Connecting Lattice QCD and Non-relativistic Effective Theory: A Multi-Scale Approach to Nuclear Physics

Wick Haxton and Tom Luu for CalLat

- Physics motivations and applications
- Scales and scale separation in nuclear physics
- Lattice QCD interface

CalLat Team

LLNL

Bronis R. de Supinski	Performance	SUPER
Robert Falgout	Solvers	FASTMath
Tom Luu	LQCD, effective theory	Co-Dir., Science
Ron Soltz	LQCD	
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Andre Walker-Loud	LQCD	
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Chao Yang	Linear algebra	FASTMath

Nvidia

Michael Clark	LQCD/GPUs

LBNL/UC Merced

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Inspired by and Built on Previous SciDAC Efforts

UNEDF/NUCLEI
Nonrelativistic Nuclear Structure

NP/HEP USQCD
(Cold Lattice QCD)

Inspired by and Built on Previous SciDAC Efforts

UNEDF/NUCLEI
Nonrelativistic Nuclear Structure

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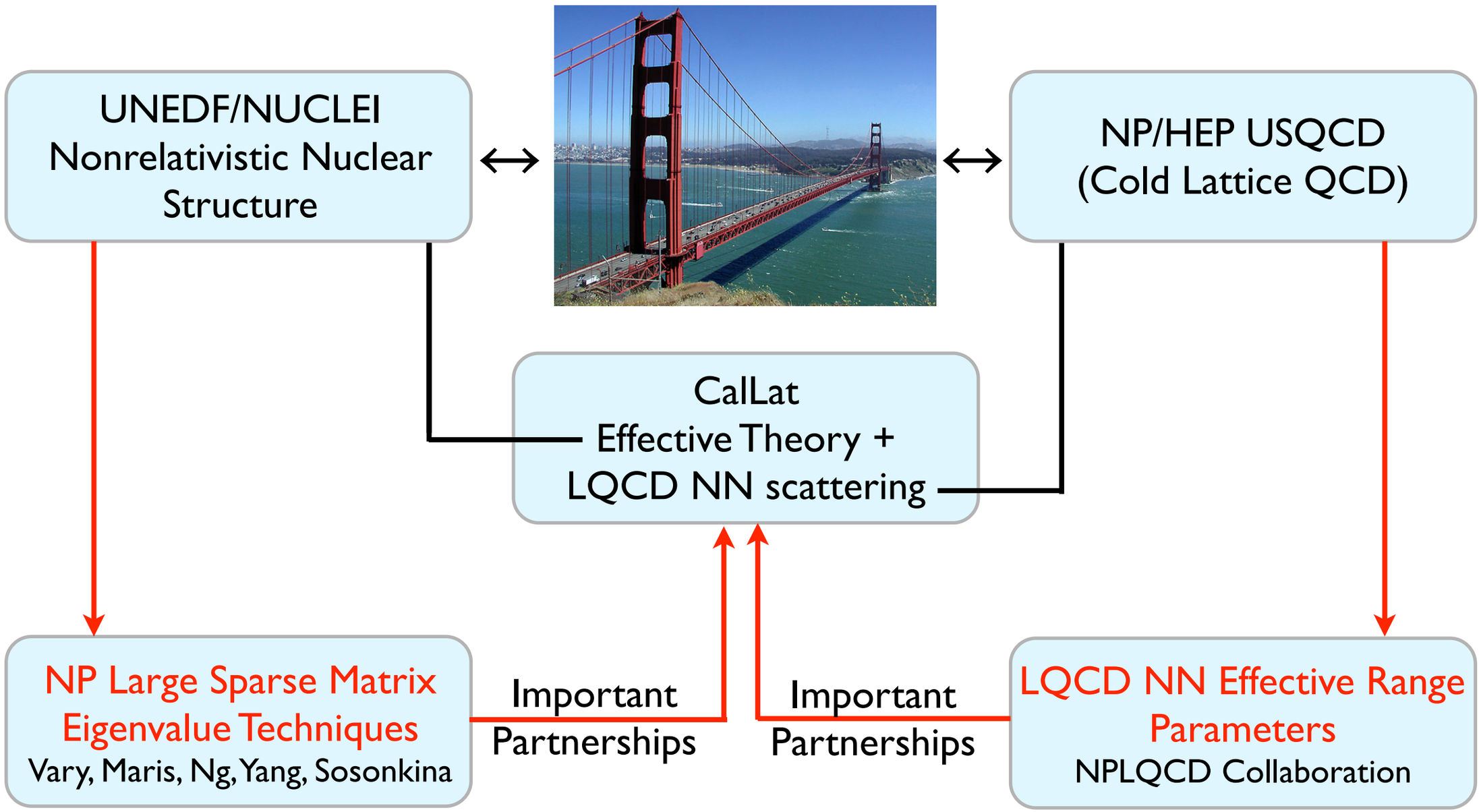
↔

NP/HEP USQCD
(Cold Lattice QCD)

CalLat
Effective Theory +
LQCD NN scattering

Inspired by and Built on Previous SciDAC Efforts



Traditional Potential-Model Framework

Parameterize the "hard" NN interaction using scattering data → V_{NN}

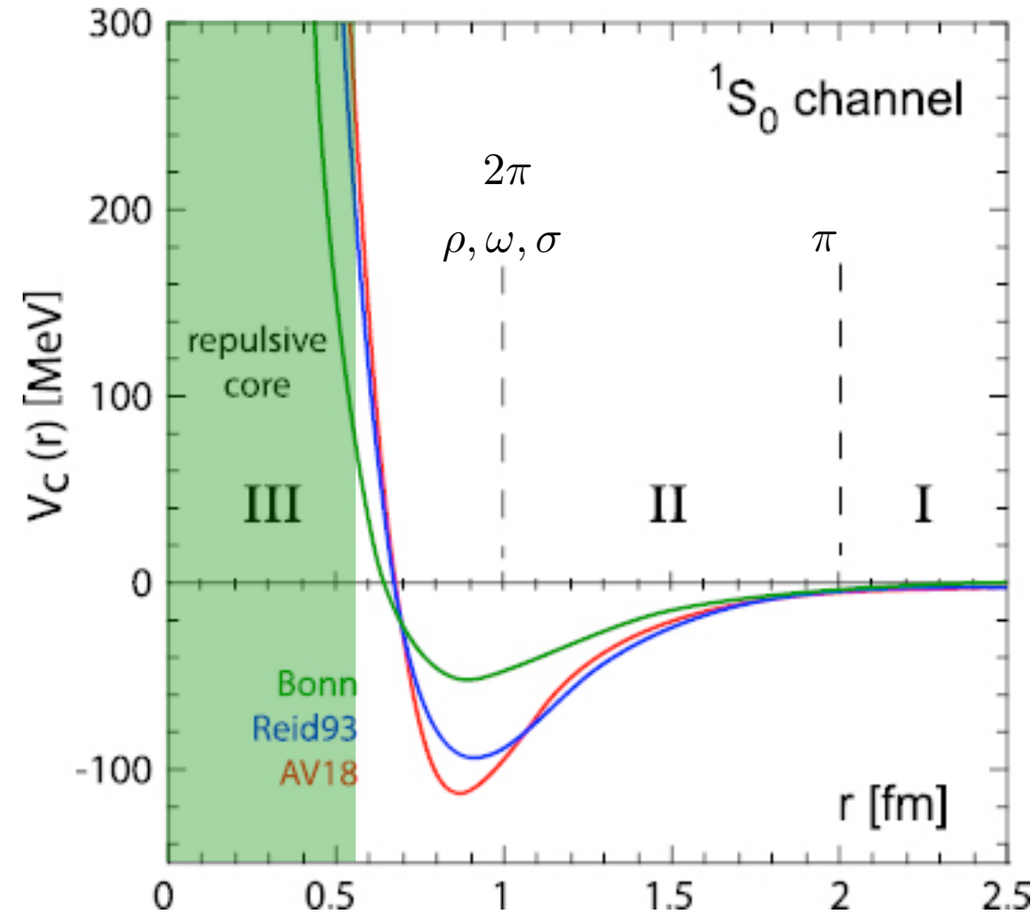
⇓

Develop an approximate "softer" V_{NN}^{eff} to enable a many-nucleon calculation in a finite P

⇓

Perform a C.I. calculation to obtain "the wave function"

⇒



- Hard (~10^3 MeV), repulsive small-distance interaction: nonperturbative and model-based

