CalLat & USQCD

USQCD All Hands Meeting

17-19 April, 2014

André Walker-Loud

for

CalLat

We formed the California Lattice (CalLat) Collaboration to take advantage of the resources (people and machines) in the Bay Area and compete for a SciDAC grant to work on low-energy nuclear physics (cold QCD)

A MultiScale Approach to Nuclear Structure and Reactions: Forming the Computational Bridge between Lattice QCD and Nonrelativistic Many-Body Theory

A Grant from the DOE Office of Science through
Scientific Discovery through Advanced Computing

PI: Wick Haxton

CalLat

SciDAC Grant

LLNL

Bronis R. de Supinski	Performance	SUPER Institute
Robert Falgout	Solvers	FASTMath Institute
Tom Luu	LQCD, effective theory	==> Bonn University + Jülich
Pavlos Vranas	LQCD	

LBNL/UC Berkeley

Wick Haxton	Effective theory	PI
Esmond Ng	Linear algebra	Co-Dir., Computing; FASTMath
André Walker-Loud	LQCD/EFT	==> William & Mary + JLab
Sam Williams	Performance	SUPER Institute
Chao Yang	Linear algebra	FASTMath Institute

Nvidia

M Clark	LQCD/GPUs

LBNL/UC Merced

Juan Meza	Performance

Young researchers:

Thorsten Kurth, Ken Mcelvain, Abjinav Sarje, Mark Strother
Evan Berkowitz, Enrico Rinaldi, Chris Schroeder
Sergey Syritsyn
Mike Buchoff

LBNL
LLNL
BNL
INT

Physics

- Hadronic Parity Violation
- Harmonic Oscillator Based Effective Theory (HOBET)

