Overlap
- Domain walls

Low-eigenmode expansion

Zero-mode dominance:

- Tool for disconnected diagrams

D-theory approach to lattice field theory

- Discrete spin formulation of lattice QCD
- Meron cluster algorithm

Contribution of low-Dirac eigenmodes to pion propagation

Two configurations of fermion occupation numbers
Jefferson Lab-MIT-Wuppertal Lattice Hadron Physics Collaboration

Founded 8/98, collaboration meetings 1/99, 4/99, 7/99, 1/00, 6/00
Collaborate on physics and cluster development

- Initial physics focus
  - Full QCD calculation of moments of structure functions
  - Calculate strange quark content of nucleon

- Cluster development
  - Performance analysis for initial clusters
  - Performance optimization
  - Network analysis and optimization

MIT
  - Started initiative 8/98
  - Purchased Alpha 164 and ES-40 clusters with startup funds
  - Sharing support of Pochinsky and Capitani

Jefferson Lab
  - Strong support by H. Grunder, C. Leemann, and N. Isgur
  - Purchased XP1000 and UP2000 clusters with startup funds
  - Hired D. Richards and R. Edwards
  - Sharing support of Pochinsky and Capitani

University of Wuppertal
  - K. Schilling, T. Lippert, postdocs, and students
  - ALiCE: 128-node, 158 Gflops cluster of DS10’s
  - NICse: 6-node, 16 Gflops cluster of dual UP2000’s
  - Sharing full QCD configurations for structure functions
  - Collaborating on network studies and performance optimization
The Lattice Hadron Physics Collaboration

Richard Brower*    Boston University
Matthias Burkardt New Mexico State University
Shailesh Chandrasekharan Duke University
Shao-Jing Dong University of Kentucky
Terrence Draper University of Kentucky
Patrick Dreher Massachusetts Institute of Technology
Robert Edwards Jefferson Laboratory
Rudolf Fiebig Florida International University
Nathan Isgur† Jefferson Laboratory
Xiangdong Ji University of Maryland
Frank Lee George Washington University
Keh-Fei Liu University of Kentucky
Colin Morningstar Carnegie Mellon University
John W. Negele† Massachusetts Institute of Technology
Andrew Pochinsky Massachusetts Institute of Technology
Claudio Rebbi Boston University
David Richards Jefferson Laboratory
Eric Swanson University of Pittsburgh
Harry B. Thacker University of Virginia
Steve Wallace University of Maryland
Chip Watson** Jefferson Laboratory
Uwe-Jens Wiese Massachusetts Institute of Technology

† Principal Investigator
* Application Software Coordinator
** Cluster Coordinator
Motivation for Alpha Cluster

- General-purpose architecture and software environment
  - Linux operating system, standard compilers
  - Source code compatibility with workstations
  - Flexibility, ability to implement innovative new approaches
  - Efficient use by everyone in community
  - Ideal for local development by dispersed collaborators
- Double-precision needed for many applications
- Commodity processors and networks offer maximal flexibility
  - Follow best technology in each generation
  - Purchase state-of-art technology any year physics or funding motivate it
- Cost-effective:
  - Market forces on processors and communications
  - Compaq entered collaboration with MIT with expectation they could bid machine for $10/sustained MFlops
  - Microway building Alpha boards with aggressive pricing – flexible in packaging and network
- For present generation, high-performance Alpha processor optimal for scaling to largest possible systems
- Next generation: EV7 computer on a chip
Prototype Clusters

Evaluated XP1000, DS10, DS20, ES40, UP2000 nodes

Incorporated Wuppertal DS10 and UP2000 cluster experience

Joint research agreement with Compaq

MIT Cluster

Optimize network and memory costs using 4-processor nodes connected by Myrinet

12 \times 4\text{-}processor \ ES40\text{'}s – 64 \text{Gflops}

\text{EV67} 667 \text{MHz processors}

8 \text{MB} \text{cache/processor}

1 \text{GB} \text{memory/SMP}

9 \text{GB} \text{disk}

500 \text{GB} \text{file server}

4 \text{Alpha 164 workstations}

Myrinet (Lanai 7)

Installed 12/99–8/00
Prototype Clusters (cont.)

Jefferson Lab Clusters

16 × 1-processor XP1000’s – 16 Gflops
500 MHz
4 MB cache
256–512 MB memory

8 × 2-processor UP2000’s – 21 Gflops
667 MHz
4 MB cache
512 MB memory / SMP
Expand to 12 or 16 SMP’s

400 GB filed server

Myrinet
Currently Lanai 7,
Ordered Lanai 9
Prototype Clusters (cont.)

