Lattice QCD from Mira or Probing Quarks at a Sustained Petaflops

Early Science Program Investigators Meeting
Argonne Leadership Computnig Facility
Argonne National Laboratory
May 17, 2013

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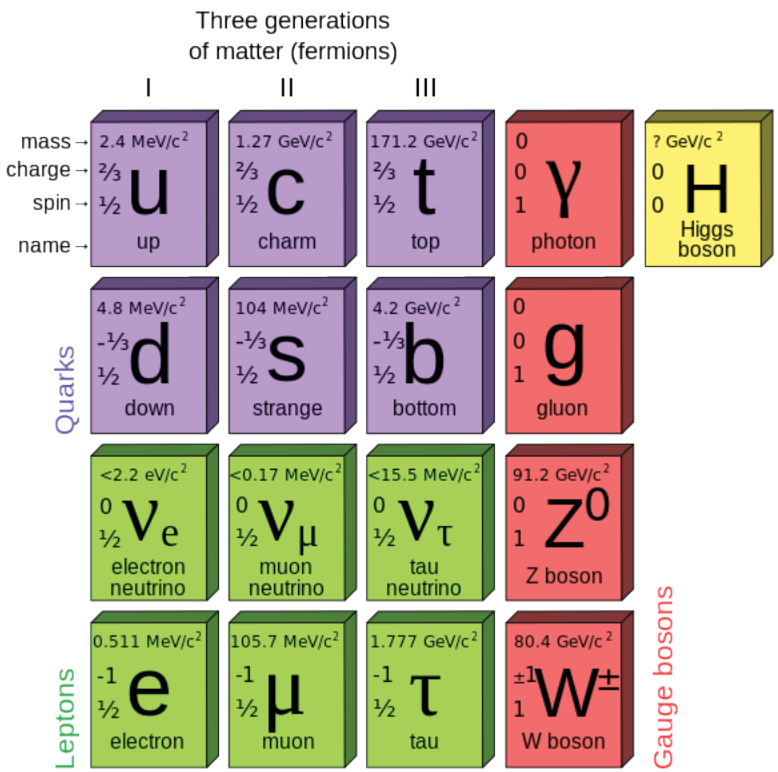
Columbia University
RBC Collaboration

USQCD is a collaboration including almost all of the US physicists working on lattice QCD and is composed of many smaller, generally long-standing, collaborations.

USQCD received an ESP allocation on Mira at the ALCF.

This allocation has been used by members of the MILC collaboration, the FNAL lattice group, the RBC collaboration and the HotQCD collaboration.

Known Elementary Particles



$$m_u = 2.19 \pm 0.15\,\text{MeV}$$

$$m_d = 4.67 \pm 0.20\,\text{MeV}$$

$$m_s = 94 \pm 3\,\text{MeV}$$

$$m_c = 1.275 \pm 0.025\,\text{GeV}$$

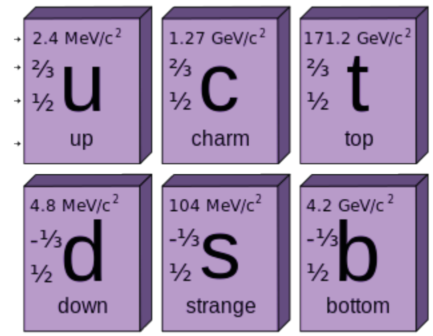
$$m_b = 4.18 \pm 0.03\,\text{GeV}$$

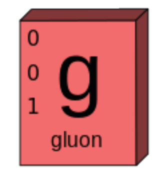
$$m_t = 173.5 \pm 0.6 \pm 0.8\,\text{GeV}$$