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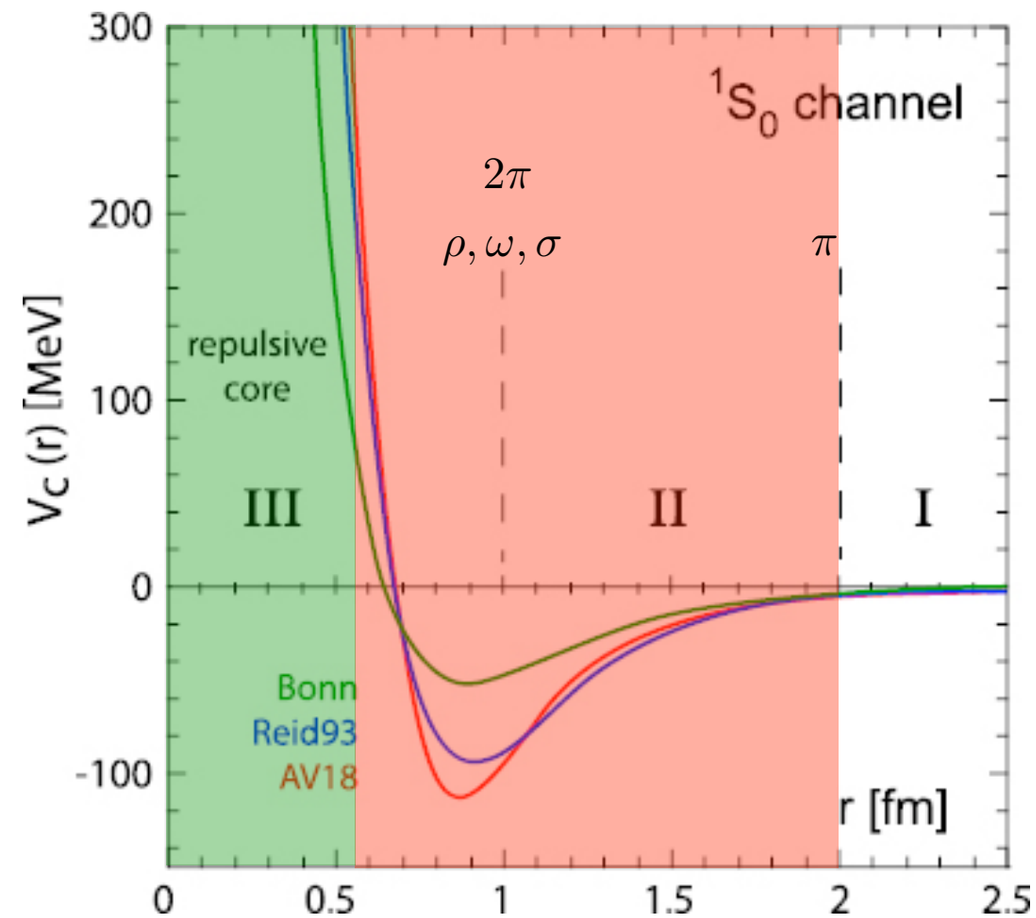

- Hard (~10^3 MeV), repulsive small-distance interaction: nonperturbative and model-based
- Weaker (~50 MeV) attractive mid-range interaction

Traditional Potential-Model Framework

Solution yields a third (anomalous) scale $1/\sqrt{M\,E_{binding}}$ → multiscale

⇓

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⇓

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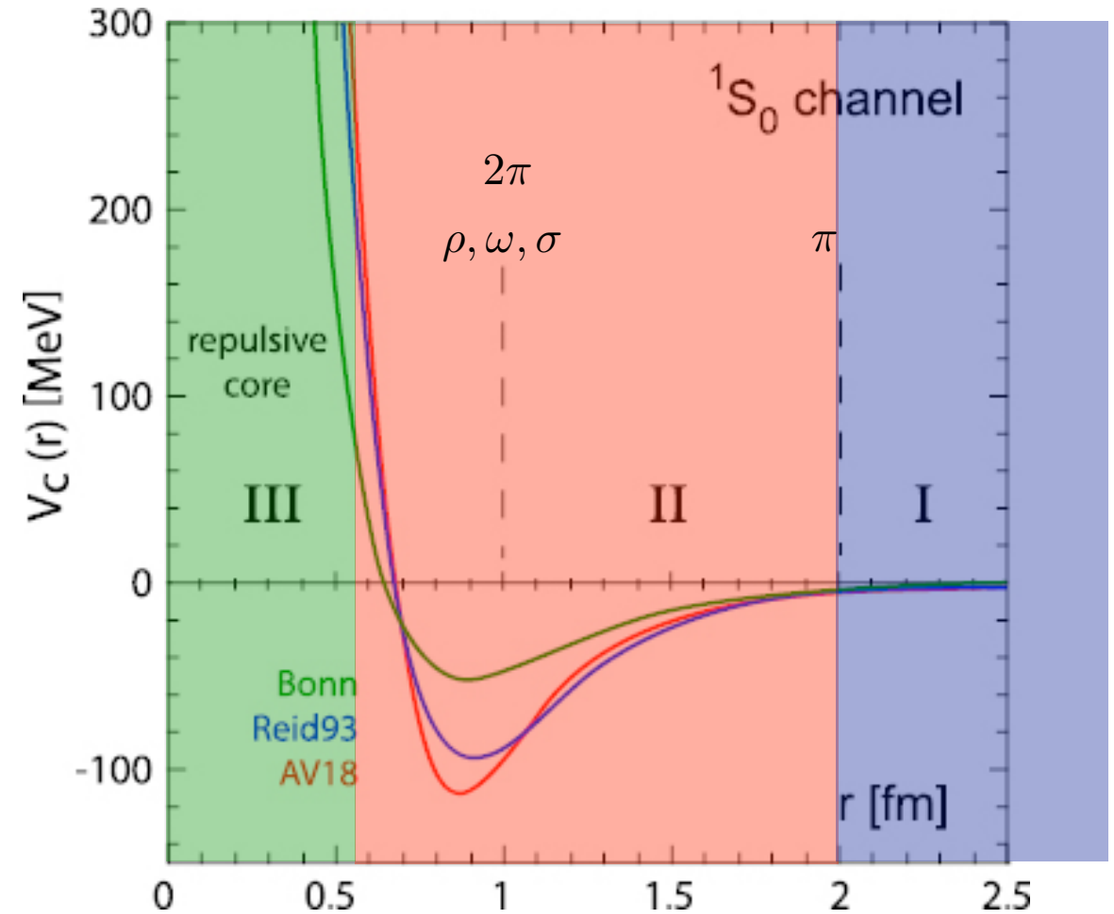

- Hard (~10^3 MeV), repulsive small-distance interaction: nonperturbative and model-based
- Weaker (~50 MeV) attractive mid-range interaction
- Finely tuned: NN $^1S_0$ state unbound by 0.066 MeV
  $^3S_1$ state bound by 2.2 MeV
- Not unique to NP: MeV → meV: NN → O_2O_2

Traditional Potential-Model Framework

Parameterize the "hard" NN interaction using scattering data → V_{NN}

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Develop an approximate "softer" V_{NN}^{eff} to enable a many-nucleon calculation in a finite P

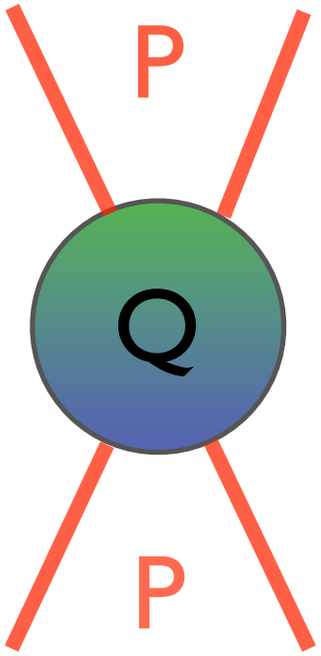
⇓

Perform a C.I. calculation to obtain "the wave function"

- Cannot solve the many-body Schroedinger equation in an infinite Hilbert space
- Work in a truncated, finite space P -- generally a C.I. space of low-momentum or -energy basis states
- Must renormalize the interaction to account for the omitted Q =1-P space

⇒

- Both semi-analytic and phenomenological approaches are pursued



UV and IR integration

energy-dependent

generally done poorly

Traditional Potential-Model Framework

Parameterize the "hard" NN interaction using scattering data → V_{NN}

⇓

Develop an approximate "softer" V_{NN}^{eff} to enable a many-nucleon calculation in a finite P

