USQCD

SciDAC
Scientific Discovery through Advanced Computing

Searching for Physics Beyond the Standard Model with Strongly Coupled Field Theories

Project Director: Paul B. Mackenzie, Fermilab

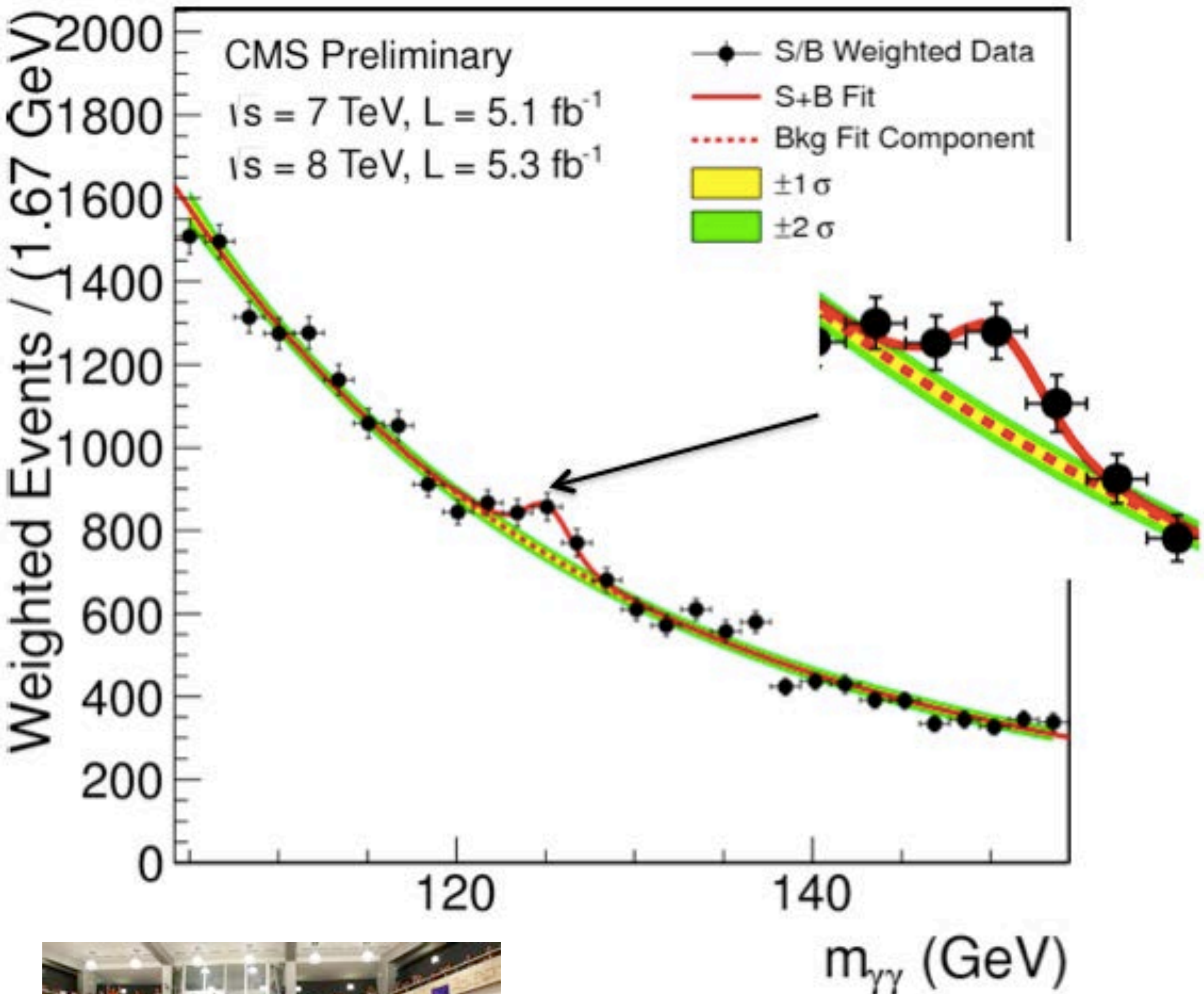
Project Co-director for Science: Stephen Sharpe, University of Washington

Project Co-Director for Computation: Richard Brower, Boston University

Participating Institutions and Principal Investigators:
Argonne National Laboratory, James Osborn
Boston University, Richard Brower
Brookhaven National Laboratory, Frithjof Karsch
Columbia University, Norman Christ
Fermi National Accelerator Laboratory, Paul Mackenzie
Lawrence Livermore National Laboratory, Pavlos Vranas
Syracuse University, Simon Catterall
University of Arizona, Doug Toussaint
University of California, Santa Barbara, Robert Sugar
University of California, San Diego, Julius Kuti
University of Utah, Carleton DeTar
University of Washington, Stephen Sharpe

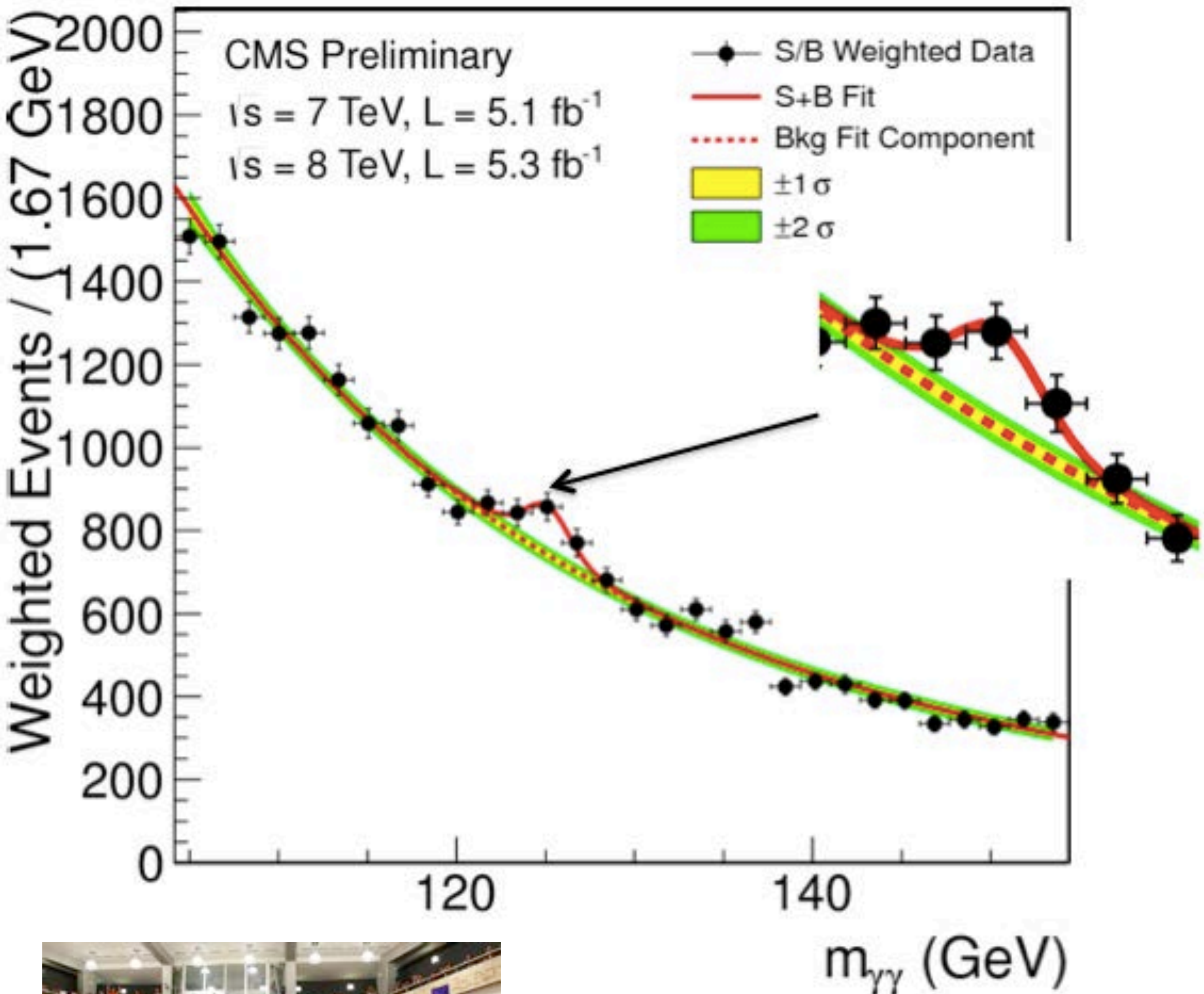
SciDAC-3 PI Meeting
Washington DC
July 30-Aug. 1, 2014

July 4, 2012: LHC discovers a “Higgs-like” particle



Is it the hypothesized “Higgs”particle?
We knew that the standard model needed at least one additional ingredient to make it mathematically consistent.

July 4, 2012: LHC discovers a “Higgs-like” particle



Is it the hypothesized “Higgs”particle?
We knew that the standard model needed at least one additional ingredient to make it mathematically consistent.

In 2012, I told you I hoped it was something more interesting!

Why?

The Standard Model

consists of numerous bells and whistles and 20 or 30 random numbers.

- Three forces (strong, weak, and electromagnetic), with coupling strengths:

$$\alpha_{\rm s},\ \alpha_{\rm w},\ \alpha_{\rm em}$$

- Six quark and six lepton masses

$$m_u,\ m_d,\ m_c,\ m_s,\ m_t,\ m_b$$

$$m_e,\ m_\mu,\ m_\tau,\ m_{\nu_1},\ m_{\nu_2},\ m_{\nu_3}$$

- Mixings among the quarks, the Cabibbo-Kobayashi-Maskawa matrix (2008 Nobel Prize), and (as of the last few years) among the leptons:

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \qquad \begin{pmatrix} V_{e\nu_1} & V_{e\nu_2} & V_{e\nu_3} \\ V_{\mu\nu_1} & V_{\mu\nu_2} & V_{\mu\nu_3} \\ V_{\tau\nu_1} & V_{\tau\nu_2} & V_{\tau\nu_3} \end{pmatrix}$$

The Standard Model

consists of numerous bells and whistles and 20 or 30 random numbers.

- Three forces (strong, weak, and electromagnetic), with coupling strengths:

$$\alpha_{\mathrm{s}},\ \alpha_{\mathrm{w}},\ \alpha_{\mathrm{em}}$$

Domain of lattice QCD

- Six quark and six lepton masses

$$m_u,\ m_d,\ m_c,\ m_s,\ m_t,\ m_b$$

$$m_e,\ m_\mu,\ m_\tau,\ m_{\nu_1},\ m_{\nu_2},\ m_{\nu_3}$$

- Mixings among the quarks, the Cabibbo-Kobayashi-Maskawa matrix (2008 Nobel Prize), and (as of the last few years) among the leptons:

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \qquad \begin{pmatrix} V_{e\nu_1} & V_{e\nu_2} & V_{e\nu_3} \\ V_{\mu\nu_1} & V_{\mu\nu_2} & V_{\mu\nu_3} \\ V_{\tau\nu_1} & V_{\tau\nu_2} & V_{\tau\nu_3} \end{pmatrix}$$

Where do these parameters come from?
Can we predict them with a more fundamental theory?

