

Computational Infrastructure for Lattice Gauge Theory

A Strategic Plan

Scientific Objectives

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Scientific Objectives

- **Understand the physical phenomena encompassed by quantum chromo-dynamics (QCD)**
- **Make precision calculations of the predictions of QCD**

Lattice QCD is an integral part of research in high energy and nuclear physics, and is closely coupled to the DOE's experimental program in these fields.

Close Coupling with the Experimental Program

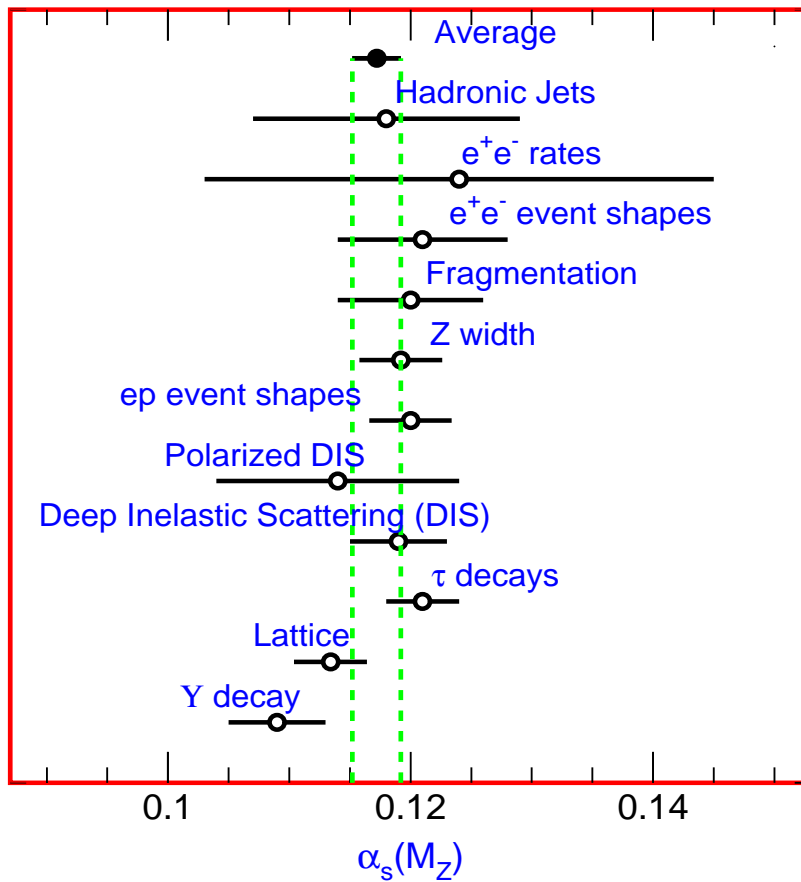
- **Weak Decays of Strongly Interacting Particles**
 - **BaBar (SLAC)**
 - **Tevatron B-Meson Program (FNAL)**
 - **CLEO-c Program (Cornell–Proposed)**

- **Quark–Gluon Plasma**
 - **RHIC (BNL)**

- **Structure and Interactions of Hadrons**
 - **Bates BNL FNAL JLab SLAC**

Some Lattice QCD Achievements

- **Qualitative features of QCD**
 - **Quark confinement**
 - **Chiral symmetry breaking**
 - **Quark–gluon plasma**
- **Examples of quantitative results**
 - **Temperature of the chiral symmetry restoration phase transition**
 - **Accurate determination of the light hadron spectrum (quenched)**
 - **Determination of $\alpha_s(M_Z)$ and masses of the c and b quarks to a few percent.**
 - **Determination of B and D meson decay constants, and $\bar{B}B$ and $\bar{K}K$ mixing matrix elements to a precision of about 10–20%.**



Summary of the determinations of $\alpha_s(M_Z)$ from the Particle Data Group.

