Lattice QCD: current status and future perspectives

C. Rebbi

Physics Department

and

Center for Computational Science

Boston University

Cornell University, February 27, 2008

A brief overview of lattice QCD

QCD: quark fields $\psi_{c,s,f}(x)$ and gluon fields $A_{\mu,i}(x)$

$A_\mu(x) = \sum_i A_{\mu,i}\lambda^i, \qquad \bar\psi(x)e^{\imath g\int_x^y A_\mu(x)\,dx^\mu}\psi(y)$

Wilson 1974: discretize the theory on a space-time Euclidean lattice and use as fundamental gauge variables the finite group elements

$U_\mu(x) = e^{\imath g\int_x^{x+\hat\mu a} A_\mu(x)\,dx^\mu}$ where a is the lattice spacing.

Quantum mechanical expectation values: $\langle \mathcal{O} \rangle = Z^{-1} \times$

$$\int \prod_{x,\mu} dU_\mu(x) \prod_x (d\bar{\psi}(x)\, d\psi(x)) \mathcal{O}(\psi, \bar{\psi}, U) e^{-S_g(U) - \bar{\psi} D(U) \psi}$$

$S_g(U)$ discretizes $\int d^4x \, \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$

$\bar{\psi} D(U) \psi$ discretizes $\int d^4x \, \bar{\psi}(x) [\sum_\mu \gamma_\mu (\partial_\mu + \imath g A_\mu) + m] \psi(x)$

Integrate over $\bar{\psi}, \psi$ explicitly: $\langle \mathcal{O} \rangle = Z^{-1} \times$

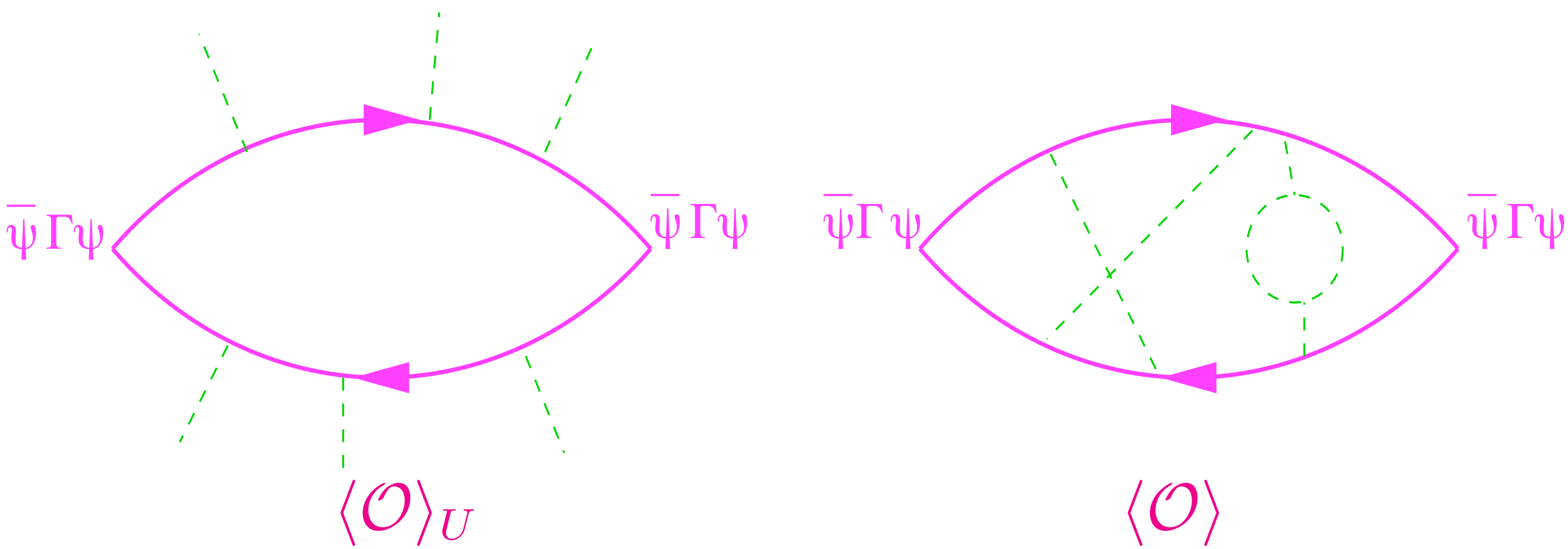
$$\int \prod_{x,\mu} dU_\mu(x) \langle \mathcal{O} \rangle_U e^{-S_g(U)} \mathrm{Det}[D(U)]$$

Approximate the integral over U by stochastic simulation.

From $\langle \mathcal{O} \rangle$ derive experimentally measurable quantities, e.g.

