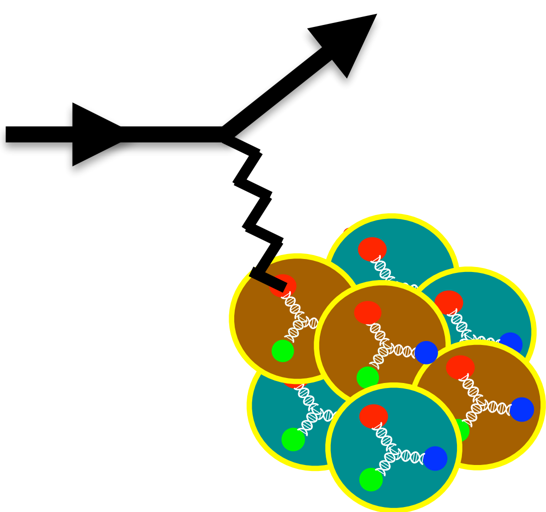
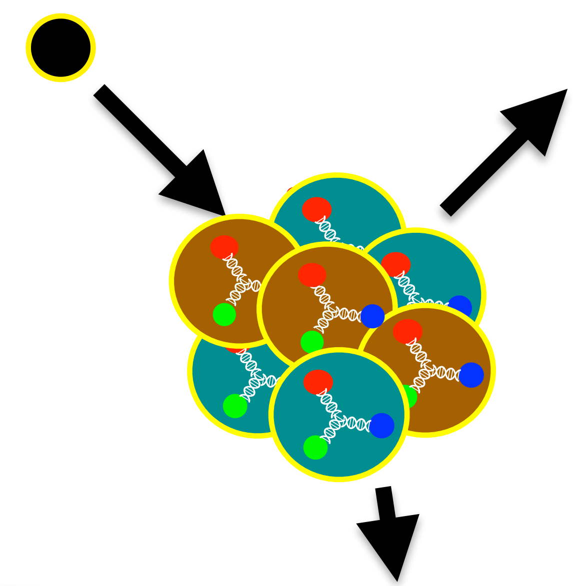
Nuclear and Nucleon Matrix Elements



Michael Wagman



USQCD All Hands Meeting

May 1, 2021

Fermilab

NPLQCD

Many-quark bound-state structure

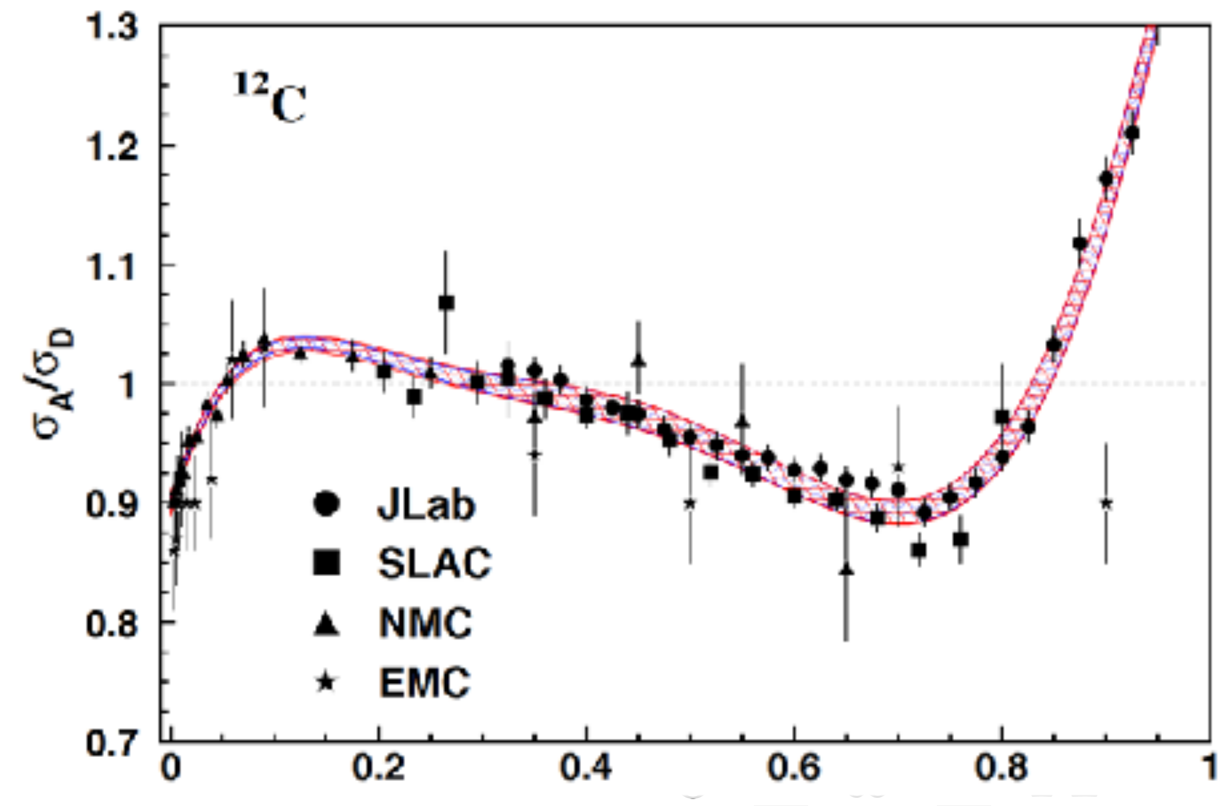
LQCD calculations of nucleon matrix elements are revealing fundamental aspects of hadron structure

See talks this afternoon, this talk will focus on nuclei in particular

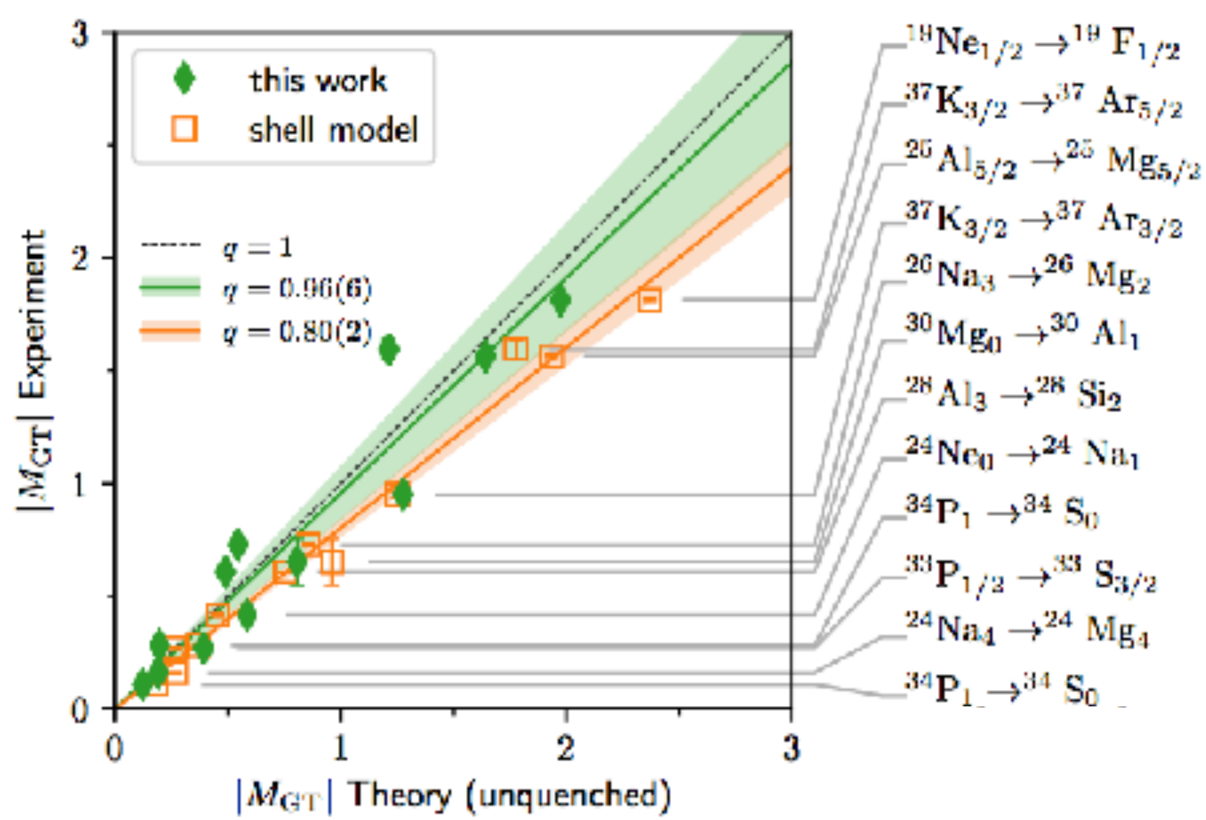
The partonic structure of nuclei is noticeably different from the nucleon

Aubert et al (EMC), Phys. Lett. 123B (1983)

The emergence of the EMC effect and it's analogs from QCD is not yet understood



Malace et al, Int. J. Mod. Phys. E 23 (2014)



Gysbers et al, Nature Phys. 15 (2019)