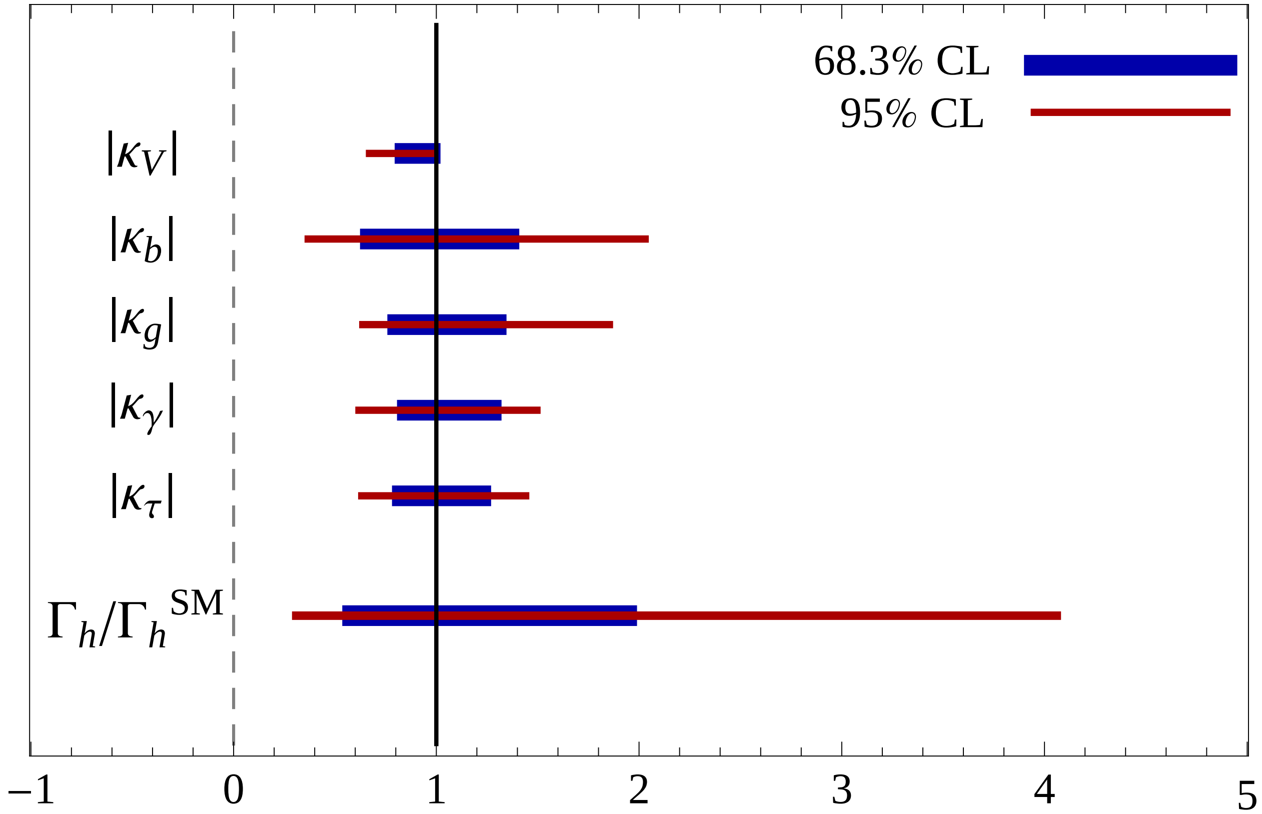
The Standard Model is *maddeningly* successful. It accounts for every particle physics experiment performed so far, sometimes to great precision (one part in a billion for the electron anomalous magnetic moment).

Why maddeningly? It contains obvious gaps and puzzles!

- Why is there more than one generation of quark?
- What is the relation between the three forces?
- No gravity.
- No explanation for dark matter.
- ...

July 4, 2012 - July 31, 2014

- Q: Does the observed new particle have spin 0 like the predicted Higgs, or does it have some other spin?
- Q: Are the quantum amplitudes of its decays the same as their mirror images like the Higgs ("positive parity"), or are they different?
- Are the probabilities for it to decay in various ways as predicted for the Higgs, or are they different?



Dobrescu and Lykken, arxiv:1210.3342

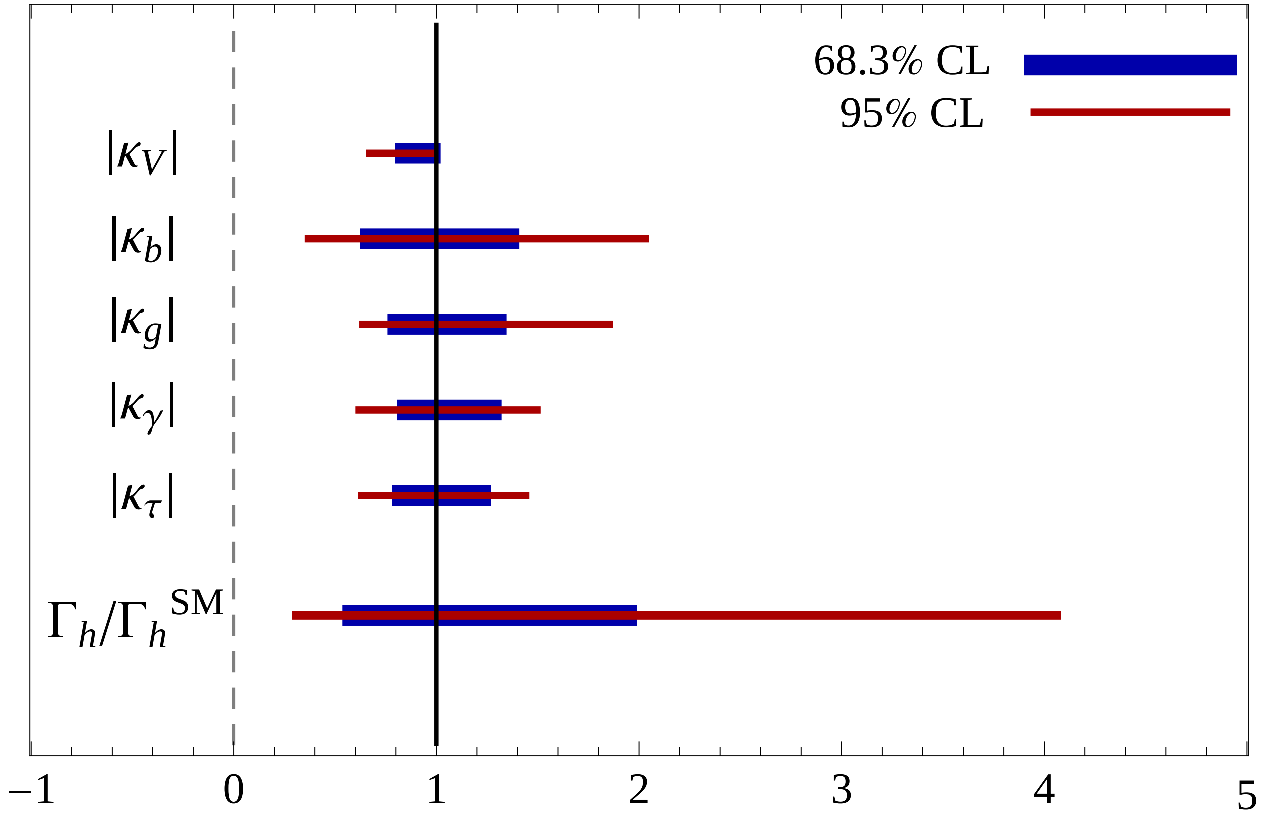
July 4, 2012 - July 31, 2014

- Q: Does the observed new particle have spin 0 like the predicted Higgs, or does it have some other spin?

A: Like the Higgs.

- Q: Are the quantum amplitudes of its decays the same as their mirror images like the Higgs (“positive parity”), or are they different?

- Are the probabilities for it to decay in various ways as predicted for the Higgs, or are they different?



Dobrescu and Lykken, arxiv:1210.3342

July 4, 2012 - July 31, 2014

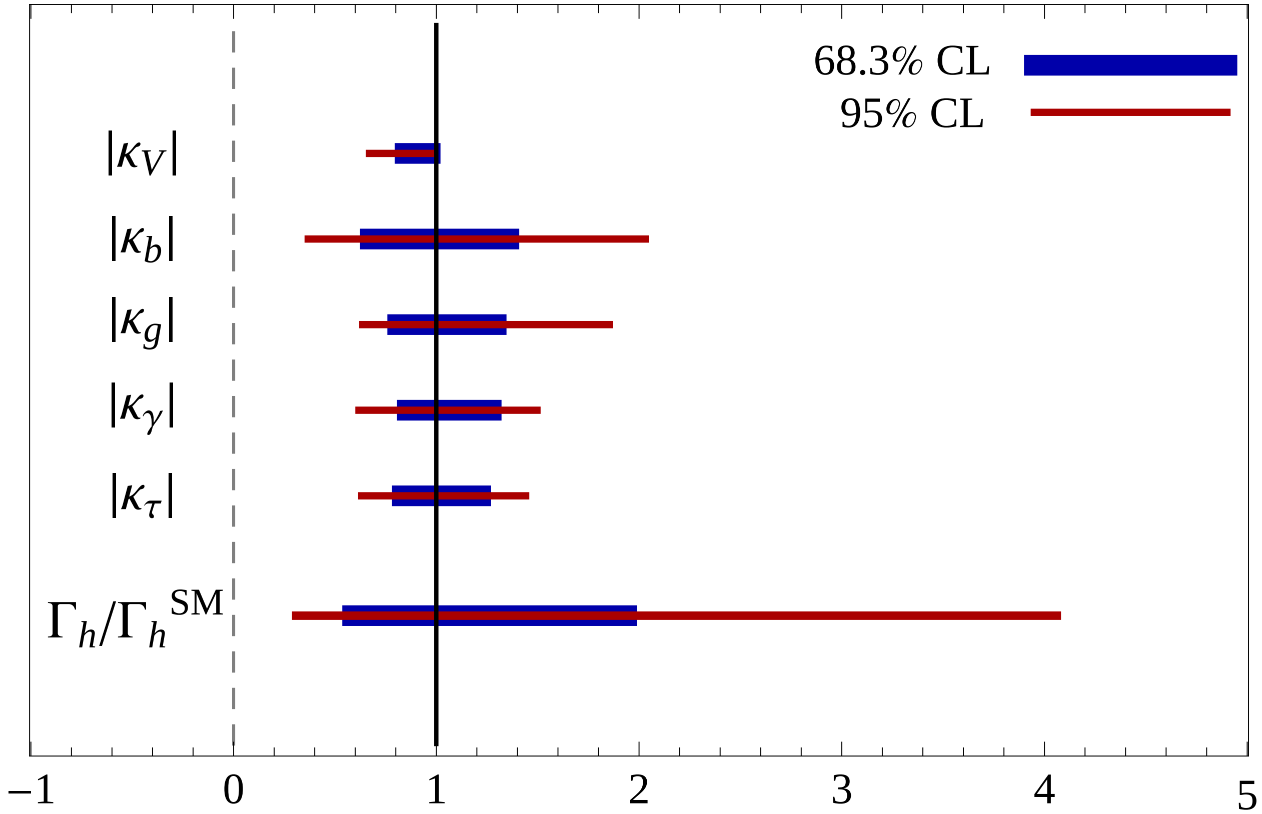
- Q: Does the observed new particle have spin 0 like the predicted Higgs, or does it have some other spin?