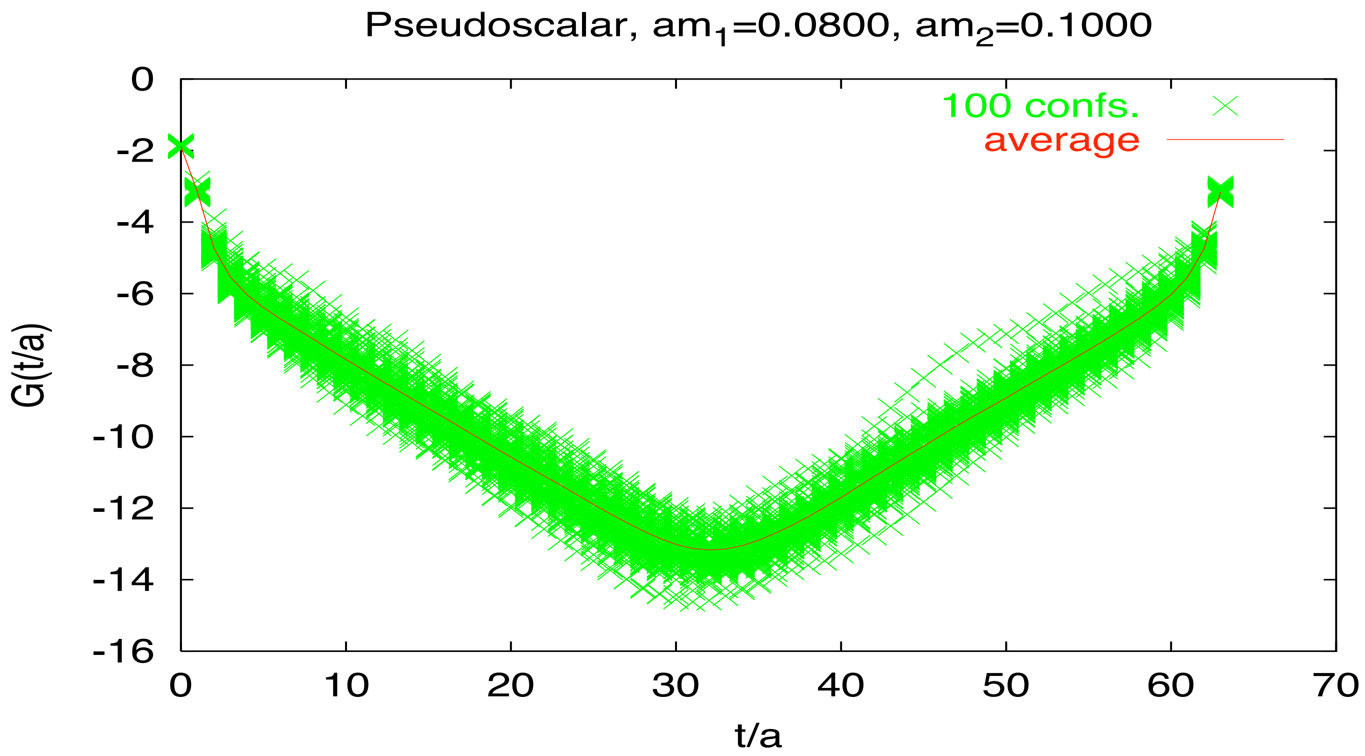
consider

$$\mathcal{O} = \bar{\psi}(0)\Gamma\psi(0)\sum_{\vec{x}}\bar{\psi}(\vec{x},t)\Gamma\psi(\vec{x},t)$$



$$\langle \mathcal{O} \rangle \equiv G(t) = \sum_n |\langle 0|\bar{\psi}\Gamma\psi|n,\vec{p}=0\rangle|^2 e^{-m_n t}$$

Example with $\Gamma = \gamma_5 \ \longrightarrow$ pseudoscalar spectrum:



(from a work with R. Babich, F. Berruto, N. Garron, Ch. Hoelbling, J. Howard, L. Lellouch, N. Shoresh)

Formidable calculations: a lattice of size $50^3 \times 100$ gives origin to a quark field with $50^3 \times 100 \times 12 = 150\mathrm{M}$ degrees of freedom and to a discretized Dirac operator given by a $150\mathrm{M} \times 150\mathrm{M}$ (sparse) matrix.

$\mathrm{Det}\, D(U)$ cannot be stochastically sampled (not directly), rather reformulate:

$$\int \prod dU \langle \mathcal{O} \rangle_U E^{-S_g(U)} \mathrm{Det}[D(U)] =$$
$$\int \prod dU \prod d\pi_U \prod d\phi e^{-S_G(U) - \pi_U^2 - \phi^* D(U)^{-1} \phi}$$

the whole set U, π_U, ϕ is then sampled by a stochastic simulation which uses a Hamiltonian evolution of U, π_U through group space as an intermediate step (hybrid Monte Carlo calculation); this requires multiple solutions of $D(U)\chi = \phi$.

Additional complication: a naive discretization of the Dirac equation

$$\sum_\mu \gamma_\mu(\partial_\mu + \imath g A_\mu) \rightarrow \sum_\mu \frac{U_\mu(x)\psi(x+\hat{\mu}a) - U_\mu^\dagger(x-\hat{\mu}a)\psi(x-\hat{\mu}a)}{2a}$$

introduces 15 extra fermion modes.

Solve by: - removing the extra modes with counterterms (Wilson fermions, breaks chiral invariance)

- splitting the fermion Dirac components through the lattice (staggered fermions, reduces the number of fermionic modes from 16 to 4, keeps one non-singlet $U(1)$ chiral symmetry)

- introducing a fifth dimension or equivalently trading the sparse Wilson Dirac matrix $D_W(U)$ for a much more challenging operator $D_O(U) = I + D_W(U)[D_W(U)^\dagger D_W(U)]^{-1/2}$ (domain wall or overlap fermions, no extra modes and chiral symmetry is preserved at the cost of much more demanding calculations.)

Forefront calculations in the U.S.

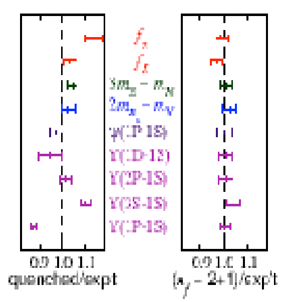
http://www.usqcd.org/

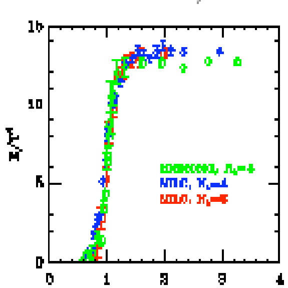
USQCD

US Lattice Quantum Chromodynamics

USQCD home | Physics program | Software | Hardware | USQCD Collaboration | Links and resources

Particle and Nuclear Physics





USQCD is a collaboration of US scientists developing and using large-scale computers for calculations in lattice quantum chromodynamics.

Lattice QCD calculations allow us to understand the results of particle and nuclear physics experiments in terms of QCD, the theory of quarks and gluons.