QCD

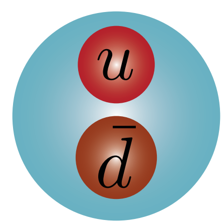
Theory of interactions of quarks

Interactions mediated by gluons

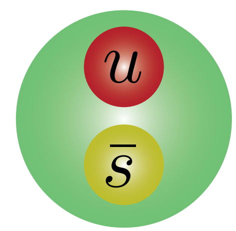




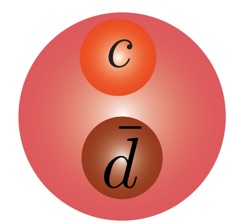
π^+



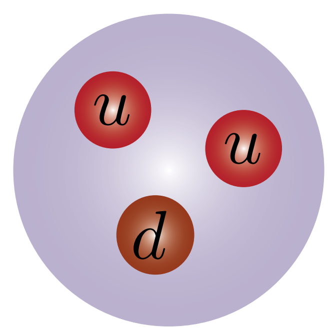
K^+



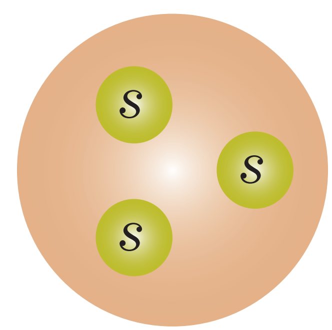
D^+ meson



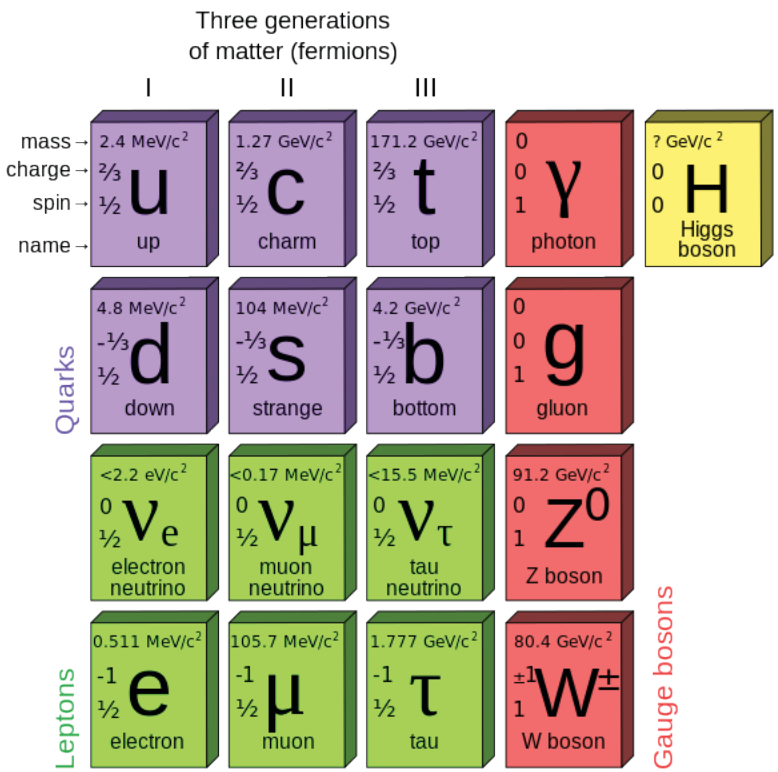
p^+



Ω^-



Known Elementary Particles

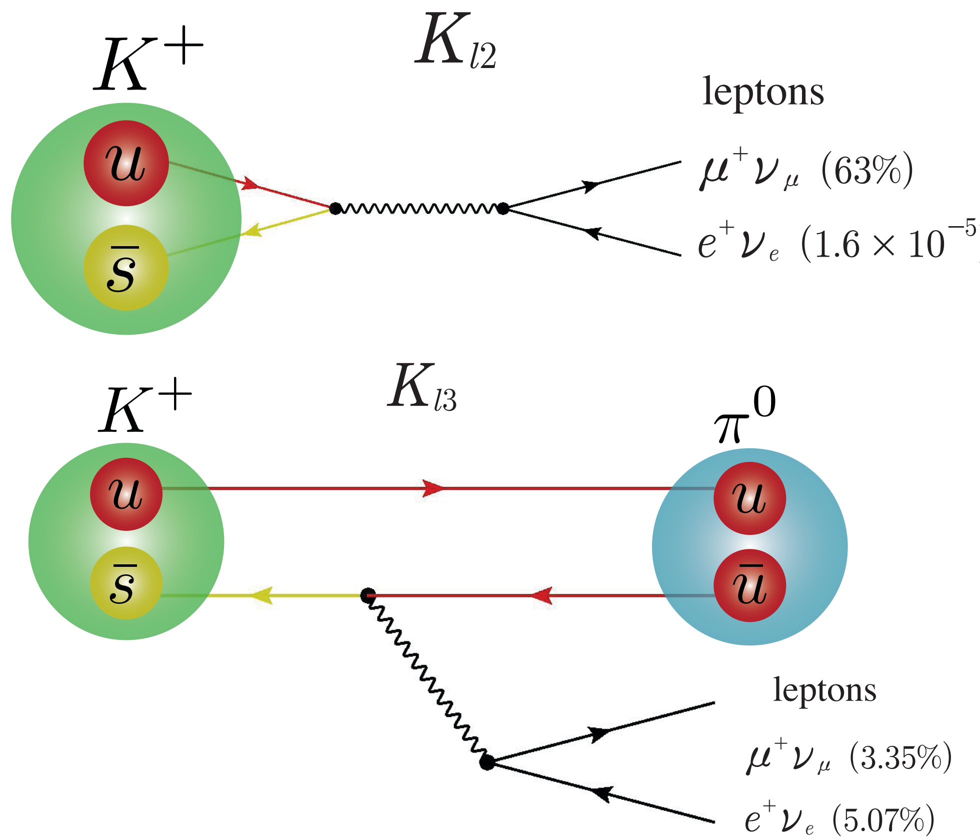


Standard Model quark decays involve elements of a 3 by 3 unitary matrix, the CKM matrix, described by 4 parameters

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

QCD + Electroweak

- Decays of quarks via weak interactions predicted by Standard Model.
- Experiments measure decays of hadrons

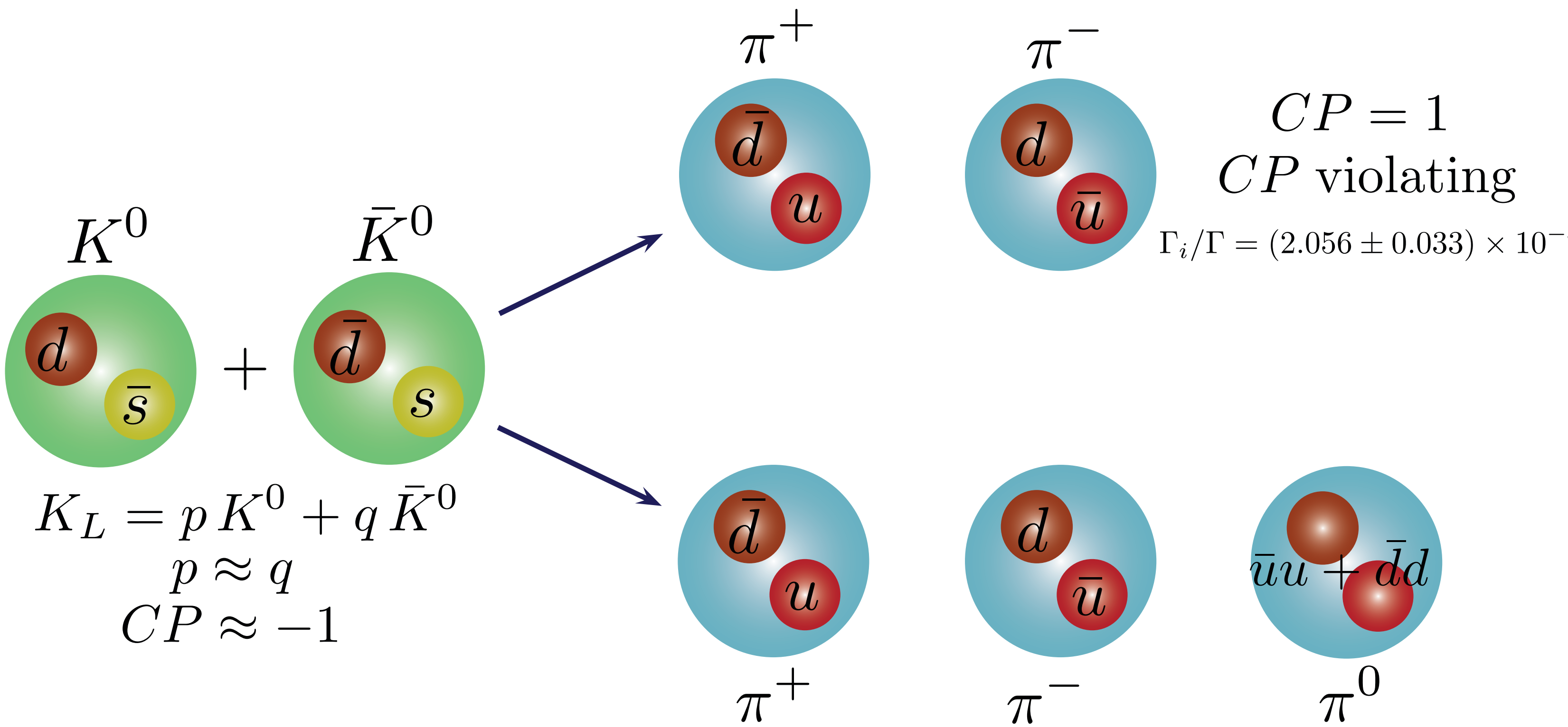


For K_{l3} we have: $\Gamma_{K\to\pi l\nu} = C_K^2 \frac{G_F^2 m_K^5}{192\pi^3} I\, S_{EW}[1 + 2\Delta_{SU(2)} + 2\Delta_{EM}]|V_{us}|^2|f_+(0)|^2$

Experiments observe kaon decays to pions which violate charge conjugation and parity symmetry (CP).

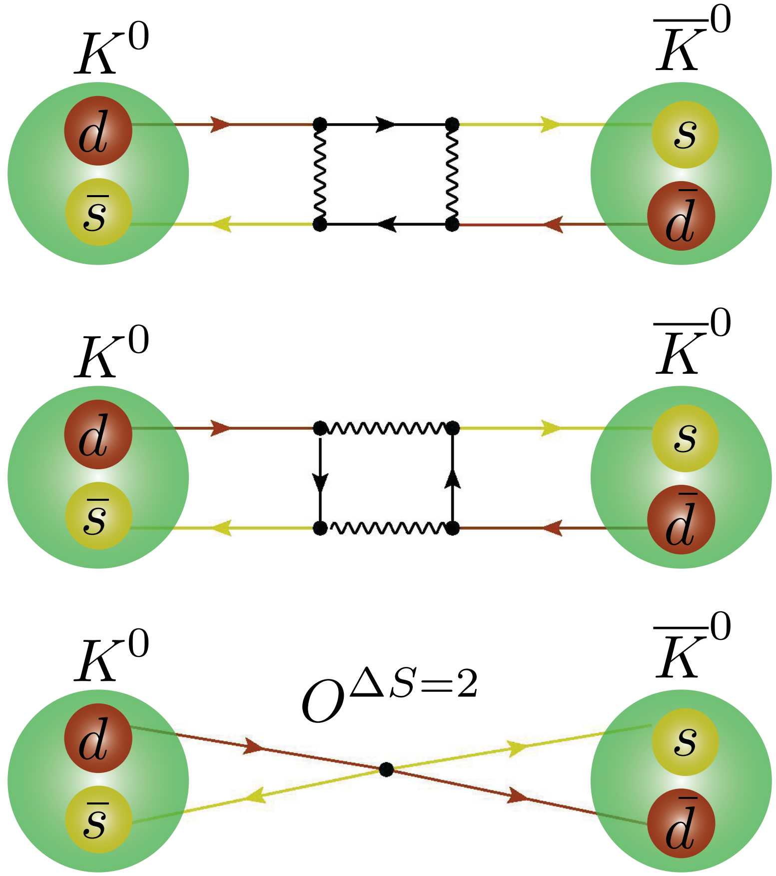
K_L is a mixture of K^0 and $\bar{K}^0$

$$K_L \longrightarrow \pi\pi$$



Direct CP Violation Measured in 1964
(Nobel Prize to Cronin and Fitch)