A: Like the Higgs.

- Q: Are the quantum amplitudes of its decays the same as their mirror images like the Higgs (“positive parity”), or are they different?

A: Like the Higgs.

- Are the probabilities for it to decay in various ways as predicted for the Higgs, or are they different?



Dobrescu and Lykken, arxiv:1210.3342

July 4, 2012 - July 31, 2014

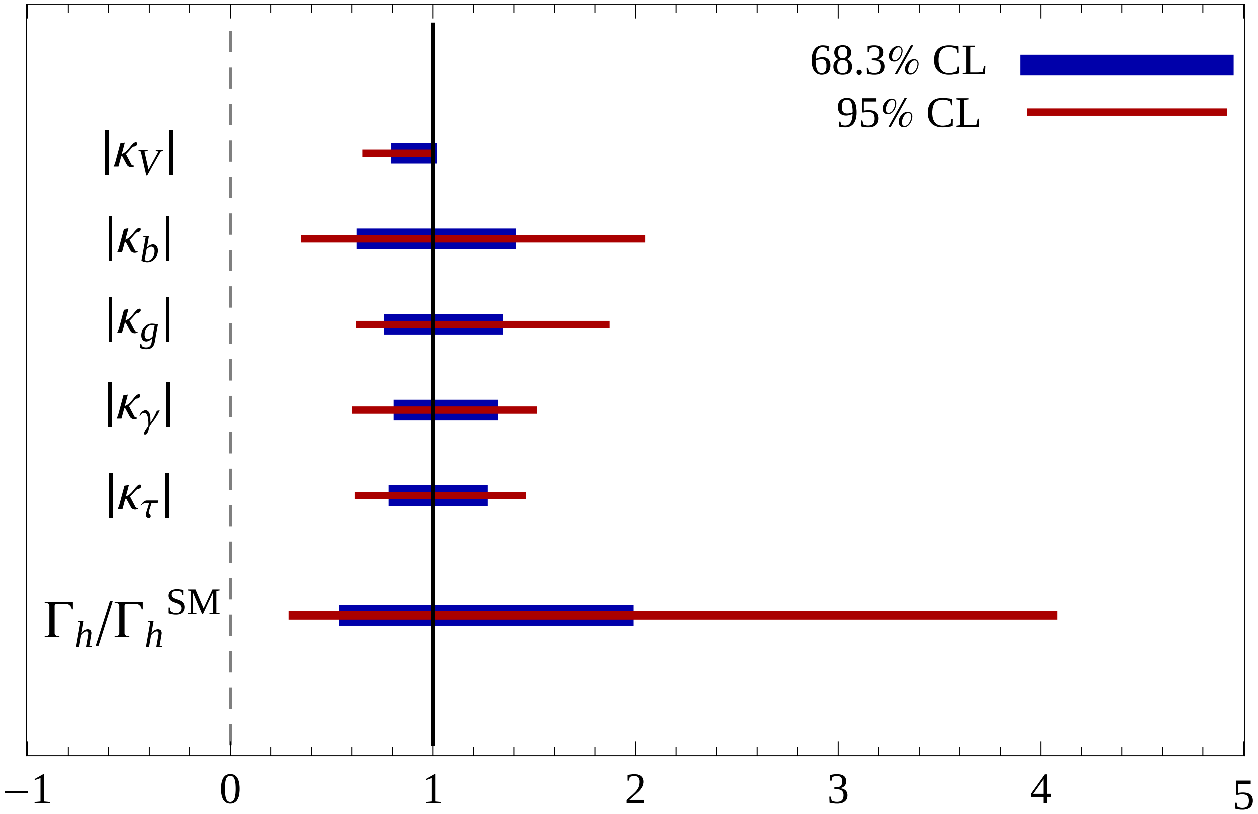
- Q: Does the observed new particle have spin 0 like the predicted Higgs, or does it have some other spin?

A: Like the Higgs.

- Q: Are the quantum amplitudes of its decays the same as their mirror images like the Higgs ("positive parity"), or are they different?

A: Like the Higgs.

- Are the probabilities for it to decay in various ways as predicted for the Higgs, or are they different?



A: Like the Higgs.

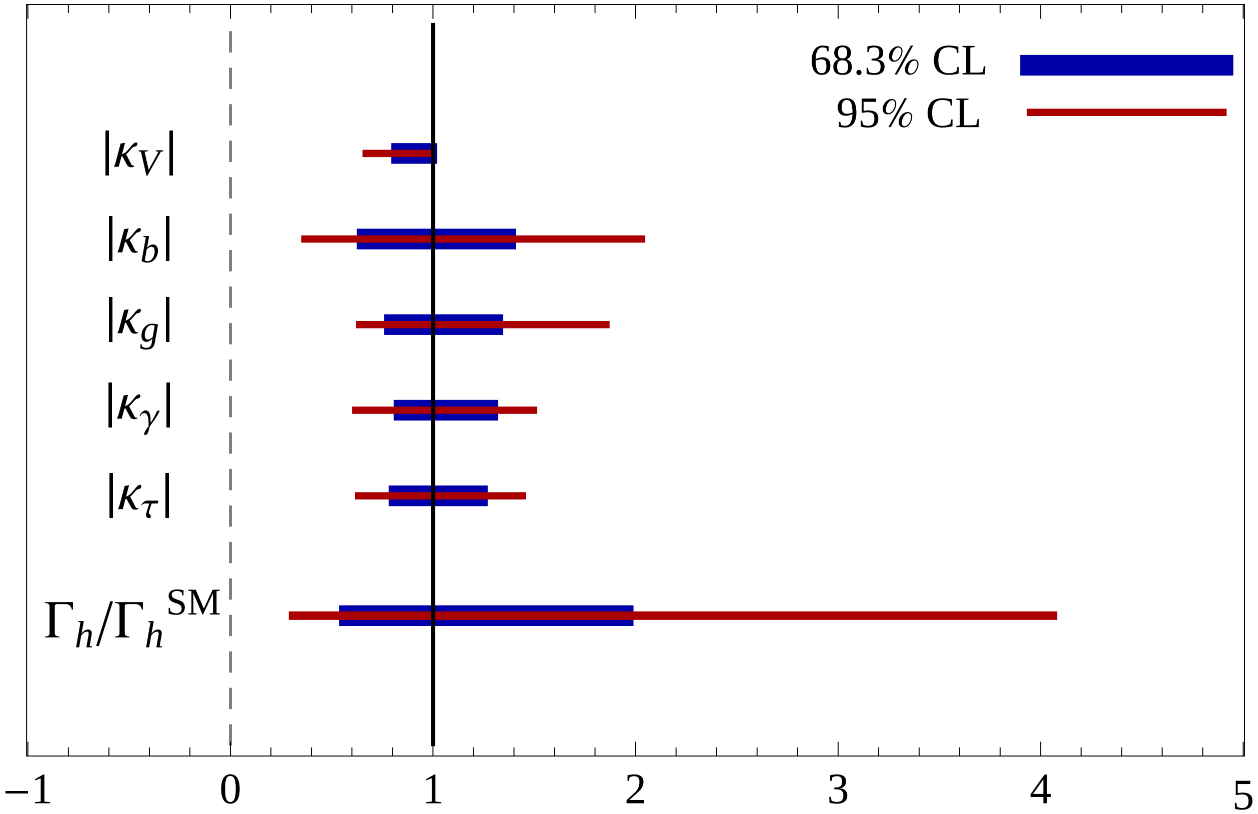
The new particle looks exactly like the expected Higgs to the accuracy we can measure.

Dobrescu and Lykken, arxiv:1210.3342

July 4, 2012 - July 31, 2014

- Q: Does the observed new particle have spin 0 like the

The agreement with the standard model is awesome and terrible. Terrible because we don't get any hints about beyond-the-standard-model physics without new experimental clues.



A: Like the Higgs.

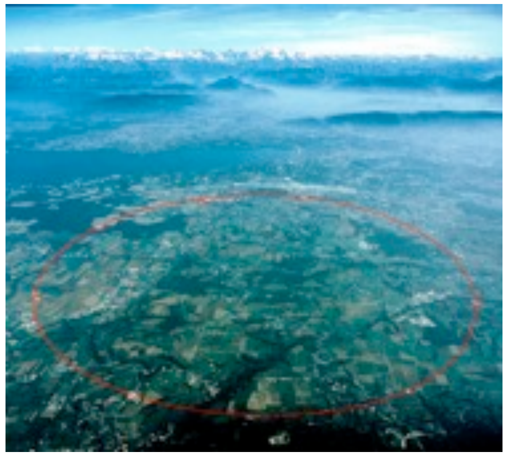
The new particle looks exactly like the expected Higgs to the accuracy we can measure.

Dobrescu and Lykken, arxiv:1210.3342

The search for a more fundamental theory underlying the Standard Model is the central task of particle physics today.

Two complementary approaches:

- The Energy Frontier: direct search for new particles and forces.
  - The LHC at CERN collides protons at the highest possible energies to push the search for direct evidences of new physics to the highest possible energies. --A new run starts in 2015 at double the energy.



- The Intensity Frontier: search for small, indirect effects of new physics in interactions of known particles.
  - Since the early 2000s, heavy flavor factories at CERN, KEK, Fermilab, and elsewhere have been pouring out huge amounts of high precision data to pin down the CKM matrix elements.

Lattice gauge theory in the SciDAC-1, -2 eras

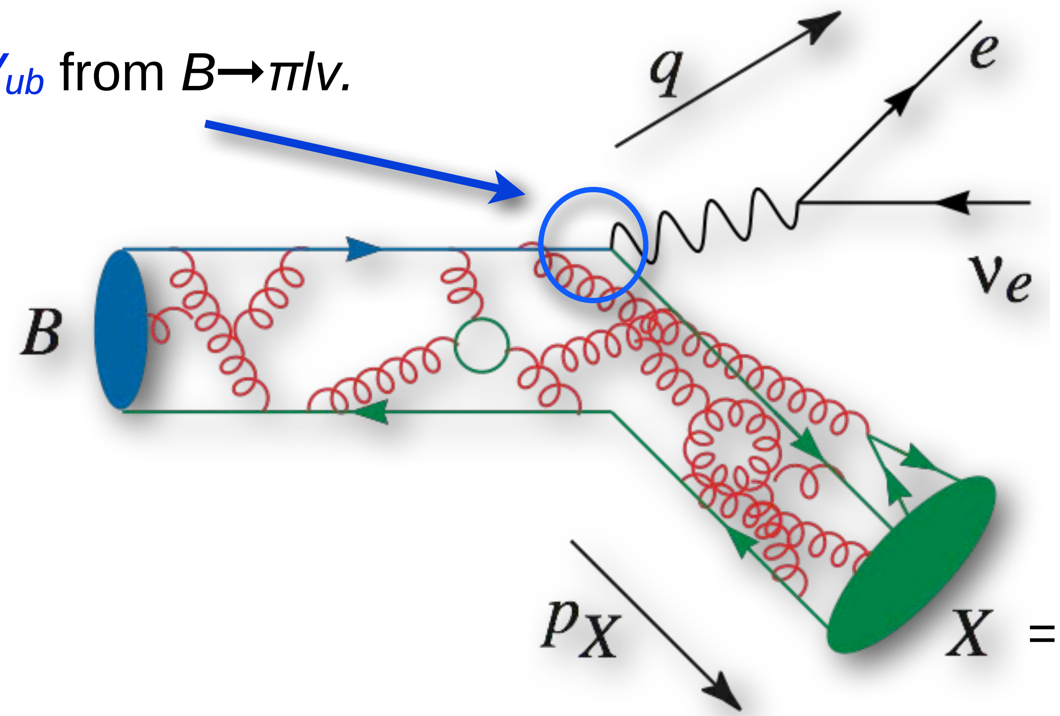
The theory of the strong interactions is quantum chromodynamics (QCD), the theory of quarks and gluons. Quarks and gluons cannot be directly observed because the forces of QCD are strongly interacting.