USQCD All Hands Meeting, April 4-5, 2008, JLab

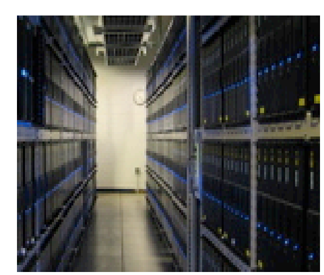
Call for proposals for USQCD resources, due Feb. 29, 2008

Lattice QCD Meets Experiment Workshop 2007, Dec. 10-11, Fermilab

SciDAC 2007 Lattice QCD Software Workshop

2007 White papers

Computing



With an effort that started in 1999 the U.S. lattice community, led by Bob Sugar and the USQCD Executive Committee (R. Brower, M. Creutz, N. Christ, P. Mackenzie, J. Negele, C. R., D. Richards, S. Sharpe), has organized itself in a national USQCD collaboration.

With DOE SciDAC support the collaboration has produced a suite of software tools which help writing code for efficient lattice QCD simulations, with DOE HEP and NP support it has deployed dedicated computers for LQCD calculations, and it has been able to secure large allocations of supercomputer time at the DOE facilities managed by DOE ASCR.

The dedicated resources are allocated by the collaboration's Scientific Program Committee and are used for large scale projects, which generate sets of gauge field configurations available to the whole collaboration, as well as for medium and small scale projects.

Examples of available or planned configurations by the MILC collaboration (with staggered fermions):

a(fm)	m_l/m_s	size	L(fm)
0.09	0.10	$40^3 \times 96$	3.6
0.09	0.05	$56^3 \times 96$	5.0
0.06	0.05	$84^3 \times 144$	5.0
0.06	$1/27$	$100^3 \times 144$	6.0
0.045	0.05	$112^3 \times 192$	5.0
0.045	$1/27$	$124^3 \times 192$	5.6

In 2007 the USQCD Executive Committee, with major contributions also from T. Applequist, C. Bernard, S. Catterall, C. DeTar, G. Fleming, J. Hetrick, F. Karsch, R. Mawhinney, C. Morningstar, R. Narayanan, H. Neuberger, K. Orginos, M. Savage, M. Schmaltz, M. Unsal and P. Vranas, has produced four White papers illustrating near term goals for lattice QCD calculations (see http://www.usqcd.org/collaboration.html#2007Whitepapers).
The following areas have been identified:

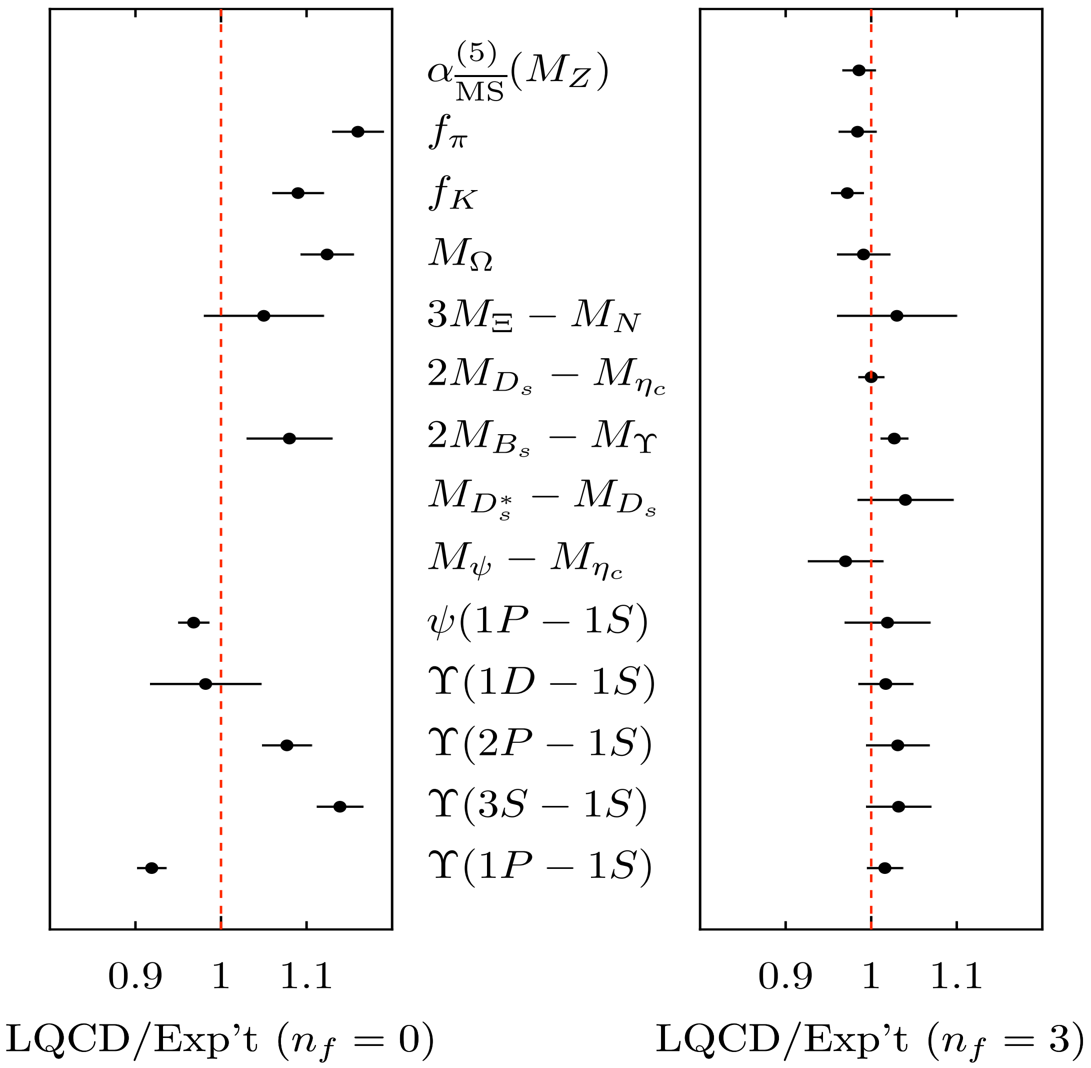
- Fundamental constants and hadronic matrix elements for electroweak interactions.