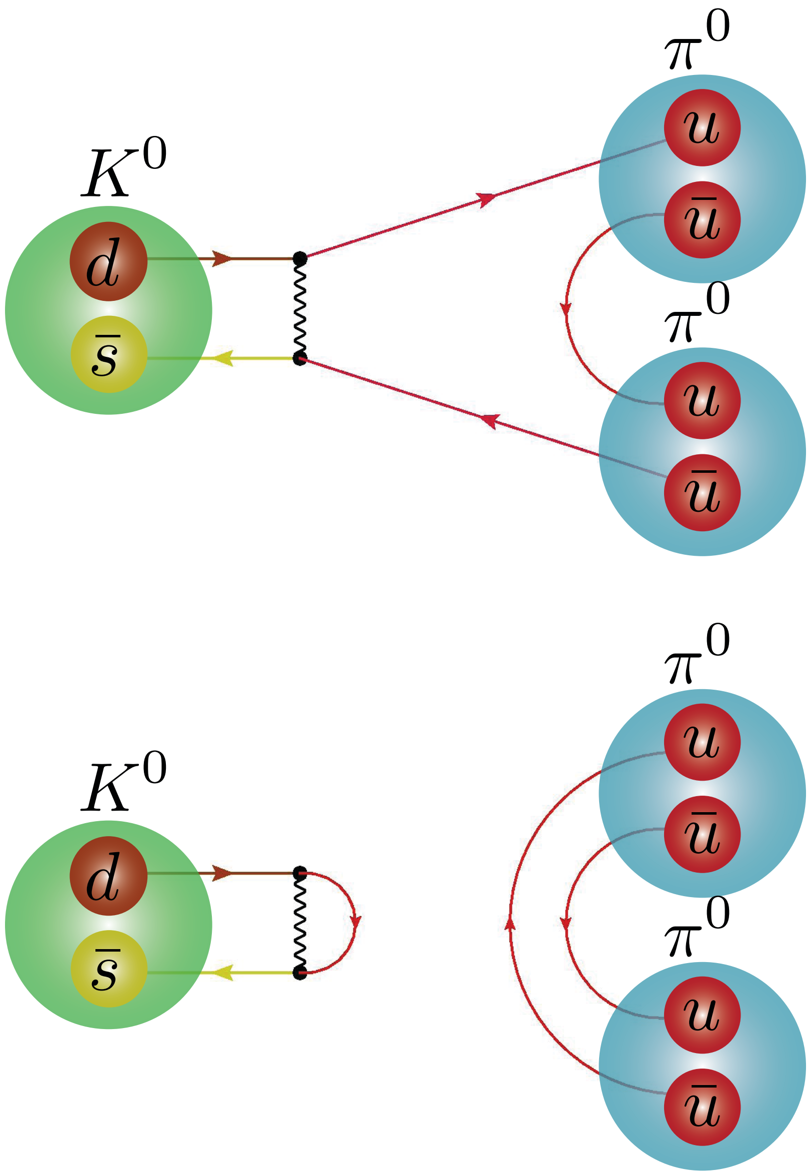
$$K^0 \leftrightarrow \overline{K}^0$$



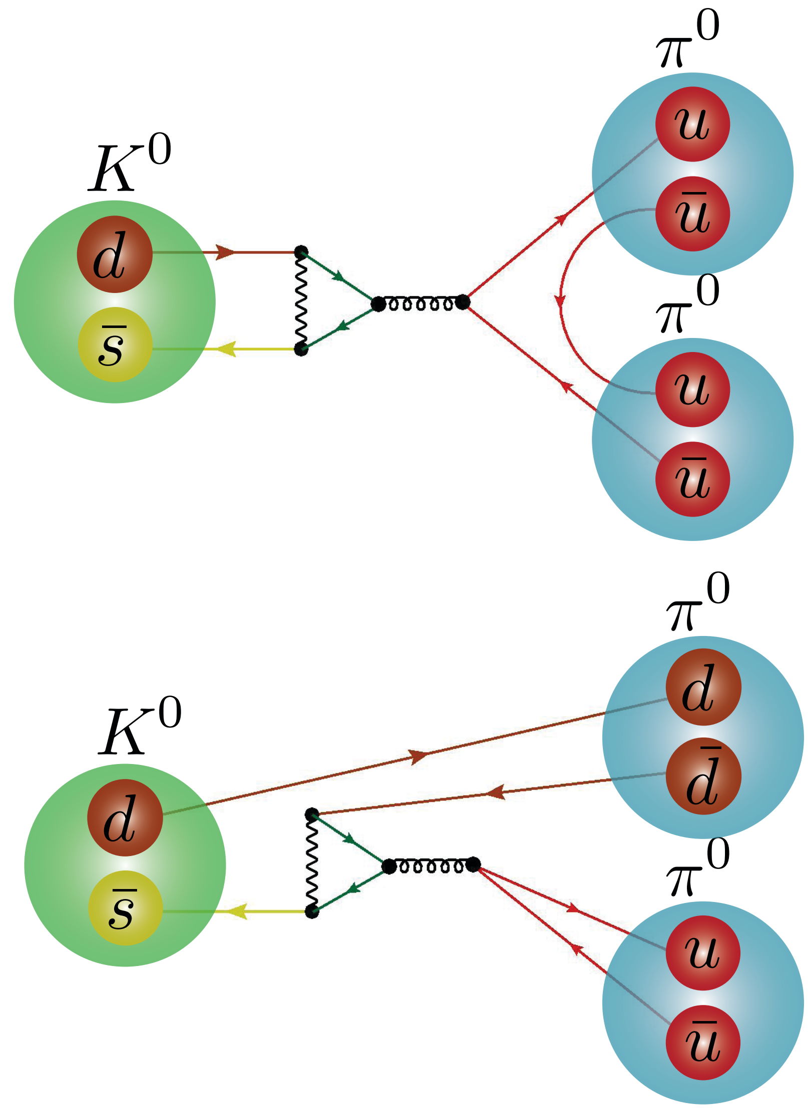
$$\varepsilon = \frac{e^{i\pi/4}}{\sqrt{2}\,\Delta M_K}\left(\mathrm{Im}(M_{12}) + 2\frac{\mathrm{Im}(A_0)}{\mathrm{Re}(A_0)}\mathrm{Re}(M_{12})\right) = \kappa_\varepsilon \frac{e^{i\phi_\varepsilon}}{\sqrt{2}}\left[\frac{\mathrm{Im}(M_{12}^{O^{\Delta S=2}})}{\Delta m_K}\right]$$

$$\varepsilon_K = \kappa_\varepsilon\, C_\varepsilon\, \hat{B}_K\, \mathrm{Im}(\lambda_t)\,\{\mathrm{Re}(\lambda_c)[\eta_1\, S_0(x_c) - \eta_3\, S_0(x_c,x_t)] - \mathrm{Re}(\lambda_t)\,\eta_2\, S_0(x_t)\}\, e^{i\pi/4}$$