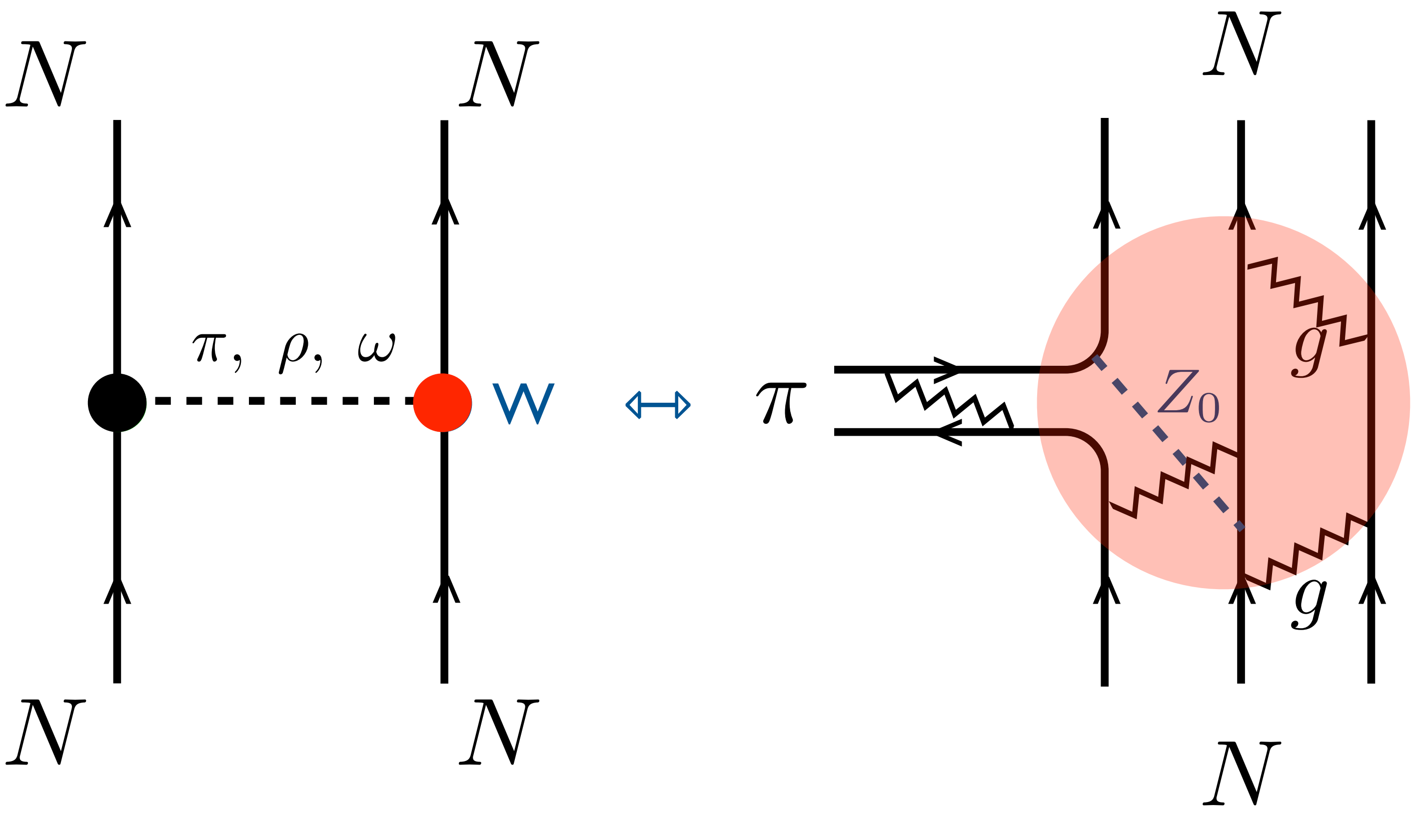
Service

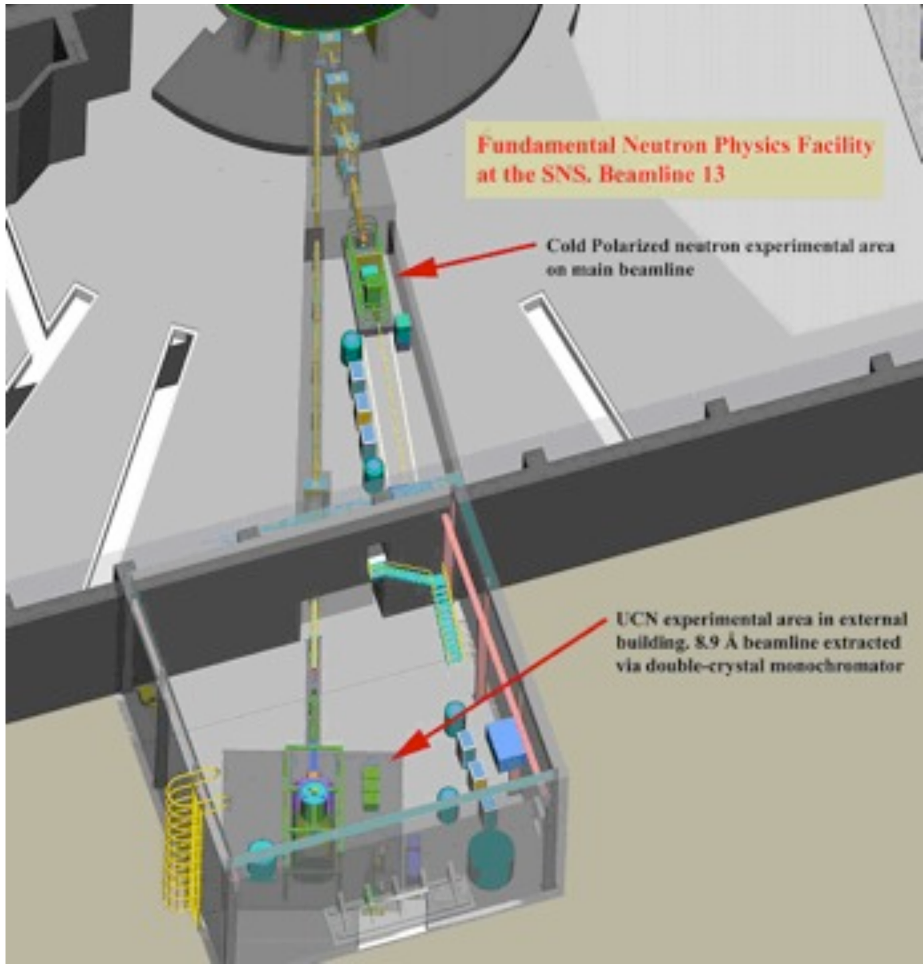
- Configuration Generation
- High-Performance I/O: HDF5 for Lattice QFT

Physics: Hadronic Parity Violation

First application: Hadronic parity nonconservation

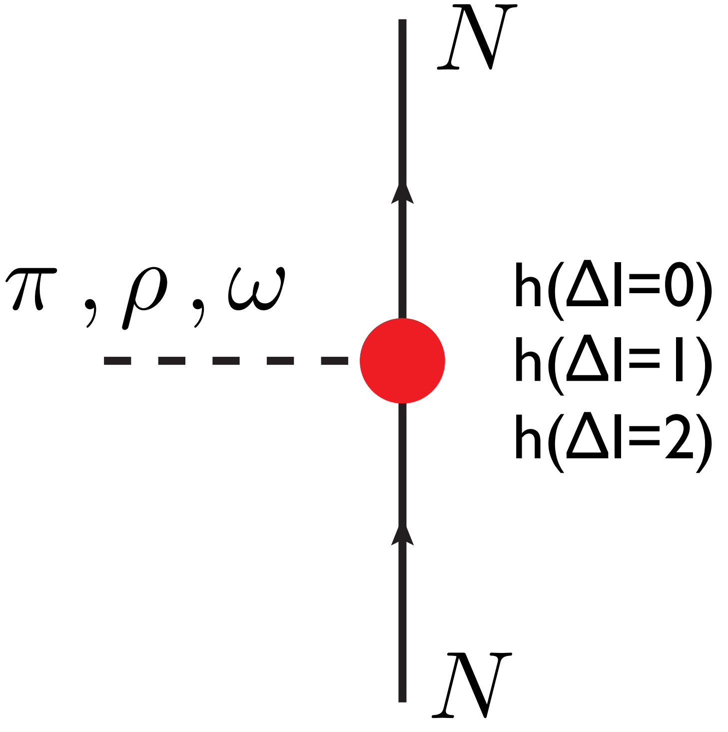
- Main goal: Neutral-current-mediated weak NN interaction (not yet isolated exp.)
- Attractive target for us because
  - there is a significant new experimental program underway at the cold neutron beam-line of the SNS
  - the bridge from NN LQCD to light nuclei is critical to the global analysis
  - new application for LQCD
  - challenging calculations but 20% uncertainties significant advancement