- QCD thermodynamics.

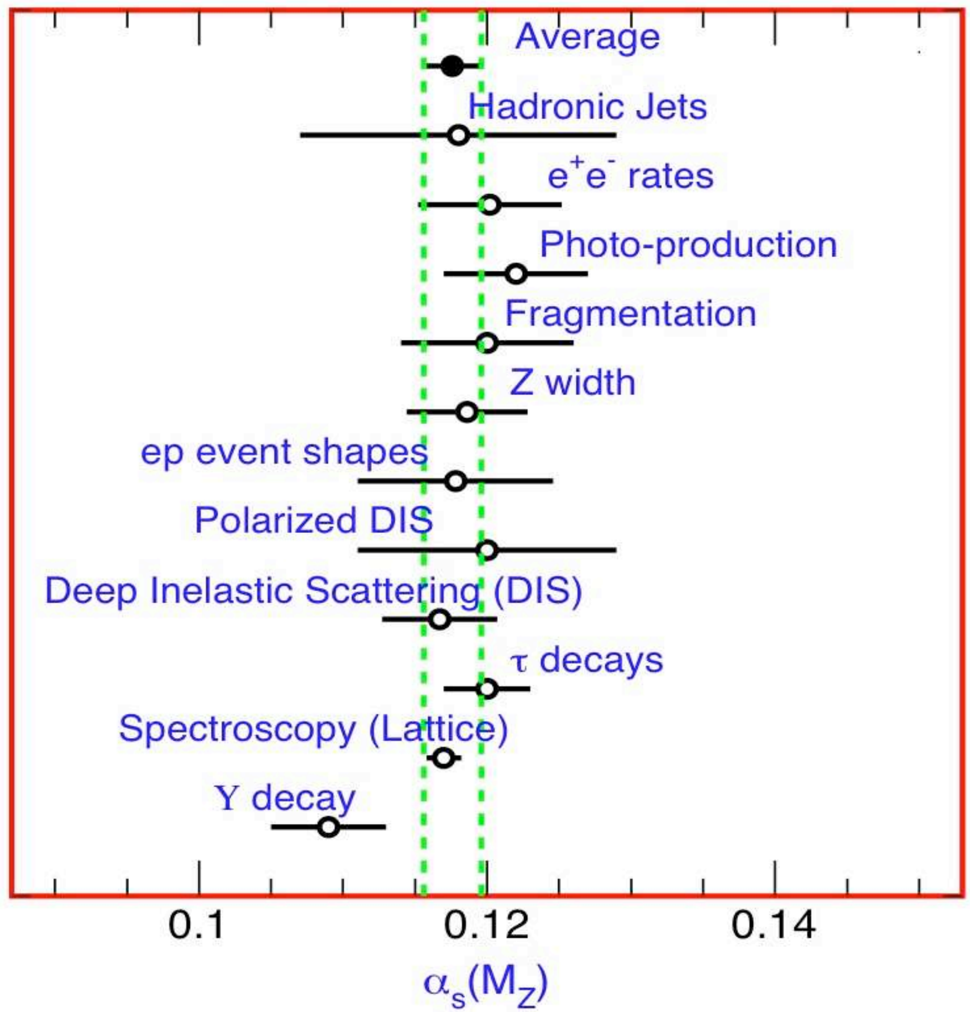
- Hadron spectrum, structure and interactions.

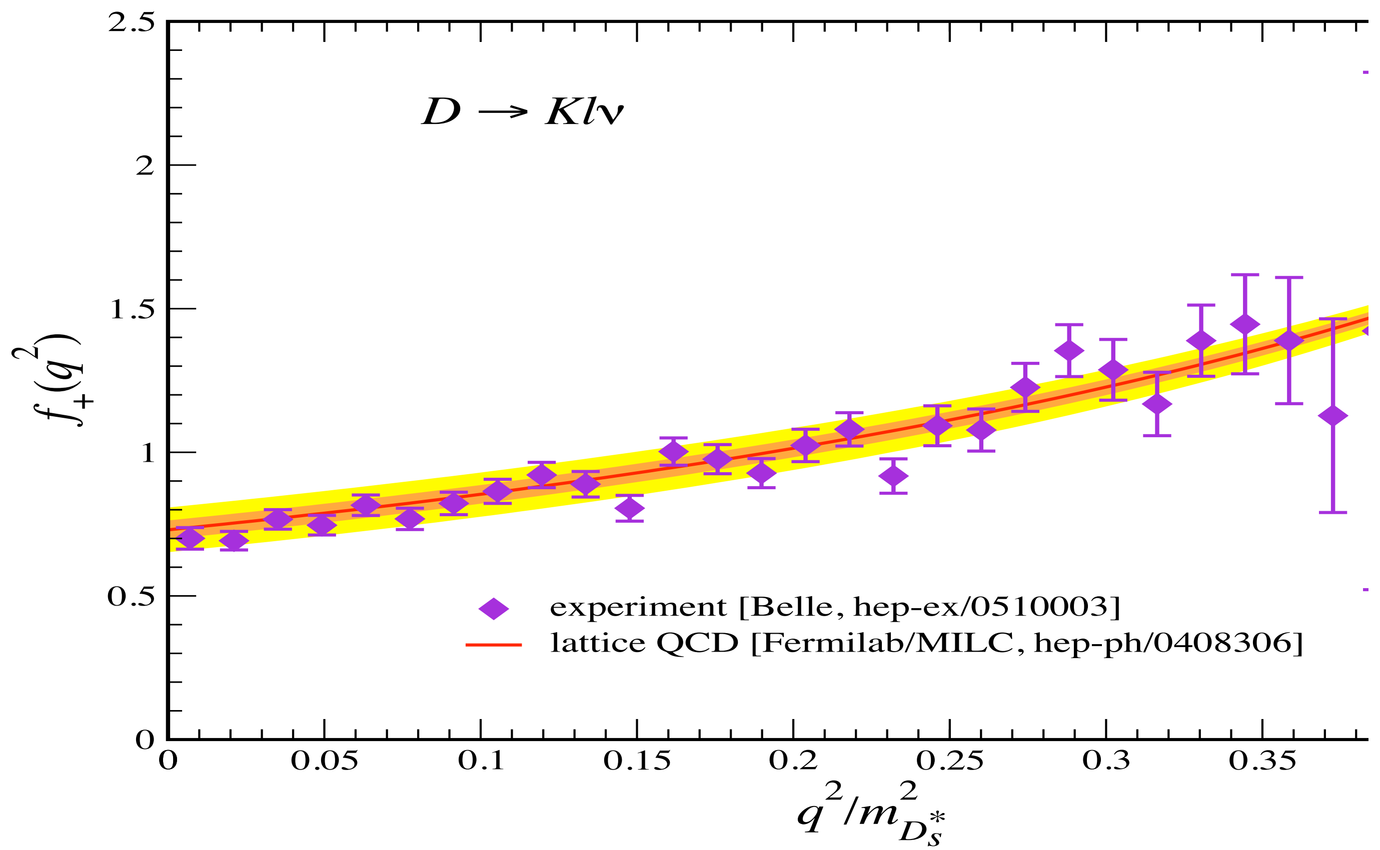
- Strong dynamics for physics beyond the standard model.