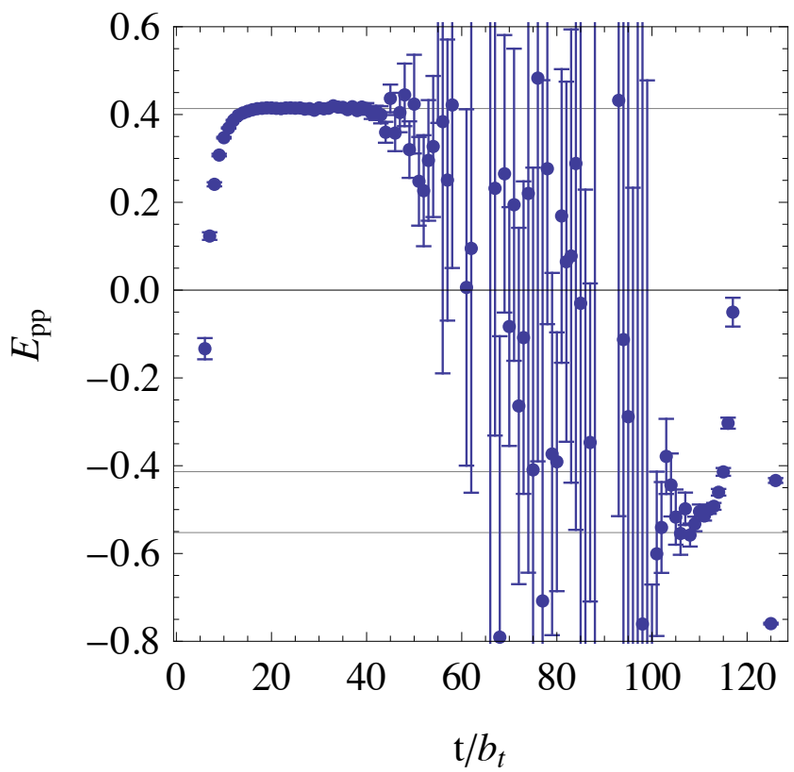
⇓

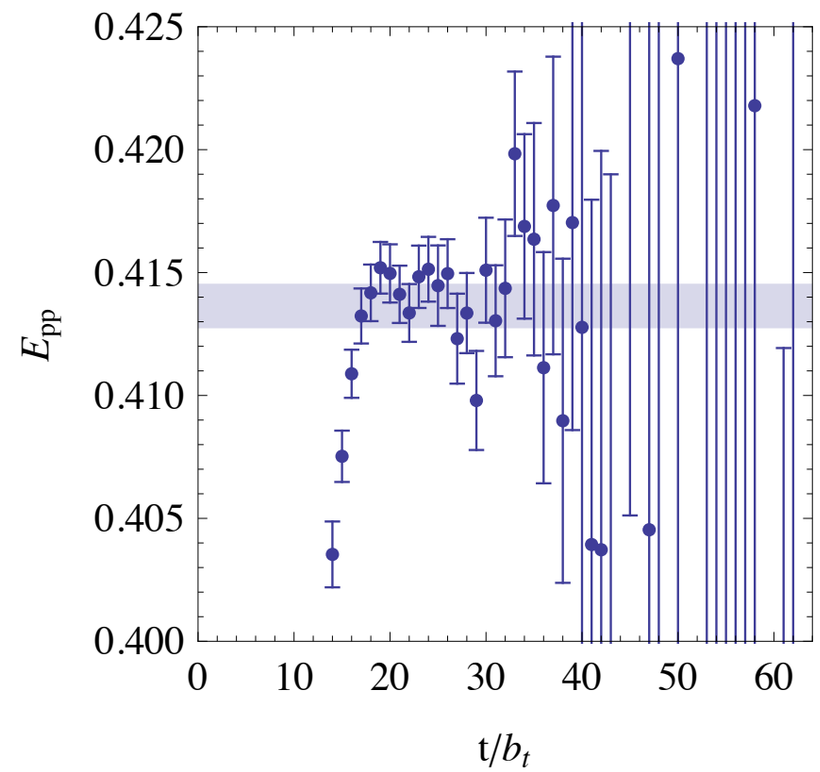
Perform a C.I. calculation in P to obtain "the wave function"

- Bases ~ 10^{10} are currently employed in NP (e.g., UNEDF/NUCLEI)
- The basis is explicitly anti-symmetric (Slater determinants)

Lattice QCD

- Employs the exact Lagrangian of the strong interaction
- Discretizes the continuum in space and time
- Sums QM paths by Monte Carlo: has been applied to NN system





pp ($^1S_0$)

S. Beane, W. Detmold, H.-W. Lin, T. Luu, K. Orginos, M. Savage, A. Torok, A. Walker-Loud (NPLQCD)

- While there is a fermion sign problem in such Monte Carlo simulations, well-defined plateau found in NN system prior to decay to the bosonic state

The Bridge: HOBET

- Conventional C.I. bases are explicitly antisymmetry, but converge slowly
  - the range in r that a C.I. basis spans grows as ~ $\sqrt{\Lambda}$

- Consider the C.I. basis - Slater determinants in an harmonic oscillator basis - as a tool to numerically enhance an effective theory: H.O. *P* space
  - only compact basis that preserves the translational invariance of the full S.E.

- Conventionally $P\Psi$ taken from self-consistent solution of Bloch-Horowitz equation

$$H^{\rm eff} P\Psi = EP\Psi \qquad H^{\rm eff} = P\left[H + \frac{1}{E-QH}QH\right] \qquad H = T + V$$

- In HOBET, this is reorganized to separate out distinct UV and IR corrections to $H^{\rm eff}$

$$H^{\rm eff} = P\frac{E}{E-TQ}\left[T - T\frac{Q}{E}T + V + V\frac{1}{E-QH}QV\right]\frac{E}{E-QT}P$$

$$\updownarrow$$

The ET NN substitution: $e^{r^2/2}\left[a^{3S1}_{LO}\delta(\vec{r}) + a^{3S1}_{NLO}(\overleftarrow{\nabla}^2\delta(\vec{r}) + \delta(\vec{r})\overrightarrow{\nabla}^2) + \ldots\right]e^{r^2/2}$
(finite, exact expansion)

- If a substantial numerical calculation is done in *P*: 1) expansion converges rapidly, can be truncated at low order, NNLO and 2) the a(E)s → constants (scale separation)

- The treatment is analytically continuous in E: can be extended to E>0 (scattering)

- For E>0 or E<0 the ET provides only $P_\Lambda \Psi$

- If this program is executed faithfully, however, one has two long-range projections

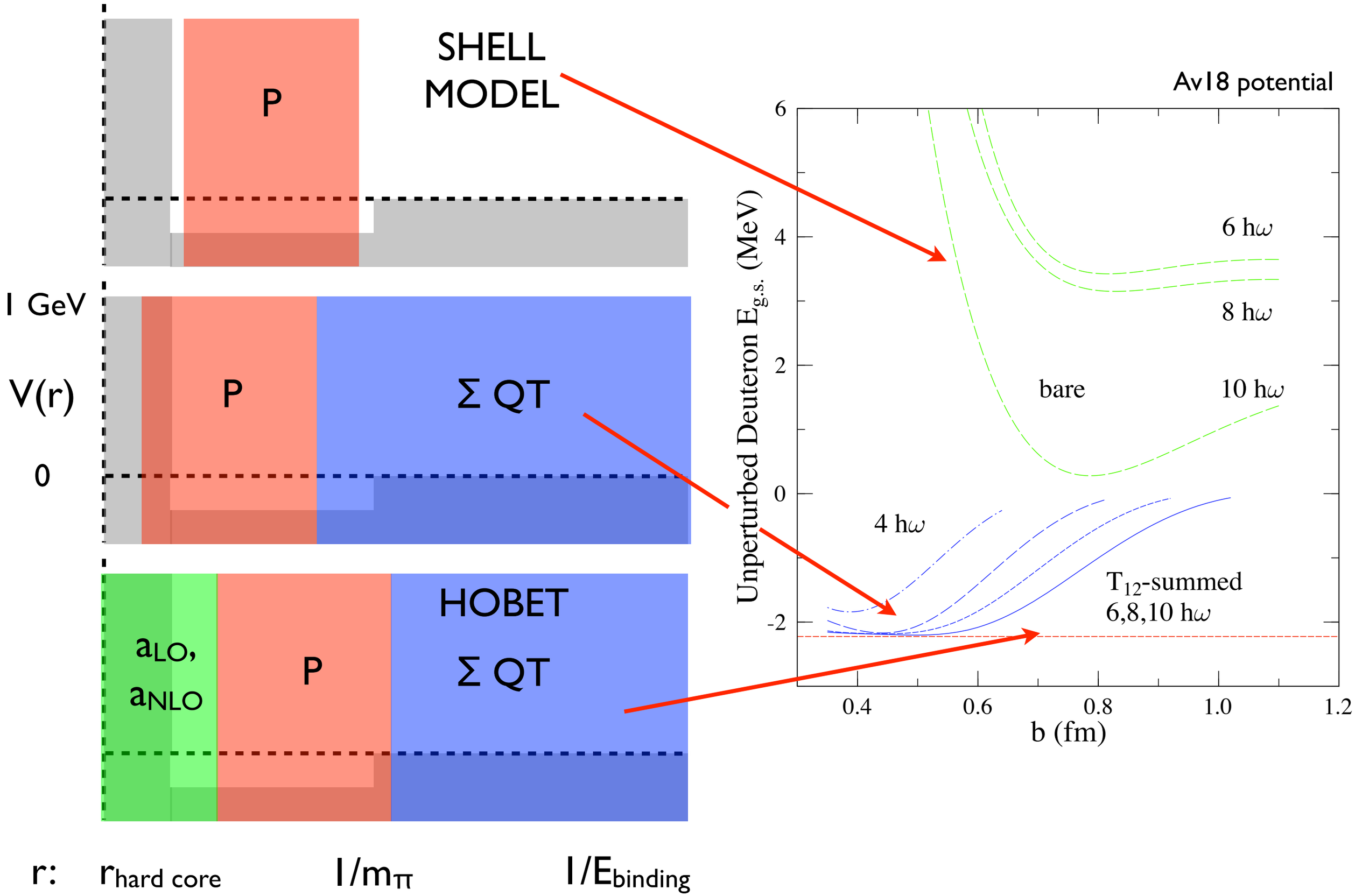
$$\int d\vec{r}\, r^\Lambda e^{-r^2/2}\Psi(r) \qquad \int d\vec{r}\, r^{\Lambda-2} e^{-r^2/2}\Psi(r)$$

- By equating the ratio of these projections to the corresponding ratio of the projections of the asymptotic wave function, one obtains an implicit relation

$$\{a^{3S1}_{LO}, a^{3S1}_{NLO}, \ldots\} \leftrightarrow k\cot\delta = -\frac{1}{a} + \frac{1}{2}r_0 k^2 + \ldots \leftrightarrow \{a, r_0, \ldots\}$$

Provided $\Lambda \gtrsim 8$ this matching can be carried out through NNLO with high accuracy

- The bridge: This matching can be done to experiment or to LQCD. Two "wins"
  - The UV/IR scale separation has enabled a direct construction of the effective interaction in *P*: one has avoided the introduction of a NN potential and the difficult problem of integrating out its high-momentum terms
  - Have a clean matching to LQCD, but no sign problem because the effective theory is formulated in an antisymmetric C.I. basis


SHELL
MODEL
P
1 GeV
V(r)
0
P
Σ QT
a_{LO},
a_{NLO}
P
HOBET
Σ QT
r:
$r_{hard\ core}$
$1/m_\pi$
$1/E_{binding}$
Av18 potential
Unperturbed Deuteron $E_{g.s.}$ (MeV)
6
4
2
0
-2
6 hω
8 hω
10 hω
bare
4 hω
T_{12}-summed
6,8,10 hω
0.4
0.6
0.8
1.0
1.2
b (fm)