Hadronic parity nonconservation

Parity Violating Vertex



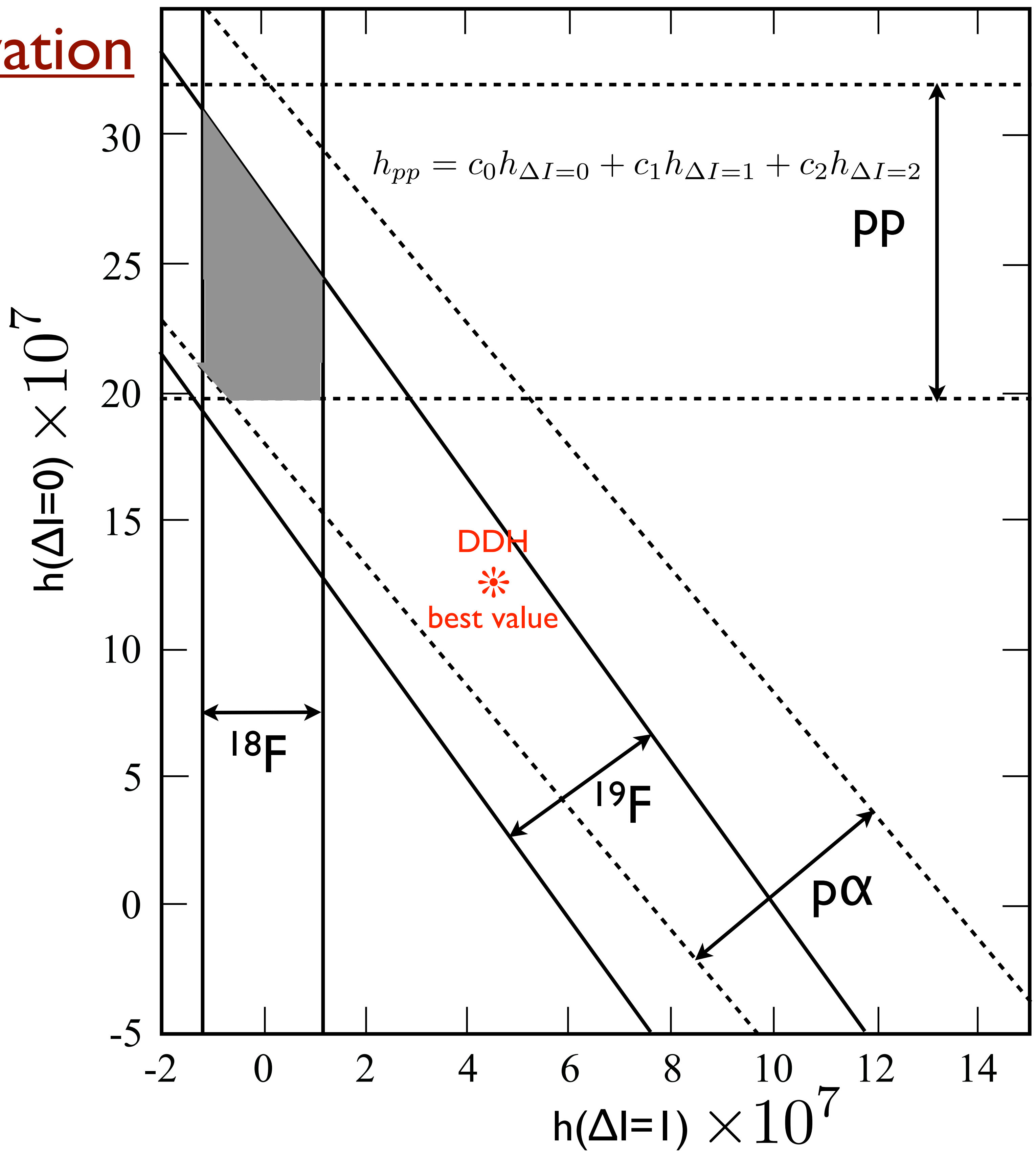
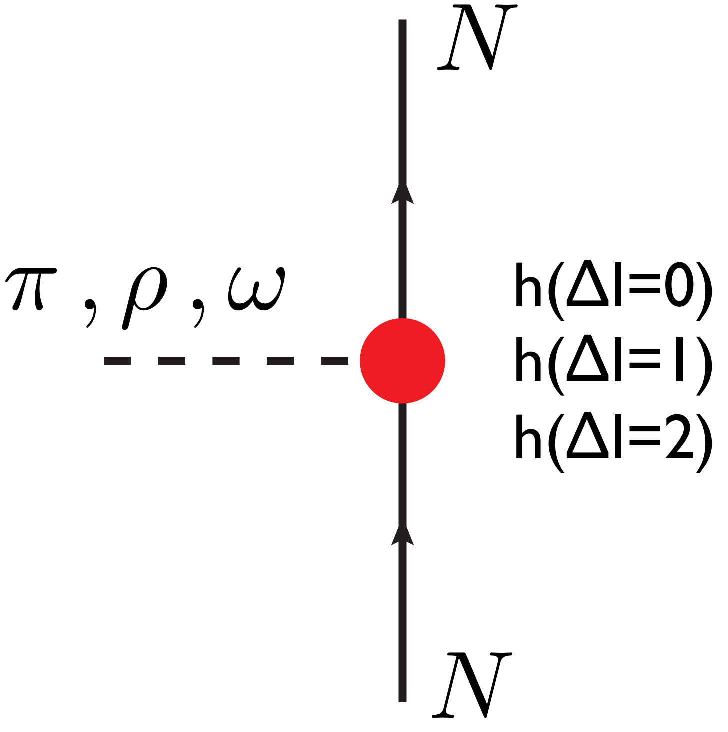
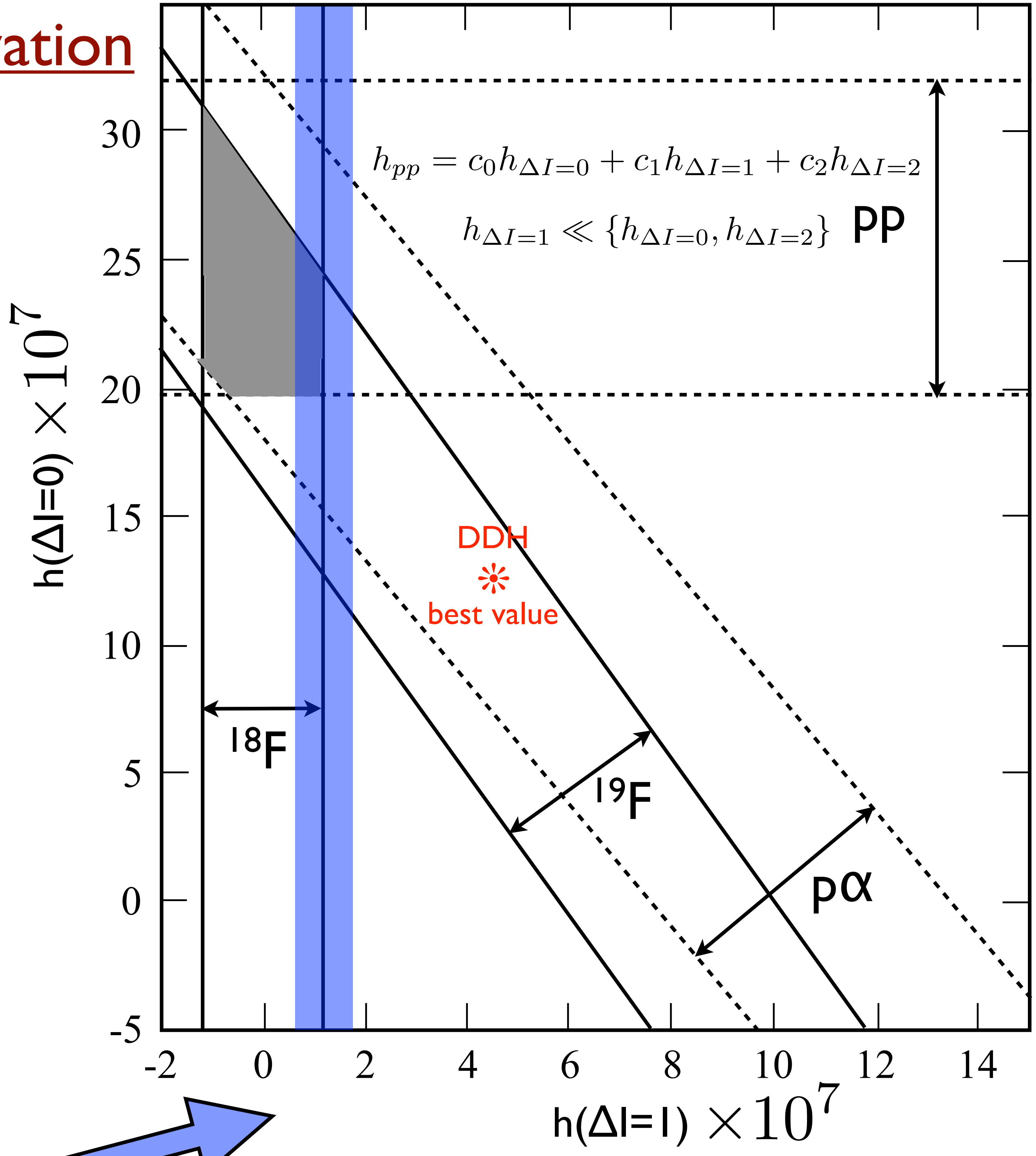