Illustrative results (data from the Fermilab Lattice, HPQCD and MILC collaborations, compilation due to P. Lepage):

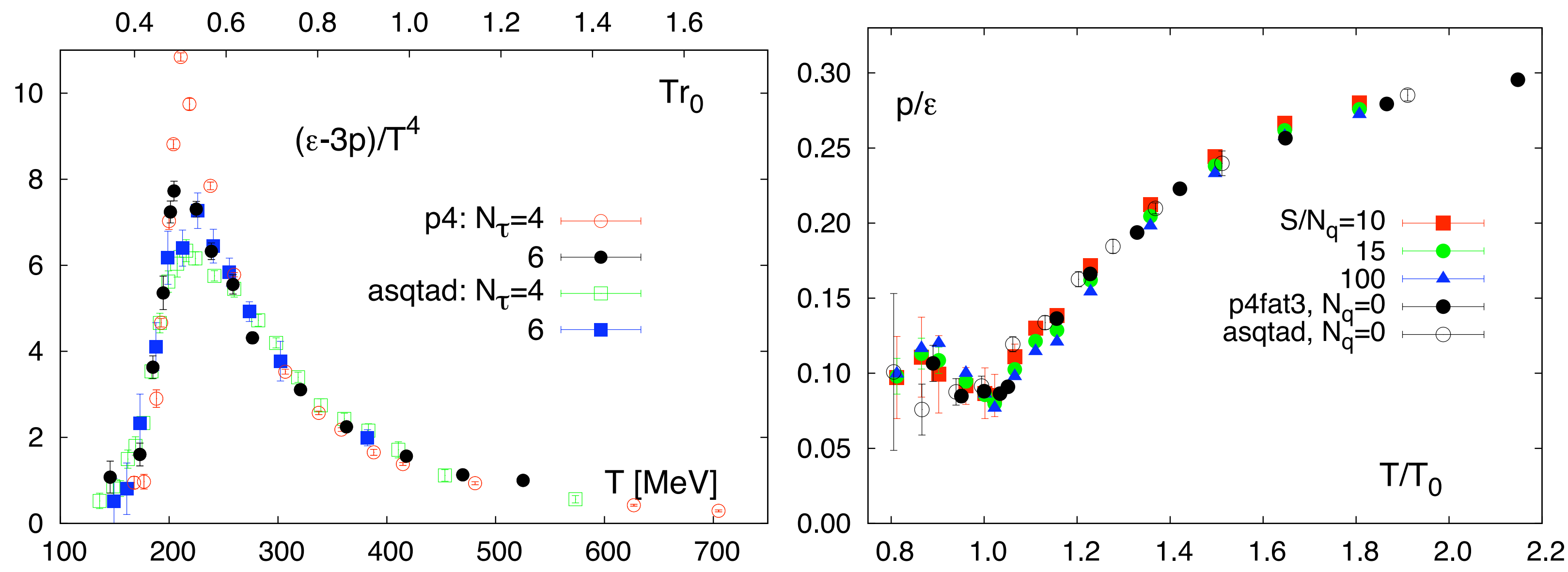


Determinations of α_s (α_L obtained by the HPQCD collaboration):