Quarks are permanently confined inside hadrons, even though they behave as almost free particles at asymptotically high energies.

"Asymptotic freedom", Gross, Politzer, and Wilczek, Nobel Prize, 2004.

Lattice QCD is used to determine the properties of quarks and gluons from the observed properties of hadrons.

Determine V_{ub} from $B \to \pi l \nu$.



$= \{\pi, K, \ldots\}$

$B \to \pi l \nu$ semileptonic decay

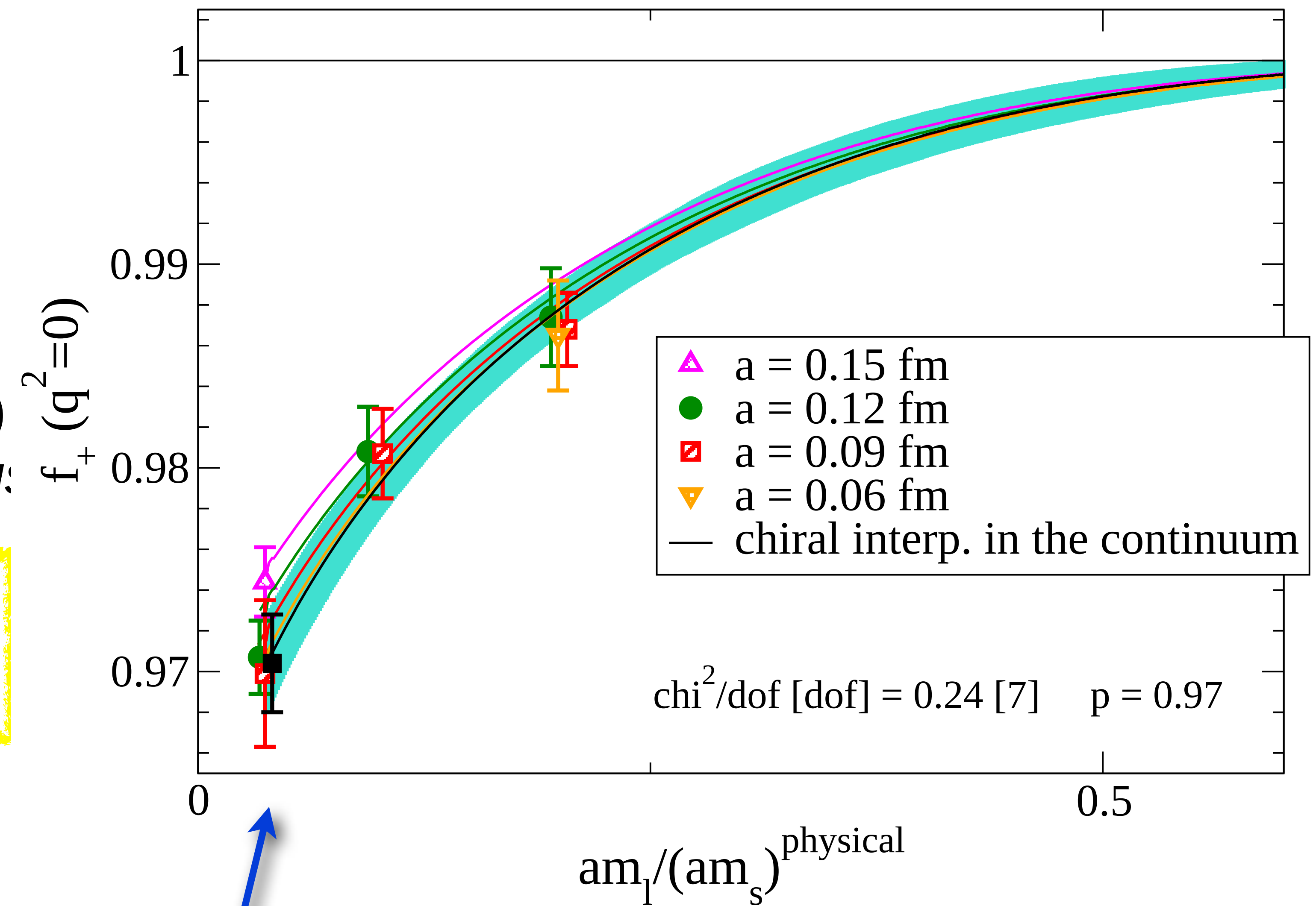
Physics achievements of 2014.

Kaon semileptonic decay:
K→πlν.

Single most precise result for *f*+(0) enables 0.4% determination of |*Vus*|

$f_+^{K\pi}(0) = 0.9704(24)_{stat}(22)_{sys}$

$|V_{us}| = 0.22290(74)_{theo}(52)_{exp}$



Uncertainty quantification in good shape.
Theoretically understood functional forms of lattice spacing dependence, volume, ...

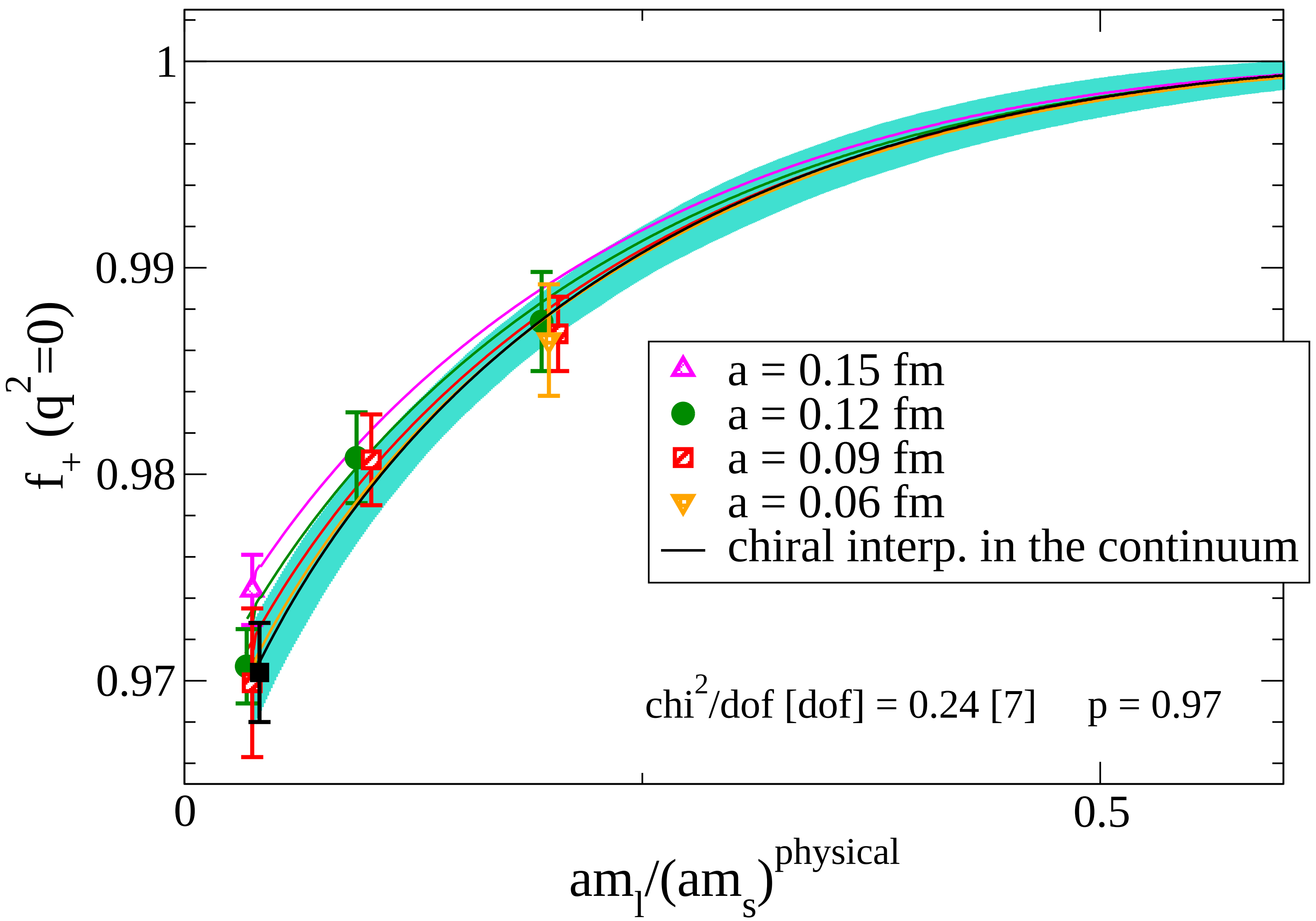
Bazavov et al. PRL 112 (2014) 112001
PRL editor's suggestion.

Calculations at the physical light quark mass only became possible with Mira and Titan.
Eliminates one of the largest uncertainties.

Physics achievements of 2014.

Kaon semileptonic decay: $K \rightarrow \pi l \nu$.

Increased precision makes visible a 2 sigma deviation from unitarity in the first row of the CKM matrix.
Will likely go away with further improved experiment and theory.
If it instead increased, might be signal of new physics.