- Software
  - Linux (Red Hat)
  - Compaq compilers available
  - PBS batch system
  - Resolving Linux and PBS difficulties

- SDAC startup support
  - Andrew Pochinsky
    - Single processor optimization
    - Single SMP optimization
    - Setting up and managing cluster

  Walt Akers and Jie Chen
  - Myrinet optimization
  - Adaptation of PBS

  Metacenter to make JLab and MIT facilities usable effectively by geographically dispersed collaboration
Preliminary performance and optimization

Single-processor performance on 667 MHz ES40 and UP2000

Conjugate gradient tests

Assembler – UKQCD optimized by Peter Boyle
Fortran – UKQCD, Peter Boyle
C – Andrew Pochinsky

CG performance as % of peak in SP

<table>
<thead>
<tr>
<th>Lattice Size</th>
<th>Assembler</th>
<th>Fortran</th>
<th>C</th>
<th>Assembler</th>
</tr>
</thead>
<tbody>
<tr>
<td>4^4</td>
<td>58</td>
<td>49</td>
<td>41</td>
<td>56</td>
</tr>
<tr>
<td>8^4</td>
<td>55</td>
<td>37</td>
<td></td>
<td>48</td>
</tr>
<tr>
<td>16^4</td>
<td>43</td>
<td>23</td>
<td></td>
<td>32</td>
</tr>
</tbody>
</table>

\[
\text{Log}(V) \quad 0 \quad 500 \quad 1000
\]

\[
\text{Mflops/sec} \quad 0 \quad 500 \quad 1000
\]

\[
\text{Log}(V) \quad 2 \quad 3 \quad 4 \quad 5 \quad 6
\]
Preliminary performance (cont.)

Multi-processor performance across SMP

Conjugate gradient tests on 1–4 processors

Pochinsky’s C code

Single and double precision

$4^4$ sites per processor

CG performance as % of peak

<table>
<thead>
<tr>
<th># Processors</th>
<th>S.P.</th>
<th>D.P.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>41</td>
<td>37</td>
</tr>
<tr>
<td>4</td>
<td>35</td>
<td>26</td>
</tr>
</tbody>
</table>

Conjugate gradient on ES40
**Preliminary performance (cont.)**

**Multi-node performance across network**

Studies just beginning with 1999 Myrinet (Lanai7) across 8 UP2000 nodes

Conjugate gradient tests on 1–8 UP2000 nodes (s.p.)

Boyle’s Assembler code using MPI

16$^4$ lattice spread over 1–8 nodes

<table>
<thead>
<tr>
<th># Nodes</th>
<th>Local size</th>
<th>Performance</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>16$^4$</td>
<td>33</td>
</tr>
<tr>
<td>2</td>
<td>16$^3 \times 8$</td>
<td>31</td>
</tr>
<tr>
<td>4</td>
<td>16$^2 \times 8^2$</td>
<td>30</td>
</tr>
<tr>
<td>8</td>
<td>16 $\times 8^3$</td>
<td>31</td>
</tr>
</tbody>
</table>

8 $\times 4 \times 4 \times 4$ local lattice

1 node \(1 \times 1 \times 1 \times 1\) 55%

8 nodes \(1 \times 1 \times 2 \times 4\) estimate 44%

with removal of excess global barriers

MPI $\rightarrow$ GM calls

reduce messages in global sums
Preliminary performance

Multi-node performance across network (cont.)

Agenda

- Optimized SMP assembler
  - threads on node
- MPI off node
- prefetching
  - optimal mult/add/load/store
  - overlapping communication and computation
- Study and optimize Myrinet performance
- Upgrade to Myrinet 2000 (Linai9)

We are confident we can exceed minimum design goal of 1/3 of peak
Physics on prototype clusters

Hadron spectroscopy: $N^*$ spectrum and exotics
Hadron-hadron interactions
Domain wall and overlap fermions
Meron cluster algorithm for nonzero chemical potential
Production of dynamical configurations
Moments of structure functions
Deep Inelastic Scattering

\[ e(k) + N(P) \rightarrow e(k') + X \]

\[ Q^2 \overset{\text{def}}{=} -q^2 = 4EE' \sin^2 \frac{\theta}{2} > 0 \]

\[ \nu \overset{\text{def}}{=} P \cdot q = M(E - E') \]

\[ x \overset{\text{def}}{=} Q^2/2\nu \]

- Cross section determined by hadronic tensor \( W_{\mu\nu} \)

\[
\left| \frac{A}{4\pi} \right|^2 = \frac{\alpha^2}{Q^4} l^{\mu\nu} W_{\mu\nu} \\
W_{\mu\nu} = \frac{1}{4\pi} \sum_X \langle PS|J^\mu|X\rangle (2\pi)^4 \delta^{(4)}(P + q - P_X) \langle X|J^\nu|PS\rangle \\
= \int d^4\xi \ e^{iq\xi} \langle PS|[J^\mu(\xi), J^\nu(0)]|PS\rangle
\]