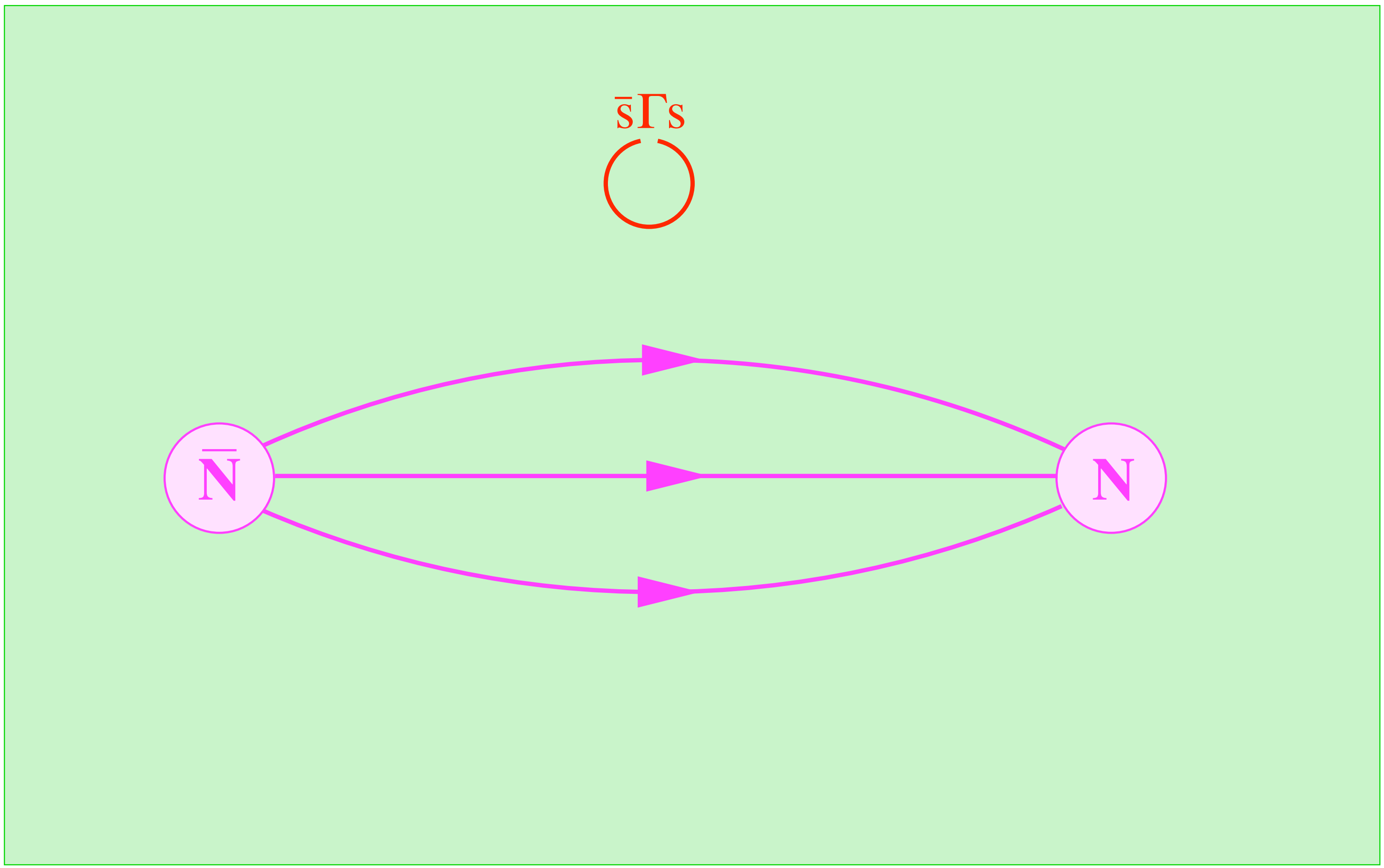
Form factor for semileptonic D decay, from the Fermilab/MILC collaboration.



Results for the QCD equation of state, from the MILC collaboration and Ejiri, Karsch, Laermann, and Schmidt.

Strange quark contribution to the nucleon form factors

Research in progress, in collaboration with R. Babich, R. Brower, M. Clark, G. Fleming, and J. Osborn



Partial results based on 386 gauge field configurations, with two flavors of dynamical quarks (Wilson discretization), on anisotropic $24^3 \times 64$ lattices ($a_s = 0.108(7)\mathrm{fm}, a_t = 0.036(2)\mathrm{fm}$), generated by the LHPC collaboration.

We must calculate $\langle N|\bar{\psi}_s \Gamma \psi_s|N\rangle =$
$\lim_{t\to\infty} \frac{\sum_{\vec{x},\vec{y}} e^{\imath(\vec{p}\cdot\vec{x}+\vec{q}\cdot\vec{y})} \langle \psi\psi\psi(\vec{x},t)\ \bar{\psi}_s\Gamma\psi_s(\vec{y},0)\ \bar{\psi}\bar{\psi}\bar{\psi}(\vec{0},-t)\rangle}{\sum_{\vec{x}}\langle \psi\psi\psi(\vec{x},t)\ \bar{\psi}\bar{\psi}\bar{\psi}(\vec{0},-t)\rangle} - \langle \bar{\psi}_s \Gamma \psi_s\rangle$

For each gauge field configuration we calculate separately the propagators $P_{cs,c's'}(U; x, y)$ which solve

$$[D(U)P(U)]_{cs}(x) = \delta(x, y)\delta_{c,c'}\delta_{s,s'}$$

for the light and strange quarks. We combine the light quark propagators into nucleon propagators (with implicit sums over color and spin indices)

$$\sum_{\vec{x}} e^{\imath\vec{p}\cdot\vec{x}} \epsilon_{c_1,c_2,c_3} \epsilon_{c'_1,c'_2,c'_3} \Psi^*_{s_1,s_2,s_3} \Psi_{s'_1,s'_2,s'_3} P_{c_1 s_1,c'_1 s'_1}(U; \vec{x}, t, \vec{0}, -t)$$
$$P_{c_2 s_2,c'_2 s'_2}(U; \vec{x}, t, \vec{0}, -t) P_{c_3 s_3,c'_3 s'_3}(U; \vec{x}, t, \vec{0}, -t)$$

and the strange quark propagators into

$$\sum_{\vec{y}} e^{\imath\vec{q}\cdot\vec{y}} \mathrm{Tr}[P(U; \vec{y}, 0, \vec{y}, 0)\Gamma]$$