Kaon Decays Via Exchange
CP Conserving



Kaon Decays Via "Penguin" Diagrams
Give Indirect CP violation

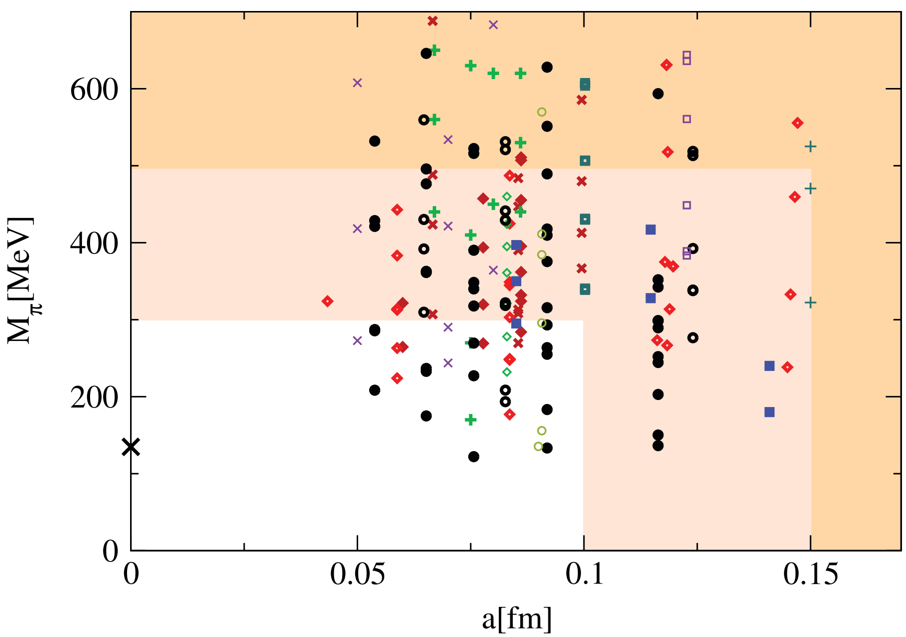


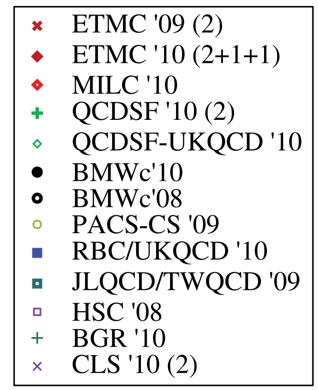
Parts of both the exchange and penguin mediated decays have recently been calculated by the RBC collaboration and improved calculations are running on Mira now

Generic Process	Examples	Experiment	LQCD calculates
$Kl2$	$K^+ \to \mu^+ \nu_\mu$ $K^+ \to e^+ \nu_e$	f_K	f_K (also f_π)
$Kl3$	$K^+ \to \pi^0 l^+ \nu_l$ $K^0 \to \pi^- l^+ \nu_l$	$\|V_{us} f^+(0)\|^2$	$f^+(0)$
$Kl4$	$K \to \pi \pi l \bar{\nu}_l$		??
$K \to \pi\pi$ (CP conserving)	$K^0 \to \pi^+ \pi^-$ $K^+ \to \pi^+ \pi^0$	$\|A_0\|$ $\|A_2\|$	$\|A_0\|$ $\|A_2\|$ (SM_{cpc} inputs)
Δm_K (CP conserving)	$K^0 \leftrightarrow \pi\pi \leftrightarrow \overline{K}^0$ (LD) $K^0 \leftrightarrow O_{\Delta S=2} \leftrightarrow \overline{K}^0$ (SD)	Δm_K	Δm_K (SM_{cpc} inputs)
$K^0 \to \pi \pi$ (indirect CP violation)	$K_L \to \pi\pi$ $\left(K^0 \leftrightarrow \overline{K}^0\right) \to \pi\pi$ independent of $\pi\pi$ isospin	$\epsilon = \frac{\hat{B}_K F_K^2 \, \mathrm{SM}}{\Delta m_K}$	$B_K, \frac{\mathrm{Im}(A_0)}{\mathrm{Re}(A_0)}$
$K^0 \to \pi \pi$ (direct CP violation)	$K_L \to \pi\pi$ depends on $\pi\pi$ isospin	$\mathrm{Re}(\epsilon'/\epsilon)$ $= f(A_0, A_2, \mathrm{SM})$	A_0 A_2 (SM_{cpc} inputs)
$K \to \pi ll$	$K_L \to \pi^0 l^+ l^-$ $K_S \to \pi^0 l^+ l^-$		??

SM_{cpc} = Standard Model CP-conserving parameters

Major Development: Ensembles with Physical Quark Masses

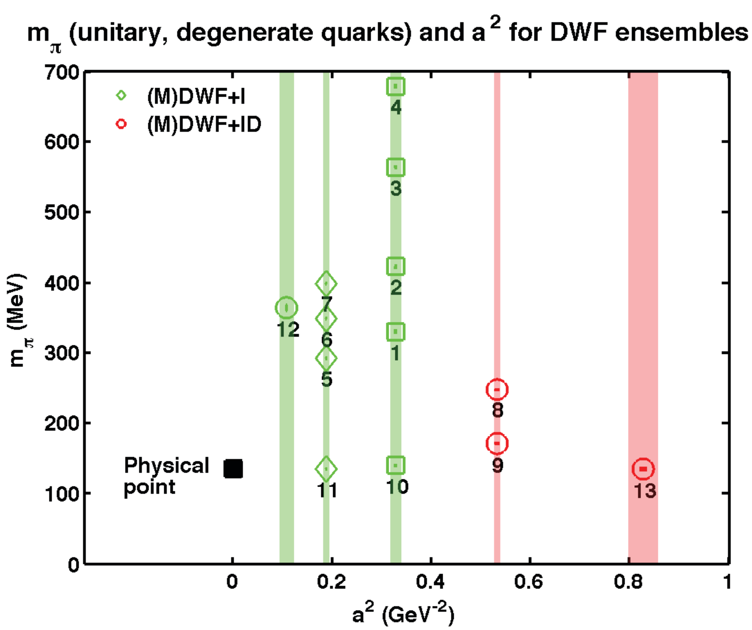




Fodor and Hoelbling,
Rev. Mod. Phys.
84 (2012) 449

$\approx a$ (fm)	m_l/m_s	$N_s^3 \times N_t$	$M_\pi L$	M_π (MeV)	N_{lats}
0.15	1/5	$16^3 \times 48$	3.78	306.9(5)	1021
0.15	1/10	$24^3 \times 48$	3.99	214.5(2)	1000
0.15	1/27	$32^3 \times 48$	3.30	131.0(1)	1020
0.12	1/5	$24^3 \times 64$	4.54	305.3(4)	1040
0.12	1/10	$24^3 \times 64$	3.22	218.1(4)	1020
0.12	1/10	$32^3 \times 64$	4.29	216.9(2)	1000
0.12	1/10	$40^3 \times 64$	5.36	217.0(2)	1029
0.12	1/27	$48^3 \times 64$	3.88	131.7(1)	1000
0.09	1/5	$32^3 \times 96$	4.50	312.7(6)	1011
0.09	1/10	$48^3 \times 96$	4.71	220.3(2)	1000
0.09	1/27	$64^3 \times 96$	3.66	128.2(1)	235 + 467
0.06	1/5	$48^3 \times 144$	4.51	319.3(5)	1000
0.06	1/10	$64^3 \times 144$	4.25	229.2(4)	435 + 227
0.06	1/27	$96^3 \times 192$	3.95	135.5(2)	240

2+1+1 flavors, HISQ Staggered,
MILC Phys. Rev. D87 (2013) 054505



2+1 flavors, (M)DWF
RBC and UKQCD Collaborations

Large Vol. Ensembles with Physical Quark Masses

- BMW Hex-smeared clover fermions
- MILC/FNAL HISQ Staggered fermions
- RBC/UKQCD DWF fermions

MILC/FNAL and RBC/UKQCD have made extensive use of ESP time to generate large volume ensembles, with physical quark masses at a variety of lattice spacings.