Figure: Haxton, Holstein, Prog.Part.Nucl.Phys. 71 (2013)

Hadronic parity nonconservation

Parity Violating Vertex





first LQCD calculation of h_π^1 for

L=2.5 f a=0.123f m$_\pi$= 389 MeV

many systematics not addressed

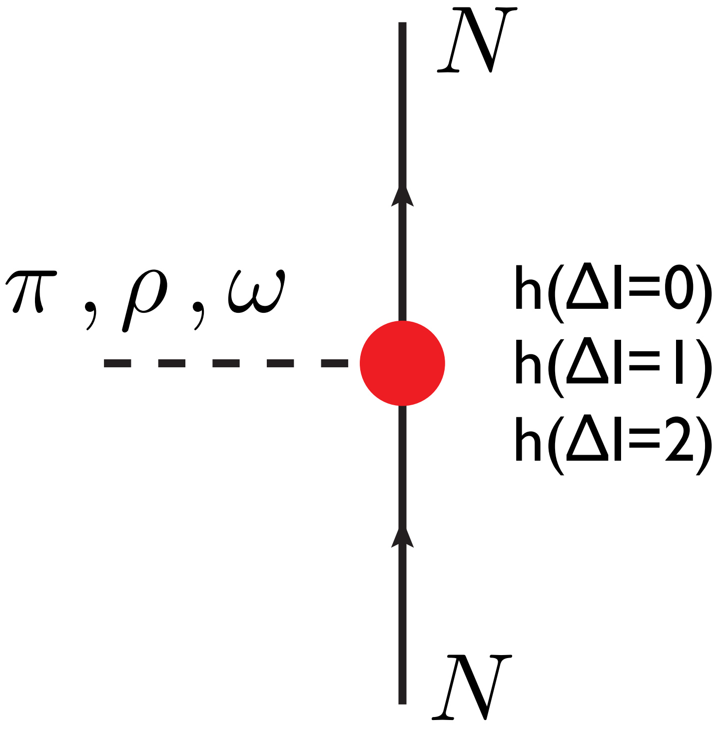
J. Wasem Phys. Rev. C85 (2012) 022501

Figure: Haxton, Holstein, Prog.Part.Nucl.Phys. 71 (2013)