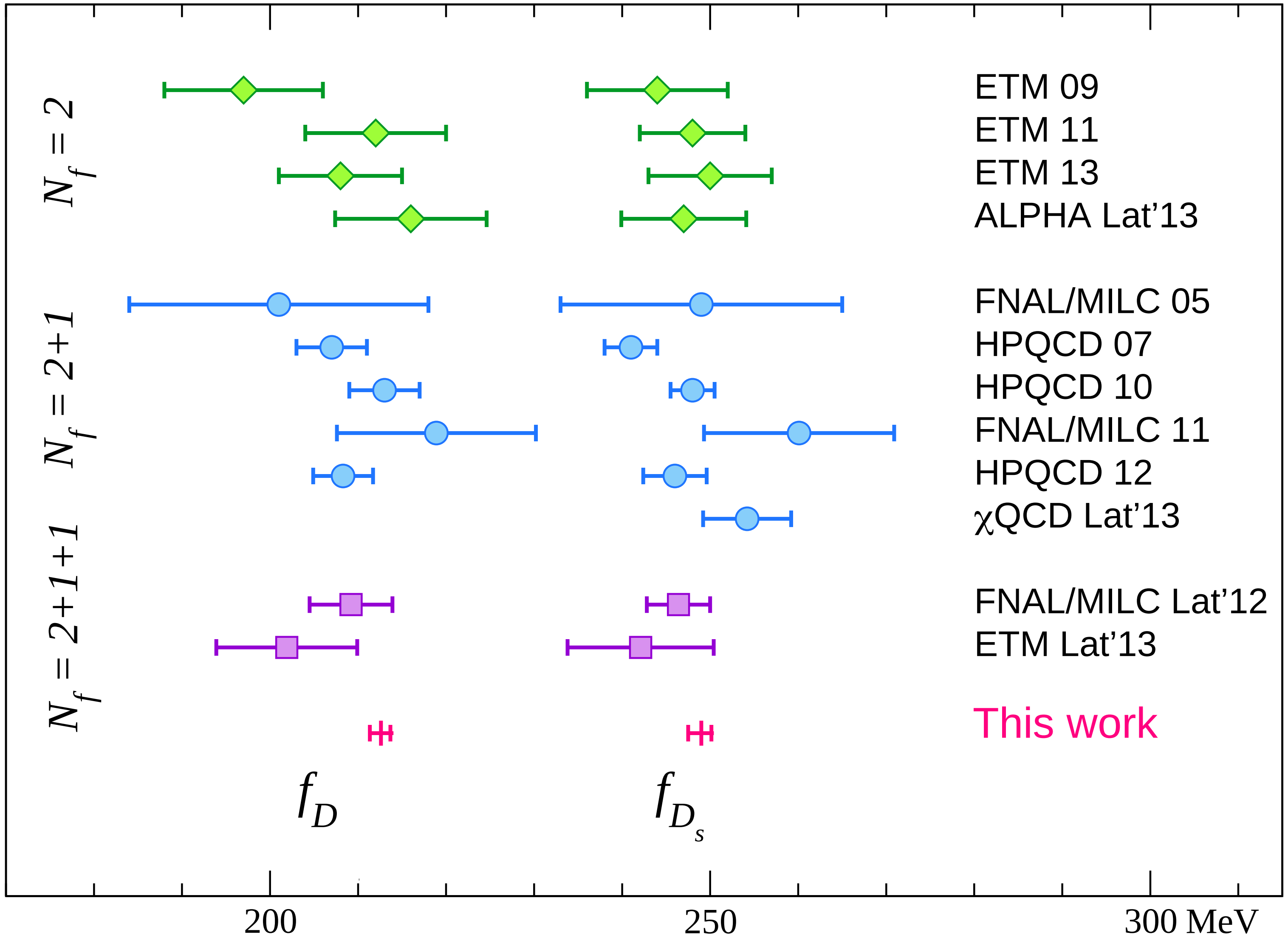
$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 - 1 = -0.00115(40)_{Vus}(43)_{Vud}.$$

Bazavov et al. PRL 112 (2014) 112001
PRL editor's suggestion.

This calculation was made possible by SciDAC work making structural improvements in the MILC code that made it easy to generate the large variety of three-point and two-point functions and interpolating operators required by the project.

D and D_s meson pure leptonic decay: $D \to l\nu$ and $D_s \to l\nu$.

Decreased the uncertainty in the form factors for *D* and *Ds* lepton decay, producing a corresponding improvement of our knowledge of the CKM matrix elements V_{cs} and V_{cd}.



Bazavov et al., arXiv:1407.3772, submitted to PRD.

Lattice QCD CKM determinations

Those were the three most recent examples of the 13 quantities on this table of lattice determinations of CKM matrix elements.

Lattice calculation determine or contribute to the determine of 8 out of the nine CKM matrix elements.

$$
\begin{pmatrix}
\mathbf{V_{ud}} & \mathbf{V_{us}} & \mathbf{V_{ub}} \\
\pi \to \ell\nu & K \to \ell\nu & B \to \ell\nu \\
 & \boxed{K \to \pi\ell\nu} & B \to \pi\ell\nu \\
\mathbf{V_{cd}} & \mathbf{V_{cs}} & \mathbf{V_{cb}} \\
\boxed{D \to \ell\nu} & \boxed{D_s \to \ell\nu} & B \to D\ell\nu \\
D \to \pi\ell\nu & D \to K\ell\nu & B \to D^*\ell\nu \\
\mathbf{V_{td}} & \mathbf{V_{ts}} & \mathbf{V_{tb}} \\
\langle B_d|\bar{B}_d\rangle & \langle B_s|\bar{B}_s\rangle &
\end{pmatrix}
$$

For all of these quantities, the best and most precise calculations were done by US groups benefited by SciDAC software.

Whither for particle physics?

In 2014, a long-term planning exercise by US particle physicists: The Particle Physics Project Prioritization Panel (P5)., and a year-long community-wide planning exercise, the Snowmass Process.

Based on this comprehensive work by the broad community, we have identified five compelling lines of inquiry that show great promise for discovery over the next 10 to 20 years. These are the science Drivers:

- **Use the Higgs boson as a new tool for discovery**
- **Pursue the physics associated with neutrino mass**
- **Identify the new physics of dark matter**
- **Understand cosmic acceleration: dark energy and inflation**
- **Explore the unknown: new particles, interactions, and physical principles**

P5 HEP priorities in terms of projects

1. The LHC experiments
   - The US is the largest participating state in the LHC experiments CMS and Atlas.
   - One of the two LHC PIs announcing the Higgs discovery was an American.
2. Neutrino experiments
   - Large Baseline Neutrino Facility at Fermilab
3. Cosmic surveys and dark matter
4. Muon experiments
   - g-2, mu2e
5. ...

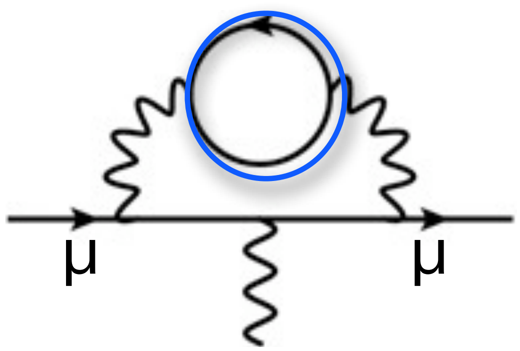
Where will lattice gauge theory calculations be needed in the new program?

Almost everywhere!

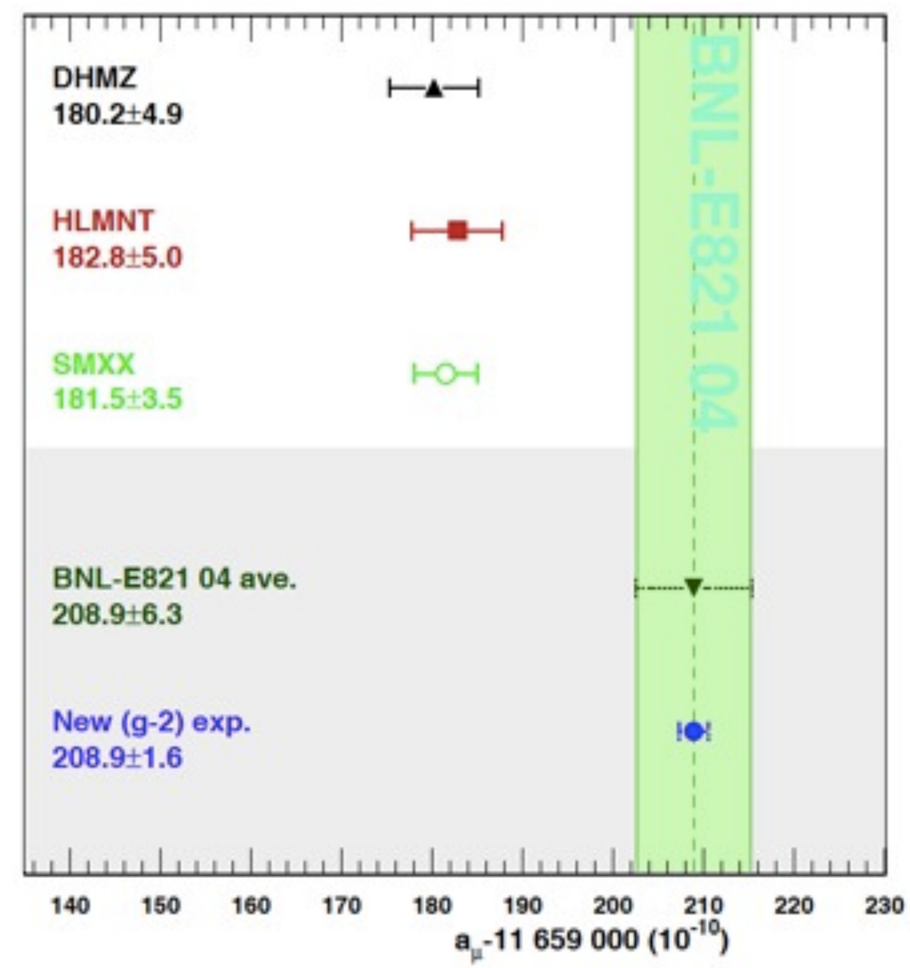
- This initially surprised us during the Snowmass planning process in 2013.
- All physical processes have higher-order corrections involving quark loops.
- All experiments are constructed out of materials containing protons and neutrons.
- It's likely you'll need lattice calculations for most future experiments

Muon anomalous magnetic moment, g-2

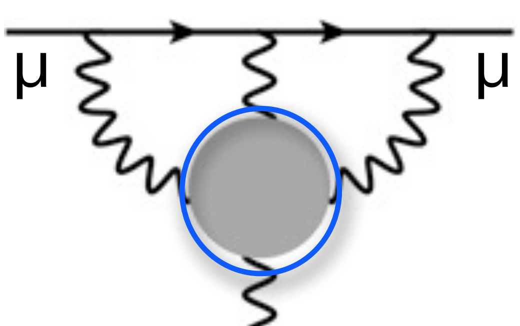
The electron anomalous magnetic moment has been predicted and observed to a part in a billion, most accurate quantity there is. The muon magnetic moment would be too, except that its larger mass allows higher energy processes to cause corrections.



Loops of quarks and leptons are included, but loops of supersymmetric particles, etc., could also cause corrections.



BNL experiment observed 3 σ deviation from SM.
New Fermilab exp. will reduce error by X4.
Theory error must also be reduced by X4.