QCD Ensembles Generated by USQCD using ESP

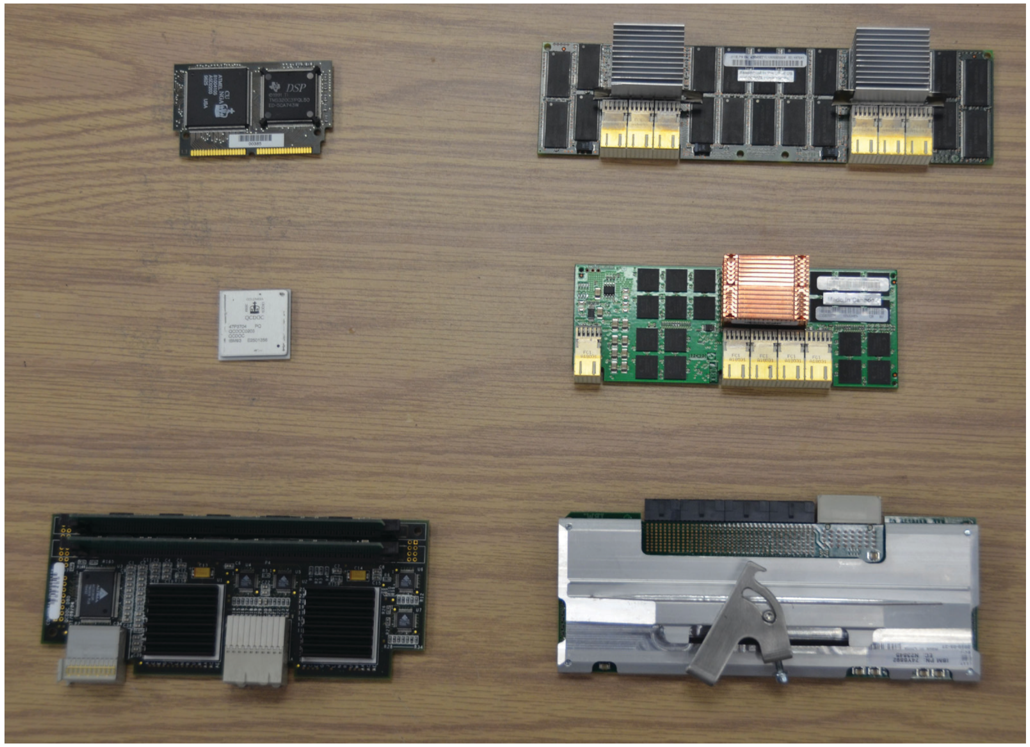
RBC/UKQCD	MILC/FNAL	HotQCD
Domain Wall Fermions	HISQ Fermions	HISQ Fermions
2+1 flavors	2+1+1 flavors	2+1 flavors
Zero temperature	Zero temperature	Finite temperature
$64^3 \times 128 \times 12$	$96^3 \times 192$	$64^3 \times 16$
Time per trajectory: 5700 seconds on 4 racks 2400 seconds on 8 racks 1350 seconds on 16 racks		
1700 trajectories produced 170 M core-hours		

Very good performance and uptime for Mira during ESP has allowed USQCD to use 530 M BGQ core-hours during ESP. We were allocated 150 M BGQ core-hours.

Computers

Columbia/RBRC
QCDSP 1998-2005
0.050 GFlops/node

Columbia/RBRC/
UKQCD
QCDOC 2005-2011
0.8 GFlops/node



IBM BGL 2005-2013
2.8 GFlops/node

IBM BGP 2007-
13.6 GFlops/node

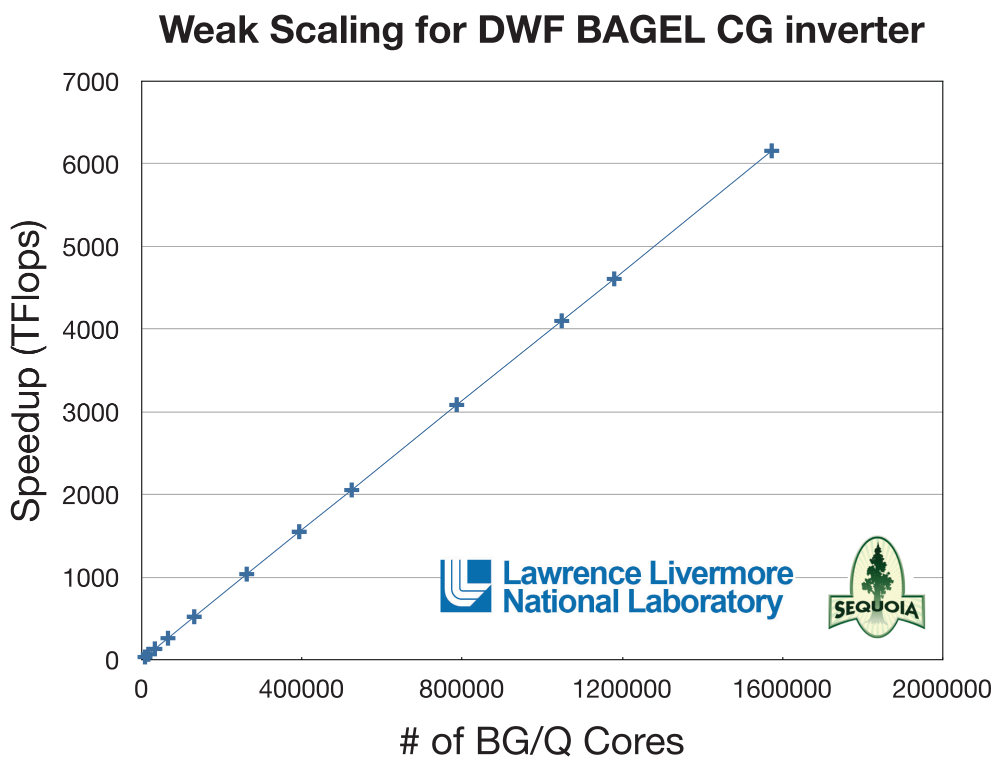
IBM BGQ 2012-
200 GFlops/node

~ 4,000× speed-up per node in 15 years, for QCD
~ 700× speed-up in Flops/$ in 15 years (no inflation)
~ 1,000x speed-up in Flops/(inflation adjusted $)

