Ab initio nuclear structure
with chiral interactions

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All interactions are “effective” until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD, is an effective theory valid below the Planck scale
\[ \lambda < 10^{19} \text{ GeV/c} \]

The “bare” NN interaction, usually with derived quantities, is thus an effective interaction valid up to some scale, typically the scale of the known NN phase shifts and Deuteron gs properties
\[ \lambda \sim 600 \text{ MeV/c } (3.0 \text{ fm}^{-1}) \]

Effective NN interactions can be further renormalized to lower scales and this can enhance convergence of the many-body applications
\[ \lambda \sim 300 \text{ MeV/c } (1.5 \text{ fm}^{-1}) \]

“Consistent” NNN and higher-body forces, as well as electroweak currents, are those valid to the same scale as their corresponding NN partner, and obtained in the same renormalization scheme.

\begin{frame}
\begin{center}
\textbf{ab initio renormalization schemes}
\end{center}
\begin{itemize}
  \item SRG: \textbf{S}imilarity \textbf{R}enormalization \textbf{G}roup
  \item LSO: \textbf{L}ee-\textbf{S}uzuki-\textbf{O}kamoto
  \item Vlowk: \textbf{V} with low k scale limit
  \item UCOM: \textbf{U}nitary \textbf{C}orrelation \textbf{O}perator \textbf{M}ethod
\end{itemize}
and there are more!
Chiral perturbation theory ($\chi$PT) allows for controlled power series expansion

Expansion parameter: \( \left( \frac{Q}{\Lambda_{\chi}} \right)^\nu \), \( Q \) – momentum transfer,

\( \Lambda_{\chi} \approx 1 \text{ GeV}, \chi\) - symmetry breaking scale

Within $\chi$PT $2\pi$-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs \( \{c_i\} \).

Terms suggested within the Chiral Perturbation Theory

Regularization is essential, which is obvious within the Harmonic Oscillator wave function basis.

R. Machleidt, D. R. Entem, nucl-th/0503025
No Core Shell Model
A large sparse matrix eigenvalue problem

\[
H = T_{rel} + V_{NN} + V_{3N} + \cdots
\]
\[
H|\Psi_i\rangle = E_i|\Psi_i\rangle
\]
\[
|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle
\]
Diagonalize \{\langle \Phi_m | H | \Phi_n \rangle \}

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, \( \alpha, \beta, \ldots \)
- Evaluate the nuclear Hamiltonian, \( H \), in basis space of HO (Slater) determinants (manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body \( H \) in its “m-scheme” basis where \([\alpha = (n,l,j,m_j,\tau_z)]\)

\[
|\Phi_n\rangle = [a^+_{\alpha} \cdots a^+_{\varsigma}]_n |0\rangle
\]
\[
n = 1, 2, \ldots, 10^{10} \text{ or more!}
\]

- Evaluate observables and compare with experiment

Comments
- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to \( A = 20 \) (40) today with largest computers available
Effective Hamiltonian in the NCSM
Lee-Suzuki-Okamoto renormalization scheme

- \( n \)-body cluster approximation, \( 2 \leq n \leq A \)
- \( H^{(n)}_{\text{eff}} \) \( n \)-body operator
- Two ways of convergence:
  - For \( P \to 1 \) \( H^{(n)}_{\text{eff}} \to H \)
  - For \( n \to A \) and fixed \( P \): \( H^{(n)}_{\text{eff}} \to H_{\text{eff}} \)
Strong correlation between \( c_D \) and \( c_E \) for exp’l properties of \( A = 3 \) & \( 4 \)

\( \Rightarrow \) Retain this correlation in applications to other systems

Range favored by various analyses & values are “natural”

**FIG. 1** (color online). Relations between \( c_D \) and \( c_E \) for which the binding energy of \( ^3\text{H} \) (8.482 MeV) and \( ^3\text{He} \) (7.718 MeV) are reproduced. (a) \( ^4\text{He} \) ground-state energy along the averaged curve. (b) \( ^4\text{He} \) charge radius \( r_c \) along the averaged curve. Dotted lines represent the \( r_c \) uncertainty due to the uncertainties in the proton charge radius.
**ab initio NCSM with $\chi_{EFT}$ Interactions**