- Unpolarized scattering measures symmetric part with 2 structure functions:

\[ W_{(\mu\nu)} = (-g^{\mu\nu} + \frac{q^\mu q^\nu}{q^2})F_1(\nu, Q^2) + \frac{1}{\nu} [((P^\mu - \frac{\nu}{q^2} q^\mu)(P^\nu - \frac{\nu}{q^2} q^\nu)]F_2(\nu, Q^2) \]

- Polarized scattering measures antisymmetric part with 2 structure functions:

\[ W_{[\mu\nu]} = -ie^{\mu\nu\lambda\rho} q_\lambda \left( \frac{S_\rho}{\nu} (g_1(\nu, Q^2) + g_2(\nu, Q^2)) - \frac{q \cdot SP_\rho}{\nu^2} g_2(\nu, Q^2) \right) \]

- In parton model

\[ F_1 = \frac{1}{2} \sum_q e_q^2 (q^\dagger(x) + q^\dagger(x)) \quad F_2 = 2xF_1 \quad g_1 = \frac{1}{2} \sum_q e_q^2 (q^\dagger(x) - q^\dagger(x)) \quad g_2 = 0 \]
Moments of Structure Functions

\[ \int _{0}^{1} dx x^{n-1} F_{1}(x, Q^2) = \frac{1}{2} C_{n}^{v}(Q^2/\mu^2) v_{n}(\mu) \quad v_{n} \equiv x^{n-1}q \]

\[ \int _{0}^{1} dx x^{n-2} F_{2}(x, Q^2) = C_{n}^{v}(Q^2/\mu^2) v_{n}(\mu) \]

\[ \int _{0}^{1} dx x^{n} g_{1}(x, Q^2) = \frac{1}{4} C_{n}^{a}(Q^2/\mu^2) a_{n}(\mu) \quad \frac{1}{2} a_{n} \equiv x^{n} \Delta q \]

\[ \int _{0}^{1} dx x^{n} g_{2}(x, Q^2) = \frac{1}{4} \frac{n}{n+1} (C_{n}^{d}(Q^2/\mu^2) d_{n}(\mu) - C_{n}^{a}(Q^2/\mu^2) a_{n}(\mu)) \]

\[ 2 v_{n} P_{\mu_1}...P_{\mu_n} = \frac{1}{2} \sum_{S} \langle PS| \left( \frac{i}{2} \right)^{n-1} \bar{\psi}_{\gamma_{\mu_1}} \overrightarrow{D}_{\mu_2}...\overrightarrow{D}_{\mu_n} \psi | PS \rangle \]

\[ a_{n} S_{\{\sigma P_{\mu_1}...P_{\mu_n}\}} = \langle PS| \left( \frac{i}{2} \right)^{n} \bar{\psi}_{\gamma_{5} \gamma_{\sigma}} \overrightarrow{D}_{\mu_1}...\overrightarrow{D}_{\mu_n} \psi | PS \rangle \]

\[ d_{n} S_{\{\sigma P_{\{\mu_1\}...P_{\mu_n}\}} = \langle PS| \left( \frac{i}{2} \right)^{n} \bar{\psi}_{\gamma_{5} \gamma_{\{\sigma}} D_{\mu_1}...\overrightarrow{D}_{\mu_n} \} \psi | PS \rangle \]

\[ \sqrt{\sigma P} \{ \mu_1, ... \mu_n \} \} P \} \]
More convenient notation – moments of Parton Distribution Functions (PDFs)

\[ x^n q \equiv \int_0^1 dx \ x^n (q_\downarrow(x) + q_\uparrow(x)) \]

\[ x^n \Delta q \equiv \int_0^1 dx \ x^n (q_\downarrow(x) - q_\uparrow(x)) \]

\[ x^n \delta q \equiv \int_0^1 dx \ x^n (q_\perp(x) - q_\perp(x)) \]

Relation to \( a_n^{(q)} \) and \( v_{n-1}^{(q)} \)

\[ x^n q = v_{n+1}^{(q)} \]