The Applied Math/CS Problems in HOBET

- Calculation in P a self-consistent version of the usual C.I. large-sparse-matrix problem

$$H^{eff}(E)\ P\Psi = E\ P\Psi$$

  - this must be iterated to convergence
  - it must be executed for each needed state (or E): not finite-dimensional in E despite the finite H^{eff} for any given E
  - the underlying expansion in short-range operators is both in derivatives and in number of nucleons interacting at short range in Q at one time: more complicated interactions must be treated to demonstrate convergence numerically

- The ultraviolet physics is embedded in the kinetic energy Lee-Suzuki operator

$$\frac{E}{E-QT}|\alpha\rangle = \left[P\left(\frac{E}{E-T}\right)P\right]^{-1}\frac{E}{E-T}|\alpha\rangle$$

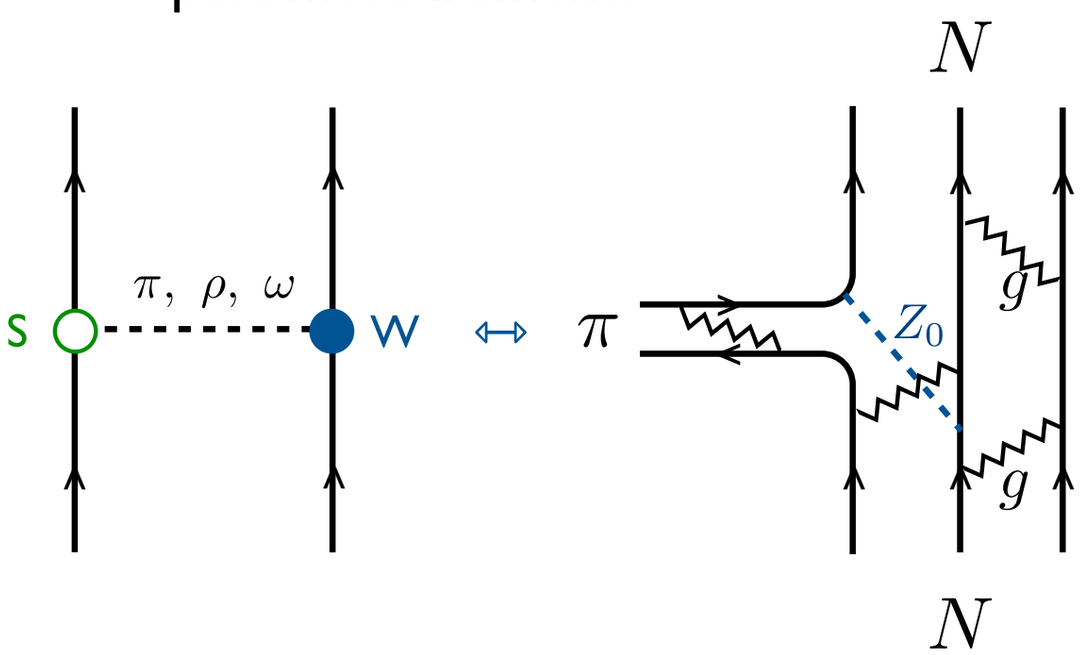
  - this requires an inversion of a sparse, one-parameter matrix in P

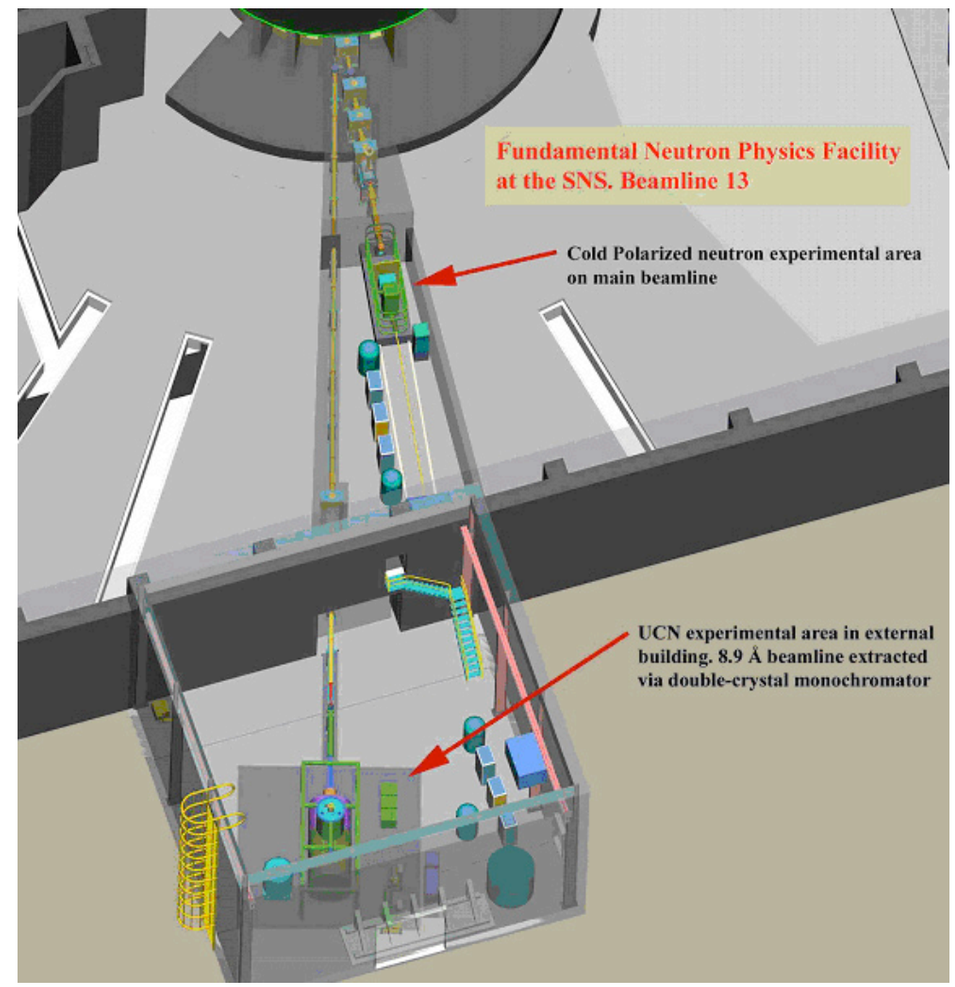
- The fitting of the $\{a_{LO}, a_{NLO}, a^1_{NNL0}\cdots\}$ to $\{a, r_0, v_2, \ldots\}$ is nontrivial because $P\Psi$ is an implicit function of the former
  - need to find methods to do this systematically

First application: Hadronic parity nonconservation (see poster)

- Main goal: Neutral-current-mediated weak NN interaction (not yet isolated exp.)

- Attractive target for us because
  - strong interaction can be matched to experiment, weak couplings to LQCD
  - the bridge from NN LQCD to light nuclei is critical to the global analysis
  - there is a significant new experimental program underway at the cold neutron beam-line of the SNS
  - an anomaly is apparent in past measurements