Multi-nucleon correlations are essential for modern nuclear theory calculations to reproduce nuclear β -decay measurements

LQCD can constrain nuclear forces, two-body currents, and nuclear PDF modifications using calculations of the lightest nuclei

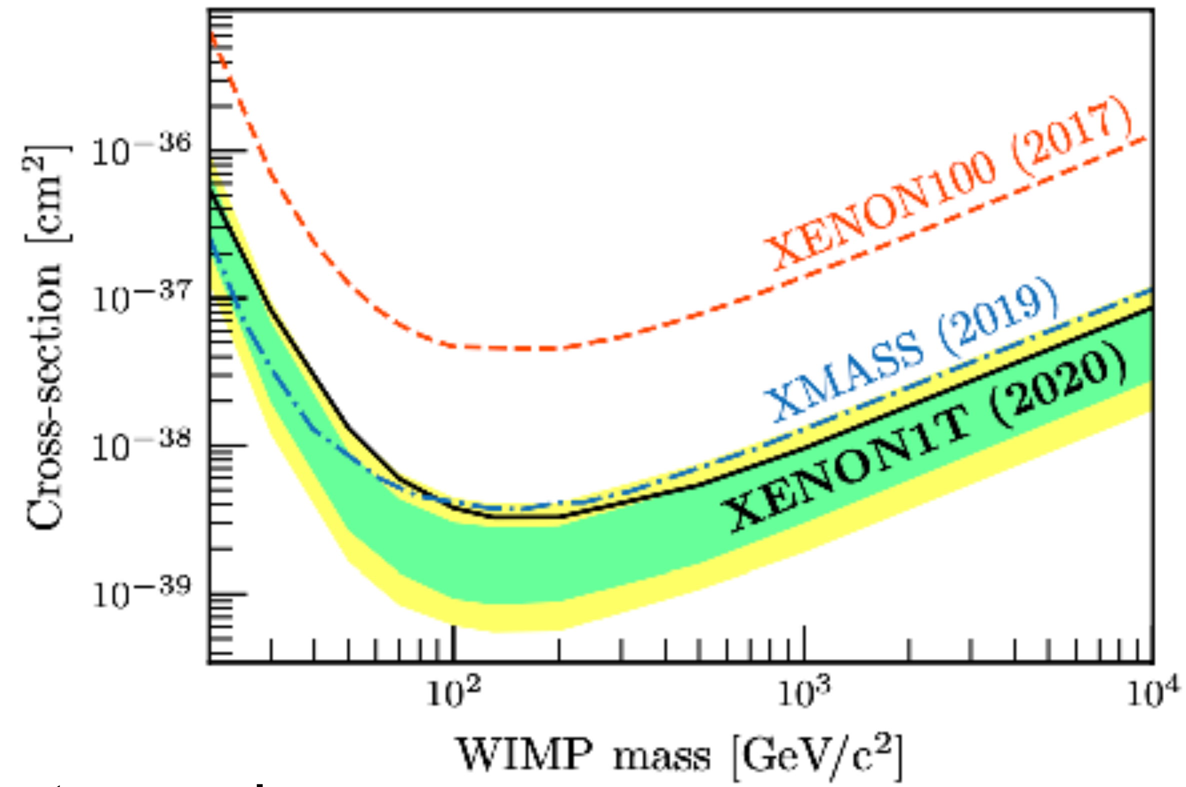
New physics and nuclei

Nuclei are abundant and useful experimental targets

Converting between nuclear- and nucleon-level cross-sections requires

- Nuclear models (error bar ?s)
- Direct LQCD calculations (impractical)
- LQCD informed EFT + modeling

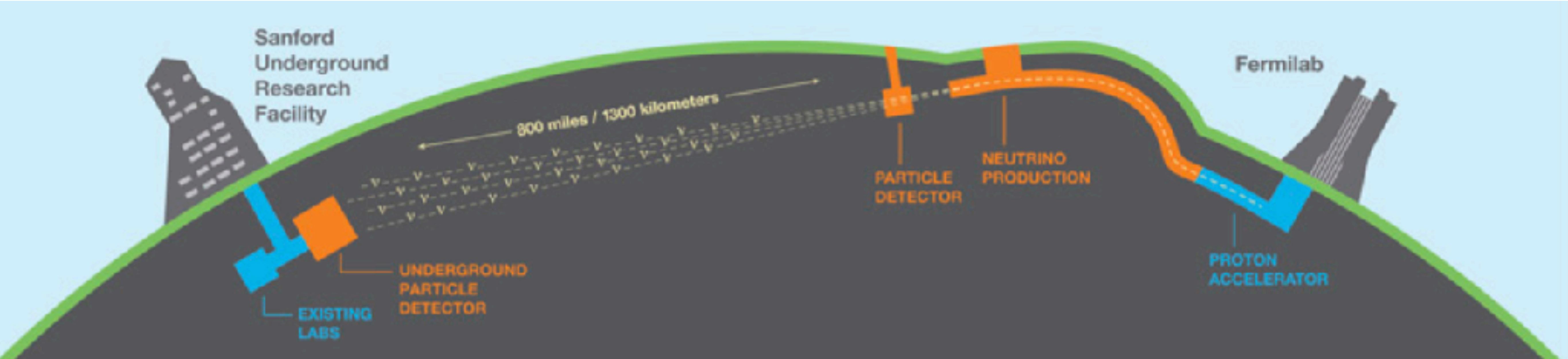
Xenon1T constraint on Dark Matter-nucleus



Next-generation accelerator neutrino experiments require few-percent level control of nuclear cross-sections

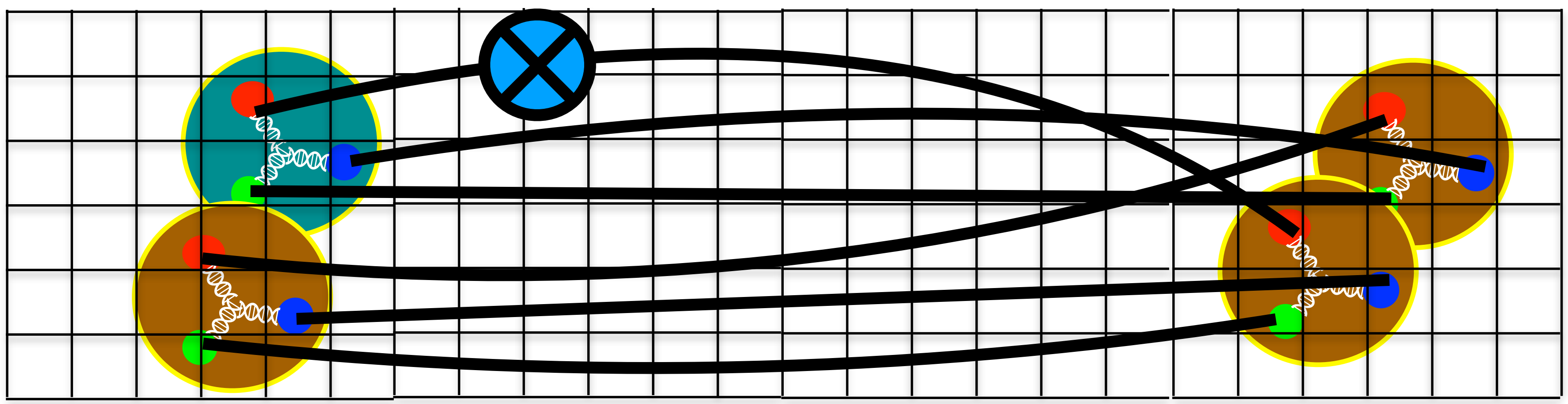
Standard Model predictions with controlled uncertainties essential

DUNE



Nuclear matrix elements from LQCD

Electroweak nuclear matrix elements and nuclear PDF moments extracted from
3pt / 2pt function ratios, “just” need (often multi-local) nuclear interpolating operators



Fixed-order background field method simplifies three-point function contractions

Lattice methods, EFT matching strategies, and early nuclear ME results reviewed:

Davoudi et al, *Phys.Rept.* 900 (2021)

New results this year with $m_\pi \sim 450\ \mathrm{MeV}$ and $m_\pi \sim 800\ \mathrm{MeV}$

Detmold et al [NPLQCD]
arXiv:2009.05522
(accepted to PRL, in prep)

Illa et al [NPLQCD] PRD 103 (2021)
arXiv:2009.12357

Parreño et al [NPLQCD] PRD 103 (2021)
arXiv:2102.03805

Nuclear matrix elements from LQCD

Electromagnetic structure and $np \rightarrow d\gamma$

Beane et al [NPLQCD] PRL 113 (2014)

Beane et al [NPLQCD] PRL 115 (2015)

Detmold et al [NPLQCD] PRL 116 (2016)

Proton-proton fusion and $2\nu\beta\beta$ computed using fixed-order background field method

Savage et al [NPLQCD], PRL 119 (2017)

Shanahan et al [NPLQCD], PRL 119 (2017)

Tiburzi et al [NPLQCD], PRD 96 (2017)