Hadronic parity nonconservation

potential impact of a future calculation of $h_{\Delta I=2}$

Parity Violating Vertex



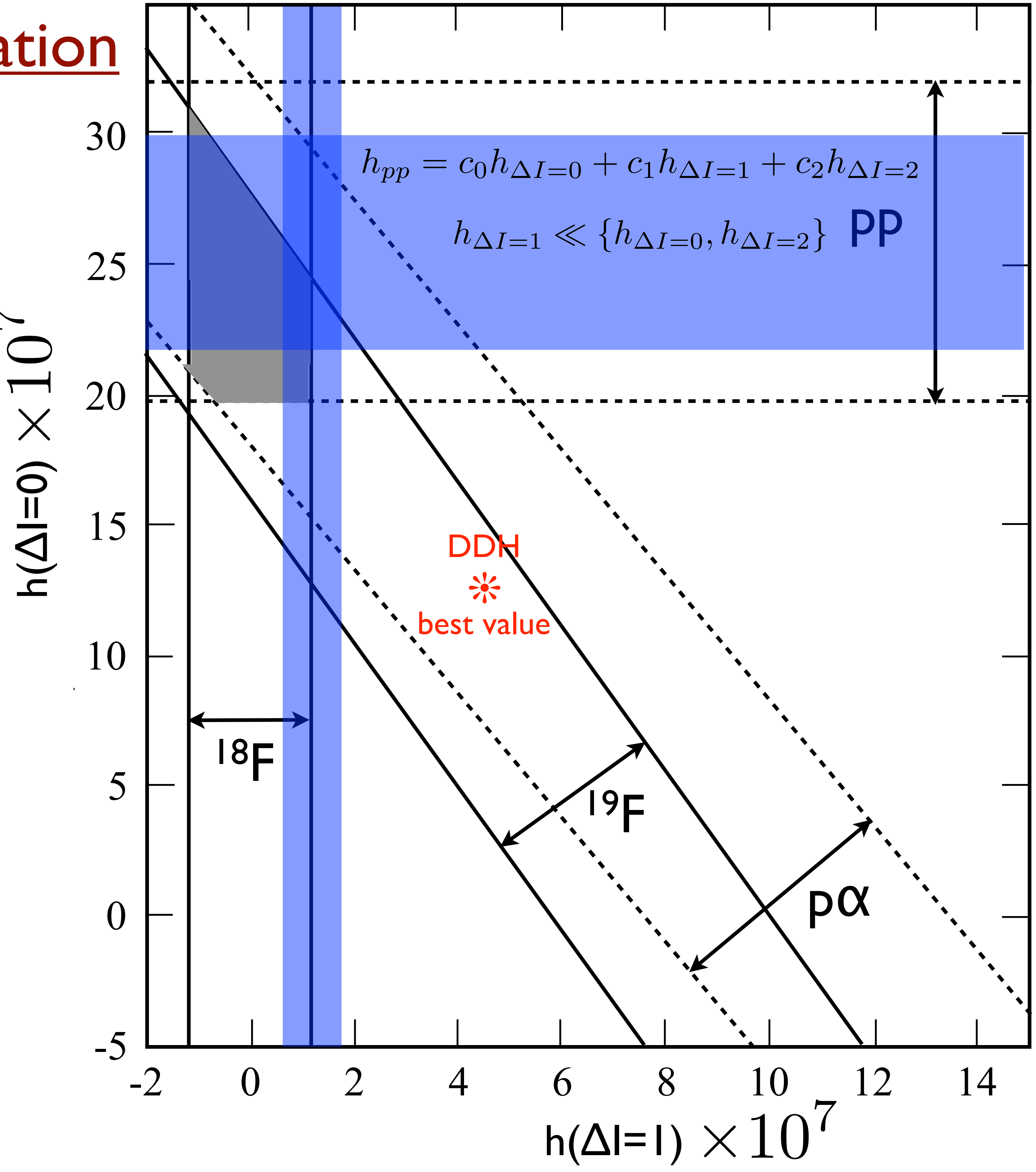


Figure: Haxton, Holstein, Prog.Part.Nucl.Phys. 71 (2013)

Physics: Hadronic Parity Violation

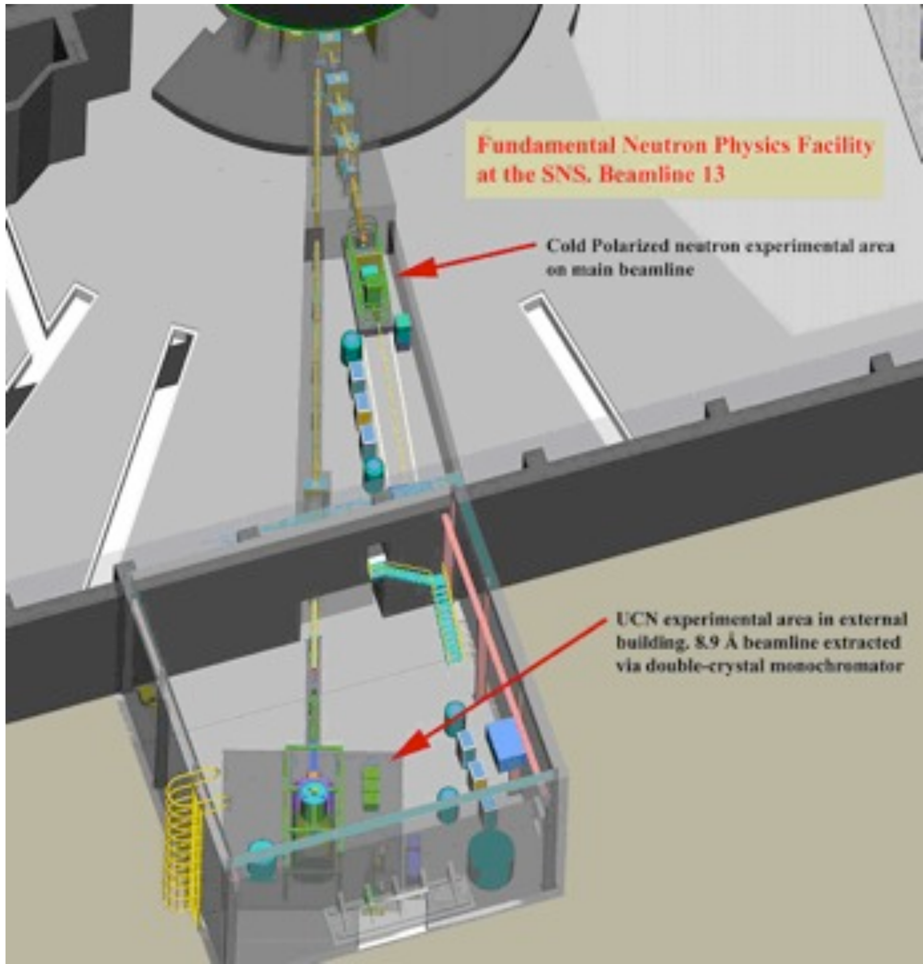
NPDGamma Experiment is designed to measure $h_{\Delta I=1} \quad (h^1_{\pi NN})$