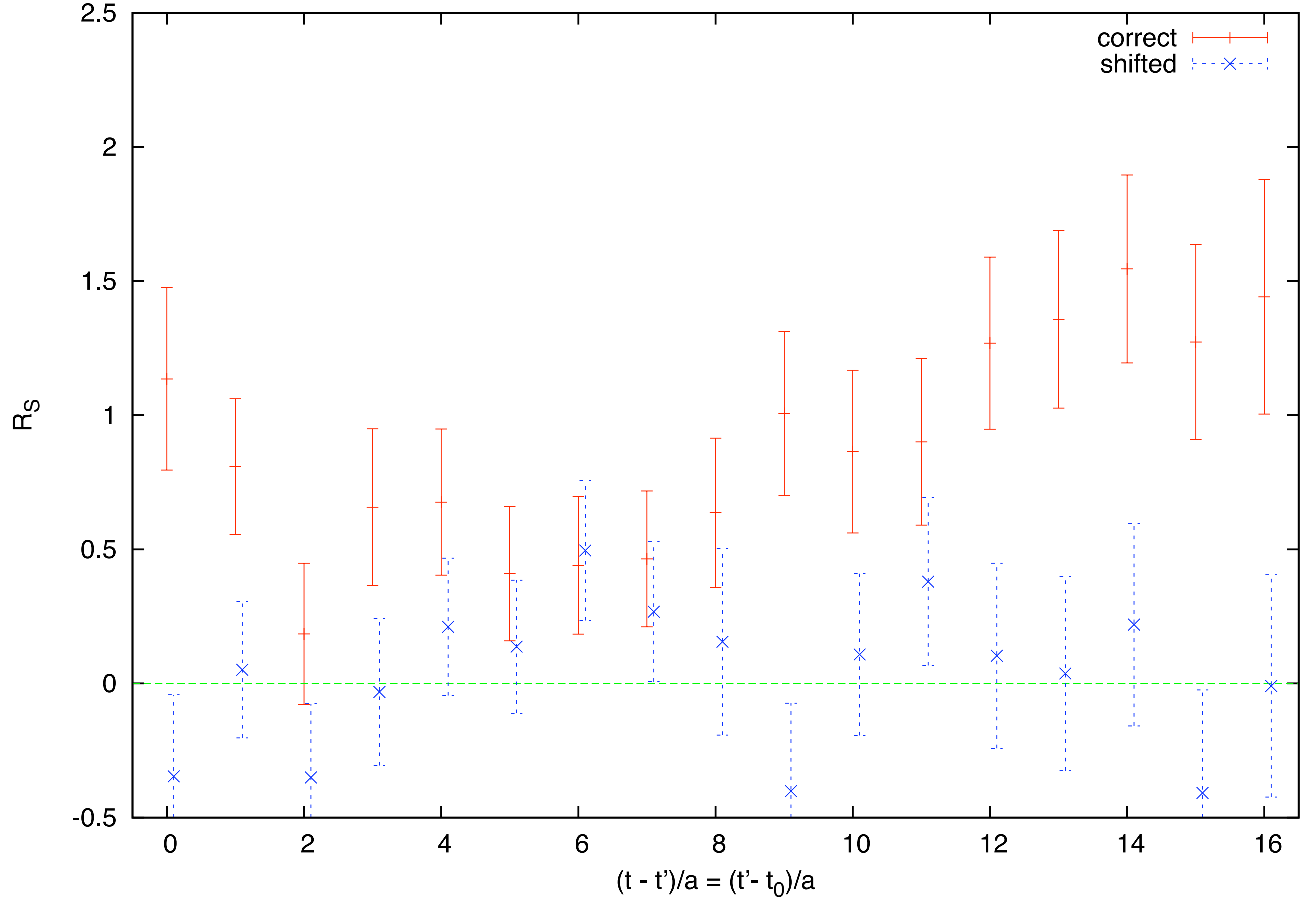
and average the product of the two over the gauge field configurations.

Note that this would require the calculation of $24^3 = 13,824$ strange quark propagators per configuration (prohibitive). Various techniques can be used to reduce the computational cost. We calculate the strange quark propagators with 64 sources staggered through the lattice, separated by $16a_t$ in time and $6\sqrt{3}a_s$ in space. We have verified that the non-diagonal contributions largely cancel because of the fall off of the propagators and gauge averaging. The number of propagators which we calculate per configuration is 864.

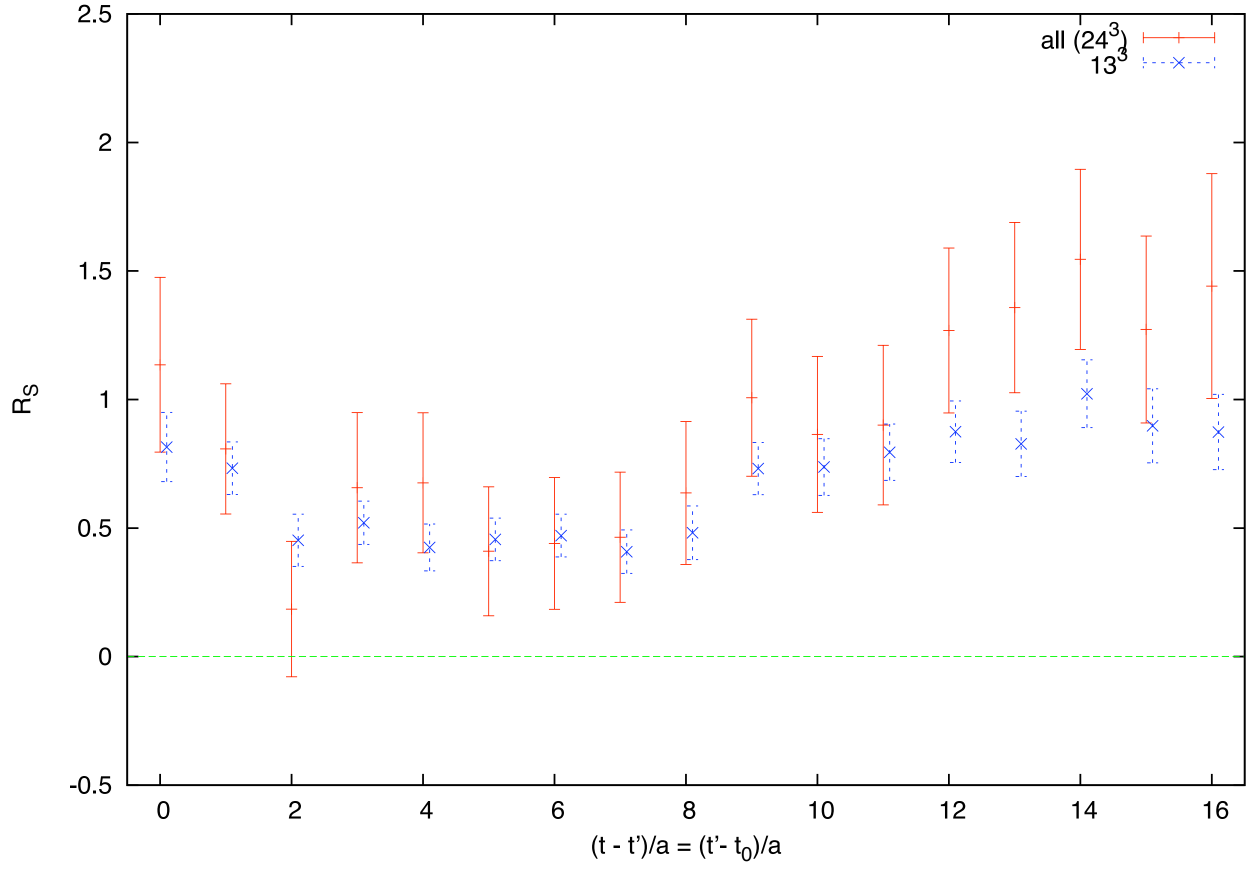
Other computational improvements are under study.