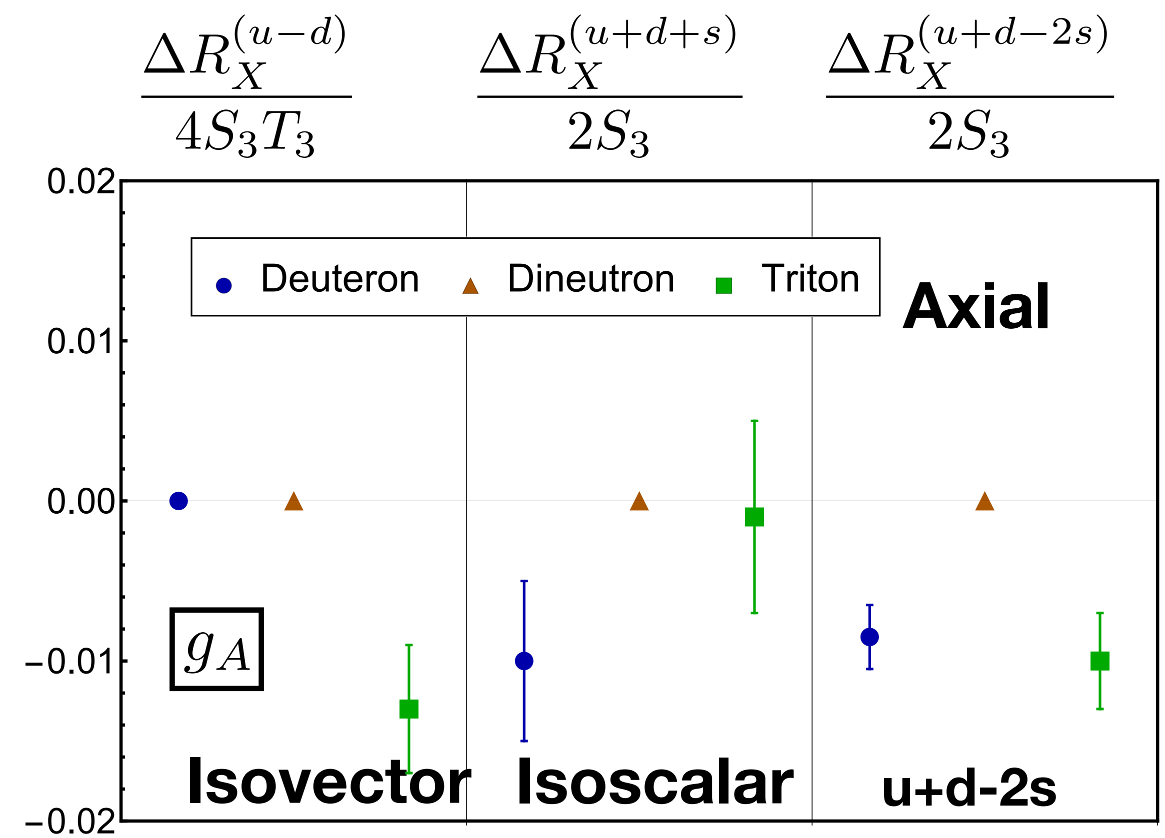
Gluonic structure of light nuclei

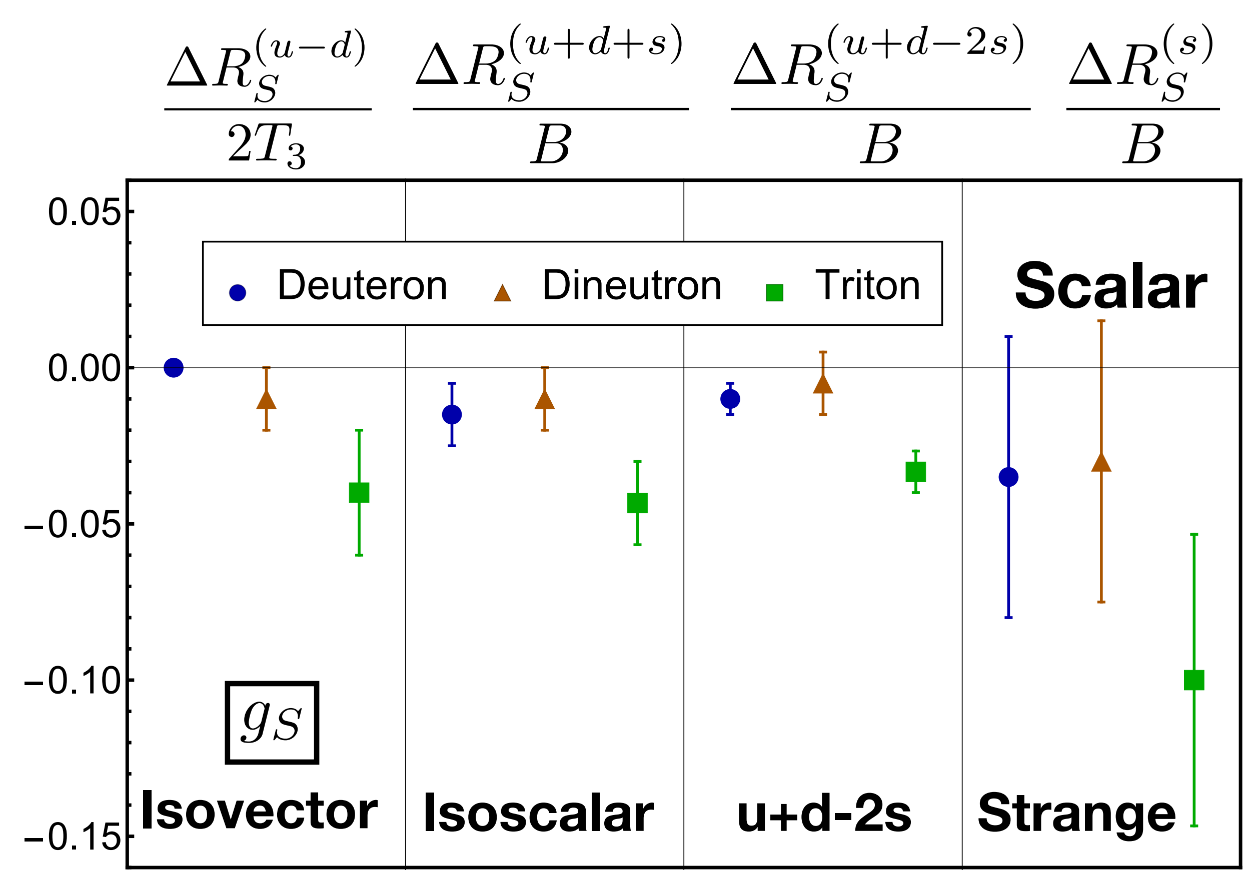
Winter et al [NPLQCD], PRD 96 (2017)

Scalar, axial, and tensor matrix elements

Chang et al [NPLQCD], PRL 120 (2018)

$$m_\pi \sim 800 \text{ MeV}$$





Momentum fractions of light nuclei

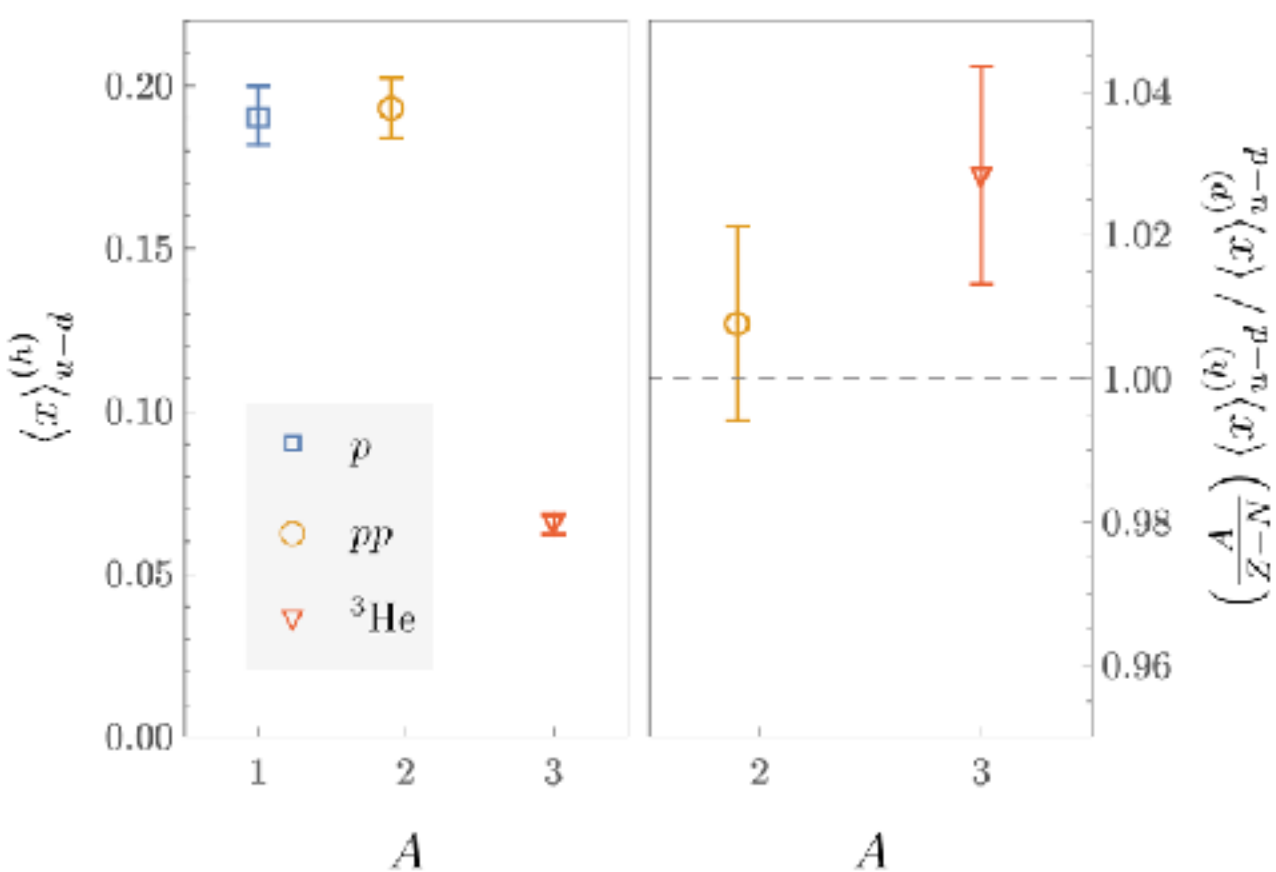
Momentum fraction carried by any quark flavor (or gluons) calculable from local matrix elements in generic hadrons