$$(N \rightarrow N + \pi)$$

J. Wasem made the first pioneering calculation of this quantity

- unphysical pion mass $m_\pi \sim 400 \text{ MeV}$
- three quark operator $N^{(-1/2)}$ used for $N\pi$ state
  (need multi-hadron operators)
- disconnected loops not determined
  (potentially large strange loops)
- no operator renormalization
  (operator mixing)

We are working to address all these systematics

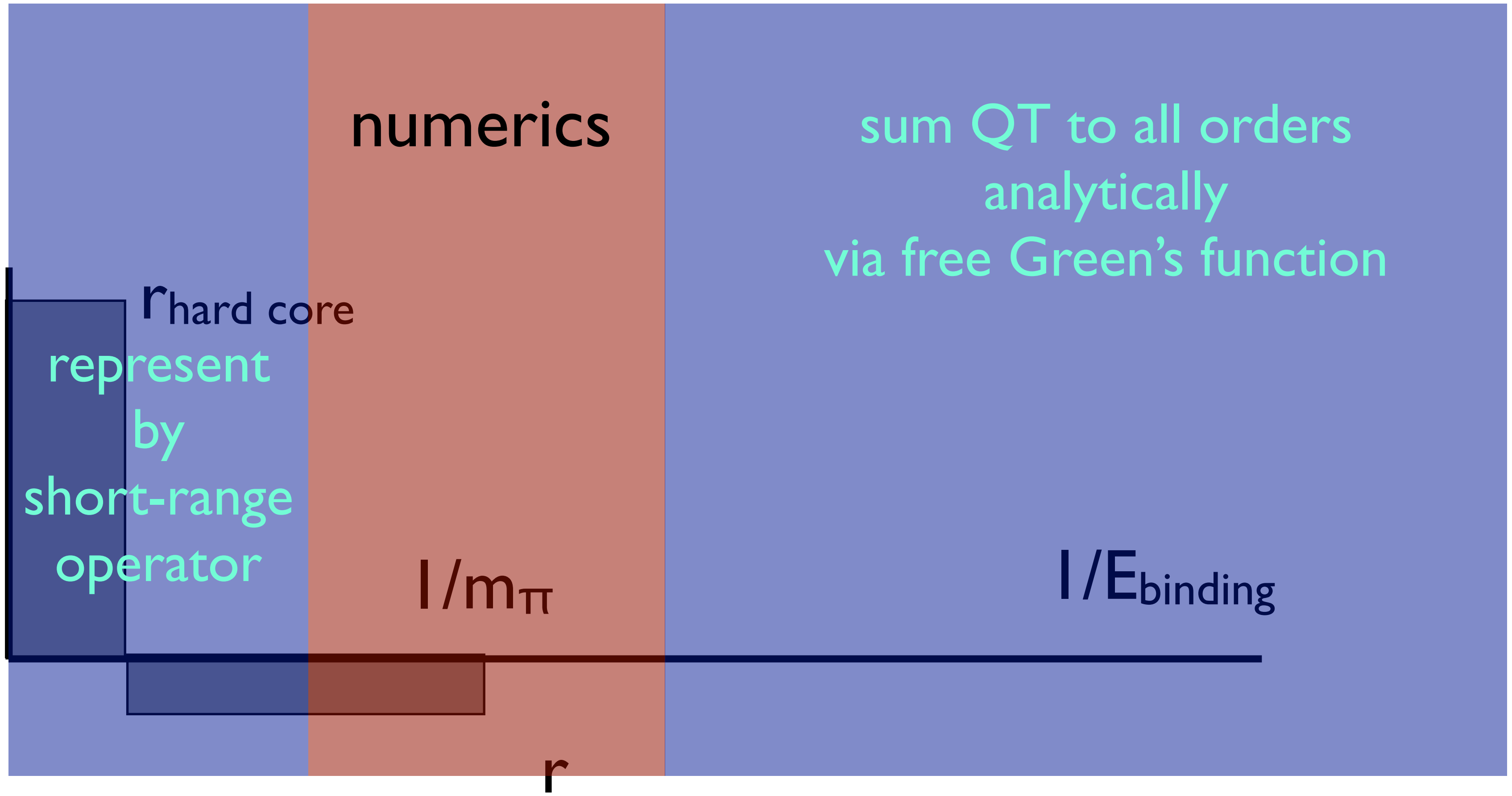


Physics: Harmonic Oscillator Based Effective Theory

Haxton & Luu
E. Ng & C. Yang & S. Williams

Coupling LQCD to a Nonrelativistic Effective Theory

CalLat is coupling LQCD results to a nonrelativistic effective theory (HOBET) constructed in an explicitly antisymmetric basis:


numerics

sum QT to all orders analytically via free Green's function

$r_{\text{hard core}}$

represent by short-range operator

$1/m_\pi$

$1/E_{\text{binding}}$

r

Goal is to create an apparatus that can make predictions in more complicated nuclear systems, taking from LQCD that which is unknown. Themes: separations of scale, avoidance of the sign problem

Physics: Harmonic Oscillator Based Effective Theory

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The Bloch-Horowitz Equation

Strategy: Use LQCD to calculate uncertain quantities (like hadronic PNC)
But use experiment to constrain other nuclear effects