\[ x^n \Delta q = \frac{1}{2} a_n^{(q)} \]
<table>
<thead>
<tr>
<th></th>
<th>H(4)</th>
<th>mixes</th>
<th>$\vec{p}$</th>
<th>lattice operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$xq_v^{(a)}$</td>
<td>$6_3^+$</td>
<td>no</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma_{{1} D_4} q$</td>
</tr>
<tr>
<td>$xq_v^{(b)}$</td>
<td>$3_1^+$</td>
<td>no</td>
<td>0</td>
<td>$\bar{q}\gamma_4 D_4 q - \frac{1}{3}(\bar{q}\gamma_1 D_1 q + \bar{q}\gamma_2 D_2 q + \bar{q}\gamma_3 D_3 q)$</td>
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<tr>
<td>$x^2q_v$</td>
<td>$8_1^-$</td>
<td>yes</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma_{{1} D_1 D_4} q - \frac{1}{2}(\gamma_{{2} D_2 D_4} + \gamma_{{3} D_3 D_4})q$</td>
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<tr>
<td>$x^3q_v$</td>
<td>$2_1^+$</td>
<td>yes</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma_{{1} D_1 D_4 D_4} q + \bar{q}\gamma_{{2} D_2 D_3 D_3} q - (3 \leftrightarrow 4)$</td>
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<tr>
<td>$\Delta q_v$</td>
<td>$4_4^+$</td>
<td>no</td>
<td>0</td>
<td>$\bar{q}\gamma^5\gamma_{3} q$</td>
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<tr>
<td>$x\Delta q_v^{(a)}$</td>
<td>$6_3^-$</td>
<td>no</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma^5\gamma_{{1} D_3} q$</td>
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<tr>
<td>$x\Delta q_v^{(b)}$</td>
<td>$6_3^-$</td>
<td>no</td>
<td>0</td>
<td>$\bar{q}\gamma^5\gamma_{{3} D_4} q$</td>
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<tr>
<td>$x^2\Delta q_v$</td>
<td>$4_2^+$</td>
<td>no</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma^5\gamma_{{1} D_3 D_4} q$</td>
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<tr>
<td>$\delta q_v$</td>
<td>$6_1^+$</td>
<td>no</td>
<td>0</td>
<td>$\bar{q}\gamma^5\sigma_{34} q$</td>
</tr>
<tr>
<td>$x\delta q_v$</td>
<td>$8_1^-$</td>
<td>no</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma^5\sigma_{34} D_1 q$</td>
</tr>
<tr>
<td>$d_1$</td>
<td>$6_1^+$</td>
<td>no*</td>
<td>0</td>
<td>$\bar{q}\gamma^5\gamma_{{3} D_4} q$</td>
</tr>
<tr>
<td>$d_2$</td>
<td>$8_2^-$</td>
<td>no*</td>
<td>$\neq 0$</td>
<td>$\bar{q}\gamma^5\gamma_{{1} D_3 D_4} q$</td>
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</tbody>
</table>
Plateaus for SESAM ($\kappa = 0.1560$) $p = 0$
Plateaus for SESAM ($\kappa = 0.1560$)  $p \neq 0$
Unpolarized PDF: Full QCD (open), quenched (solid)
Polarized PDF: Full QCD (open), quenched (solid)
Unpolarized PDF: Full QCD (open), cooled full QCD (solid)
Comparison with Phenomenology