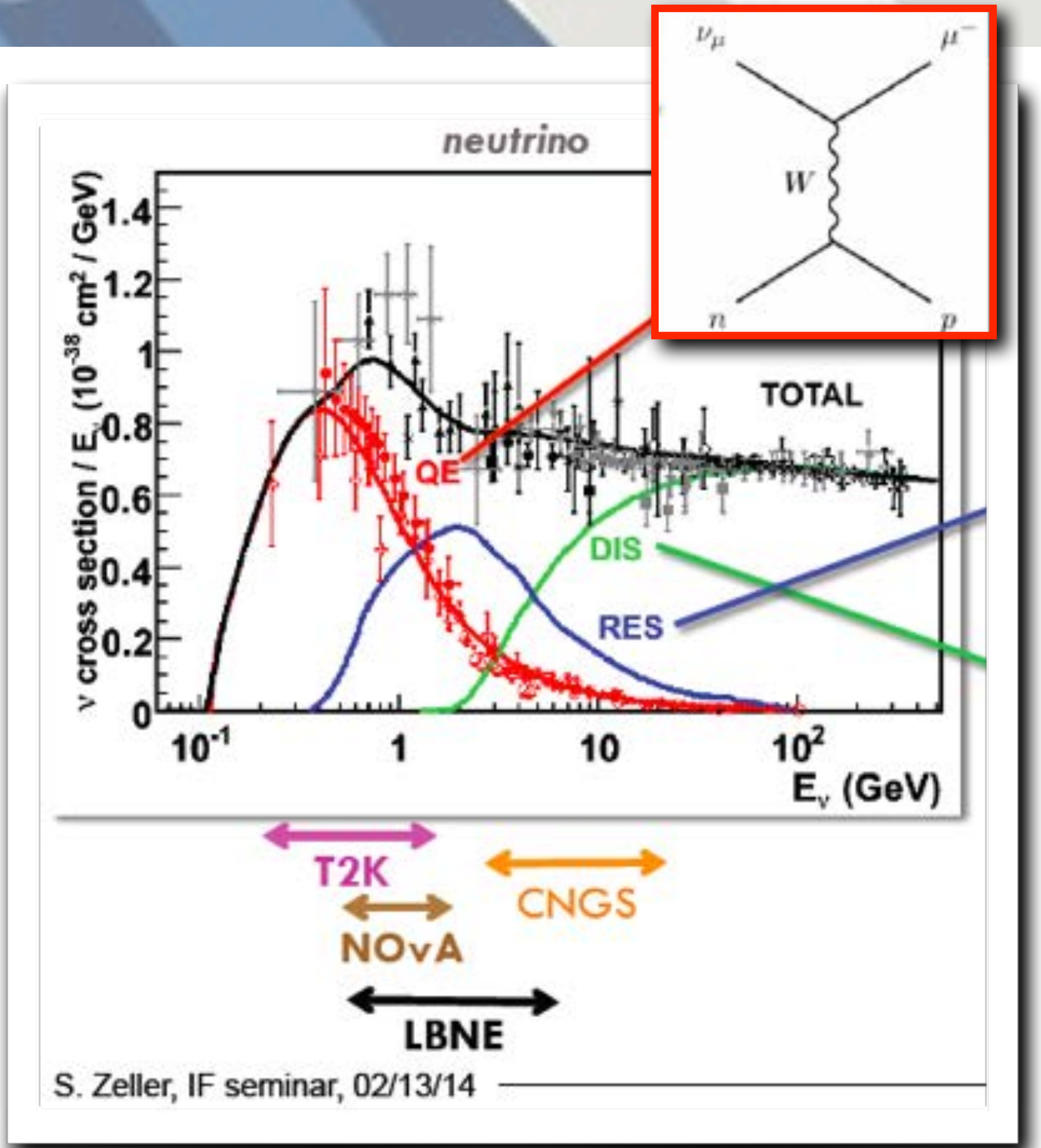


Theory error includes this diagram,
requires lattice QCD if the loop is a quark loop.
This calculation is harder than any done so far in lattice QCD.
The experiment will fail if we can't figure it out.

Neutrino physics

- ✦ Measurement of ν-oscillation parameters & possible discovery of new ν states limited by understanding of charged-current quasielastic scattering on bound neutron.

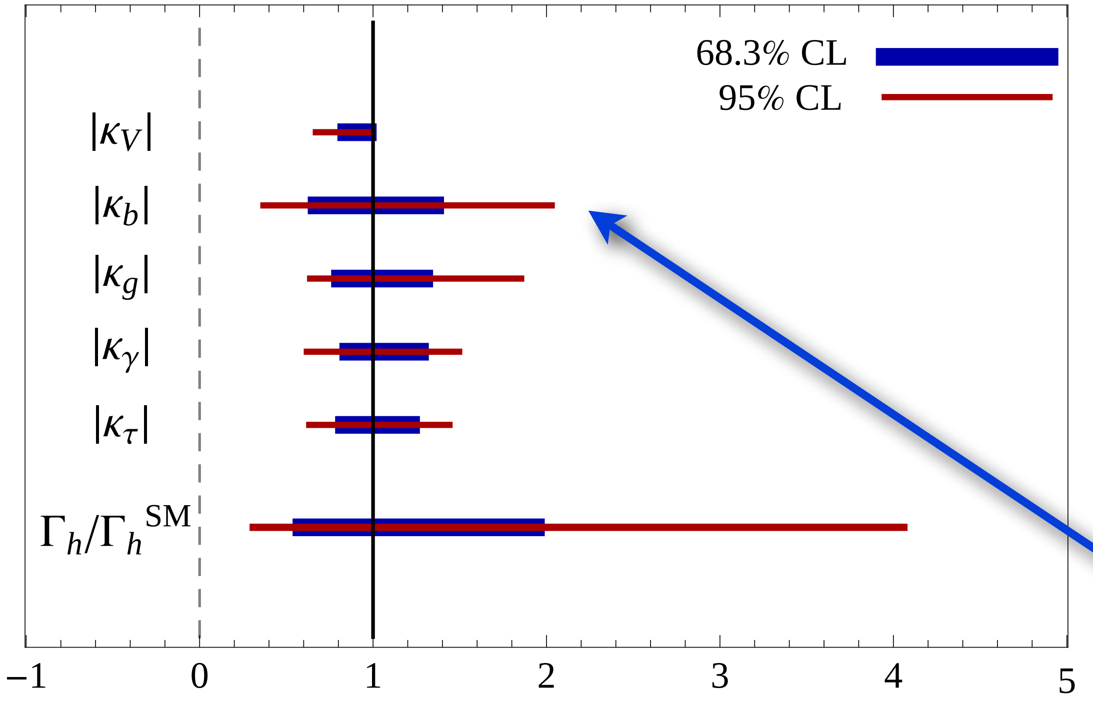
- ✦ **Obtain CCQE X-section from nucleon axial-vector form-factor $F_A(q^2)$ + nuclear models.**
  - ❖ $F_A(q^2)$ usually treated in dipole approximation, but dipole fits over different q^2 ranges & by different experiments inconsistent.



- ✦ Kronfeld co-supervising U. Chicago student on first-principles calculation of $F_A(q^2)$ merging analyticity constraints with lattice QCD
  - ❖ Completing work with Minerνa experimentalists implementing z-parameterization & external QCD input into standard GENIE Monte Carlo
  - ❖ Will soon begin lattice calculation on MILC (2+1+1)-flavor HISQ ensembles with physical pions to avoid steep chiral extrapolations.

The LHC and beyond

Strong focus of current BSM physics: composite theories approximately consistent with the observed Higgs: spin 0 particles with the same properties as those observed (even parity, about the same decay properties,..). In such theories (Ex: SU(2) gauge theory with 2 massless fermions), we expect to be able to compute additional new particles at higher mass, small deviations in decay strengths from standard model expectations.



The high-luminosity LHC will measure these branching fractions to a few % in a few years.
A high-luminosity International e+e- Collider (ILC) may measure them to a few tenths % in 10-20 years.
The standard model expectation of the Higgs total decay strength is dominated by its main decay channel, the *b*-quark channel, whose strength is governed by the *b* quark mass.
m_b is known to ~1% now from lattice QCD, but will easily known in ten years to the required 0.25%.

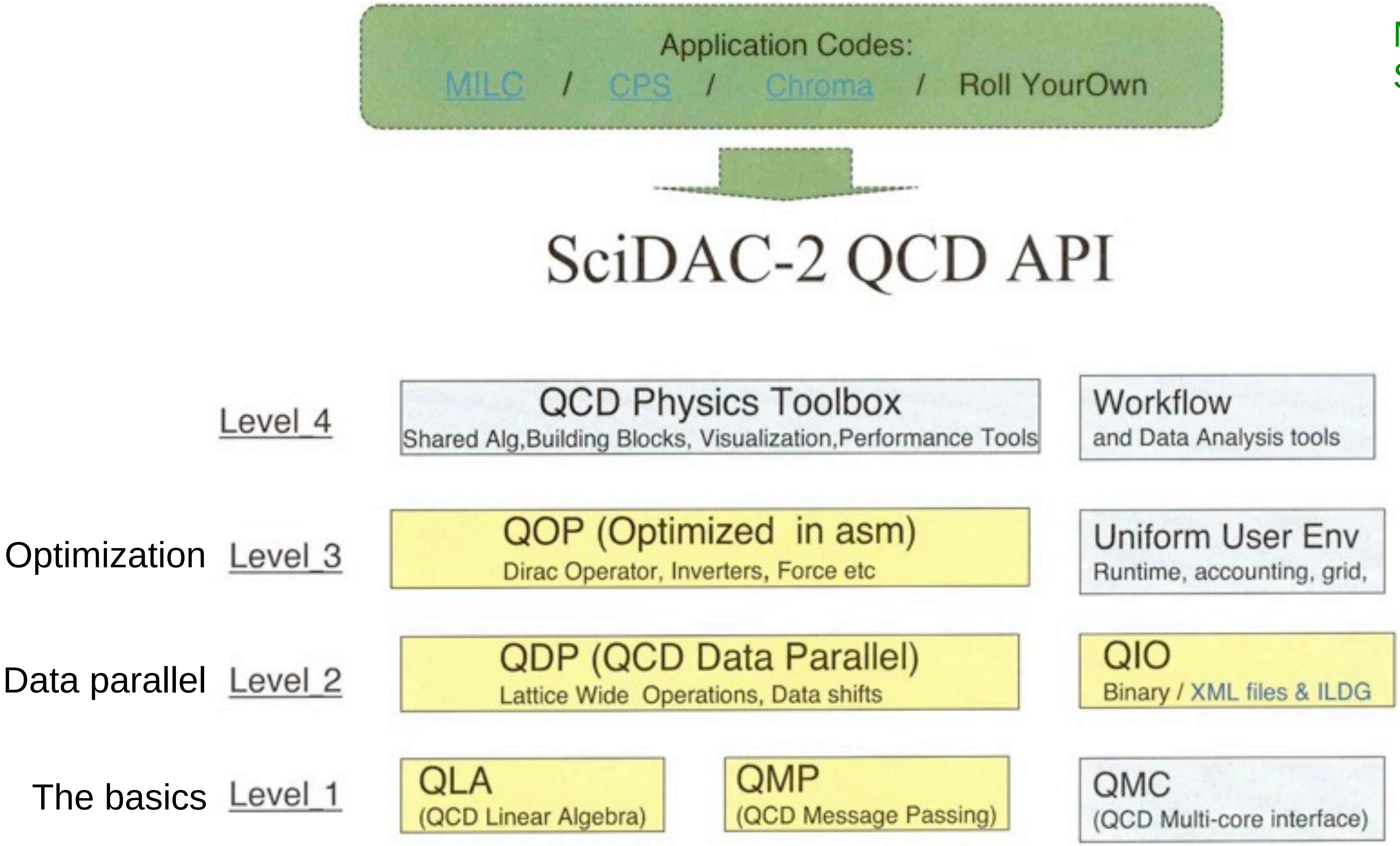
Lepage, Mackenzie, and Peskin, arXiv:1404.0319.

Current physics achievements have been built on foundation of previous SciDAC software

- USQCD software community ~20-30 people.
- Achievements include
  - community libraries for QCD programming, called the QCD API,
  - optimized high-level QCD codes and software packages,
  - porting to new platforms,
  - work with SciDAC centers and institutes and with computer scientists and applied mathematicians.
- Such sharing is not universal in HEP. The 2013 Topical Panel on Computing and Simulations:
  - recommended that an HEP Center for Computational Excellence be set up to facilitate more HEP-wide solutions to common problems and interactions with external entities (ASCR, NSF).