Formalism based on the Bloch-Horowitz equation

Given $H|\Psi\rangle = E|\Psi\rangle \Rightarrow H_{eff}P|\Psi\rangle = EP|\Psi\rangle$

where if $H = T + V$ it can be shown

$$H_{eff} = \frac{E}{E - TQ}\left(T - \frac{TQT}{E} + V + V\frac{1}{E - QH}QV\right)\frac{E}{E - QT}$$

P+Q=1, P finite   Nonlinear eigenvalue problem: self-consistent solution

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This resummation builds in the correct long-distance behavior:
can be derived from the free Green's function + a matrix inversion in P

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$$H_{eff} = \frac{E}{E-TQ}\left(T - \frac{TQT}{E} + V + \boxed{V\frac{1}{E-QH}QV}\right)\frac{E}{E-QT}$$

Short range, nearly energy independent: rapidly converging expansion

$$V_{eff} = a_{LO}^{3S1}\delta(\vec{r}) + a_{NLO}^{3S1}\left[\delta(\vec{r}), \vec{\nabla}^2\right] + \ldots$$

Physics: Harmonic Oscillator Based Effective Theory

Haxton & Luu
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The low-energy constants can be determined directly from experiment

P is a compact basis of harmonic oscillator Slater determinants

Pick an energy E >0, for which the phase shift $\delta(E)$ is known

In the continuum, a solution must exist at each E: $P|\Psi(E)\rangle$

Build in the correct outgoing wave (the correct infrared behavior)

$$\frac{E}{E-QT} \to G(E,\delta(E)) \quad \text{then} \quad \frac{E}{E-QT}P|\Psi\rangle \to |\Psi(\delta)\rangle_{asymptotic}$$

But in general the solution in P will not yield an eigenvalue at E

Thus adjust a_{LO}^{3S1} until a solution is obtained at E

Short-range physics can be determined because correct infra-red behavior has been built in

Physics: Harmonic Oscillator Based Effective Theory

Connection to LQCD

Haxton & Luu
E. Ng & C.Yang & S.Williams

We are free to take $\delta(E)$ from LQCD, for this matching

But as experiment precisely determines the strong-interaction phase shifts, using experiment would give us more accurate results

But the hadronic weak phase shift is not known experimentally

Thus we must compute $\delta_{weak}^{LQCD}(E)$

One computed, we can then determine the PNC potential that generates this phase shift

$$a_{weak}^{LO}\ \vec{\sigma}\cdot\left[\vec{\nabla},\delta(\vec{r})\right]$$

The technique for accomplishing this has to do with the fact that certain long-distance moments of $|\Psi\rangle$ are equivalent to those of $P|\Psi\rangle$

$$\int d\vec{r}\ r^{\Lambda}e^{-r^2/2}\ \Psi(\vec{r})\equiv\int d\vec{r}\ r^{\Lambda}e^{-r^2/2}\ P\Psi(\vec{r})$$

Physics: Harmonic Oscillator Based Effective Theory

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As the details are a bit involved, here we just show the results of this method, applied to a realistic strong interaction "toy model," for a case where P consists of $\Lambda \leq 8\hbar\omega$ shells

The effective range expansion is reconstructed to high orders, very accurately, using just the P-space information we have described:

Parameter	Projected	Exact
a	1.26707	1.26735
r_0	0.700041	0.700083
v_2	0.0186633	0.0186273
v_3	9.94282×10^{-3}	9.92127×10^{-3}
v_4	3.24082×10^{-5}	3.28324×10^{-5}

Service: Configuration Generation

We are coordinating with JLAB+WM+ to generate an ensemble of Isotropic-Clover Wilson configurations (see new proposal) using LLNL resources which are designed for "nuclear physics" (NN,NNN,NNN..., spectroscopy, N-structure,...)

Details of releasing these configurations are still being worked out, but we plan to release them to USQCD modulo some exclusive projects

Service: High-Performance I/O: HDF5 for Lattice QFT

See next talk!

(Andrew & André)

Service: High-Performance I/O: HDF5 for Lattice QFT

High-Performance I/O: HDF5 for Lattice QCD

Thorsten Kurth[*], Abhinav Sarje[†], Andrew Pochinsky[‡] and André Walker-Loud[§][¶]

[*] Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. Email: tkurth@lbl.gov
[†] Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA. Email: asarje@lbl.gov
[‡] Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA, USA. Email: avp@mit.edu
[§] Physics Department, The College of William & Mary, Williamsburg, VA, USA. Email: walkloud@wm.edu
[¶] Theory Division, Jefferson Laboratory, Newport News, VA, USA.

Thanks to Sergey Syritsyn, I got introduced to and fell in love with HDF5 (2012?).

Since then, I have been proselytizing and incorporating it into all my work.

The SciDAC effort seemed perfect for incorporating HDF5 into our software stack

Why HDF5?

- It is professionally maintained (HDF Group)
- The code is free and "open source"
- HDF5 is one of the codes used to stress test new machines/file systems @ the Leadership Class HPC centers
- standardized file type
- portable/backwards compatible
- hooks from C, C++, Python, Matlab, "Mathematica", ...
- alleviates us from needing to worry about I/O
- replaces involved QIO with simple calls to HDF5 routines

Why HDF5?