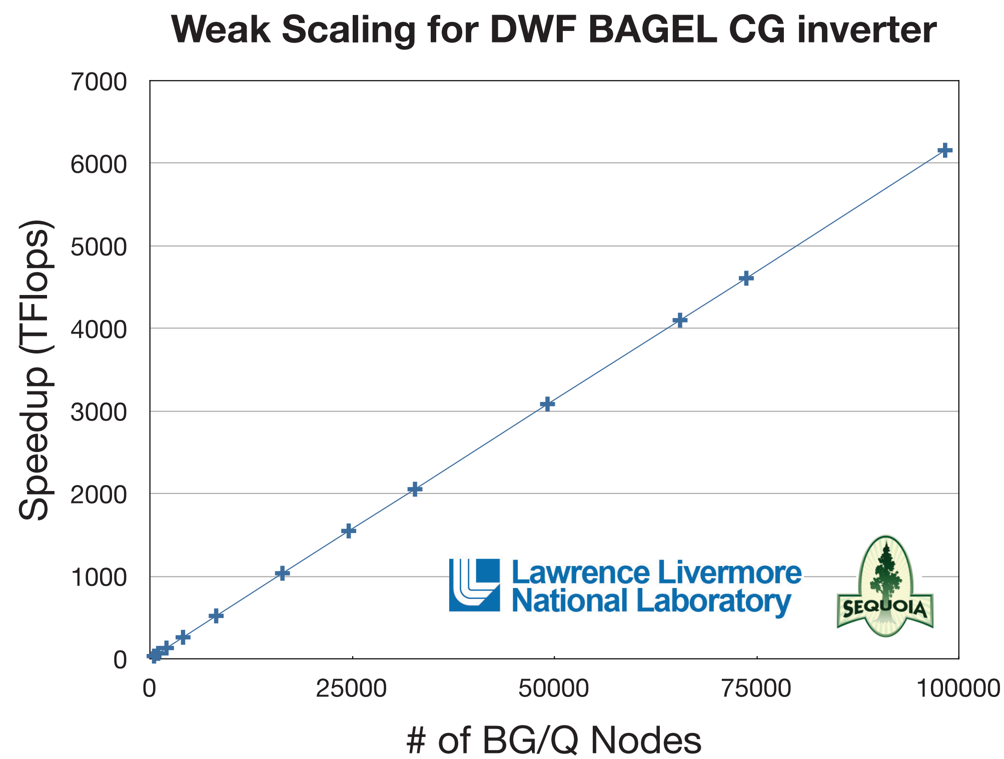
RBC/UKQCD have production jobs on the Argonne ALCF BGQ that sustain 1 PFlops on 32 racks = 32k nodes = 0.5 M cores.

This performance comes from very carefully tuned assembly code on BGQ, produced by Peter Boyle, using his BAGEL code generator

Scaling for Dirac Equation Solver



Code developed by Peter Boyle at the STFC funded DiRAC facility at Edinburgh



Code developed by Peter Boyle at the STFC funded DiRAC facility at Edinburgh

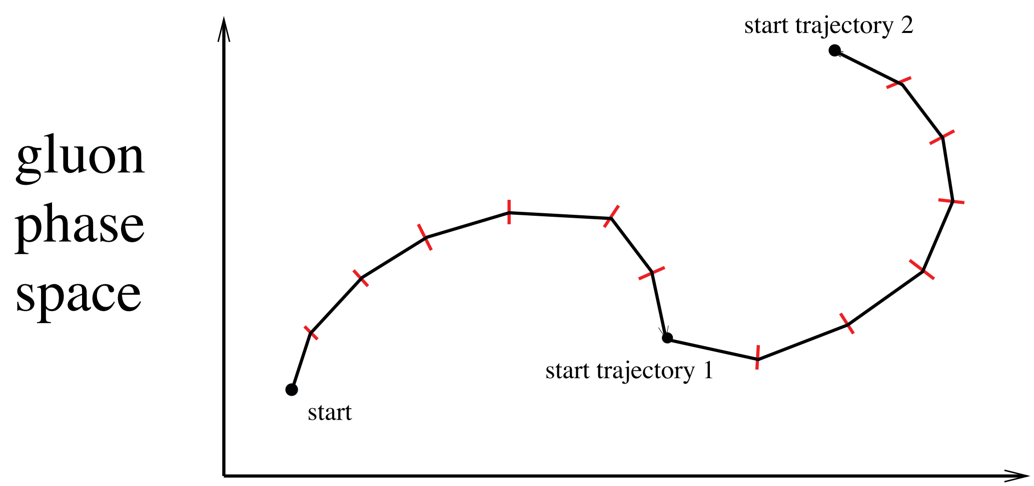
Quantum Chromodynamics

- Like QED, but with SU(3) local gauge symmetry

$$Z = \int [dA] \prod_{i=1}^{3} \det \left[D(A, g_0, m_0^i) \right] \exp \left\{ -\frac{i}{4} (\partial_\mu A_\nu - \partial_\nu A_\mu + g_0 f^{abc} A_\mu^b A_\nu^c)^2 \right\}$$

$$D(A, g_0, m_0^i) \equiv i\gamma^\mu (\partial_\mu - igA_\mu^a t^a/2) - m_0^i$$

- Good approximation: Only include three (or four) light quarks in path integral
- Gluon self-interaction yields a very non-linear system.
- Chiral symmetry of system broken by vacuum state
- Quarks bound in hadrons



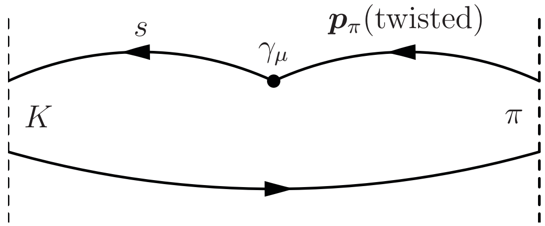
Algorithms for Gauge Field Production

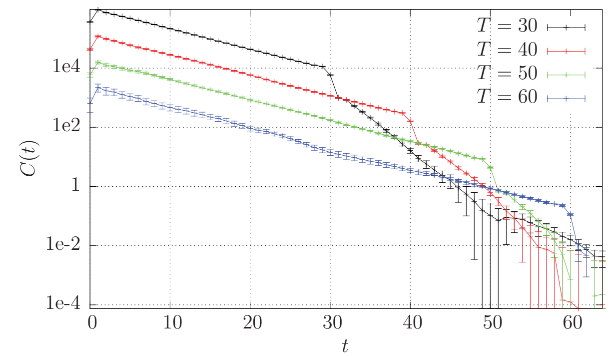
- Producing gauge fields:
  - * Use classical molecular dynamics to move through gauge field space
  - * Quark loops give back reaction on gauge fields by solving Dirac equation
  - * Hasenbusch mass preconditioning allows tuning back reaction

$$\det[D(m)] = \underbrace{\frac{\det[D(m)]}{\det[D(m_1)]}}_{\text{For } m \approx m_1 \text{ gives small force but expensive to calculate}} \times \underbrace{\frac{\det[D(m_1)]}{\det[D(m_2)]}}_{\text{Control force size from } m_1 \text{ and } m_2\text{, less expensive to calculate}} \cdots \det[D(m_n)]$$

  - * RBC/UKQCD uses 7 levels of intermediate masses
  - * Integrate different d.o.f on different time scales (Sexton-Weingarten integrators)
  - * Use higher order integrators, currently RBC/UKQCD use force gradient, $O(dt^4)$
- These are giving 10-100× speed-up over a decade ago.
  - * Hard to be completely quantitative here, since without these algorithmic speed-ups, we could not even try current simulations

Algorithms for Measurements





$$T = |t_K - t_\pi|$$

- Time translated the n-point function, on a fixed background gauge field, are sufficiently decorrelated (independent enough) to make them worth calculating
- This means many solutions of the Dirac equation $D[U_\mu]\ \Psi = s$ for fixed U_μ
- Calculating eigenvectors of $D[U_\mu]$ with small eigenvalues (low-modes) speeds up subsequent solves. Can be done with EigCG or Lanczos algorithms
- Alternatives for Wilson fermions are domain decomposition and multigrid, giving similar speed-up with smaller memory requirements.
- Further improvement from all-mode-averaging of Blum, Izubuchi and Shintani
  - * Separates measurements into expensive parts, with small statistical errors after a few measurements, and inexpensive parts, where many measurements are needed.