<table>
<thead>
<tr>
<th></th>
<th>QCDSF</th>
<th>QCDSF(a = 0)</th>
<th>Wuppertal</th>
<th>DD60Q</th>
<th>SESAM (4 pts)</th>
<th>SESAM (3 pts)</th>
<th>Phenom. (q_{\text{val}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x_u)</td>
<td>0.452(26)</td>
<td>0.454(29)</td>
<td>0.454(18)</td>
<td>0.504(18)</td>
<td>0.459(29)</td>
<td>0.284</td>
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<tr>
<td>(x_d)</td>
<td>0.189(12)</td>
<td>0.203(14)</td>
<td>0.213(11)</td>
<td>0.190(17)</td>
<td>0.190(17)</td>
<td>0.104</td>
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</tr>
<tr>
<td>(x_u - x_d)</td>
<td>0.263(17)</td>
<td>0.251(18)</td>
<td>0.291(14)</td>
<td>0.269(23)</td>
<td>0.269(23)</td>
<td>0.180</td>
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<tr>
<td>(x^2_u)</td>
<td>0.104(20)</td>
<td>0.119(61)</td>
<td>0.115(44)</td>
<td>0.176(63)</td>
<td>0.176(63)</td>
<td>0.083</td>
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<tr>
<td>(x^2_d)</td>
<td>0.037(10)</td>
<td>0.029(32)</td>
<td>0.0251(209)</td>
<td>0.0314(303)</td>
<td>0.0314(303)</td>
<td>0.025</td>
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<tr>
<td>(x^3_u)</td>
<td>0.022(11)</td>
<td>0.037(36)</td>
<td>0.0500(247)</td>
<td>0.0685(392)</td>
<td>0.0685(392)</td>
<td>0.032</td>
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<tr>
<td>(x^3_d)</td>
<td>−0.001(7)</td>
<td>0.009(18)</td>
<td>0.00472(1179)</td>
<td>−0.00989(1529)</td>
<td>−0.00989(1529)</td>
<td>0.008</td>
<td></td>
</tr>
<tr>
<td>(\Delta u)</td>
<td>0.830(70)</td>
<td>0.889(29)</td>
<td>0.816(20)</td>
<td>0.888(80)</td>
<td>0.719(48)</td>
<td>0.860(69)</td>
<td>0.918</td>
</tr>
<tr>
<td>(\Delta d)</td>
<td>−0.244(22)</td>
<td>−0.236(27)</td>
<td>−0.237(9)</td>
<td>−0.241(58)</td>
<td>−0.179(31)</td>
<td>−0.171(43)</td>
<td>−0.339</td>
</tr>
<tr>
<td>(\Delta u - \Delta d)</td>
<td>1.074(90)</td>
<td>1.14(3)</td>
<td>1.053(27)</td>
<td>1.129(98)</td>
<td>0.898(57)</td>
<td>1.031(81)</td>
<td>1.257</td>
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<tr>
<td>(x \Delta u)</td>
<td>0.198(8)</td>
<td>0.215(25)</td>
<td>0.215(25)</td>
<td>0.243(17)</td>
<td>0.242(22)</td>
<td>0.150</td>
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<tr>
<td>(x \Delta d)</td>
<td>−0.048(3)</td>
<td>−0.054(16)</td>
<td>−0.054(16)</td>
<td>−0.0347(86)</td>
<td>−0.0290(129)</td>
<td>−0.055</td>
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<tr>
<td>(x^2 \Delta u)</td>
<td>0.087(14)</td>
<td>0.027(60)</td>
<td>0.027(60)</td>
<td>0.113(34)</td>
<td>0.116(42)</td>
<td>0.050</td>
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<tr>
<td>(x^2 \Delta d)</td>
<td>−0.025(6)</td>
<td>−0.003(25)</td>
<td>−0.003(25)</td>
<td>−0.00515(936)</td>
<td>−0.00142(2515)</td>
<td>0.016</td>
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<tr>
<td>(\delta u)</td>
<td>0.93(3)</td>
<td>0.980(30)</td>
<td>1.01(8)</td>
<td>0.898(46)</td>
<td>0.963(59)</td>
<td>−0.0202(36)</td>
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<tr>
<td>(\delta d)</td>
<td>−0.20(2)</td>
<td>−0.234(17)</td>
<td>−0.20(5)</td>
<td>−0.213(29)</td>
<td>−0.228(81)</td>
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</tr>
<tr>
<td>(d_2^u)</td>
<td>−0.206(18)</td>
<td>−0.233(86)</td>
<td>−0.233(86)</td>
<td>−0.224(60)</td>
<td>−0.228(81)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(d_2^d)</td>
<td>−0.035(6)</td>
<td>0.040(31)</td>
<td>0.040(31)</td>
<td>0.0658(222)</td>
<td>0.0765(310)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Summary

- Moments of structure functions in full QCD
  \[ \beta = 5.6, \ a_n = 0.085 \ \text{fm} \quad \beta = 5.5, \ a_n = 0.115 \ \text{fm} \]
- Close agreement between full QCD and quenched connected diagrams
- Principal Puzzles
  \[ xu - xd \sim 0.24-0.28 \ (0.18) \]
  \[ \Delta u - \Delta d \sim 1.0-1.1 \ (1.26) \]
- General agreement between full QCD and cooled at small \( m_q \)
  instanton and zero-mode dominance

Future

- Disconnected diagrams (exploiting zero-mode dominance)
- Gluon matrix elements
- Chiral fermions
- Finite volume corrections
Physics on prototype clusters (cont.)

Lessons from calculating moments of structure functions

Pion cloud essential for nucleon structure: $\mu, g_A$

$\Rightarrow$ large volume

light quark mass

Large statistics for $p_x, p_y, p_z, p_t \neq 0$

Disconnected diagrams

Gluon operators

Terascale machine essential
Phase I Clusters

One component of coherent national plan by Lattice QCD Executive Committee for 2000–2001
Proposal submitted to DOE, March 1999
ftp://www-ctp.mit.edu/pub/negele/LatProp/

Hardware

256-processor cluster at JLab $\geq 384$ Gflops

65 4-way SMP nodes

$\geq 750$ MHz Alpha 21264

4 MB cache/processor

1 GB memory/SMP

Myrinet

64 port switch

64 interconnect cards (64 bit, 66 MHz, $\geq 140$ MB/s)

4 Alpha servers

Ethernet switch

64-processor cluster at MIT (32 new + 32 current) $\geq 90$ Gflops

Combined with prototype clusters,

$> 1/2$ Tflops peak, $1/6$ Tflops sustained
Phase I Clusters (cont.)