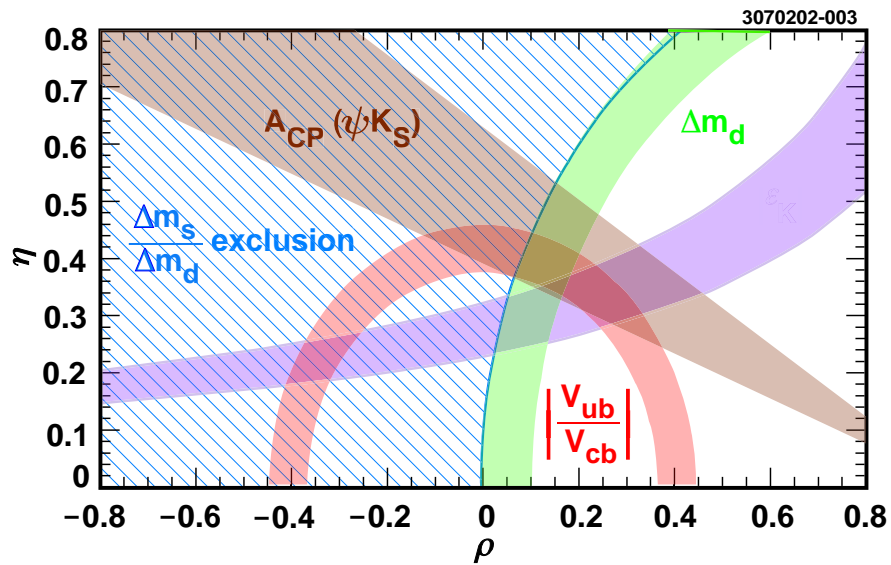
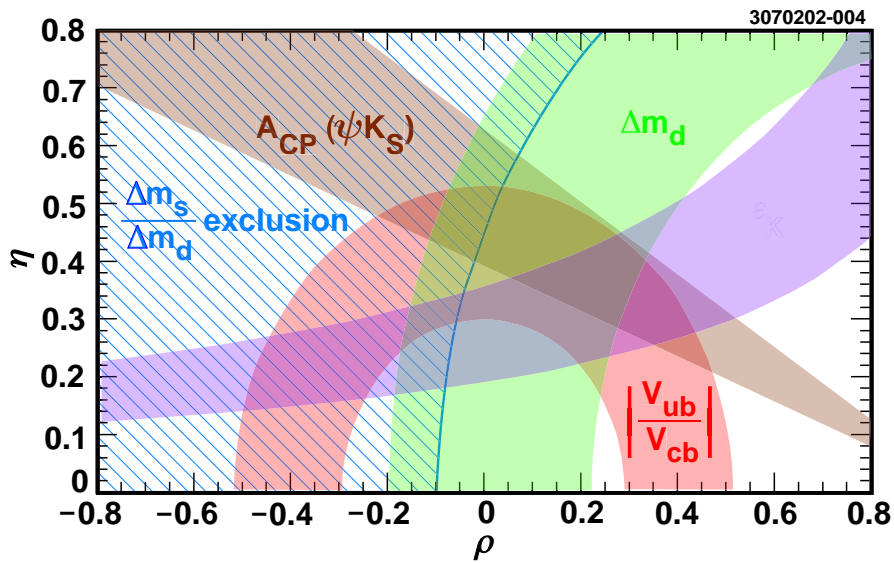
Precision Tests of the Standard Model

- Lattice calculations of weak matrix elements are needed to relate experimental results to underlying parameters of the Standard Model.
- Multiple measurements of the same Standard Model parameters in different experiments and calculations will lead to crucial consistency tests.
- In many cases the greatest challenge is to reduce the uncertainties in the lattice calculations.

Impact of Lattice QCD on CKM Matrix Elements

Measurement	CKM Matrix Element	Hadronic Matrix Element	Expt. Error	Current Lattice Error	Lattice Error 0.5 TF-Yr	Lattice Error 10 TF-Yr
ΔM_{B_d} ($\bar{B}B$ mixing)	$ V_{td} ^2$	$f_{B_d}^2 B_{B_d}$	4%	35%	18%	9%
$\Delta M_{B_s}/\Delta M_{B_d}$	$ V_{ts}/V_{td} ^2$	$f_{B_s}^2 B_{B_s}/f_{B_d}^2 B_{B_d}$	Not yet measured	10%	5%	3%
ε ($\bar{K}K$ mixing)	$\text{Im} V_{td}^2$	B_K	2%	20%	10%	5%
$B \rightarrow (\rho/\pi) l \nu$	$ V_{ub} ^2$	$\langle \rho/\pi (V-A)_\mu B \rangle$	25%	Calc. in progress	15%	5–10%

In the table above, f_X is the leptonic decay amplitude for the indicated meson, and B_X is proportional to the matrix element of $\Delta S = 2$ or $\Delta B = 2$ four-quark operators. The last two columns show the improvements in lattice errors that we estimate would be obtained with computers sustaining 0.5 and 10 Tflops for one year.



Constraints on the Standard Model parameters ρ and η (one sigma confidence level). For the Standard Model to be correct, they must be restricted to the region of overlap of the solidly colored bands. The figure on the top shows the constraints as they exist today. The figure on the bottom shows the constraints as they would exist with no improvement in the experimental errors, but with lattice gauge theory uncertainties reduced to 3%. R. Patterson, Cornell University.

The Quark Gluon Plasma

- At high temperatures and/or baryon densities one expects a phase transition or crossover from the state of strongly interacting matter to a plasma of quarks and gluons.
- Lattice QCD simulations are required to calculate properties of strongly interacting matter in the vicinity of the transition.