- Only method capable to apply the $\chi_{EFT}$ NN+NNN interactions to all p-shell nuclei
- Importance of NNN interactions for describing nuclear structure and transition rates

**Extensions and work in progress**

- **Better determination of the NNN force itself, feedback to $\chi_{EFT}$** (LLNL, OSU, MSU, TRIUMF/GSI)
- **Implement Vlowk & SRG renormalizations** (Bogner, Furnstahl, Maris, Perry, Schwenk & Vary, NPA 801, 21(2008); ArXiv 0708.3754)
- **Response to external fields - bridges to DFT/DME/EDF (SciDAC/UNEDF)**
  - Axially symmetric quadratic external fields - in progress
  - Triaxial and spin-dependent external fields - planning process
- **Cold trapped atoms** (Stetcu, Barrett, van Kolck & Vary, PRA 76, 063613(2007); ArXiv 0706.4123) and applications to other fields of physics (e.g. quantum field theory)
- **Effective interactions with a core** (Lisetsky, Barrett, Navratil, Stetcu, Vary)
- **Nuclear reactions-scattering** (Forssen, Navratil, Quaglioni, Shirokov, Mazur, Luu, Savage, Schwenk, Vary)
Note additional predicted states! Shown as dashed lines.

C_D = -0.2
- Solves the puzzle of the long but useful lifetime of $^{14}$C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments

- Dimension of matrix solved for 8 lowest states $\sim 1\times10^9$
- Solution takes $\sim 6$ hours on 215,000 cores on Cray XT5 Jaguar at ORNL
Detailed results and estimated corrections due to chiral 2-body currents

TABLE I. Decomposition of $p$-shell contributions to $M_{CT}$ in the LS scheme for the beta decay of $^{14}$C without and with 3NF. The 3NF is included at two values of $c_D$ where $c_D \approx -0.2$ is preferred by the $^3$H lifetime and $c_D \approx -2.0$ is preferred by the $^{14}$C lifetime. The calculations are performed in the $N_{\text{max}} = 8$ basis space with $\hbar \Omega = 14$ MeV.

<table>
<thead>
<tr>
<th>$(m_l, m_s)$</th>
<th>$NN$ only</th>
<th>$NN + 3NF$ $c_D = -0.2$</th>
<th>$NN + 3NF$ $c_D = -2.0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1, + \frac{1}{2})$</td>
<td>0.015</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td>$(1, - \frac{1}{2})$</td>
<td>-0.176</td>
<td>-0.296</td>
<td>-0.280</td>
</tr>
<tr>
<td>$(0, + \frac{1}{2})$</td>
<td>0.307</td>
<td>0.277</td>
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<td>0.015</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td><strong>Subtotal</strong></td>
<td>0.292</td>
<td>-0.019</td>
<td>0.024</td>
</tr>
<tr>
<td><strong>Total sum</strong></td>
<td>0.275</td>
<td>-0.063</td>
<td>-0.013</td>
</tr>
</tbody>
</table>

$2$-body current quenching (est'd)\(^*\) $\times 0.75 \Rightarrow -0.047$ $\times 0.93 \Rightarrow -0.012$

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Tritium half-life

$c_D = -0.20$ $-2.0$

Thy/Exp. = 1.00 0.80

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*J. Menéndez, D. Gazit and A. Schwenk, PRL (to appear); arXiv 1103.3622; (estimated using their effective 1-body quenching approximation)
Innovations underway to improve the NCSM with aims:
(1) improve treatment of clusters and intruders
(2) enable *ab initio* solutions of heavier nuclei
Initially, all follow the NCFC approach = extrapolations

**Importance Truncated – NCSM**
Extrapolate full basis at each Nmax using a sequence with improving tolerance
Robert Roth and collaborators

“Realistic” single-particle basis - Woods-Saxon example
Control the spurious CM motion with Lagrange multiplier term
A. Negoita, ISU PhD thesis project
Alternative sp basis spaces – Mark Caprio collaboration