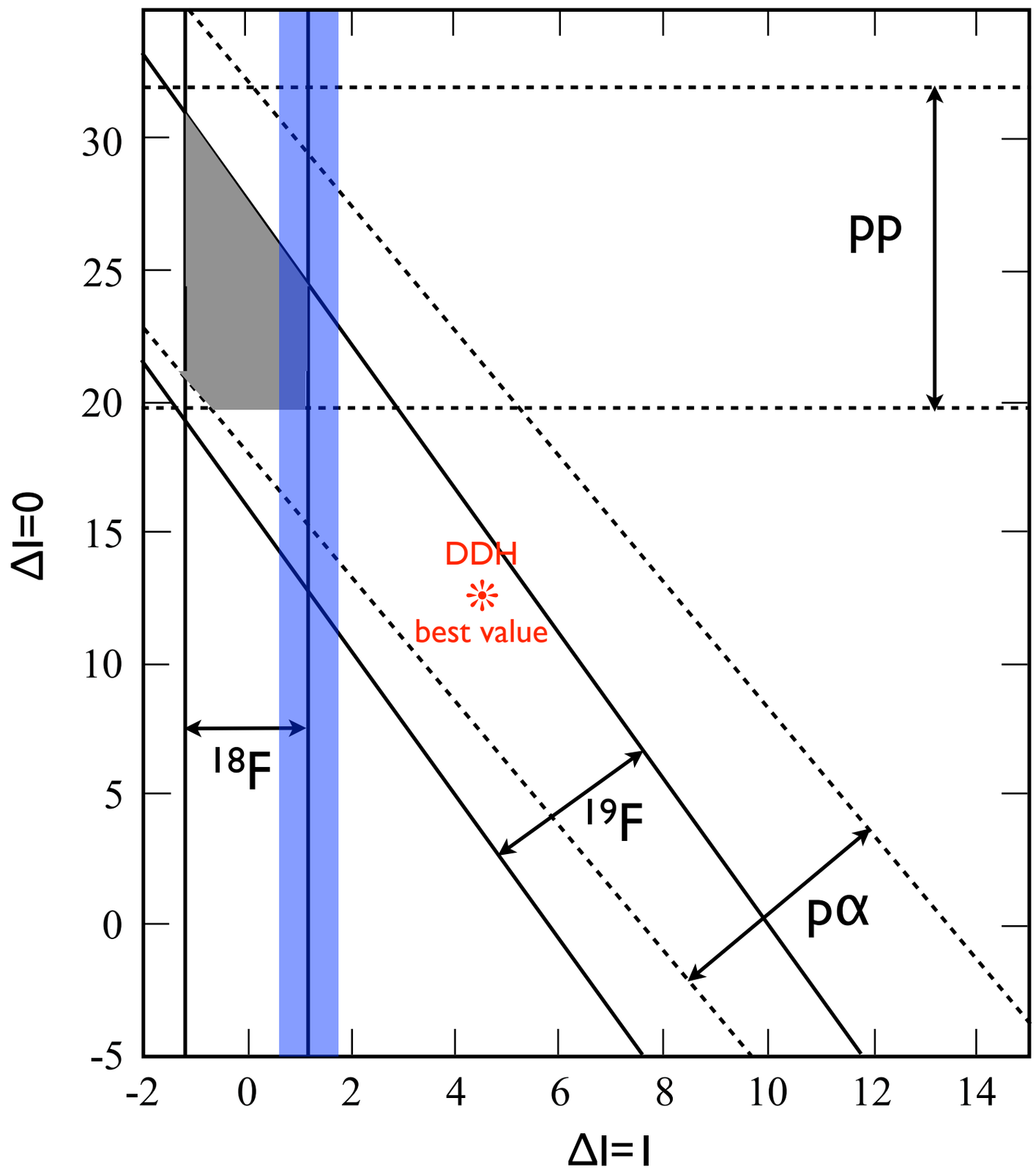


current LQCD calculation of for h_π^1

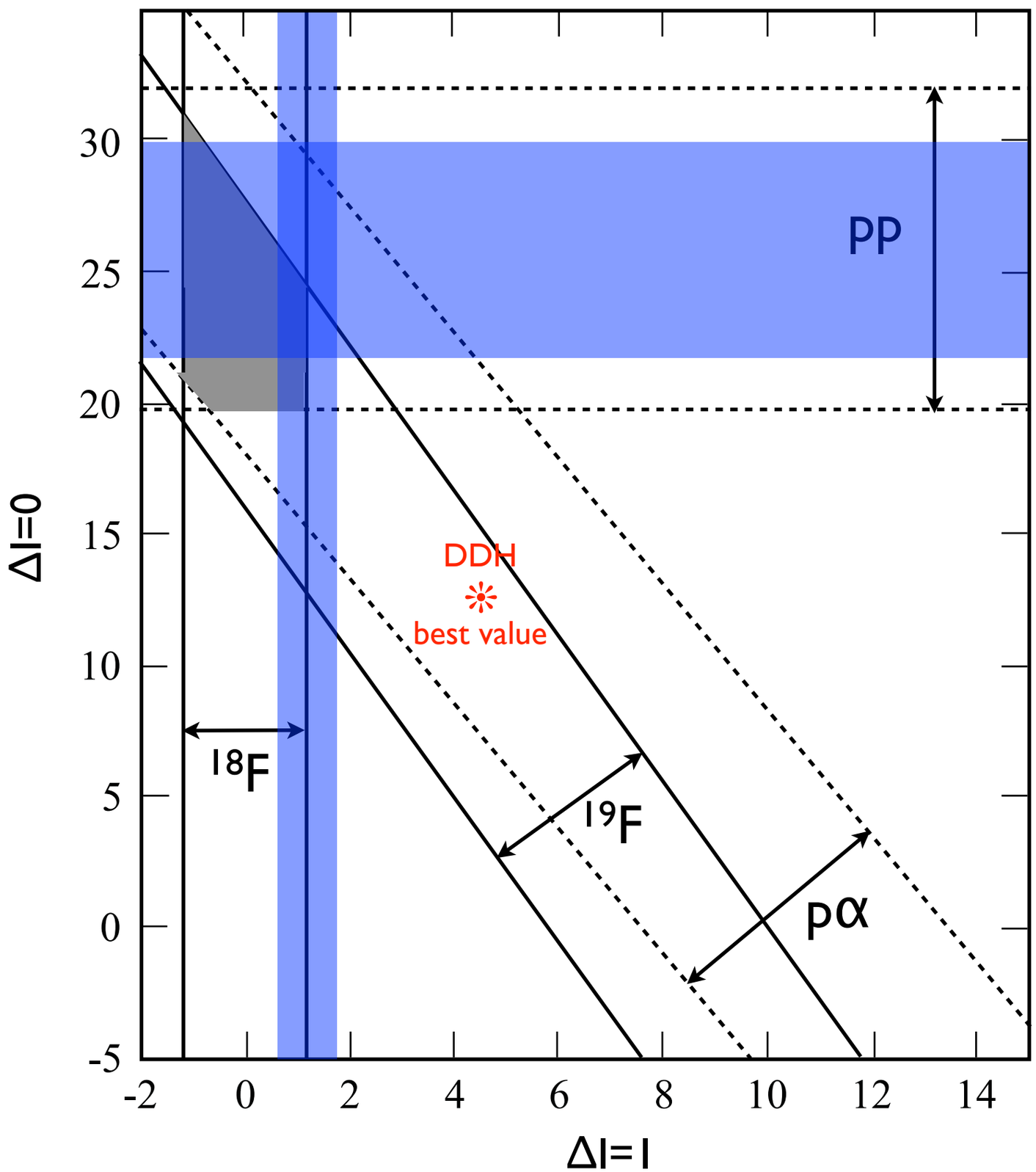
L=2.5 f
a=0.123f
m_π= 389 MeV

no quark loops

J. Wasem

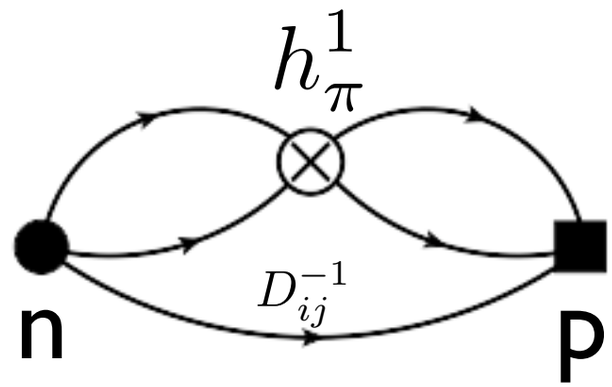


potential impact
of a future
calculation of h_ρ^2

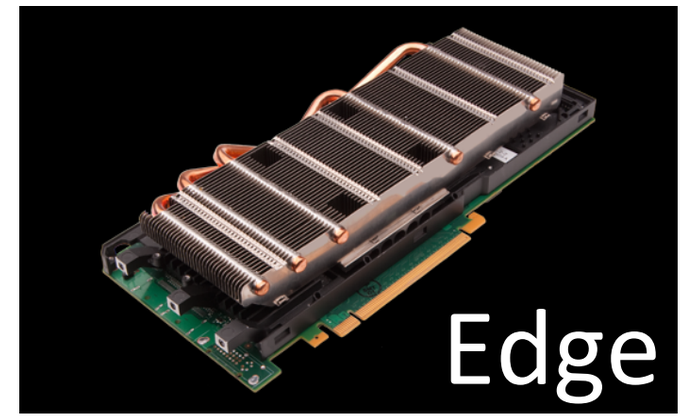


HPC Resources at LLNL have enabled these calculations

LCF



ΔI=1



GPU capacity

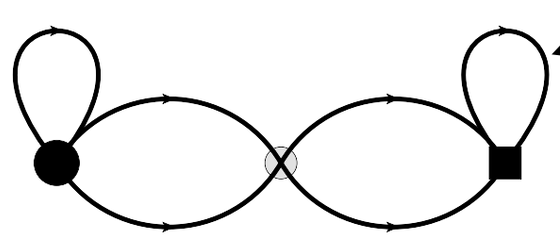
To confront experiment, will need to look at other channels