RBC/UKQCD 2+1 flavor MDWF ensembles

- Force gradient integrator and evolution code by Hantao Yin, solvers by Peter Boyle. BGQ: 30-50 Gflops/node (15-25% of peak) depending on local volume.
    - * 48^3 ensemble: 1200 MD time units produced (100 M BGQ core hours) with RBRC/BNL BGQ, Mira and 2 rack BGQ at Edinburgh.
    - * 64^3 ensemble: 1700 MD time units (180 M BGQ core hours) produced at Mira
- We are at the physical point to a few percent accuracy!
    - * 48^3 ensemble

Quantity	Physical Value	Simulation Value	Deviation (Sim. - Phys.)/Phys.
m_π/m_K	0.2723	0.2793(6)	2.5%
m_π/m_Ω	0.0807	0.0835(5)	3.3%
m_K/m_Ω	0.2964	0.2989(16)	0.8%

- * 64^3 ensemble (3 measurements now, most recent finished yesterday)

$m_\pi/m_K = 0.275$ $\qquad$ $m_\pi = 137$ MeV $\qquad$ $m_K = 499$ MeV

- * We are very close to the physical point!

- Two different lattice spacings will allow us to take the continuum limit.

Measurement Times

- RBC/UKQCD has measurements of $f_\pi, f_K, B_K, m_{ud}, m_s, f^+_{K\pi}(0), K \to (\pi\pi)_{I=2}$ all in a single executable, using EigCG deflation and all mode averaging,
- In production on ensemble 10, using RBRC/BNL and Edinburgh BGQ's.
  In production on ensemble 11 on Mira at the ALCF
- Ensemble 10 runs on 1 rack, ensemble 11 on 32 racks.
  Number of EigCG low modes is 600 for ensemble 10, 1500 for ensemble 11

	Ensemble 10	Ensemble 11
EigCG setup time	29.5	66
Exact light quark time	18.7	13
Sloppy light quark time	64	55
Exact strange quark time	8	17
Contraction time	3	16
Total time	123	167
Total time on partition	5.2 days	5.3 hrs

- With more deflation, the ensemble 11 calculation is only 1.3× ensemble 10

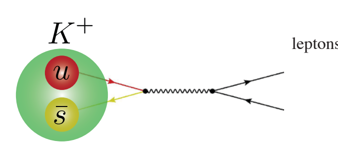
Very Recent Results

- Results from previous calculations by RBC and UKQCD

Quantity		Value		Stat		Chiral		Finite V		Pert Match	Units
f_π	=	127.1	$\pm$	2.7	$\pm$	0.9	$\pm$	2.5			MeV
f_K	=	152.4	$\pm$	3.0	$\pm$	0.7	$\pm$	1.5			MeV
f_K/f_π	=	1.199	$\pm$	0.012	$\pm$	0.007	$\pm$	0.012			
$\hat{m}_{ud}^{\mathrm{RGI}}$	=	8.78	$\pm$	0.24	$\pm$	0.17	$\pm$	0.03	$\pm$	0.07	MeV
$\hat{m}_{s}^{\mathrm{RGI}}$	=	240.1	$\pm$	4.8	$\pm$	2.4	$\pm$	1.2	$\pm$	2.0	MeV
$\hat{B}_{K}^{\mathrm{RGI}}$	=	0.758	$\pm$	0.011	$\pm$	0.010	$\pm$	0.004	$\pm$	0.016	
Re A_2	=	(1.436	$\pm$	0.062	$\pm$	$0.258_{\mathrm{syst}}) \times 10^{-8}$					GeV
Im A_2	=	-(6.83	$\pm$	0.51	$\pm$	$1.30_{\mathrm{syst}}) \times 10^{-13}$					GeV
$f_+(0)$	=	0.962	$\pm$	0.002		(Preliminary)					

- Results from 26 ensemble 10 configurations (statistical errors only)

	m_π	m_K	f_π	f_K	f_K/f_π	Z_A	m_Ω
AMA	0.08056(17)	0.28845(25)	0.07594(16)	0.09047(12)	1.1914(21)	0.71184(13)	-
Exact	0.08064(21)	0.28889(38)	0.07622(28)	0.09052(42)	1.1876(57)	0.71278(63)	0.9649(50)

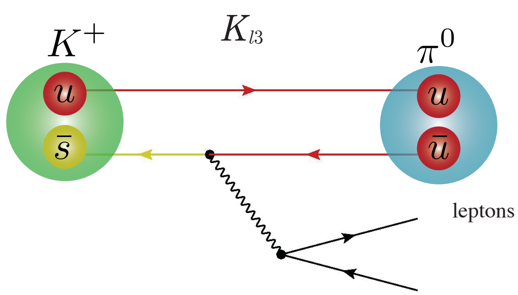


- Recent MILC result (arXiv:1301.5855): $f_{K^+}/f_{\pi^+} = 1.1970(26)(37)$
- Recent HPQCD result (arXiv:1303.1670): $f_{K^+}/f_{\pi^+} = 1.1916(21)$. (MILC HISQ lattices)
- Largest volume, physical quark mass DWF and MILC lattices used in f_K/f_π generated at ALCF on Mira

Improvement from All Mode Averaging

- For $f^+_{K\pi}(0)$ RBC/UKQCD statistical errors are 5× smaller with AMA than exact only. With 26 configurations, have 0.5% statistical error for $f^+_{K\pi}(0)$

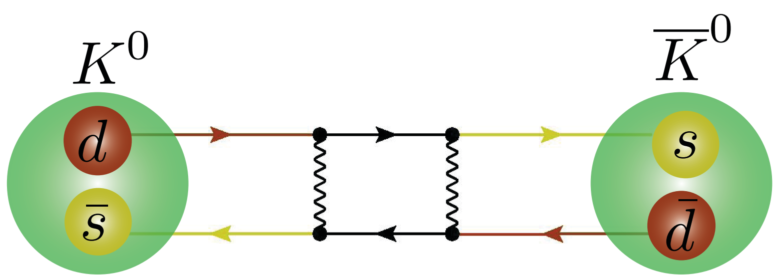
$K-\pi$ sep	AMA?	$f^+_{K\pi}(0)$	$f^-_{K\pi}(0)$	Z_V
20:24	AMA	0.9672(45)	-0.1327(123)	0.7123(13)
20:28	AMA	0.9602(52)	-0.1254(97)	0.7089(17)
20:32	AMA	0.9639(49)	-0.1318(96)	0.7093(16)
24:28	AMA	0.9598(59)	-0.1230(112)	0.7087(18)
24:32	AMA	0.9646(52)	-0.1322(106)	0.7092(17)
20:24	exact	1.0018(253)	-0.1206(320)	0.7315(150)
20:28	exact	0.9552(227)	-0.0850(205)	0.7016(157)
20:32	exact	0.9537(246)	-0.1004(215)	0.6971(162)
m_{res}		0.0006148(59)		



- FNAL/MILC (arXiv:1212.4993) has $f^+_{K\pi}(0) = 0.9667 \pm 0.0023_{stat} \pm 0.0033_{sys}$

- B_K has 0.2% statistical errors as well, 10× smaller than without AMA

$K-K$ sep	AMA?	B_K
20:4:24	AMA	0.5836(11)
20:4:28	AMA	0.5844(12)
20:4:32	AMA	0.5839(12)
20:4:24	exact	0.5712(109)
20:4:28	exact	0.5870(110)
20:4:32	exact	0.5845(116)