**SU(3) No Core Shell Model**
Add symmetry-adapted many-body basis states
Preserve exactly the CM factorization
LSU - ISU – OSU collaboration

**No Core Monte Carlo Shell Model**
Invokes single particle basis (FCI) truncation
Separate spurious CM motion in same way as CC approach
Scales well to larger nuclei
U. Tokyo - ISU collaboration
**Novel approach**
- Sp-CI: exploiting symmetries of nuclear dynamics
- Innovative workload balancing techniques & representations of multiple levels of parallelism for ultra-large realistic problems

**Impact**
- Applications for nuclear science and astrophysics

**Goals**
- Ab initio calculations of nuclei with unprecedented accuracy using basis-space expansions
- Current calculations limited to nuclei with $A \leq 16$ (up to 20 billion basis states with 2-body forces)

**Progress**
- Scalable CI code for nuclei
- Sp(3,R)/SU(3)-symmetry vital

**Challenges/Promises**
- Constructing hybrid Sp-CI code
- Publicly available peta-scale software for nuclear science

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**Taming the scale explosion in nuclear calculations**
*NSF PetaApps - Louisiana State, Iowa State, Ohio State collaboration*
$^8$Li translationally invariant 1-body density distributions

2+ Ground State

1$^{\text{st}}$ 4+ Excited State

Chase Cockrell, ISU PhD student
Fig. 15. Plot of the ground-state energy of $^4$He and $^6$He vs. $\lambda$ for potentials evolved by the SRG from the 500 MeV N$^3$LO $NN$-only potential from Ref. [13]. Conservative error bars have been included with the larger $\lambda$’s, for which an extrapolation is needed. The arrow marks the experimental binding.

R. Roth: Include 3NF within SRG renormalization

IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions.
Descriptive Science

Predictive Science
**Objectives**

- Apply *ab initio* microscopic nuclear theory’s predictive power to major test case

**Impact**

- Deliver robust predictions important for improved energy sources
- Provide important guidance for DOE-supported experiments
- Compare with new experiment to improve theory of strong interactions

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**Experiment confirms our published predictions!**

- Dimension of matrix solved for 14 lowest states \( \sim 2 \times 10^9 \)
- Solution takes \( \sim 2.5 \) hours on 30,000 cores (Cray XT4 Jaguar at ORNL)

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Ab Initio Neutron drops in traps

\[ \text{UNEDF} \]
Properties of trapped neutrons interacting with realistic nuclear Hamiltonians

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Pieter Maris and James Vary
Iowa State University, Ames, Iowa, 50011

Steven C. Pieper
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(Dated: April 20, 2011)

Preliminary
Ab initio Nuclear Structure

Ab initio Nuclear Reactions
Figure 7. Calculated $p-^4\text{He}$ differential cross section (bottom panels) and analyzing power (top panels) for proton laboratory energies $E_p = 12, 14.32$ and $17$ MeV compared to experimental data from Refs. [29, 30, 31, 32]. The SRG-$N^3$LO NN potential with $\lambda = 2.02$ fm$^{-1}$ was used.

Figure 8. Calculated inelastic $^7\text{Be}(p,p')^7\text{Be}(1/2^-)$ cross section with indicated positions of the $P$-wave resonances (left figure). Calculated S-factor of the $^3\text{He}(d,p)^4\text{He}$ fusion reaction compared to experimental data (right figure). Energies are in the center of mass. The SRG-$N^3$LO NN potential with $\lambda = 1.85$ fm$^{-1}$ ($\lambda = 1.5$ fm$^{-1}$) was used, respectively.