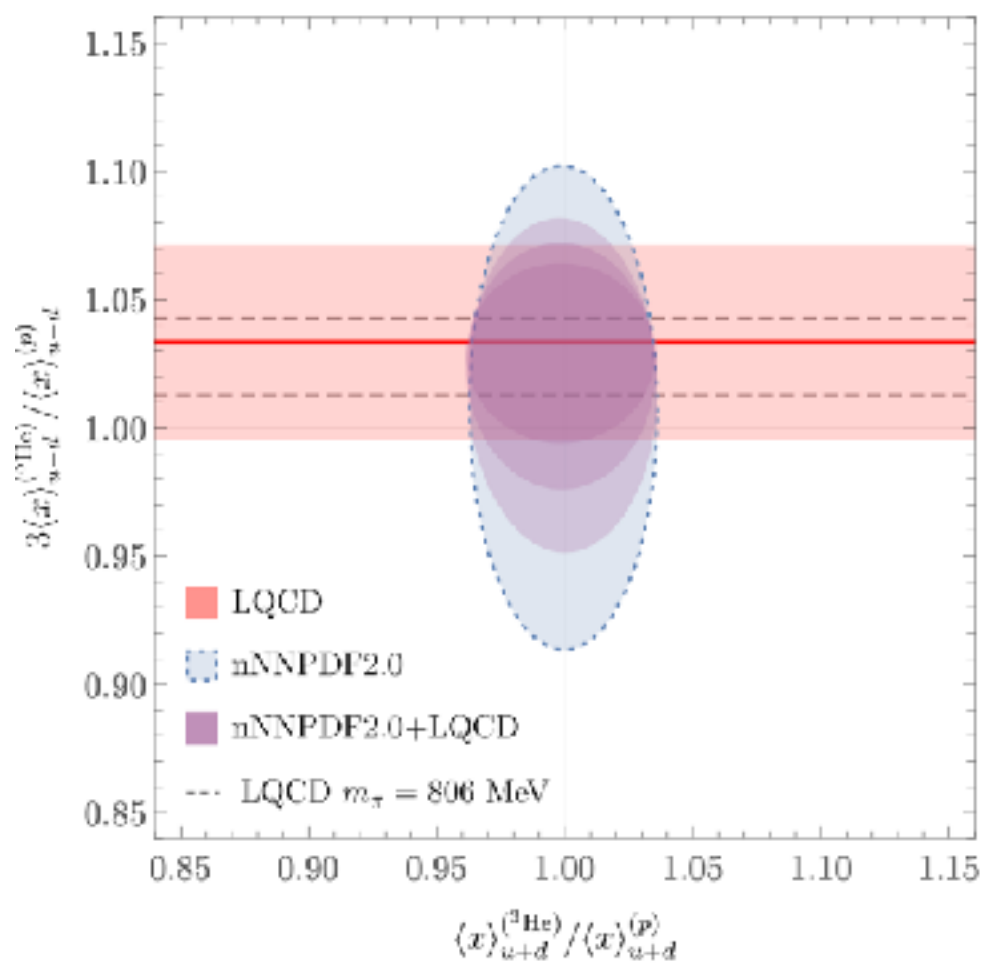
$$\langle x \rangle_h^i = \int_{-1}^{1} dx\ x\ q_h^i(x) = C(M_h, \vec{p}, J) \sum_{\lambda=-J}^{J} \langle h, \vec{p}, \lambda | T^i_{\mu\nu} | h, \vec{p}, \lambda \rangle$$

First calculation of isovector quark momentum fractions of light nuclei performed

Detmold et al [NPLQCD] PRL.xx arXiv:2009.05522

Although systematic uncertainties are not fully controlled (one lattice spacing, volume, quark mass, …) demonstrates potential for LQCD to usefully constrain nuclear PDFs





Matching to nuclear EFT

New analysis of baryon-baryon correlation functions allows (hyper-)nuclear forces to be constrained using pionless EFT

Illa et al [NPLQCD] PRD 103 (2021)

Approximate symmetries including SU(6) spin-flavor observed, though less pronounced than at SU(3) symmetric quark masses

$$
\begin{aligned}
\mathcal{L}_{BB}^{(0),SU(3)} =& - c_1 \mathrm{Tr}(B_i^\dagger B_i B_j^\dagger B_j) - c_2 \mathrm{Tr}(B_i^\dagger B_j B_j^\dagger B_i) - c_3 \mathrm{Tr}(B_i^\dagger B_j^\dagger B_i B_j) \\
& - c_4 \mathrm{Tr}(B_i^\dagger B_j^\dagger B_j B_i) - c_5 \mathrm{Tr}(B_i^\dagger B_i)\mathrm{Tr}(B_j^\dagger B_j) - c_6 \mathrm{Tr}(B_i^\dagger B_j)\mathrm{Tr}(B_j^\dagger B_i)\,, \\
\mathcal{L}_{BB}^{(2),SU(3)} =& - \tilde{c}_1 \mathrm{Tr}(B_i^\dagger \nabla^2 B_i B_j^\dagger B_j + \mathrm{h.c.}) - \tilde{c}_2 \mathrm{Tr}(B_i^\dagger \nabla^2 B_j B_j^\dagger B_i + \mathrm{h.c.}) \\
& - \tilde{c}_3 \mathrm{Tr}(B_i^\dagger B_j^\dagger \nabla^2 B_i B_j + \mathrm{h.c.}) - \tilde{c}_4 \mathrm{Tr}(B_i^\dagger B_j^\dagger \nabla^2 B_j B_i + \mathrm{h.c.}) \\
& - \tilde{c}_5 [\mathrm{Tr}(B_i^\dagger \nabla^2 B_i)\mathrm{Tr}(B_j^\dagger B_j) + \mathrm{h.c.}] - \tilde{c}_6 [\mathrm{Tr}(B_i^\dagger \nabla^2 B_j)\mathrm{Tr}(B_j^\dagger B_i) + \mathrm{h.c.}]\,, \\
\mathcal{L}_{BB}^{(2),SU(3)} =& - c_1^\chi \mathrm{Tr}(B_i^\dagger \chi B_i B_j^\dagger B_j) - c_2^\chi \mathrm{Tr}(B_i^\dagger \chi B_j B_j^\dagger B_i) - c_3^\chi \mathrm{Tr}(B_i^\dagger B_i \chi B_j^\dagger B_j) \\
& - c_4^\chi \mathrm{Tr}(B_i^\dagger B_j \chi B_j^\dagger B_i) - c_5^\chi \mathrm{Tr}(B_i^\dagger \chi B_j^\dagger B_i B_j + \mathrm{h.c.}) - c_6^\chi \mathrm{Tr}(B_i^\dagger \chi B_j^\dagger B_j B_i + \mathrm{h.c.}) \\
& - c_7^\chi \mathrm{Tr}(B_i^\dagger B_j^\dagger \chi B_i B_j) - c_8^\chi \mathrm{Tr}(B_i^\dagger B_j^\dagger \chi B_j B_i) - c_9^\chi \mathrm{Tr}(B_i^\dagger B_j^\dagger B_i B_j \chi) \\
& - c_{10}^\chi \mathrm{Tr}(B_i^\dagger B_j^\dagger B_j B_i \chi) - c_{11}^\chi \mathrm{Tr}(B_i^\dagger \chi B_i)\mathrm{Tr}(B_j^\dagger B_j) - c_{12}^\chi \mathrm{Tr}(B_i^\dagger \chi B_j)\mathrm{Tr}(B_j^\dagger B_i)\,,
\end{aligned}
$$

$$
\mathcal{L}_{BB}^{(0),SU(6)} = -a(\Psi_{\mu\nu\rho}^\dagger \Psi^{\mu\nu\rho})^2 - b\Psi_{\mu\nu\sigma}^\dagger \Psi^{\mu\nu\tau} \Psi_{\rho\delta\tau}^\dagger \Psi^{\rho\delta\sigma}
$$