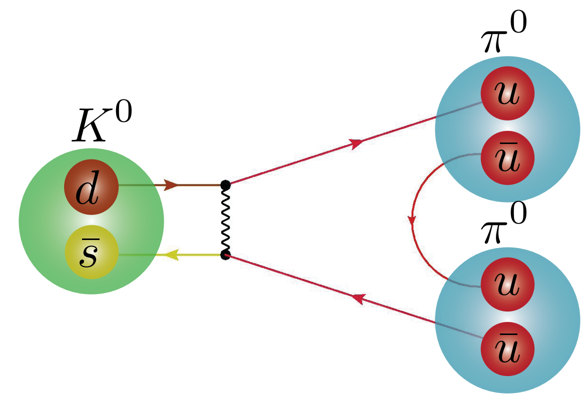


- More work can reduce perturbative matching errors

RBC/UKQCD K -> ππ, I = 2 on Ensemble 10

- Measurements on 22 configurations yield (statistical error only)

i	Re(A_2)(Gev)	Im(A_2)(Gev)
1	-4.98(10)e-09	0
2	1.913(38)e-08	0
7	2.238(36)e-11	3.761(61)e-14
8	-1.640(29)e-10	-7.99(14)e-13
9	-2.273(46)e-15	1.488(30)e-13
10	1.752(35)e-12	-4.156(84)e-14
Total	1.401(28)e-08	-6.54(13)e-13

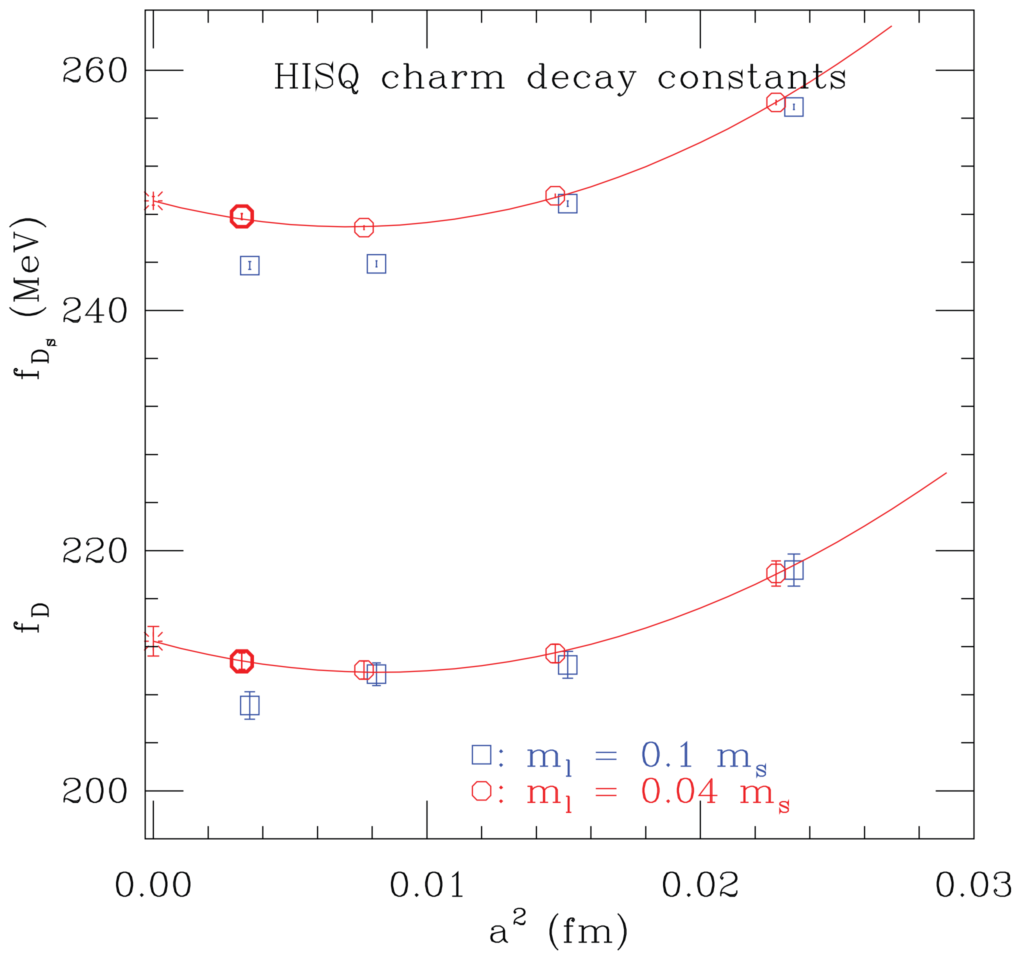


- Previous published result:

$$\mathrm{Re}\ A_2 = (1.436 \pm 0.062 \pm 0.258_{\mathrm{syst}}) \times 10^{-8}\ \mathrm{GeV}$$
$$\mathrm{Im}\ A_2 = -(6.83 \pm 0.51 \pm 1.30_{\mathrm{syst}}) \times 10^{-13}\ \mathrm{GeV}$$

- Statistical error already 2× smaller than previous result
- Much of the systematic error in previous calculation is from only one lattice spacing. Will now have 2 lattice spacings with this action.

Results from MILC/FNAL on f_D and f_{Ds}



The red points (physical quark masses) at the smallest a^2 were measured on HISQ ensembles generated at Mira using ESP time.

USQCD Goals for CKM Physics

- Recent white paper from our community detailing current and expected errors.

TABLE I. *History, status and future of selected LQCD calculations needed for the determination of CKM matrix elements. Forecasts from the 2007 white paper (where available) assumed computational resources of 10–50 TF years. Most present lattice results are taken from http://www.latticeaverages.org [28]. Other entries are discussed in the text. The quantity* ξ *is* $f_B^2 B_B/(f_{B_s}^2 B_{B_s})$.

Quantity	CKM element	Present expt. error	2007 forecast lattice error	Present lattice error	2014 lattice error	2018 lattice error
f_K/f_π	$\|V_{us}\|$	0.2%	0.5%	0.5%	0.3%	0.15%
$f_+^{K\pi}(0)$	$\|V_{us}\|$	0.2%	–	0.5%	0.35%	0.2%
f_D	$\|V_{cd}\|$	4.3%	5%	2%	1%	$< 1\%$
f_{D_s}	$\|V_{cs}\|$	2.1%	5%	2%	1%	$< 1\%$
$D \to \pi\ell\nu$	$\|V_{cd}\|$	2.6%	–	4.4%	3%	2%
$D \to K\ell\nu$	$\|V_{cs}\|$	1.1%	–	2.5%	2%	1%
$B \to D^*\ell\nu$	$\|V_{cb}\|$	1.3%	–	1.8%	1.5%	$< 1\%$
$B \to \pi\ell\nu$	$\|V_{ub}\|$	4.1%	–	8.7%	4%	2%
f_B	$\|V_{ub}\|$	9%	–	2.5%	1.5%	$< 1\%$
ξ	$\|V_{ts}/V_{td}\|$	0.4%	2-4%	4%	1.5%	$< 1\%$
ΔM_s	$\|V_{ts}V_{tb}\|^2$	0.24%	7–12%	11%	8%	5%
B_K	$\mathrm{Im}(V_{td}^2)$	0.5%	3.5–6%	1.3%	1%	$< 1\%$

- The ESP time we have used to generate DWF and HISQ ensembles has put us ahead of this schedule, perhaps by a year or more.

Conclusions

- After 30 years of QCD simulations, large volume, physical pion/kaon ensembles are begin produced by a number of collaborations.
- Many technical improvements are being used: twisted b.c. for particle states, NPR, RI-SMOM renormalization, EigCG, deflation, Lellouch-Luscher relation
- We can now do quite sophisticated field theory numerically
- 4,000× improvement in computer power in 15 years.
- Evolution algorithms to produce gauge fields are 10-100× faster
- Measurement algorithms are > 10× faster
- Our most refined measurements have total errors in the 0.2 - 1 % range
- 5 - 10% errors for much more complicated observables are now possible
- Enormous opportunity for precison comparisons of theory and experiment and, hopefully, new physics.
- ESP time has given USQCD a number of vital lattice QCD ensembles that will be used extensively for measurements for a number of years.