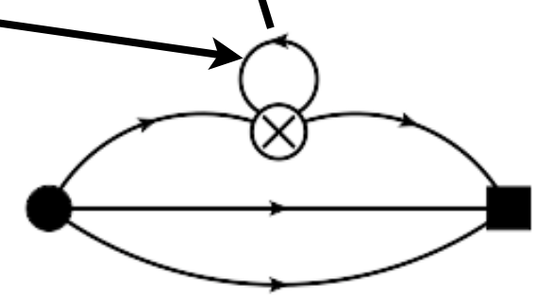
ΔI=2

ΔI=0

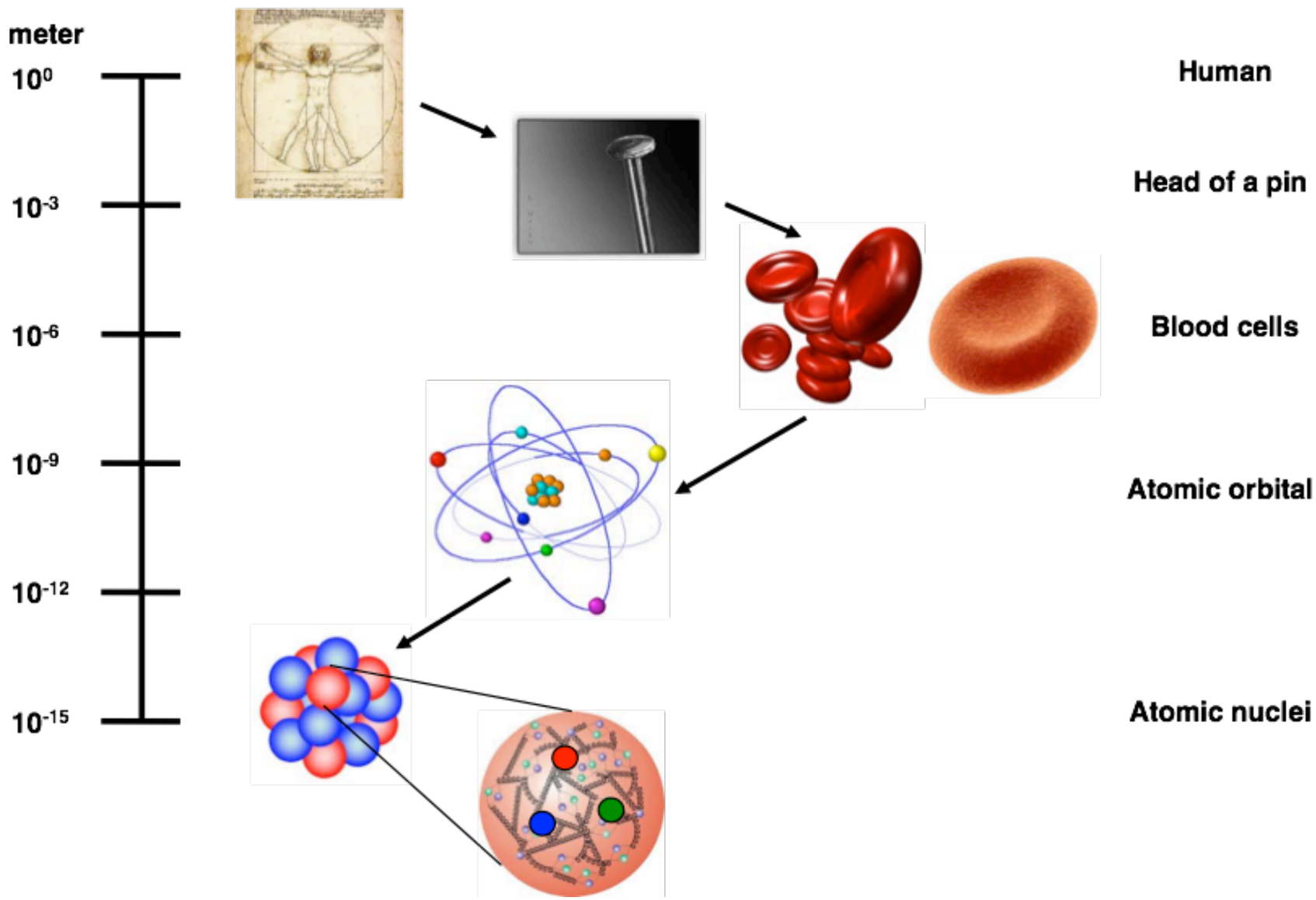
$$D_{jj}^{-1} \approx \frac{1}{N_R} \sum_r^{N_R} \sum_b X_j^{r[b]} \eta_j^{r[b]}$$

Quark loops





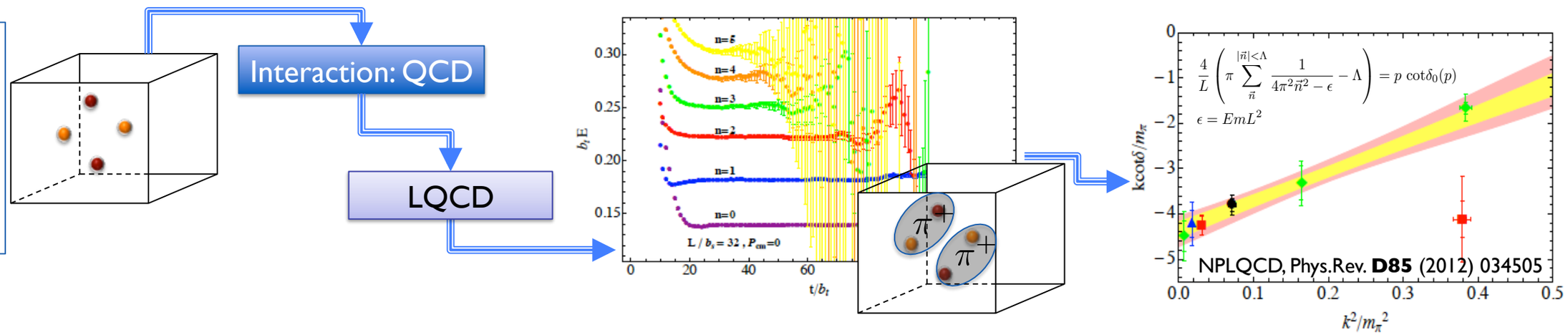
Overarching goal: Connect Cold QCD to Nuclear Many-body Physics



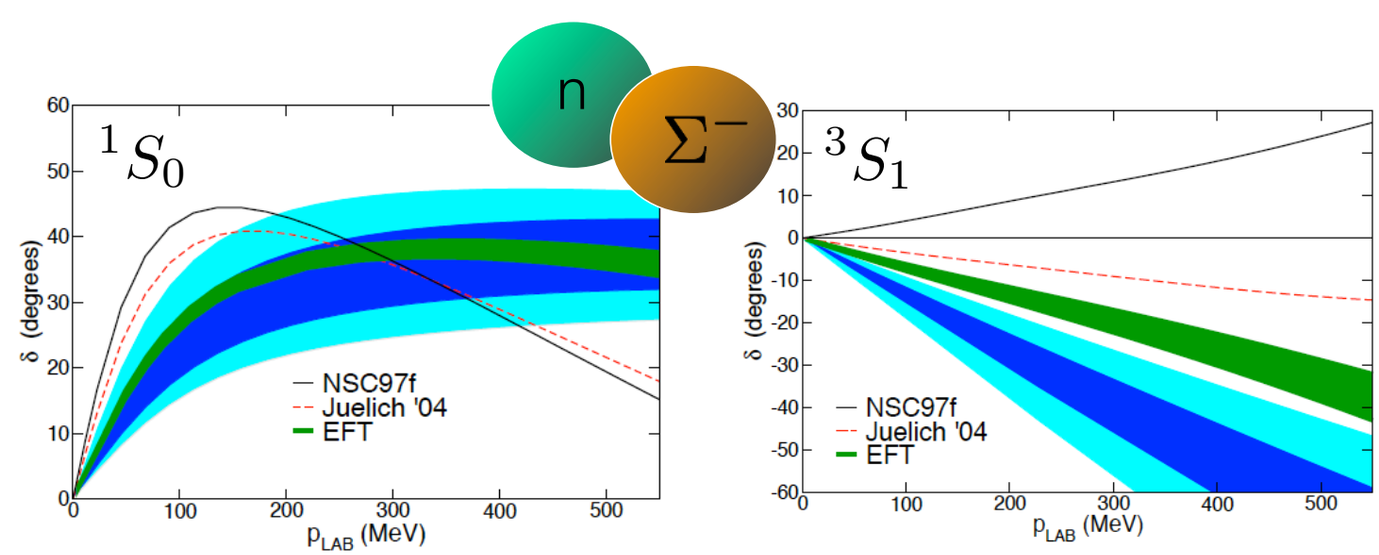
Multi-scale problem: HPC intensive

Finite-volume techniques are key

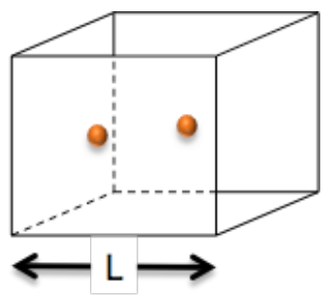
Four valence quarks in a cubic volume: 2 *u* and 2 anti-*d*

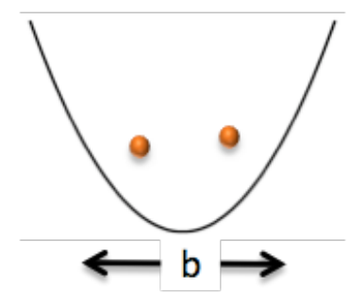


Cold QCD calculations are probing systems not accessible terrestrially



Finite-volume techniques in Nuclear Physics





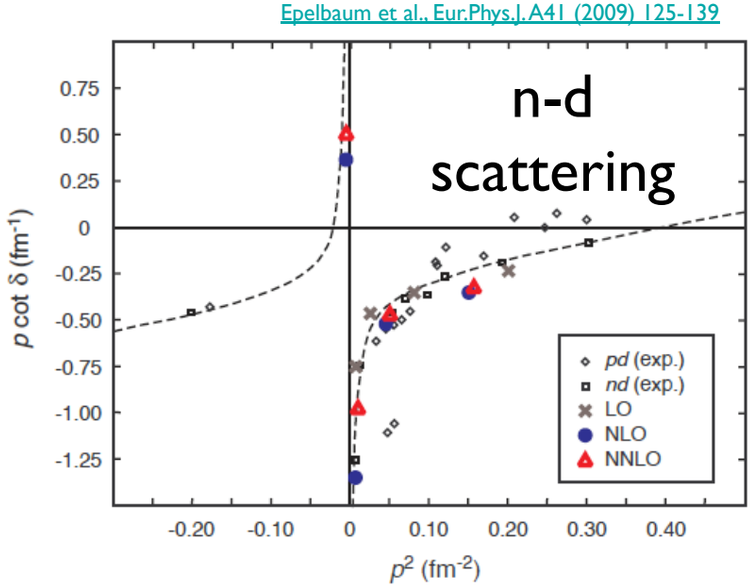
$$\frac{4}{L}\left(\pi \sum_{\vec{n}}^{|\vec{n}|<\Lambda} \frac{1}{4\pi^2\vec{n}^2-\epsilon} - \Lambda\right) = p\,\cot\delta_0(p)$$