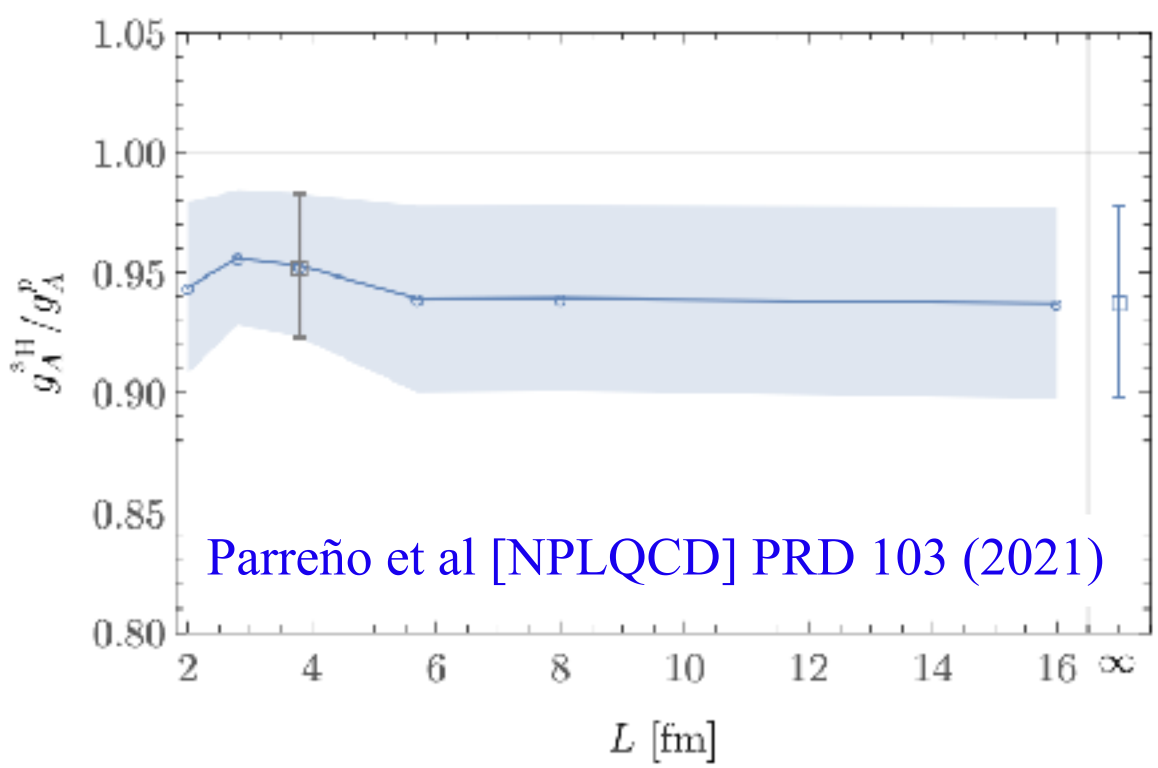
Pionless EFT can also be used as a tool to extrapolate lattice QCD results to infinite-volume

Stochastic variational approach to infinite-volume extrapolation of energies

Barnea et al, PRL 114 (2015)

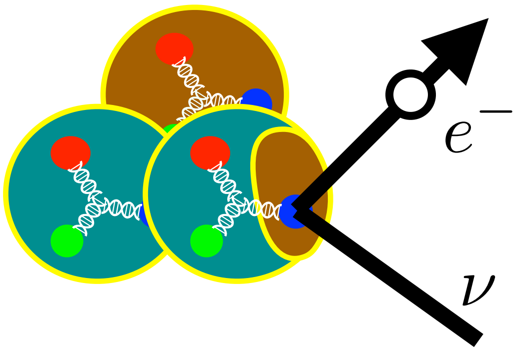
Recently extended to infinite-volume extrapolation of nuclear matrix elements

Detmold and Shanahan, PRD 103 (2021)



Parreño et al [NPLQCD] PRD 103 (2021)

Triton β- decay



Triton studied with one $m_\pi \sim 450$ MeV ensemble, 3 lattice volumes

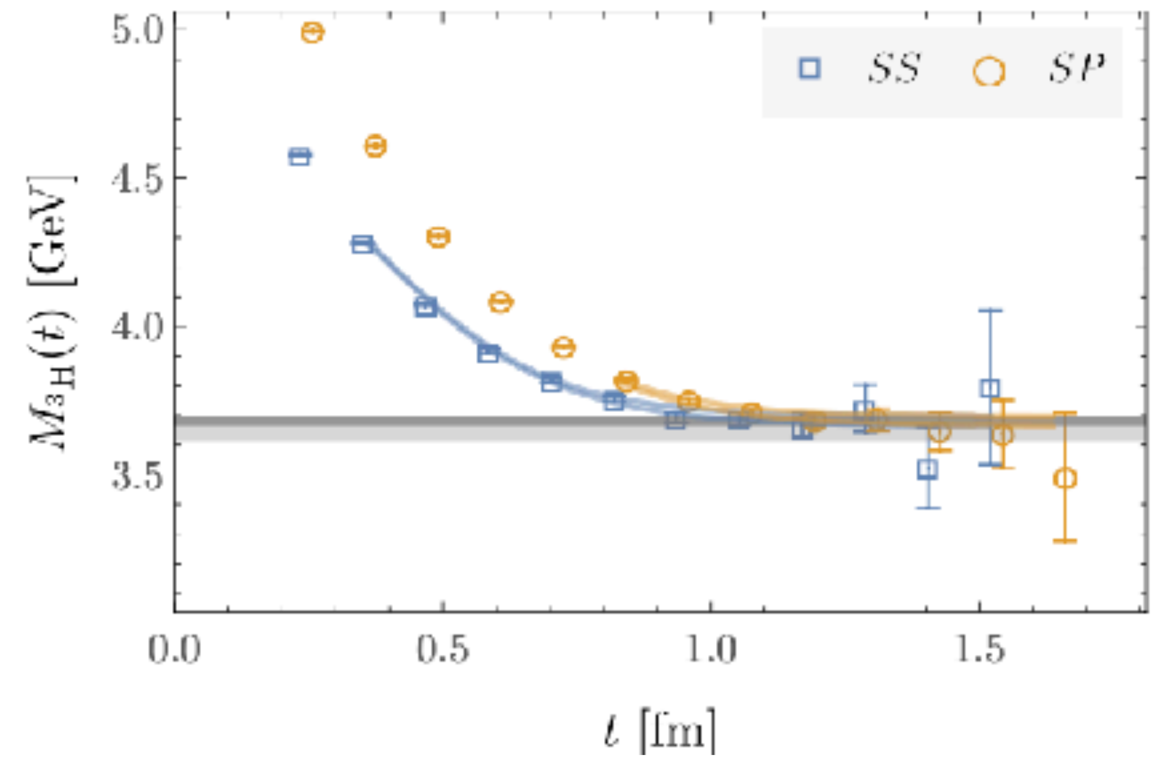
Robust fitting methodology used to study excited-state effects

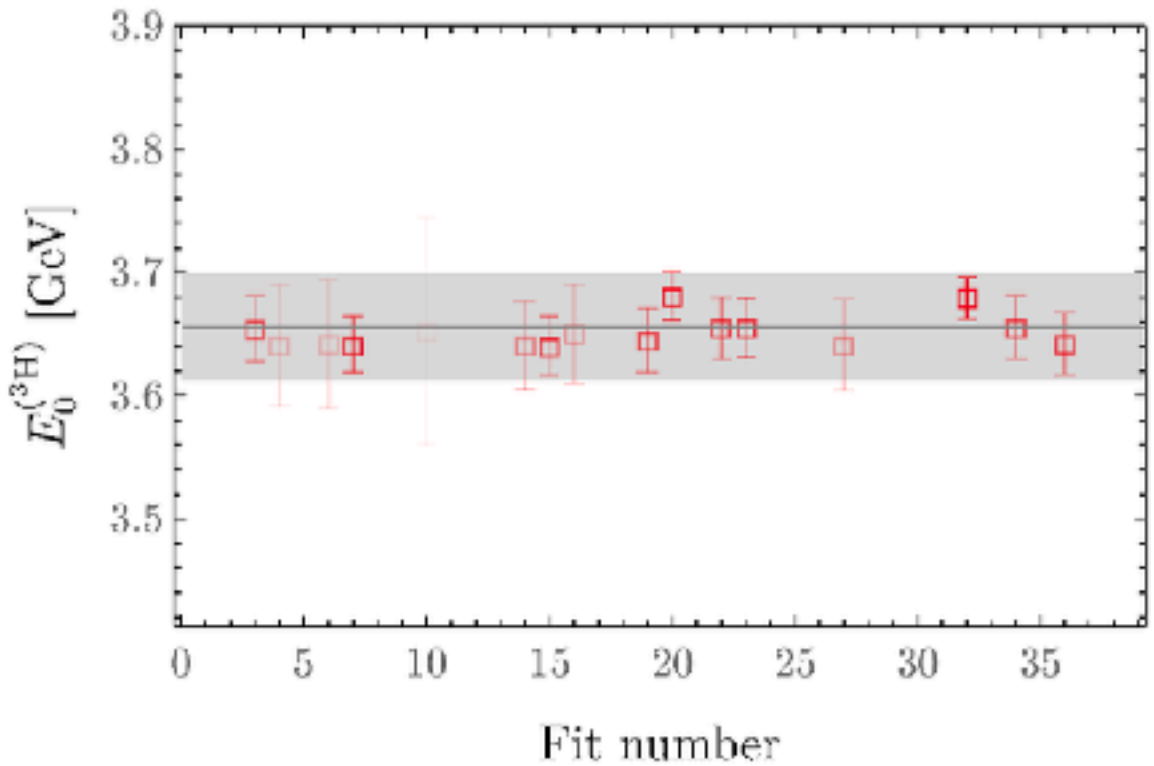
Ground-state energy consistent with a binding energy intermediate between nature and $m_\pi \sim 800$ MeV