(Different computational approaches are followed by other groups, cfr. S.J. Dong, K.-F. Liu, and A. G. Williams, 1998, R. Lewis, W. Wilcox and R. M. Woloshyn, 2003.)

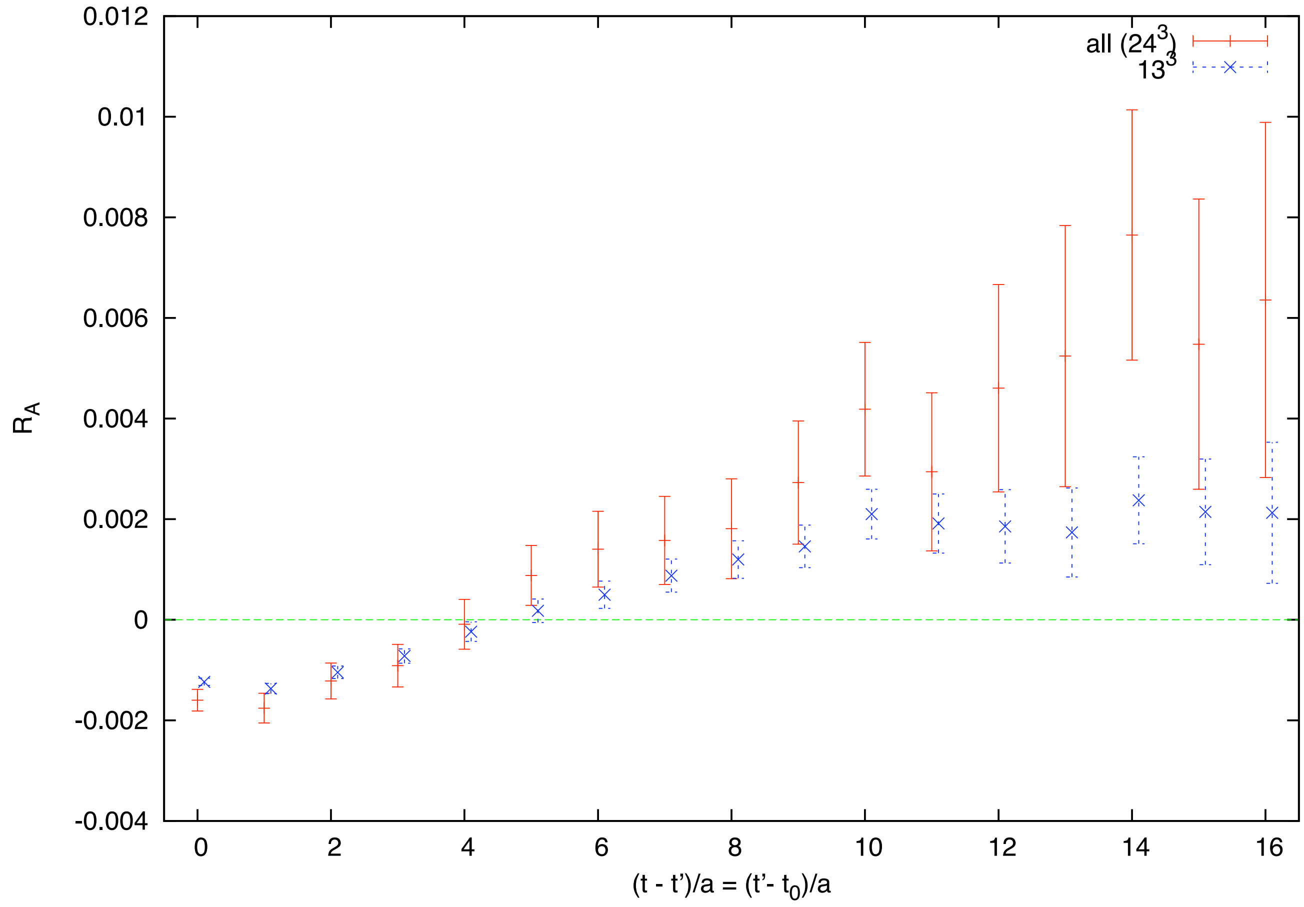
Current results for the zero-momentum scalar density $\sum_{\vec{x}} \bar{\psi}_s \psi_s(\vec{x}, 0)$, showing also the effect of decorrelating scalar density and nucleon propagators.



The contributions to $\bar{\psi}_s \psi_s$ from spatial points far away from the nucleon source add noise but very little signal. The error can be reduced by windowing (although this introduces some momentum contamination).



Current results for the zero-momentum axial-vector current $\sum_{\vec{x}} \bar{\psi}_s \gamma_5 \gamma_i \psi_s(\vec{x}, 0)$, showing also the effect of windowing.



Conclusions

- Lattice calculations provide very accurate results for a variety of QCD observables which cannot be otherwise evaluated.

- The calculation of many observables presents formidable computational challenges.

- With increasing computational power and progress in algorithms the accuracy and scope of lattice calculations continue to increase.