$$\epsilon = EmL^2$$

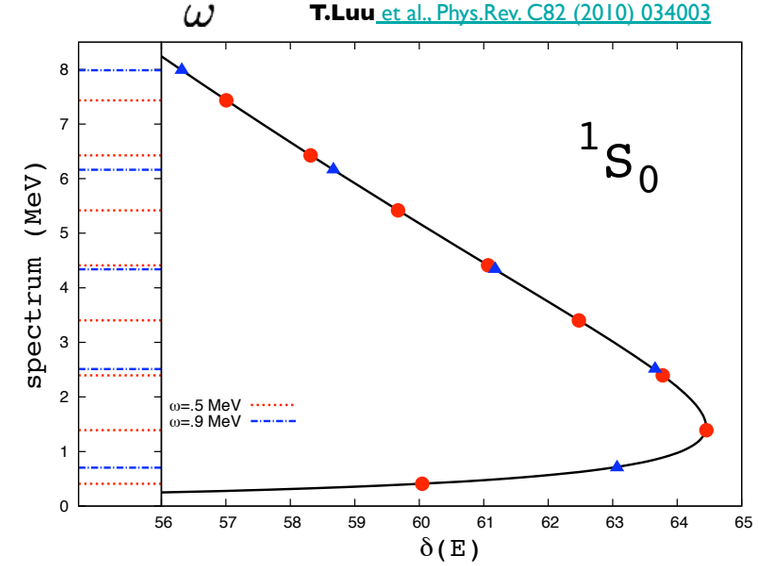
$$-\frac{2}{b}\frac{\Gamma(\frac{3}{4}-\frac{\epsilon}{2})}{\Gamma(\frac{1}{4}-\frac{\epsilon}{2})} = p\,\cot\delta_0(p)$$

$$\epsilon = \frac{E}{\omega}$$

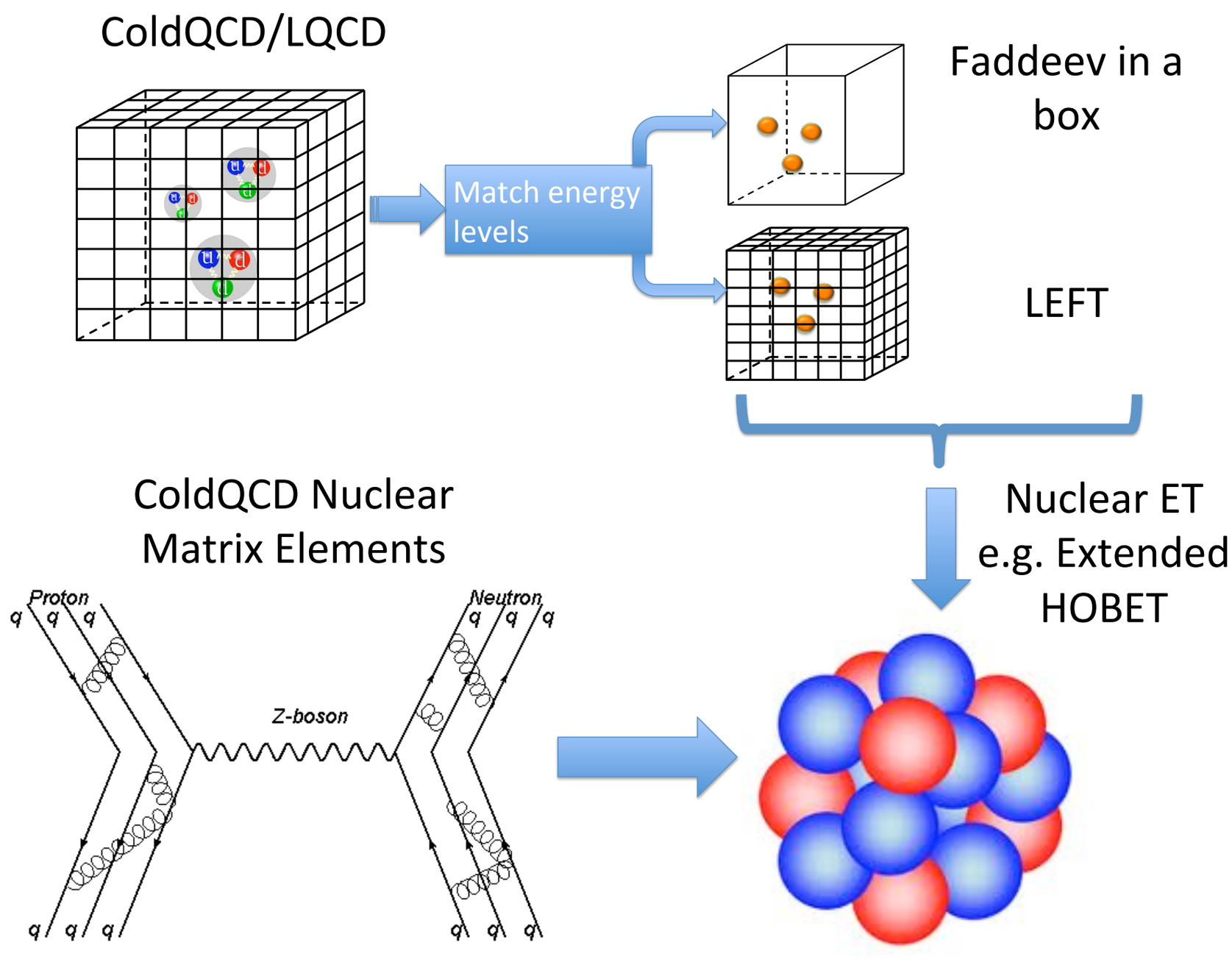
Epelbaum et al., Eur.Phys.J.A41 (2009) 125-139



T.Luu et al., Phys.Rev. C82 (2010) 034003

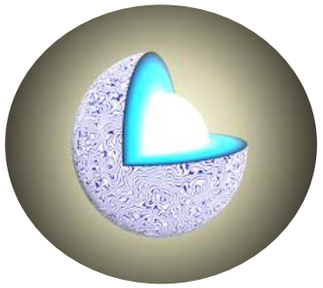


Beyond two-particle scattering

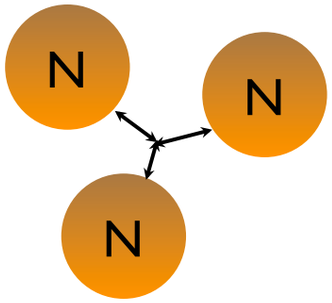


Looking forward…

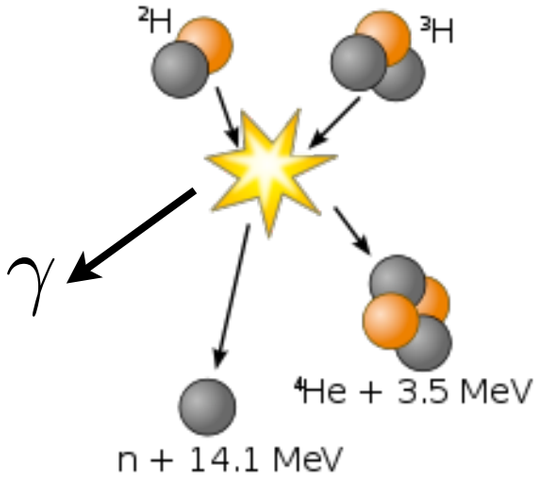
- Stochastic methods for quark loops in multi-hadron systems and quark-field tensor contractions
  - $\Delta I=0$ parity-violating interaction
  - Kaon-neutron



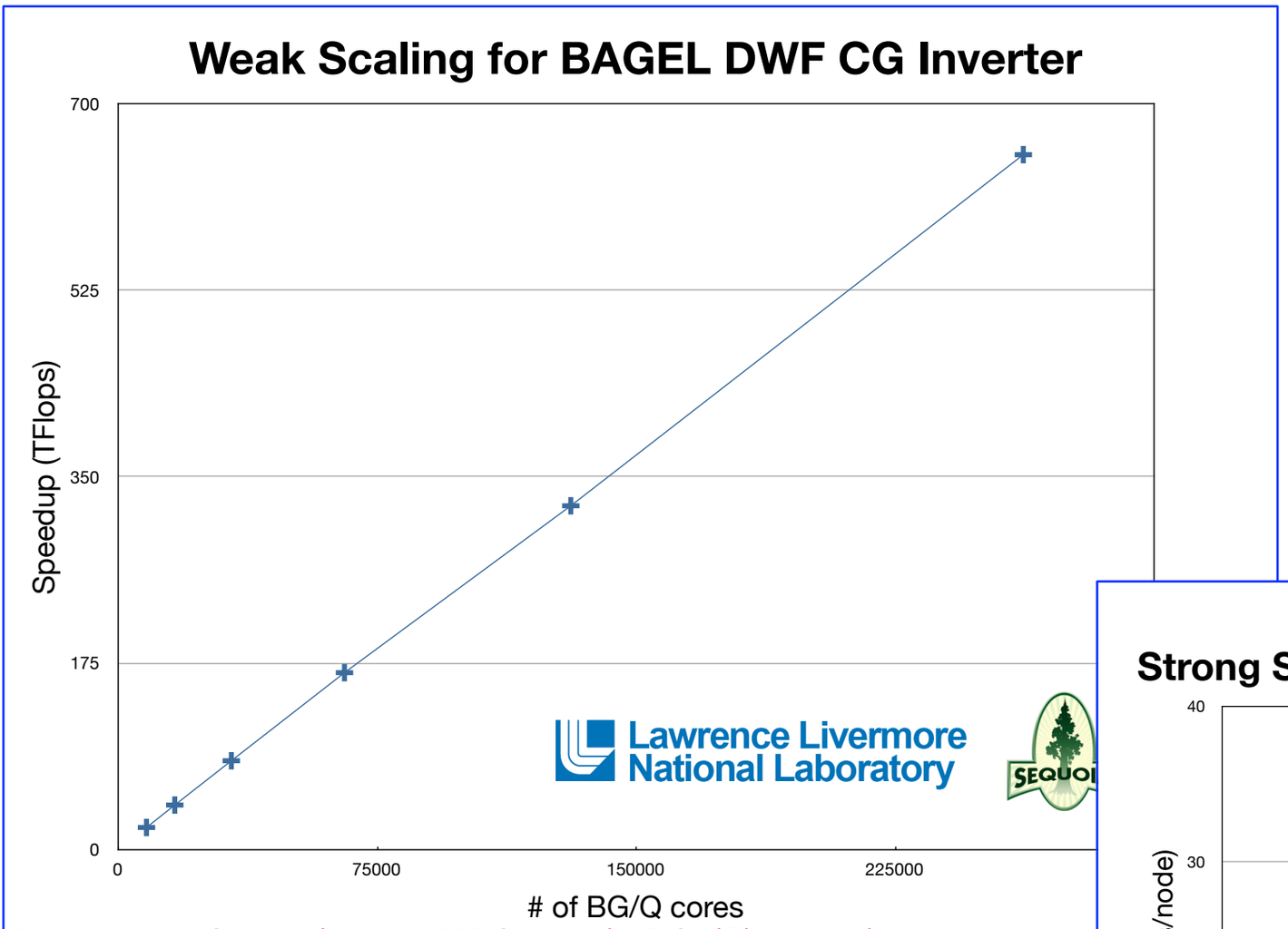
- Finite-volume effective theories for multi-hadron systems
  - Three-neutron interaction
  - Hyper-nuclei structure