Gamow-Teller matrix element governing triton β- decay rate computed

$$g_A(^3\mathrm{H}) = |\langle ^3\mathrm{He}|A_z^+|^3\mathrm{H}\rangle|$$

$$= |\langle ^3\mathrm{H}|A_z^3|^3\mathrm{H}\rangle|$$

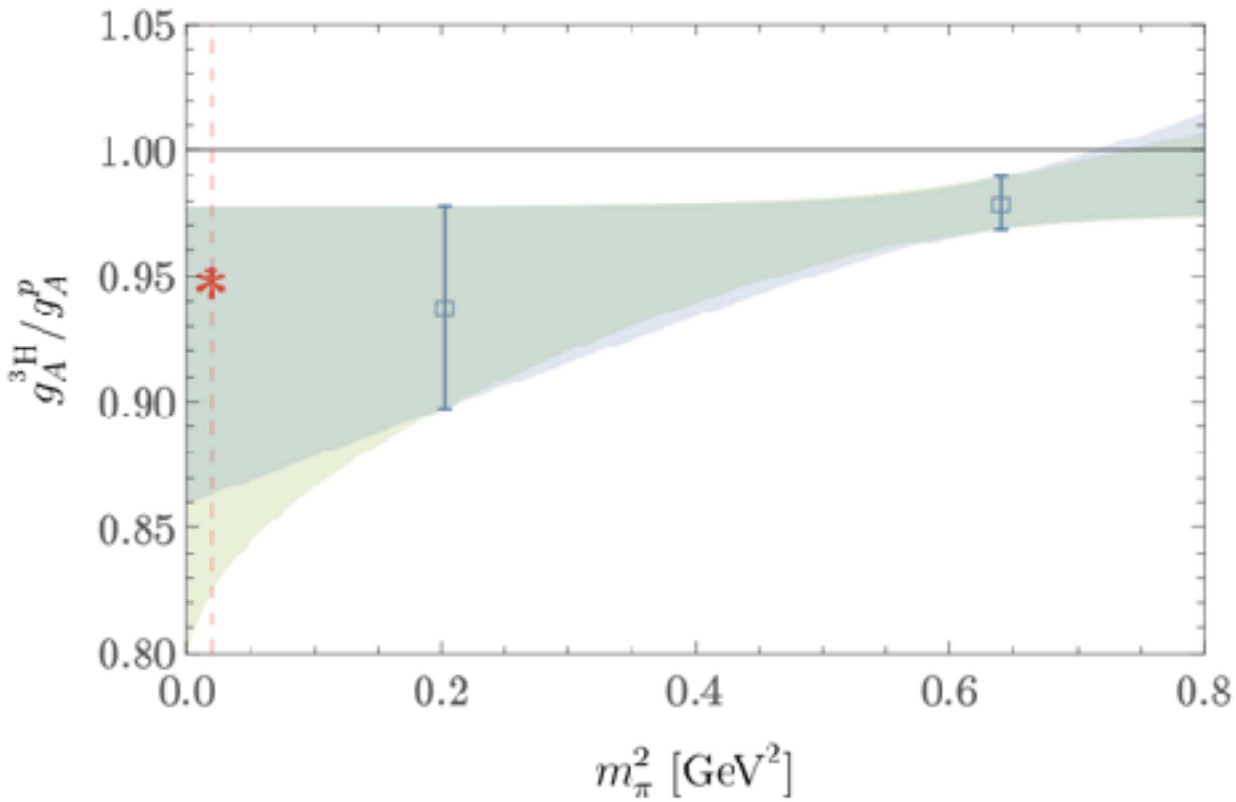




Parreño et al [NPLQCD] PRD 103 (2021)

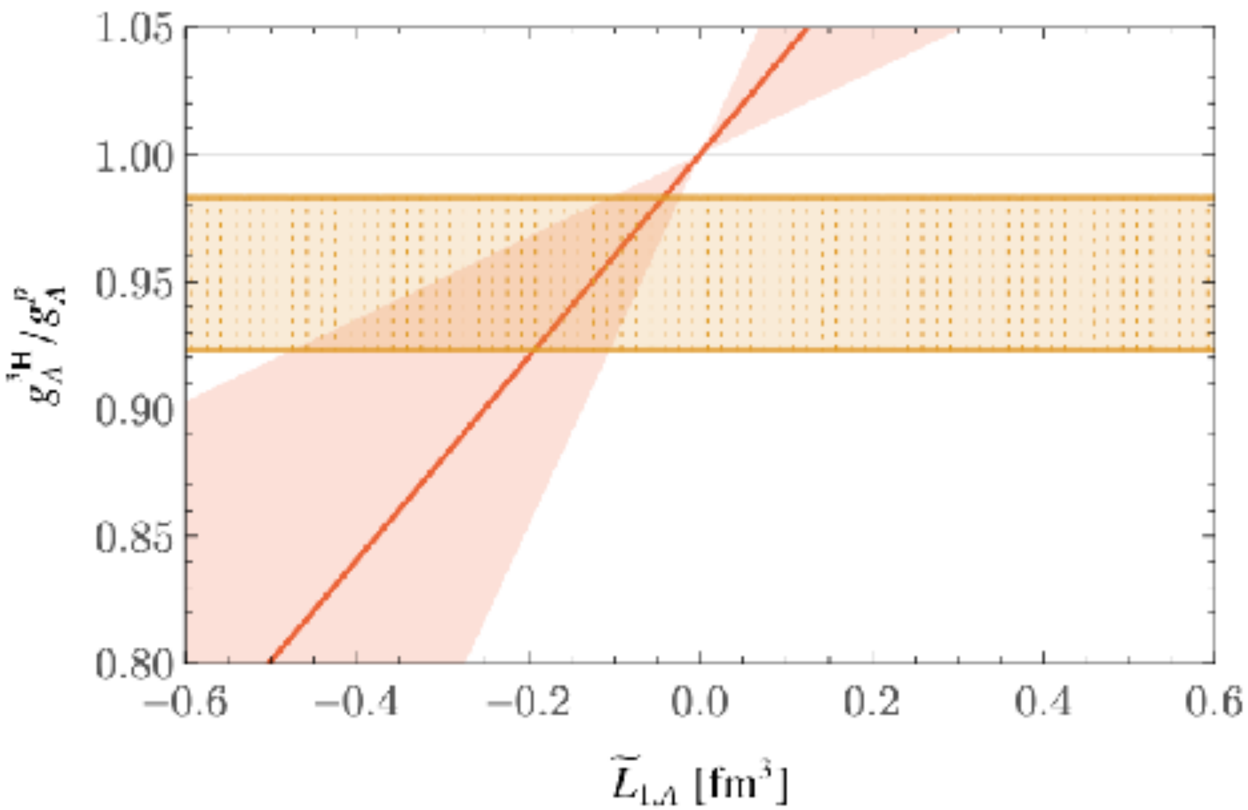
Triton β - decay

Triton β - decay results with $m_\pi \sim 450$ MeV permit first extrapolations to physical point

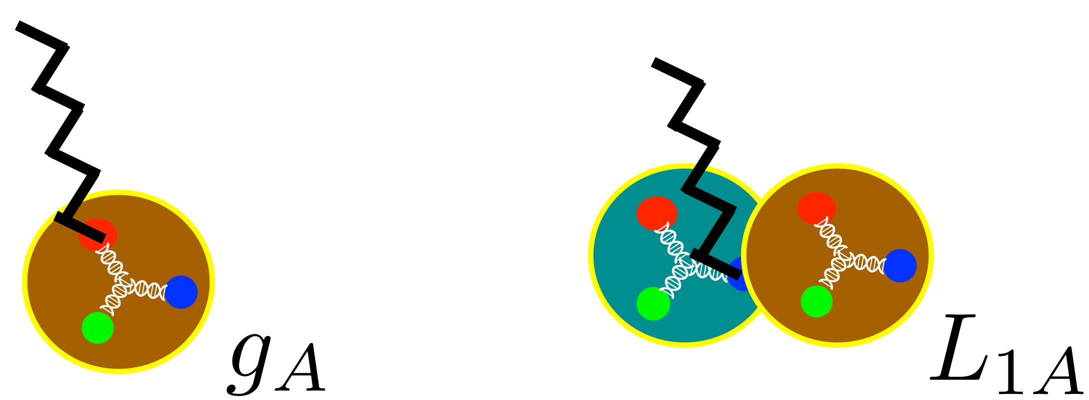


Several systematic uncertainties remain, but encouraging agreement with experiment seen