Performance estimates for 256-processor cluster

Example:

\[24^3 \times 48\] lattice divided between 256 processors

⇒ 1.3 MB/node: fits in cache

Assume 10 µs latency

Assume half of peak on node (667 MHz)

Obtain half of peak at 200 MB/s bidirectional bandwidth

Achievable with current generation Myrinet
Phase I Clusters (cont.)

Lattice QCD Metacenter

Major clusters at JLab and MIT

Highly integrated environment for ongoing joint leadership of scientific and computational effort

Follows successful Brookhaven/Columbia model

Facilitates strong coupling with vendors
Phase I Clusters (cont.)

Cost Estimates

Cost of JLab Cluster

<table>
<thead>
<tr>
<th>Item</th>
<th>Unit Cost ($K)</th>
<th>Quantity</th>
<th>Cost ($K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-way SMP, 4-MB caches, 1024 MB, 10-GB disk</td>
<td>18</td>
<td>65</td>
<td>1170</td>
</tr>
<tr>
<td>64-port switch (with 64 addt’l backside ports)</td>
<td>32</td>
<td>1</td>
<td>32</td>
</tr>
<tr>
<td>PCI cluster interconnect cards</td>
<td>0.8</td>
<td>65</td>
<td>52</td>
</tr>
<tr>
<td>Workstation/file server w/100 GB</td>
<td>12</td>
<td>4</td>
<td>48</td>
</tr>
<tr>
<td>Ethernet switch (64<em>100, 8</em>1000)</td>
<td>20</td>
<td>1</td>
<td>20</td>
</tr>
<tr>
<td>Racks</td>
<td>1.2</td>
<td>12</td>
<td>14</td>
</tr>
<tr>
<td><strong>Subtotal</strong></td>
<td></td>
<td></td>
<td><strong>1336</strong></td>
</tr>
<tr>
<td>Overhead on hardware (26% on 1st $50K of each P.O.)</td>
<td>35</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Total cluster hardware</strong></td>
<td></td>
<td></td>
<td><strong>1371</strong></td>
</tr>
</tbody>
</table>

Cost of MIT Cluster

<table>
<thead>
<tr>
<th>Item</th>
<th>Unit Cost ($K)</th>
<th>Quantity</th>
<th>Cost ($K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-way SMP, 4-MB caches, 1024 MB, 10-GB disk</td>
<td>18</td>
<td>8</td>
<td>144</td>
</tr>
<tr>
<td>PCI cluster interconnect cards</td>
<td>0.8</td>
<td>8</td>
<td>6</td>
</tr>
<tr>
<td>Myricom switch (16 port)</td>
<td>4</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>Racks</td>
<td>1.2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td><strong>Total hardware</strong></td>
<td></td>
<td></td>
<td><strong>157</strong></td>
</tr>
</tbody>
</table>

Total cost of hardware and 1 year manpower

<table>
<thead>
<tr>
<th>Item</th>
<th>Cost ($K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hardware (JLab main cluster)</td>
<td>1371</td>
</tr>
<tr>
<td>less JLab contributions</td>
<td>(86)</td>
</tr>
<tr>
<td>Hardware (MIT cluster)</td>
<td>157</td>
</tr>
<tr>
<td>JLab sys admin (1st yr, 1 FTE w/fringes + overhead)</td>
<td>102</td>
</tr>
<tr>
<td>MIT sys admin (1st yr, 1/4 FTE w/fringes + overhead)</td>
<td>40</td>
</tr>
<tr>
<td><strong>Subtotal, cluster hardware and operations</strong></td>
<td>1584</td>
</tr>
<tr>
<td>Cluster dev. manpower (1st yr w/ fringes + overhead)</td>
<td></td>
</tr>
<tr>
<td>JLab sys programmer, cluster software</td>
<td>130</td>
</tr>
<tr>
<td>MIT sys programmer, node performance, and application optimization</td>
<td>150</td>
</tr>
<tr>
<td><strong>Subtotal, software development</strong></td>
<td>280</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>1864</td>
</tr>
</tbody>
</table>
Phase I Clusters (cont.)

Project Administration

Jefferson Lab and MIT

Develop, procure, construct, and operate clusters
Host regular collaboration meetings

Lattice Hadron Physics Collaboration

Open to individual theorists who are:

Interested in solving lattice QCD to understand hadron structure

Willing to collaborate in coherently sharing computational resources

Collaborators commit to one or more core projects

Hadron structure
Hadron-hadron interactions
Spectroscopy
Lattice field theory

Collaborators determine the research projects and resource allocations
Phase I Clusters (cont.)