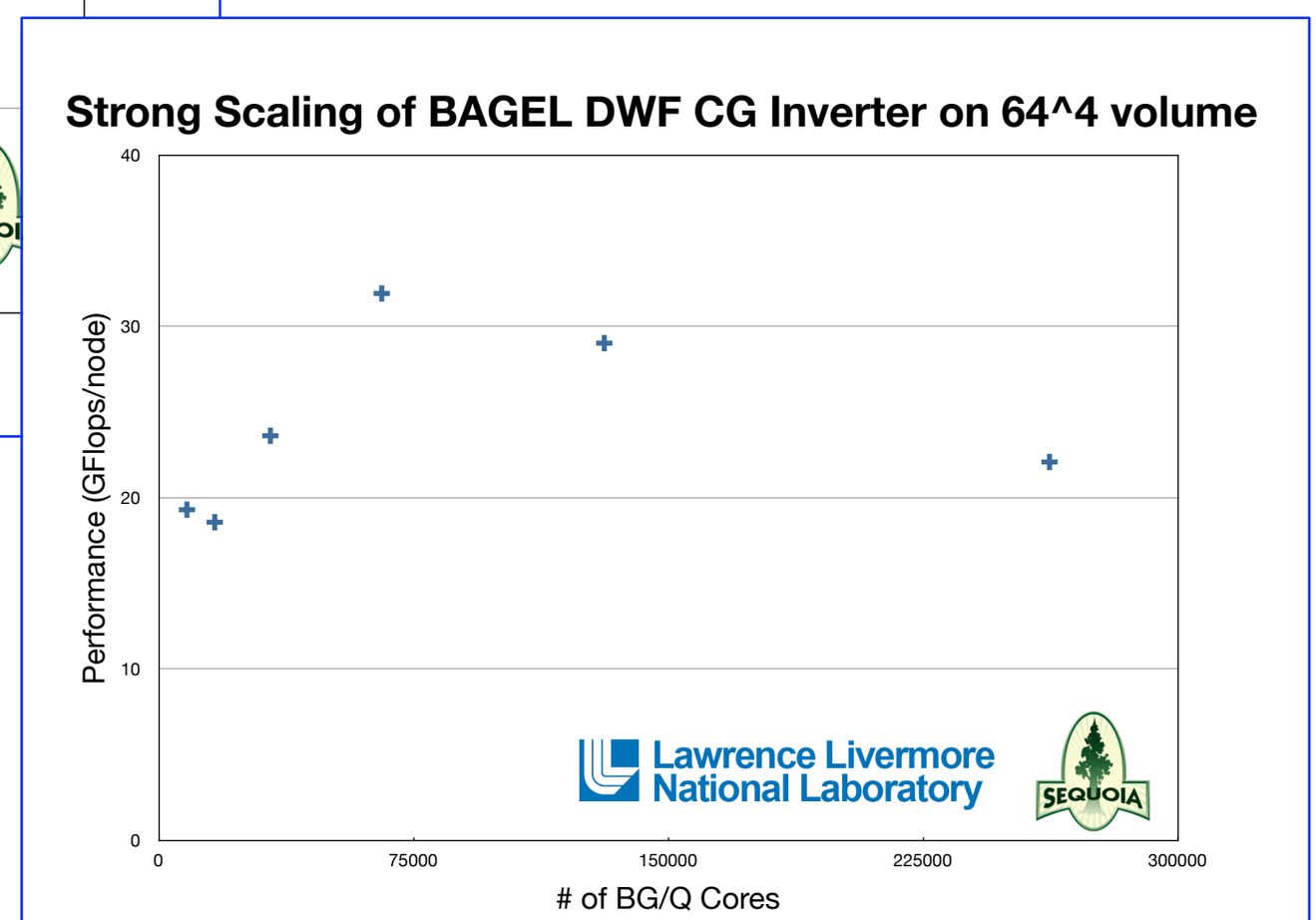
- Inelastic formalism
  - Nuclear reactions
  - ICF prompt diagnostics



. . .on the horizon



Tests were performed with the STFC funded DiRAC facility at Edinburgh



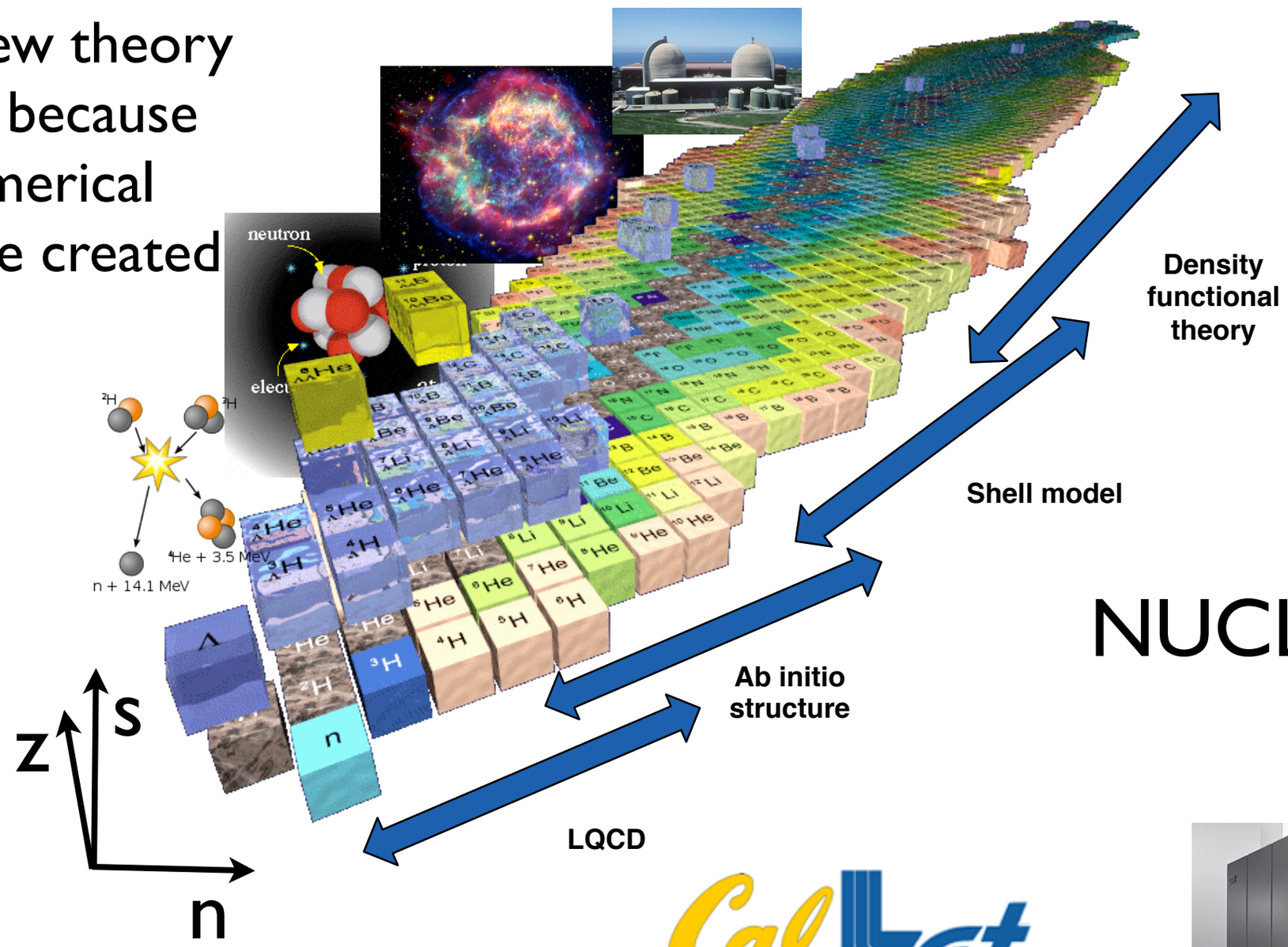
Tests were performed with the STFC funded DiRAC facility at Edinburgh

Studies performed by M. Buchoff, C. Schroeder, P. Vranas, J. Wasem

Figures courtesy of M. Buchoff

Nuclear Physics as a *Predictive Science*

CalLat shows how past SciDAC efforts can enable new theory approaches because of the numerical infrastructure created



USQCD