Parreño et al [NPLQCD] PRD 103 (2021)



Results used to constrain two-body axial current in pionless EFT



Approaching the physical point

Very high statistics required

$$e^{3(2M_N - 3m_\pi)(1\ \mathrm{fm})}$$

$m_\pi \sim 800$ MeV:	10^5
$m_\pi \sim 450$ MeV:	10^7
$m_\pi \sim 140$ MeV:	10^9

Improved Wilson fermions used for efficiency and simplicity of contractions / spin algebra

QUDA multigrid with many propagator sources per configuration

Clark et al, Proceedings SC '16 (2016)

QDP / JIT used to put all parts of propagator calculations on GPU

Winter, Clark, Edwards, Jóo, Proceedings IPDPS '14 (2014)

Sparsened quark propagators and baryon blocks allow manageable storage

Detmold et al [NPLQCD], arXiv:1908.07050

Systematic uncertainties

Several systematic uncertainties remain to be quantified in detail

- Heavier than physical quark masses only
- One lattice spacing
- Excited-state effects

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Gap between ground and two-nucleon finite-volume "scattering" states becomes small for large volumes, ground-state dominance relies on overlap factors

$$Z_0 e^{-E_0 t}\left(1 + \frac{Z_1}{Z_0} e^{-\delta t} + \dots\right) \qquad \delta \sim \frac{4\pi^2}{ML^2}$$

For non-positive-definite correlation functions, cancellations between the ground and excited-state could in principle conspire to form a "false plateau"

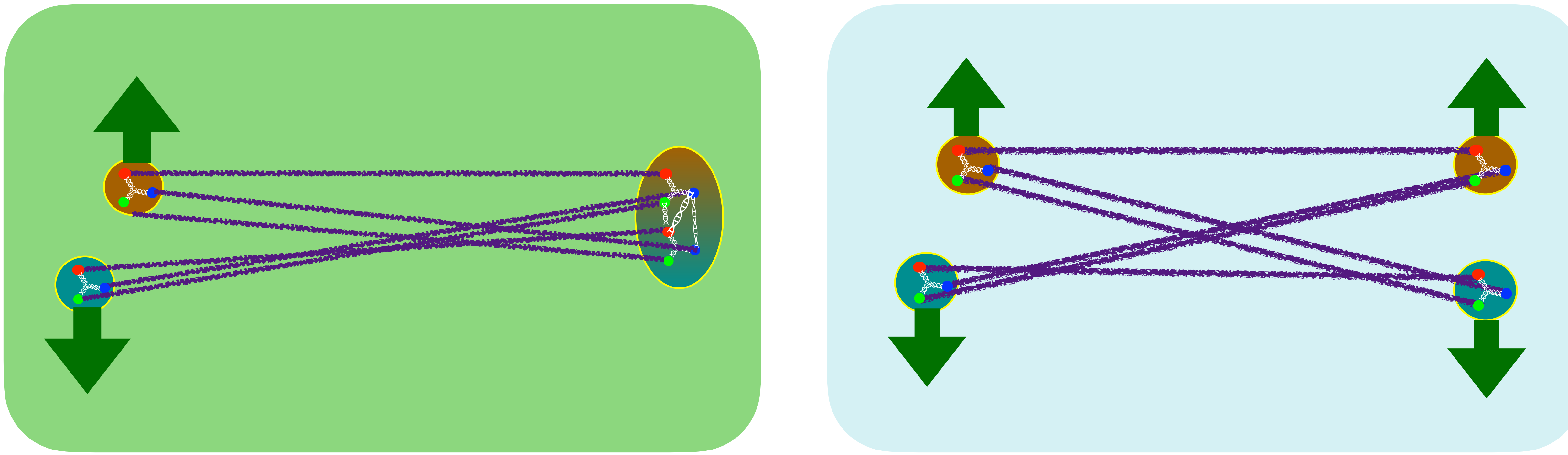
See e.g. Iritani et al, JHEP 10 (2016)

First studies using positive-definite correlation functions (enabled by distillation / stochastic LapH) give results in tension with previous studies

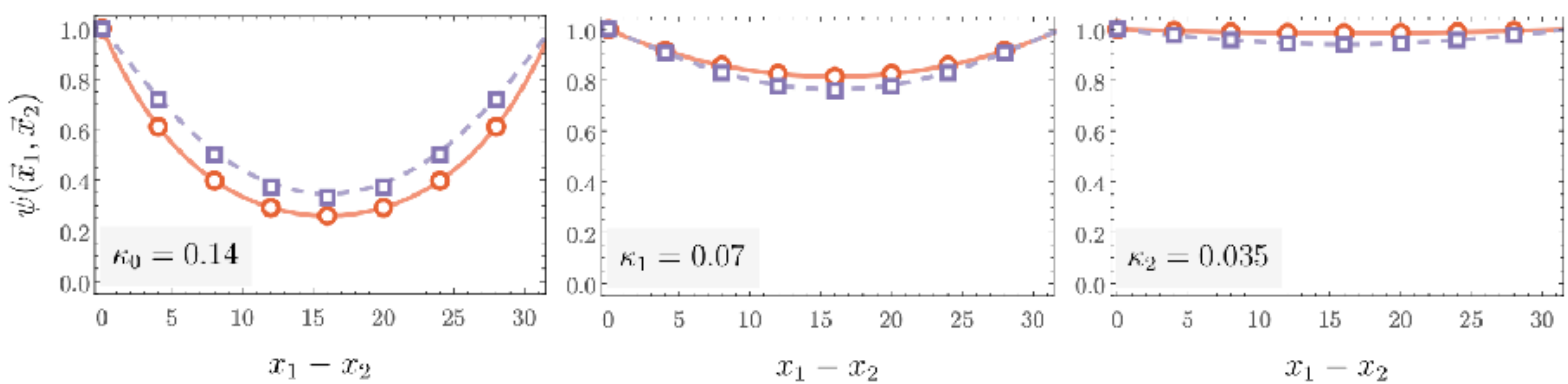
Francis et al, PRD 99 (2019) Hörz et al, PRC 103 (2021) Green et al, arXiv:2103.01054

Thinking positive

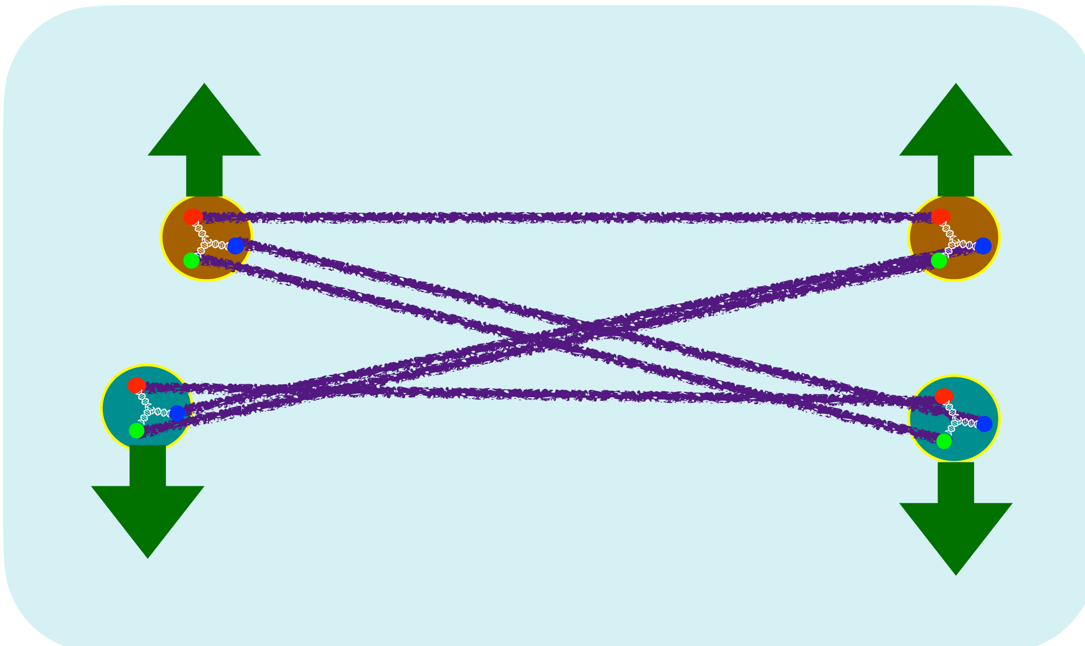
Correlation-function matrices for an interpolator set including both local "hexaquark" and bilocal "dibaryon" operators generalize calculations performed to date