Applications to Relativistic Quantum Field Theory
QED (new) and QCD (under development)


Light cone coordinates and generators

\[ M^2 = P^0 P_0 - P^1 P_1 = (P^0 - P^1)(P_0 + P_1) = P^+ P^- = KE \]
Preliminary


No External Trap

Basis params

$\omega$  $N_{\text{max}}$

- 0.5  $2n_{\text{even}}$
- 0.5  $2n_{\text{odd}}$
- 0.02  $2n_{\text{even}}$
- 0.02  $2n_{\text{odd}}$

Linear fits to $N_{\text{max}} \geq 64$

$\sqrt{\delta \mu / g^2}$

$1 / \sqrt{N_{\text{max}}}$

Observation

*Ab initio* nuclear physics maximizes predictive power & represents a theoretical and computational physics challenge

Key issues

How to achieve the full physics potential of *ab initio* theory? Can theory and experiment work more closely to define/solve fundamental physics problems?

Conclusions

We have entered an era of first principles, high precision, nuclear structure and nuclear reaction theory

Linking nuclear physics and the cosmos through the Standard Model is well underway

Pioneering collaborations between Physicists, Computer Scientists and Applied Mathematicians have become essential to progress
Challenges

- improve NN + NNN + NNNN interactions/renormalization
develop effective operators beyond the Hamiltonian
tests of fundamental symmetries
- achieve higher precision
  quantify the uncertainties - justified through simulations
  global dependencies mapped out
- proceed to heavier systems - breaking out of the p-shell
  extend quantum many-body methods
- evaluate more complex projectile-target reactions
- achieve efficient use of computational resources – improve
  scalability, load-balance, I/O, inter-process communications
- build a community aiming for investment preservation
  support/sustain open libraries of codes/data
  develop/implement provenance framework/practices
Collaborators – Nuclear Structure/Reactions

Nuclear Physics
ISU: Pieter Maris, Alina Negoita, Chase Cockrell, Miles Aronnax
LLNL: Erich Ormand, Tom Luu, Eric Jurgenson
SDSU: Calvin Johnson, Plamen Krastev
ORNL/UT: David Dean, Hai Ah Nam, Markus Kortelainen, Mario Stoitsov, Witek Nazarewicz, Gaute Hagen, Thomas Papenbrock
OSU: Dick Furnstahl, students
MSU: Scott Bogner, Heiko Hergert
WMU: Mihai Horoi
ANL: Harry Lee, Steve Pieper
LANL: Joe Carlson, Stefano Gandolfi
UA: Bruce Barrett, Sid Coon, Bira van Kolck, Michael Kruse
LSU: Jerry Draayer, Tomas Dytrych, Kristina Sviratcheva
UW: Martin Savage, Ionel Stetcu

International Collaborators
Canada: Petr Navratil
Russia: Andrey Shirokov, Alexander Mazur
Sweden: Christian Forssen
Japan: Takashi Abe, Takaharu Otsuka, Yutaka Utsuno, Noritaka Shimizu
Germany: Achim Schwenk, Robert Roth, Javier Menendez, students

Computer Science/Applied Math
Ames Lab: Masha Sosonkina, Fang (Cherry) Liu, students
LBNL: Esmond Ng, Chao Yang, Metin Aktulga
ANL: Stefan Wild
OSU: Umit Catalyurek

Collaborators – Quantum Field Theory
ISU: Heli Honkanen, Xingbo Zhao, Pieter Maris, Paul Wiecki, Young Li
Stanford: Stan Brodsky
Germany: Hans-Juergen Pirner
Costa Rica: Guy de Teramond
India: Avaroth Harindranath
Recent accomplishments of the *ab initio* no core shell model (NCSM) and no core full configuration (NCFC)

- Described the anomaly of the nearly vanishing quadrupole moment of $^6\text{Li}$
- Established need for NNN potentials to explain neutrino $^{12}\text{C}$ cross sections
- Explained quenching of Gamow-Teller transitions (beta-decays) in light nuclei
- Obtained successful description of $A=10-13$ nuclei with chiral NN+NNN potentials
- Explained ground state spin of $^{10}\text{B}$ by including chiral NNN potentials
- Successful prediction of low-lying $^{14}\text{F}$ spectrum (resonances) before experiment
- Developed/applied methods to extract phase shifts (J-matrix, external trap)
- Explained the anomalous long lifetime of $^{14}\text{C}$ with chiral NN+NNN potentials