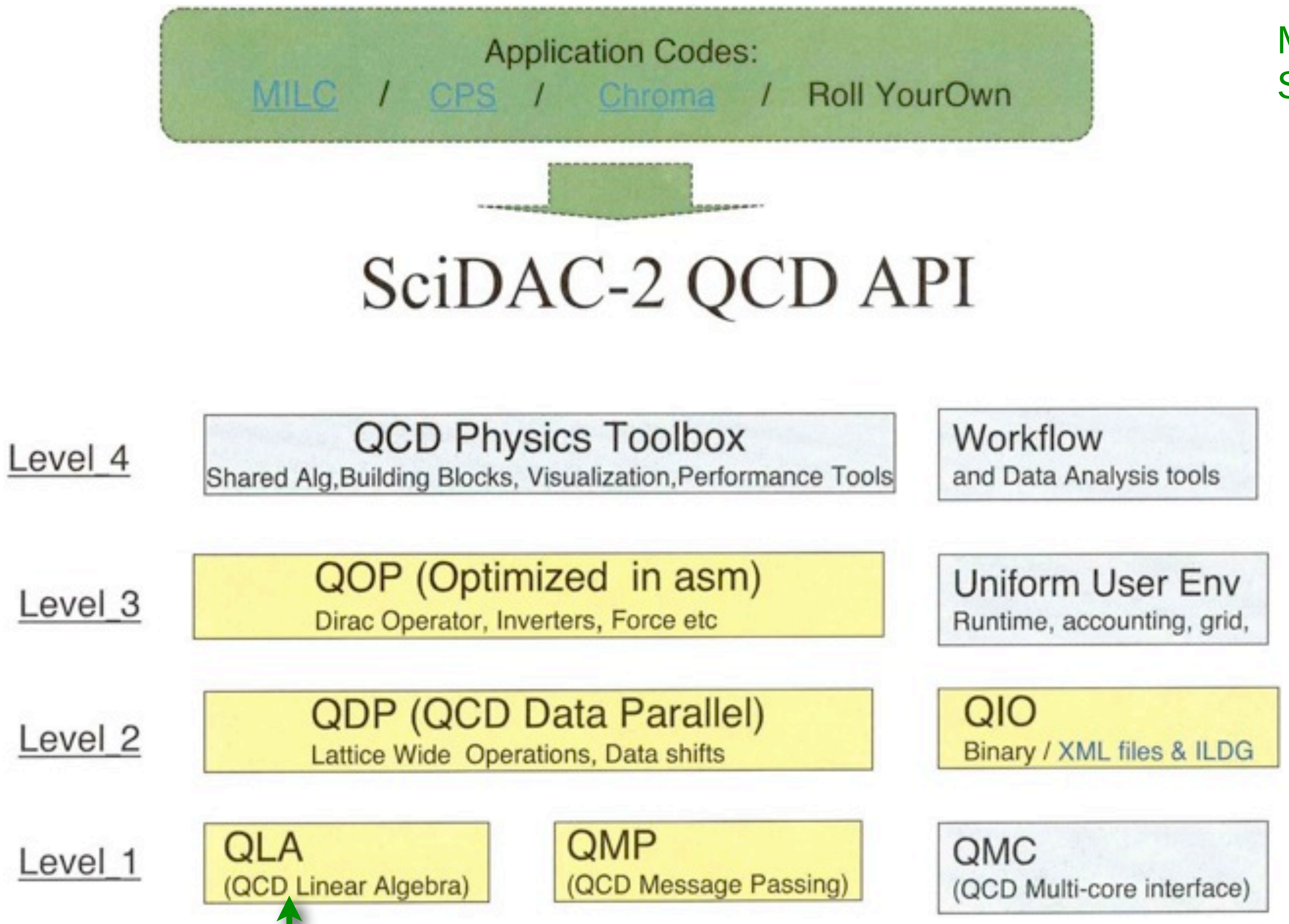
The QCD-API

Main structure was in SciDAC-1.



The QCD-API

Main structure was in SciDAC-1.



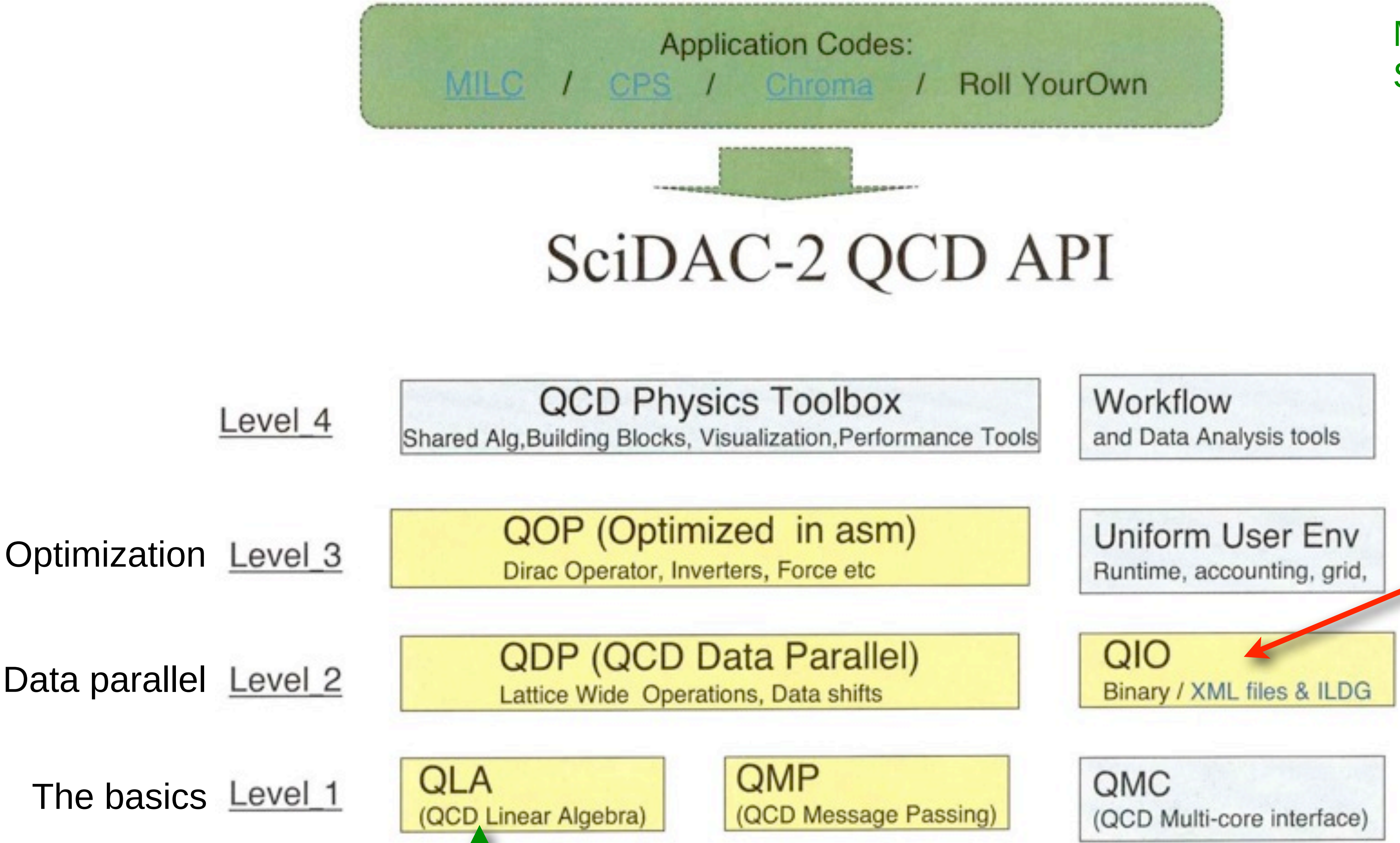
Optimization

Data parallel

The basics

Linear algebra: e.g., multiplying SU(3) matrices together

The QCD-API



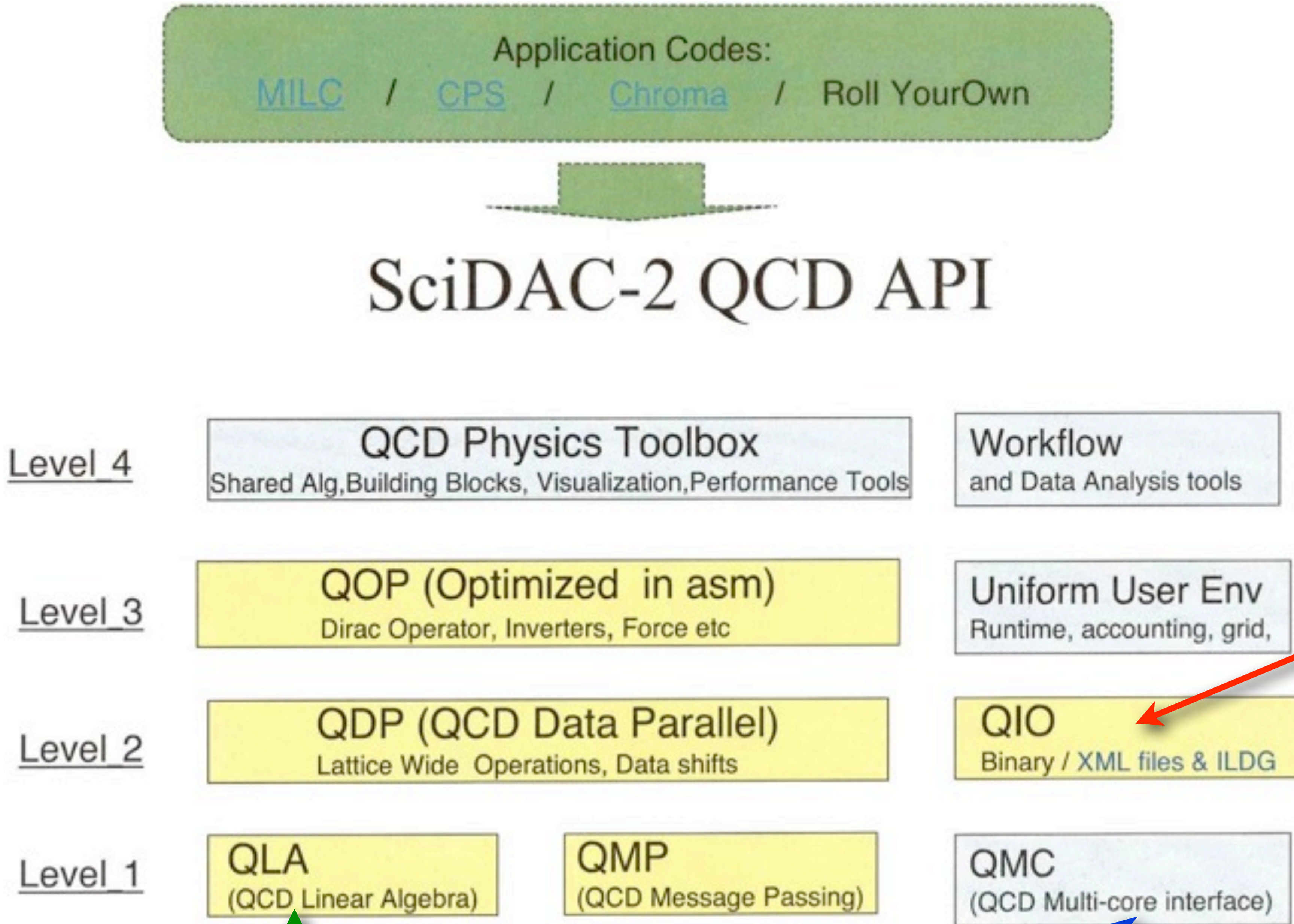
Main structure was in SciDAC-1.