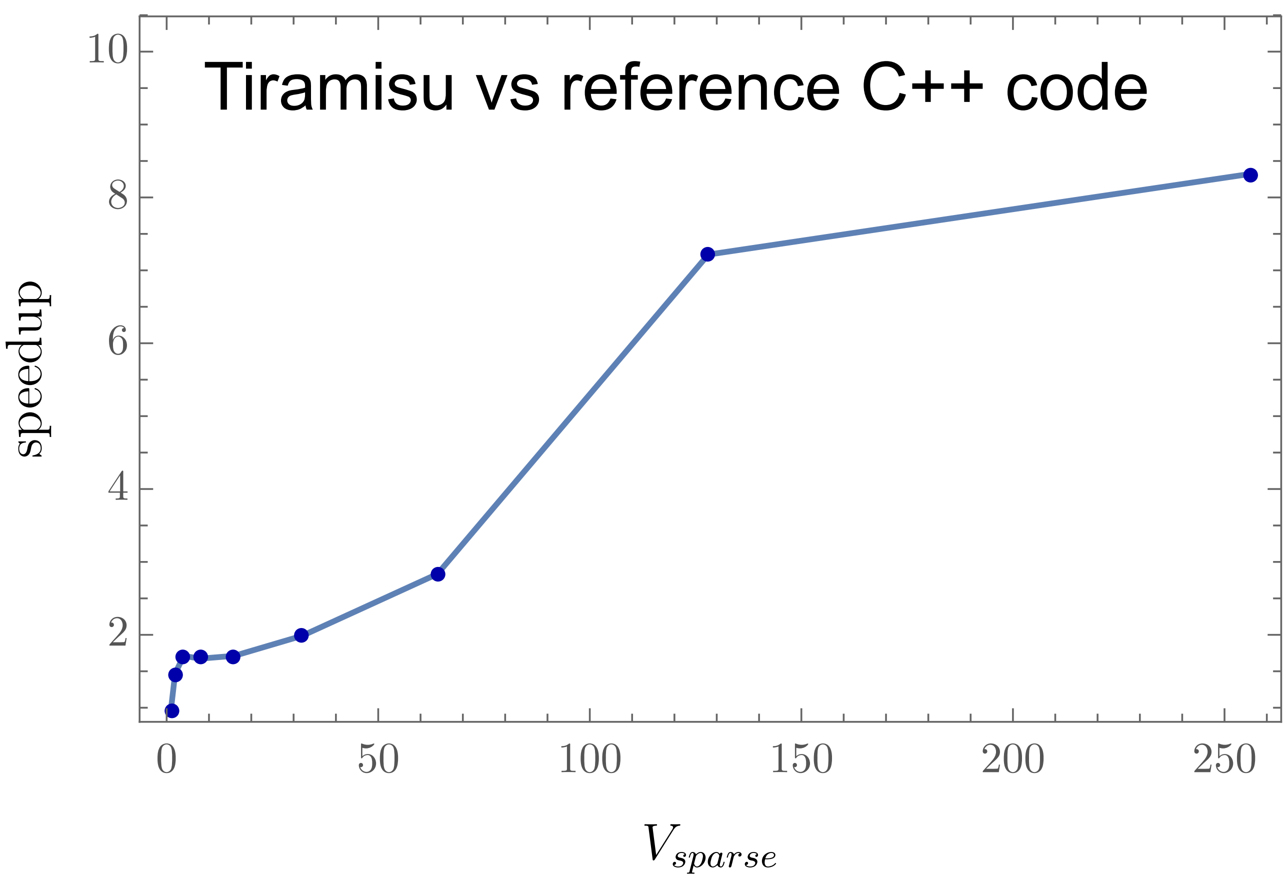


Also possible to include "quasi-local" operators with a variety of wavefunctions in an interpolating operator set, may increase overlap with loose bound states



Contractions - a piece of cake





Loops over independent spatial locations for each baryon are expensive

- Bilocal baryon blocks (product of sums)

$$V^4 \to V^3$$

- Sparsening

$$V \to V_{\text{sparse}}$$

- Tiramisu — a C++ polyhedral compiler that excels at optimizing tensor contractions

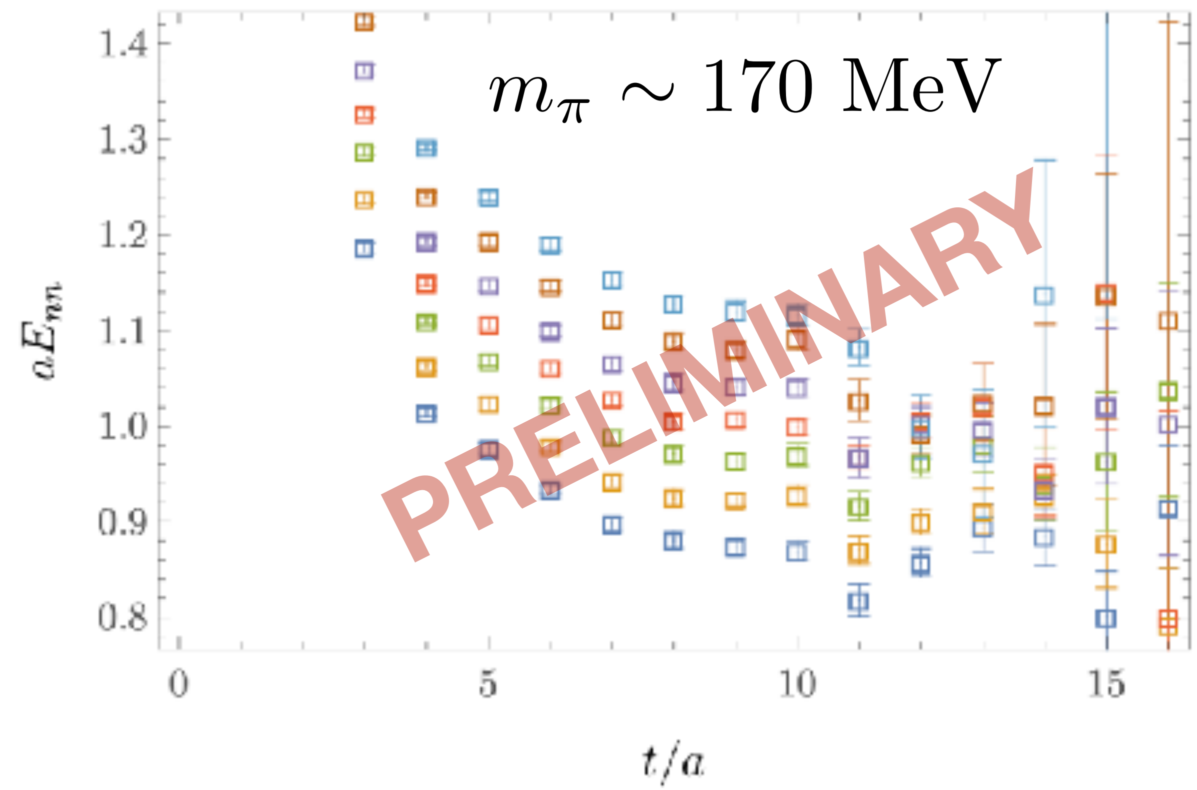
Baghdadi et al, arXiv:2005.04091

https://github.com/Tiramisu-Compiler/tiramisu

Towards variational studies of nuclei

- New contraction codes validated (including machine precision symmetry tests) and CPU version optimized

- Promising preliminary results obtained by solving Generalized Eigenvalue Problem (GEVP) with variational sets of two-nucleon interpolating operators



Flavor States	I	J	$-S$	$N_u : N_d : N_s$	Cost	Storage
np	0	1	0	3:3:0	108	3
pp	1	0	0	4:2:0	48	1
Λp, $\Sigma^0 p$, $\Sigma^+ n$	1/2	0	1	3:2:1	108	9
Λp, $\Sigma^0 p$, $\Sigma^+ n$	1/2	1	1	3:2:1	324	27
$\Sigma^+ p$	3/2	0	1	4:1:1	24	1
$\Sigma^+ p$	3/2	1	1	4:1:1	72	3
$\Xi^- p$, $\Xi^0 n$, $\Lambda\Lambda$, $\Sigma^+\Sigma^-$, $\Sigma^0\Sigma^0$	0	0	2	2:2:2	400	25
$\Xi^- p$, $\Xi^0 n$	0	1	2	2:2:2	96	12
$\Lambda\Sigma^+$, $\Xi^0 p$	1	0	2	3:1:2	48	4
$\Lambda\Sigma^+$, $\Sigma^0\Sigma^+$, $\Xi^0 p$	1	1	2	3:1:2	324	27
$\Sigma^+\Sigma^+$	2	0	2	4:0:2	48	1
$\Lambda\Xi^0$, $\Sigma^0\Xi^0$, $\Sigma^+\Xi^-$	1/2	0	3	2:1:3	108	9
$\Lambda\Xi^0$, $\Sigma^0\Xi^0$, $\Sigma^+\Xi^-$	1/2	1	3	2:1:3	324	27
$\Sigma^+\Xi^0$	3/2	0	3	3:0:3	36	1
$\Sigma^+\Xi^0$	3/2	1	3	3:0:3	108	3
$\Xi^0\Xi^-$	0	1	4	1:1:4	72	3
$\Xi^0\Xi^0$	1	0	4	2:0:4	48	1
				Total	2296	157

- Next step: variational baryon-baryon scattering including coupled-channel systems relevant for H-dibaryon and neutron star physics

- LQCD calculations of nuclear matrix elements with fully controlled systematic uncertainties on the horizon