Phase Diagram

Transition Temperature

Order of the Transition

Equation of State

Role of Instantons

Structure and Interactions of Hadrons

- **Hadron mass spectrum**
- **Electromagnetic Form Factors**
- **Quark and Gluon Distribution Functions**
- **Origin of Nucleon-Nucleon Interaction**

Hardware Plans

- Simplifying features of lattice QCD calculations make building specially designed computers far more cost effective than buying commercial ones.
 - Uniform grids
 - Regular, predictable communications
- Two hardware tracks:
 - QCD On a Chip (QCDOC)
 - Commodity Clusters
- Each track has its own strengths.
- Each track may prove optimal for different aspects of our work.
- The two track approach positions us to exploit future technological advances, and enables us to retain flexibility.

QCDOC

- The latest of the highly successful Columbia/Riken/BNL special purpose computers.
 - The Columbia group has pioneered the design and construction of special purpose computers for QCD.
 - The QC DSP won the Gordon Bell Prize in 1998 for price performance.
- The QCDOC combines processor, networking and memory on a single chip.
- Partnership with IBM provides access to its technology for chip design and fabrication.
- Targets a price–performance of \$1/Mflops for multi-teraflops machines as early as 2003.

Commodity Clusters

- **Market forces are producing rapid gains in processor and memory performance**
 - **Moore's Law \Rightarrow 60% growth in performance per year**
 - **Pentium 4 currently provides exceptional performance for QCD**
- **Market for interconnects is growing**
- **Open Source System Software**
 - **Flexible programming environment**
 - **SciDAC Scalable Systems Software**
- **Targeted price–performance**

	FY 2003	FY 2004	FY 2005	FY 2006
\$/Mflops	2.0	1.2	0.9	0.7

SciDAC Software Infrastructure Project

- **Create a programming environment that will enable very high performance on the QCDOC and clusters**

- **Principal Components**
 - **QCD Application Programming Interface**
 - **Highly optimized linear algebra routines**
 - **Highly optimized communications**
 - **Optimization of computationally intensive subroutines**
 - **Porting and optimization of major community codes**

Deployment Plan

- **QCDOC**

- **FY 2003: 1.5 Tflops (Columbia)**
- **FY 2003–4: 5.0 Tflops (BNL)**

- **Clusters**

- **FY 2002–03: 0.5 Tflops (FNAL, JLab)**
- **FY 2004: 1.0 Tflops (FNAL, JLab)**
- **FY 2005: 6.0 Tflops (FNAL, JLab)**
- **FY 2006: 8.0 Tflops (FNAL, JLab)**

Funding Profile

Year	SciDAC	QCDOC	Clusters	Total	Tflops
2003	\$2.0M	\$2.5M		\$4.5M	2
2004		\$5.4M	\$2.3M	\$7.7M	8
2005		\$1.0M	\$8.0M	\$9.0M	14
2006		\$1.0M	\$8.4M	\$9.4M	22

Collaboration and Management Structure

- **Our collaboration includes nearly all senior lattice gauge theorists in the U.S.**
 - **Sixty–four senior scientists**
 - **Lattice gauge theorists, computer scientists, computer engineers**

- **Management Structure**

Executive Committee

Richard Brower	Boston U.
Norman Christ	Columbia U.
Michael Creutz	BNL
Paul Mackenzie	FNAL
John Negele	MIT
Claudio Rebbi	Boston U.
Stephen Sharpe	U. of Washington
Robert Sugar (Chair)	UC Santa Barbara
Chip Watson	JLab

Scientific Program Committee

Peter Lepage	Cornell U.
Robert Mahwinney	Columbia U.
Colin Morningstar	Carnegie Mellon U.
John Negele	MIT
Claudio Rebbi (Chair)	Boston U.
Stephen Sharpe	U. of Washington
Doug Toussaint	U. of Arizona
Frank Wilczek	MIT

Oversight Committee

Steven Gottlieb (Chair)	Indiana U.
Anna Hasenfratz	U. of Colorado
Gregory Kilcup	Ohio State U.
Julius Kuti	UC San Diego
Robert Pennington	NCSA
Ralph Roskies	Director, PSC
Terry Schalk	UC Santa Cruz

Software Co-ordinating Committee

Richard Brower (Chair)	Boston U.
Carleton DeTar	U. of Utah
Robert Edwards	JLab
Donald Holmgren	FNAL
Robert Mawhinney	Columbia U.
Celso Mendes	U. of Illinois
Chip Watson	JLab

Conclusions

- **Lattice QCD is an integral part of research in high energy and nuclear physics, and is closely coupled to the DOE's experimental program in these fields.**
- **We need to act now to deploy the infrastructure required for terascale simulations of QCD.**
 - **Major experiments which require terascale simulations for their interpretation have recently been completed, or will be completed within the next several years.**
 - **Theorists in Europe and Japan are moving rapidly to secure resources comparable to those we propose.**

Lattice gauge theory was invented in the U.S., and U.S. theorists have traditionally been leaders of this field. If U.S. lattice gauge theorists are to play a significant role in the major advances expected in this area over the next five years, we must act now.