First-year physics projects planned by LHPC

1) Calculation of the strange quark contribution to the nucleon’s electromagnetic form factors

2) Precision calculation of nucleon form factors

3) Calculation of moments of nucleon parton distributions

4) Calculation of leading light-cone quark-distribution amplitudes of the nucleon

5) Calculation of the spectrum of lowest lying $N^*$ resonances

6) Calculation of the Born-Oppenheimer potential between heavy-light hadrons

7) Studies of chiral phase transitions of staggered fermions at finite chemical potential using the meron cluster algorithm

8) Exploratory calculations with chiral fermions, using either the domain-wall or overlap algorithm
# Phase I Clusters (cont.)

## Computational tasks for first year

<table>
<thead>
<tr>
<th>Physics project</th>
<th>Computation</th>
<th>Lattice</th>
<th>No. of $\beta$ values</th>
<th>No. of cases</th>
<th>GFyr for inversions</th>
<th>GFyr total</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Disconnected 3-pt. functions</td>
<td>$16^3 \times 32$</td>
<td>3</td>
<td>1</td>
<td>0.70</td>
<td>2.1</td>
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<tr>
<td>1</td>
<td>Disconnected 3-pt. functions</td>
<td>$16^3 \times 32$</td>
<td>3</td>
<td>1</td>
<td>0.58</td>
<td>1.7</td>
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<tr>
<td>1</td>
<td>Disconnected 3-pt. functions</td>
<td>$24^3 \times 48$</td>
<td>1</td>
<td>1</td>
<td>2.9</td>
<td>2.9</td>
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<tr>
<td>1</td>
<td>Eigenfunction calculations for preceding lattices</td>
<td></td>
<td></td>
<td>19</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2,3,4</td>
<td>2-pt. &amp; 3-pt. functions</td>
<td>$24^3 \times 48$</td>
<td>3</td>
<td>10</td>
<td>0.27</td>
<td>8.1</td>
</tr>
<tr>
<td>2,3,4</td>
<td>2 pt. &amp; 3-pt. functions</td>
<td>$32^3 \times 64$</td>
<td>1</td>
<td>10</td>
<td>2.10</td>
<td>21.0</td>
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<tr>
<td>5</td>
<td>2-pt. functions</td>
<td>$24^3 \times 48$</td>
<td>3</td>
<td>4</td>
<td>0.53</td>
<td>6.4</td>
</tr>
<tr>
<td>5</td>
<td>2-pt. functions</td>
<td>$32^3 \times 64$</td>
<td>1</td>
<td>4</td>
<td>4.19</td>
<td>16.8</td>
</tr>
<tr>
<td>6</td>
<td>All-to-all propagators</td>
<td>$24^3 \times 48$</td>
<td>3</td>
<td>1</td>
<td>2.65</td>
<td>8.0</td>
</tr>
<tr>
<td>6</td>
<td>All-to-all propagators</td>
<td>$32^3 \times 64$</td>
<td>1</td>
<td>1</td>
<td>21.0</td>
<td>21.0</td>
</tr>
<tr>
<td>7</td>
<td>Cluster algorithm calculations</td>
<td></td>
<td></td>
<td></td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Chiral-fermion exploratory studies</td>
<td></td>
<td></td>
<td></td>
<td>25</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10% Contingency</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>15</td>
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<td><strong>Total</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td><strong>150</strong></td>
</tr>
</tbody>
</table>
Phase I Clusters (cont.)

Phase I provides excellent opportunity for rapid funding

  Submitted in March 2000

  Reviewed

  Collaboration is ready to proceed

  Urgently needed for physics goals

  Commodity clusters need to be explored immediately
to be a viable option

  SDAC will be strengthened by accomplishments sooner
rather than later
Phase II Clusters

Coherent national plan by Lattice QCD Executive Committee for 2002–2005 calls for multi-Teraflops resources from a combination of QCDOC and Clusters.

We are using our collaboration with Compaq to explore the commodity cluster opportunities in this timeframe.

**Alpha 21364 (EV7)**

- Computer on a chip well suited to QCD
- Alpha 21264 core at 1250 MHz
- Integrated 1.75 MB L2 cache
- Integrated memory controller – RAMbus at 6 GB/s
- Integrated network interface
  
  - NEWS $4 \times 2 \times 3.2$ GB/s
  - I/O interface 3 GB/s

**Alpha 21464 (EV8)**

- 8-wide superscalar – 4 floats/clock
21364 Chip Block Diagram

- 16 L1 Miss Buffers
- 64K Icache
- 21264 Core
- 64K Dcache
- 16 L1 Victim Buf
- L2 Cache
- Memory Controller
- Network Interface
- 16 L2 Victim Buf
Integrated L2 Cache