I/O for lattice data types (added in SciDAC-2)

Linear algebra: e.g., multiplying SU(3) matrices together

The QCD-API

Main structure was in SciDAC-1.



Optimization

Data parallel

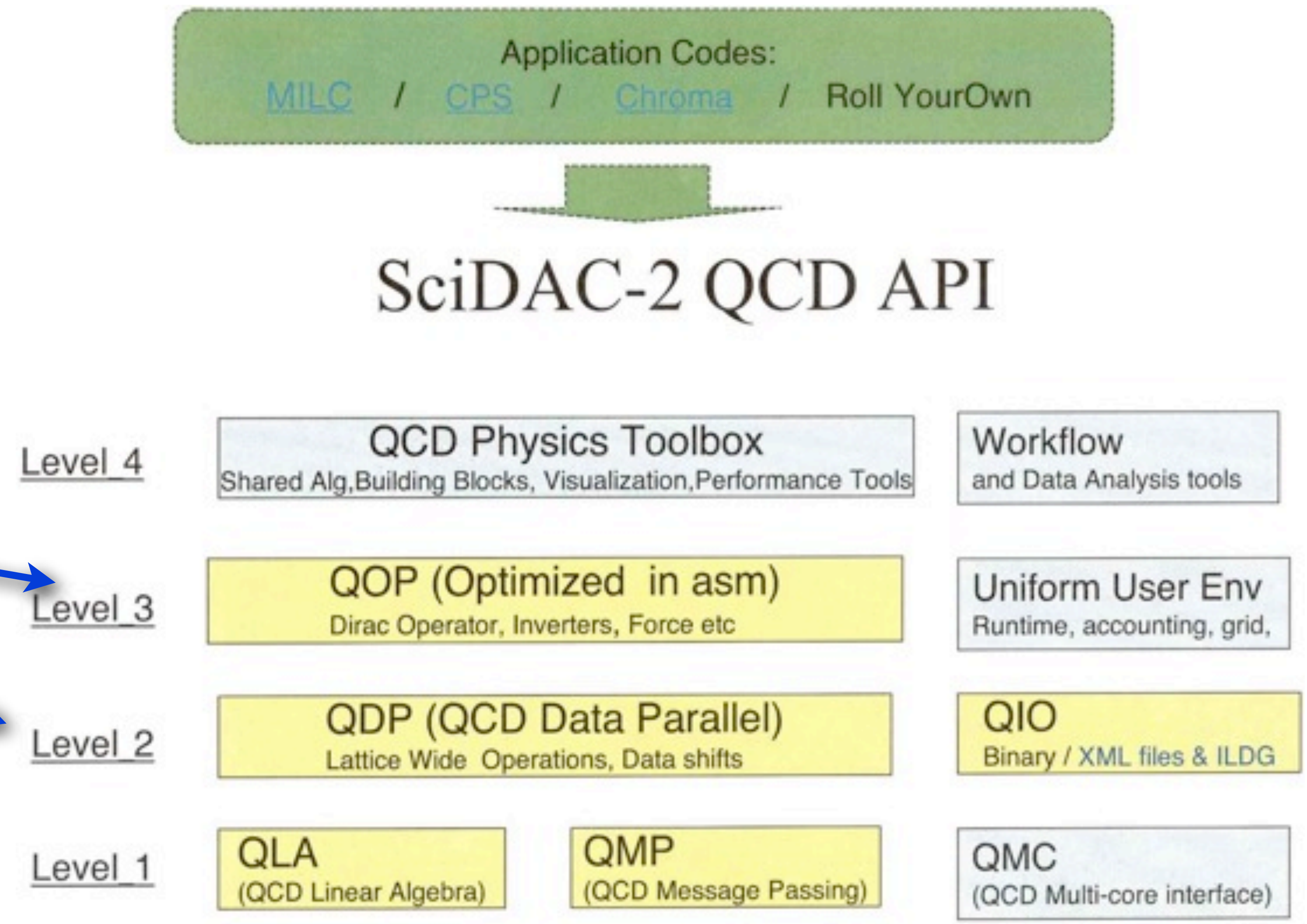
The basics

I/O for lattice data types (added in SciDAC-2)

multicore interface (active area of development now)

Linear algebra: e.g., multiplying SU(3) matrices together

Beyond-the-standard-model software



Low-level modules of the QCD API must be generalized for non-QCD gauge theories with groups other than SU(3).

This year, code for arbitrary SU(N) gauge theory has been inserted into the QOP and QDP libraries in anticipation of its use in current projects using SU(2) and SU(4) Wilson fermions.

Code for N = 4 supersymmetric Yang-Mills theory was released.

Improving software and algorithms

- Lattice calculations consist of two major parts:
  - Creating ensembles of O(1,000) gauge configurations (4D lattices with SU(3) matrices on links). A Monte Carlo process. A single large job that usually must be done on leadership-class resources.
  - Creating many quark propagators on each configuration for physics analysis. A sparse matrix problem. Requires more flops that configuration generation, but can be done in parallel in 1,000 smaller jobs. Often done efficiently on capacity resources.
- In the late ‘90s and early ‘00s, huge progress in configuration generation algorithms.
- Critical need now: improvement in quark propagators calculations.
  - g-2 and other physics challenges have essential needs here.

Quark propagator sparse matrix methods

- Intense work going on in multigrid methods.
  - Good methods have been developed and deployed.
    - Code for Wilson fermions has been deployed and is in production. (More commonly used in NP lattice QCD than in HEP.)
    - Method is being ported to staggered fermions and domain-wall fermions.
  - Working with Rob Falgout of FASTMath; Hypre code has been extended to N-dimensions and made complex, and an arbitrary Dirac operator has been implemented. Beginning go study how multigrid methods could be implemented.
- Active work going on with other approaches: domain decomposition, eigenvalue deflation, all mode averaging, ...

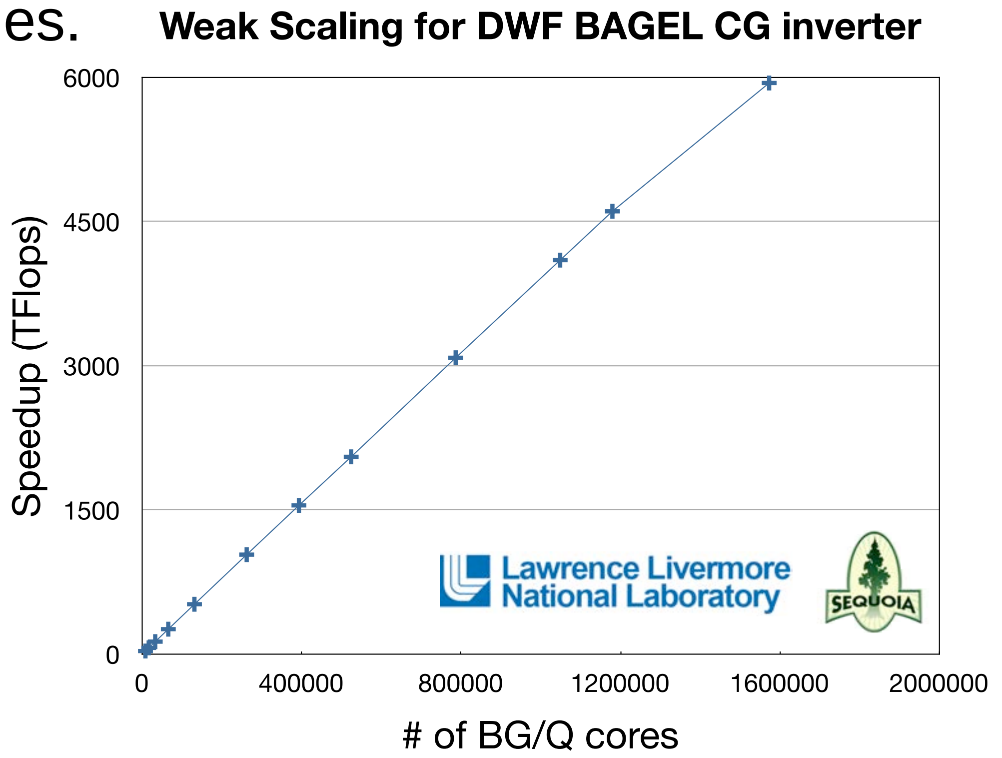
Machines

Lattice gauge theorists have been involved with the development of supercomputing from the beginning; our ability to program the largest current machines is enhanced by close relationships with vendors.

- Ken Wilson, inventor of lattice gauge theory, was an early proponent of supercomputing.
  - In the 70s, he was programming array processors in assembly language to attack critical phenomena problems for which he won the Nobel Prize. This work was in condensed matter problems like the Kondo problem. Wilson invented lattice QCD precisely in order to be able to attack particle physics problems with the methods of condensed matter.
  - Interactions have continued since, up to the recent particle physics/ condensed matter workshop in May, 2014 organized by Eduardo Fradkin and Rich Brower.
- After the introduction of Monte Carlo methods to lattice QCD in the early 80s, lattice gauge theorists worked to design machines aimed at lattice QCD
  - in academic efforts at Caltech (Cosmic Cube), Columbia, IBM (GF11, not a commercial project), Fermilab, ...

The Blue Gene line

- The Columbia University group, led by Norman Christ, won the Gordon Bell prize for price/performance in 1998 for the QCDSP, a machine purpose-built for lattice QCD.
- A team led by Al Gara that had been part of these projects went to IBM and designed the closely related (and commercial product!) BG/L, which won the Gordon Bell prize for performance in 2005.
  - The system-on-a-chip design, tightly coupled standard processor and FP unit, torus network, and style of mechanical design (small easily replaced node cards) were modeled on the Columbia machines.
- The Columbia group continued to work with the Blue Gene team throughout the Blue Gene years.
  - They designed and implemented: the interface between the processor core and the level-2 cache, and the look-ahead algorithms used to prefetch data from level-2 cache and main memory, anticipating misses in the level-1 cache.



GPUs

- Important resources at Titan, Blue Waters, dedicated QCD clusters at Fermilab and JLab.
- NVIDIA has hired two of USQCD's top GPU experts.
    - They work with academic collaborators to attain best performance,
    - Mike Clark, former BU postdoc, evaluates potential future architectures in terms of QCD (cache sizes, memory bandwidths, network bandwidth, latency sensitivity).

Intel PHIs

- Another possible path to exascale? Several USQCD groups have NDAs and very active. Cori will be a good place to learn.
    - RBC/UKQCD has begun to plan for a new generation QCD software environment that will both support high performance kernels on KNX chips and also allow more generic code to run at high performance on such many core chips.
    - Part of Fermilab/MILC effort is to investigate how useful PHIs may be in experimental HEP.
    - Our sister NP software project has active PHI project at JLab.

Summary

- US high energy physics is planning an ambitious program of new experiments over the next ten years.
- Lattice gauge theory calculations will be needed almost everywhere in this program.
- New software and algorithms will be just as critical to the success of the program of the next ten years as they have been in the last ten.