- “smart” meta-data wrapper on top of very flexible, hierarchical data structures (inside looks like linux file system)
- data is self-descriptive (real, float, double, BigEndian, ...)
- “arbitrary” sized arrays are natural data types for HDF5
- a single file could store either (or all) configuration:propagator:eigenvectors:correlators:...
- post alter data with completely different data type/size etc, delete trees, “repack” to recover space
- supports chunking/striping to optimize I/O for given file system

Service: High-Performance I/O: HDF5 for Lattice QFT

Two implementations so far:

QLUA (publicly available)

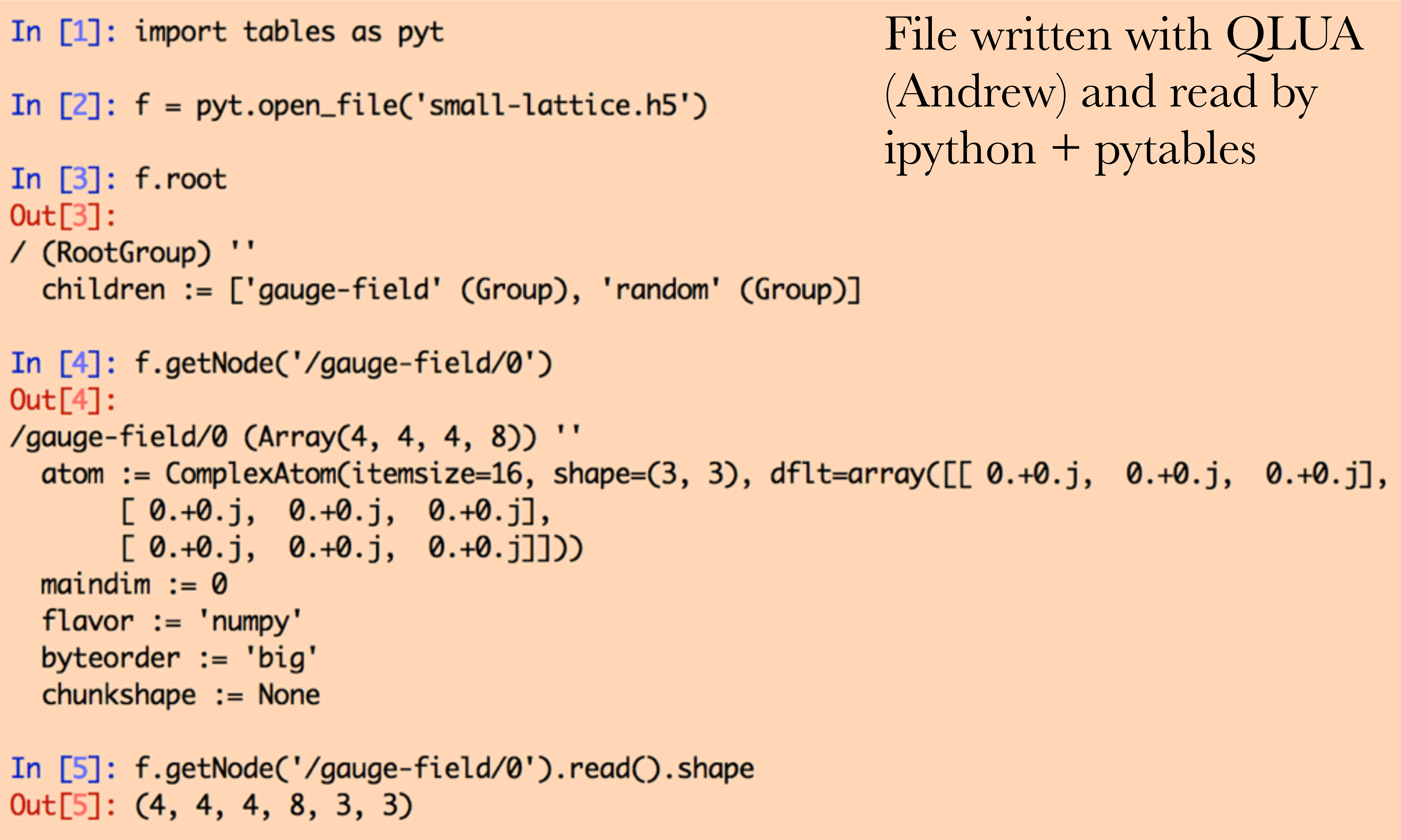
QDP++ (almost publicly available)

Service: High-Performance I/O: HDF5 for Lattice QFT

QDP++ *(Thorsten Kurth, Abhinav Sarje, AWL)*

- ☐ optional compile with qdp++ (--enable-hdf5 --with-hdf5=/path/parallel/hdf5)
- ☐ copied the xml reader/writer class
- ☐ can write any structure (LatticeColorMatrix, LatticeDiracPropagator,...) although not all implemented yet
- ☐ largely protected from job failures (closed trees can't be corrupted)
- ☐ 10-20% outperforms QIO on Hopper, Edison, Edge, Mira, ...
- ☐ more stable I/O performance
- ☐ will add "node attribute" to describe data layout so anyone can easily read in (with different code)
- ☐ code can easily be stripped-out for standalone use
- ☐ interface through Chroma
- ☐ converters for QIO/LIME <==> HDF5

Service: High-Performance I/O: HDF5 for Lattice QFT



```
In [1]: import tables as pyt

In [2]: f = pyt.open_file('small-lattice.h5')

In [3]: f.root
Out[3]:
/ (RootGroup) ''
  children := ['gauge-field' (Group), 'random' (Group)]

In [4]: f.getNode('/gauge-field/0')
Out[4]:
/gauge-field/0 (Array(4, 4, 4, 8)) ''
  atom := ComplexAtom(itemsize=16, shape=(3, 3), dflt=array([[ 0.+0.j,  0.+0.j,  0.+0.j],
        [ 0.+0.j,  0.+0.j,  0.+0.j],
        [ 0.+0.j,  0.+0.j,  0.+0.j]]))
  maindim := 0
  flavor := 'numpy'
  byteorder := 'big'
  chunkshape := None

In [5]: f.getNode('/gauge-field/0').read().shape
Out[5]: (4, 4, 4, 8, 3, 3)
```

File written with QLUA (Andrew) and read by ipython + pytables

Service: High-Performance I/O: HDF5 for Lattice QFT

QLUA *(Andrew Pochinsky)*

- See Andrew's slides