- 1.75 MB
- 7-way set associative
- 20 GB/s total read/write bandwidth
- 16 Victim buffers for L1 -> L2
- 16 Victim buffers for L2 -> Memory
- ECC SECDED code
- 9.6ns load to use latency
Integrated Memory Controller

- Direct RAMbus
  - High data capacity per pin
  - 800 Mb/s operation
  - 30ns CAS latency pin to pin
- 6 GB/sec read or write bandwidth
- 2048 open pages
- Directory based cache coherence
- ECC SECDED
Integrated Network Interface

- Direct processor-to-processor interconnect
- 4 links 2x3.2 GB/second per processor
- 18ns processor-to-processor latency
- ECC, single error correct, double error detect, per hop
- Out-of-order network with adaptive routing
- Asynchronous clocking between processors
- 3 GB/second I/O interface per processor
21364 System Interface

- Glue-less multiprocessor via directory coherence
- High-speed interconnect, 800 Mb/s
EV8 Overview

- Enhanced out-of-order execution
- 8-wide super-scalar
- New instruction fetcher and branch predictor
- On-chip L2 cache, > 3MB
- RAMBUS interface
- Sustained memory bandwidth -- 16 GB/sec
- SIMD Integer Operations
- 4-way simultaneous multi-threading (SMT)
EV8 Functional Units

- Fadd
- Fmul
- Fdiv
- Fsqrt
- Iadd
- Ilog
- Ishft
- br

- Load
- Store
- ladd
- Ilog
- Imul
- br

- Load
- Store
- ladd
- Ilog
- Imul
- br

- Load
- ladd
- Ilog
- Imm
- br

- Load
- ladd
- Ilog
- Imm
- br
System Block Diagram

EV8

M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
M
IO
Phase II Clusters (cont.)

Performance and cost estimates

Basic unit – 128 processor SMP with 2-d torus

Assume 1.25 GHz, 50% peak

1028 processors  8 nodes  1.28 Tflops sustained
4096 processors  32 nodes  5.12 Tflops sustained

Examples:

$32^3 \times 64$ lattice on 2048 processors

$8^2 \times 4^2$ per site – fits in 1.75 MB L2 cache

Requires < 1% NEWS bandwidth for CG

Requires < 32 current Myrinet interfaces/SMP

Conclusion: Ample memory and communications bandwidth

Rough cost, performance estimates

Assume $\sim$ $2K$/processor

50% peak performance

18 300 MB/s links/box

<table>
<thead>
<tr>
<th>Processor</th>
<th>EV7 Speed (GHz)</th>
<th>EV7 # Processors</th>
<th>EV7 Lattice</th>
<th>EV7 Cost, $M</th>
<th>EV7 Ttfflops sustained</th>
<th>EV7 $ / MF</th>
</tr>
</thead>
<tbody>
<tr>
<td>EV7</td>
<td>1.25</td>
<td>1024</td>
<td>$16^3 \times 24$</td>
<td>2.5</td>
<td>1.2</td>
<td>2.1</td>
</tr>
<tr>
<td>EV7</td>
<td>1.25</td>
<td>4096</td>
<td>$24^3 \times 32$</td>
<td>9.9</td>
<td>4.5</td>
<td>2.2</td>
</tr>
<tr>
<td>EV7</td>
<td>1.6</td>
<td>4096</td>
<td>$32^3 \times 48$</td>
<td>9.9</td>
<td>6.2</td>
<td>1.6</td>
</tr>
<tr>
<td>EV7</td>
<td>1.6</td>
<td>4096</td>
<td>$32^3 \times 48$</td>
<td>9.9</td>
<td>12.4</td>
<td>0.8</td>
</tr>
<tr>
<td>EV8</td>
<td>1.6</td>
<td>4096</td>
<td>$32^3 \times 48$</td>
<td>9.9</td>
<td>12.4</td>
<td>0.8</td>
</tr>
</tbody>
</table>
Principles for Consensus Report

• Support coherent national plan by Lattice QCD Executive Committee
  
  Exploration of two approaches: Clusters and QCDOC
  
  Multi-Teraflops resources comparable to Japan, Europe
  
  Ramp up – double capacity yearly for five years

• Strong science motivation for several physics-focused facilities
  
  Three national thrusts
  
  Weak Matrix Elements   Fermilab
  QCD Thermodynamics     BNL/Columbia
  Hadron Structure       JLab/MIT
  
  Collaborations can optimize resources for common physics
  
  No technical disadvantages in $3 \times 5$ Tflops instead of 15 Tflops
  
  Machines already run that way
  
  Different BC, parameters

• Keep technology choices for 2002–2005 open as long as possible

• Cost/performance-optimized commodity clusters
  
  Well suited to science
  
  Cost effective
  
  Ramp up continuously instead of five-year steps
  
  Need to be explored immediately to be viable option