From QCD to ab initio nuclear structure with point nucleons and back again

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## Ab initio nuclear physics – fundamental ?'s

> What controls nuclear saturation?



- > How the nuclear shell model emerges from the underlying theory?
- > What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- > Can nuclei provide precision tests of the fundamental laws of nature?
- Under what conditions do we need QCD to describe nuclear structure?













National Science Foundation







K-super. Blue Waters Lomonosov

+



## UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional



### The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of  $2^{A} \binom{A}{Z}$  coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Successful ab initio quantum many-body approaches (A > 6)

Stochastic approach in coordinate space Greens Function Monte Carlo (**GFMC**)

Hamiltonian matrix in basis function space No Core Shell Model (**NCSM**) No Core Full Configuration (**NCFC**)

Cluster hierarchy in basis function space Coupled Cluster (**CC**)

Lattice + EFT approach (New)

Coming - Gorkov Green's Function, ...

Comments All work to preserve and exploit symmetries Extensions of each to scattering/reactions are well-underway They have different advantages and limitations

## "Leadership Class" Computational Resources







16 "cores" on one compute "node"Total: 300,000 cores at presentTitan will have 1GPU/node

& INCITE Award 55M cpu-hrs/yr

## 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.

ab initio renormalization schemes	
SRG:	Similarity Renormalization Group
OLS:	Okubo-Lee- <mark>S</mark> uzuki
Vlowk:	V with low k scale limit
UCOM:	Unitary Correlation Operator Method
	and there are more!

## **Effective Nucleon Interaction** (Chiral Perturbation Theory)

#### Chiral perturbation theory ( $\chi$ PT) allows for controlled power series expansion



#### No Core Shell Model

A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet \bullet$$
$$H |\Psi_i\rangle = E_i |\Psi_i\rangle$$
$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$
Diagonalize {\langle \Psi\_m |H|\Psi\_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,  $\alpha$ ,  $\beta$ ,...
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where  $[\alpha = (n,l,j,m_{j},\tau_{z})]$

$$|\Phi_n\rangle = [a_{\alpha}^+ \bullet \bullet \bullet a_{\zeta}^+]_n |0\rangle$$
  
n = 1,2,...,10<sup>10</sup> 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 renormalization scheme



$$H: E_{1}, E_{2}, E_{3}, \dots E_{d_{P}}, \dots E_{\infty}$$
$$H_{\text{eff}}: E_{1}, E_{2}, E_{3}, \dots E_{d_{P}}$$
$$OXHX^{-1}P = O$$
$$M_{\text{eff}} = PXHX^{-1}P$$

- *n*-body cluster approximation,  $2 \le n \le A$
- *H*<sup>(n)</sup><sub>eff</sub> *n*-body operator
- Two ways of convergence:
  - For  $P \rightarrow 1$   $H^{(n)}_{eff} \rightarrow H$
  - For  $n \to A$  and fixed *P*:  $H^{(n)}_{eff} \to H_{eff}$



Controlling the center-of-mass (cm) motion in order to preserve Galilean invariance

Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

$$H_{eff} \left( N_{\max}, \hbar \Omega \right) \equiv P[T_{rel} + V^a \left( N_{\max}, \hbar \Omega \right)] P$$

$$H = H_{eff} \left( N_{\max}, \hbar \Omega \right) + \lambda H_{cm}$$

$$H_{cm} = \frac{P^2}{2M_A} + \frac{1}{2} M_A \Omega^2 R^2$$

$$\lambda \sim 10 \text{ suffices}$$

Along with the  $N_{max}$  truncation in the HO basis, the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.



#### Structure of A = 10-13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,<sup>1</sup> V. G. Gueorguiev,<sup>1,\*</sup> J. P. Vary,<sup>1,2</sup> W. E. Ormand,<sup>1</sup> and A. Nogga<sup>3</sup>

Strong correlation between  $c_D$  and  $c_E$ for exp' I properties of A = 3 & 4

=> 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 <sup>3</sup>H (8.482 MeV) and <sup>3</sup>He (7.718 MeV) are reproduced. (a) <sup>4</sup>He ground-state energy along the averaged curve. (b) <sup>4</sup>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)



P. Maris, P. Navratil, J. P. Vary, to be published



week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of <sup>14</sup>C

P. Maris,<sup>1</sup> J. P. Vary,<sup>1</sup> P. Navrátil,<sup>2,3</sup> W. E. Ormand,<sup>3,4</sup> H. Nam,<sup>5</sup> and D. J. Dean<sup>5</sup>



- Solves the puzzle of the long but useful lifetime of <sup>14</sup>C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding DOE-supported experiments





Figure 10. GT matrix element between the  $(1^+, 0)$  ground state and the lowest  $(0^+, 1)$  excited state of <sup>14</sup>N, using the  $(1^+, 0)$  wavefunction obtained with threebody forces, but the  $(0^+, 1)$  wavefunction obtained without three-body forces, and vice versa. For comparison, we also include the results with and without three-body forces for both wavefunctions. 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

> <u>"Realistic" single-particle basis - Woods-Saxon example</u> 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

## <sup>7</sup>Li – effect of removing spurious CM motion



## 9Be Translationally invariant gs density Full 3D densities = rotate around the vertical axis



Shows that one neutron provides a "ring" cloud around two alpha clusters binding them together

Chase Cockrell, ISU PhD student









<sup>8</sup>Li

# Descriptive Science

## **Predictive Science**

## **"Proton-Dripping Fluorine-14"**

## **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



Light cone coordinates and generators



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

J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng and C. Yang, "Hamiltonian light-front field theory in a basis function approach", Phys. Rev. C 81, 035205 (2010); arXiv nucl-th 0905.1411

H. Honkanen, P. Maris, J. P. Vary and S. J. Brodsky, "Electron in a transverse harmonic cavity", Phys. Rev. Lett. 106, 061603 (2011); arXiv: 1008.0068

<u>Basis Light Front Quantization (BLFQ) in brief</u>
 Derive LF Hamiltonian density from Lagrangian density
 Invoke canonical quantization
 Evaluate H (kinetic term + vertices) in transverse 2D HO basis with longitudinal plane waves
 Setup associated multi-parton Fock space basis
 Diagonalize -> invariant mass spectra and LF amplitudes
 Evaluate suite of observables and compare with experiment



## **Sample planned Applications for BLFQ**

Strong pulsed laser fields – electron-positron pair creation

Quarkonia – structure & transitions - including exotics

Baryons – mass spectra, spin content, Generalized Parton Distributions (GPDs) Under what conditions do we need quarks & gluons to describe nuclear structure?

- 1. Spin crisis in the proton
- 2. Proton RMS radius
- 3. DIS on nuclei Bjorken x > 1
- 4. Nuclear Equation of State
- 5. Q > 1 GeV/c

#### New Measurements of High-Momentum Nucleons and Short-Range Structures in Nuclei

N. Fomin,<sup>1,2,3</sup> J. Arrington,<sup>4</sup> R. Asaturyan,<sup>5,\*</sup> F. Benmokhtar,<sup>6</sup> W. Boeglin,<sup>7</sup> P. Bosted,<sup>8</sup> A. Bruell,<sup>8</sup> M. H. S. Bukhari,<sup>9</sup>
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P. Markowitz,<sup>7</sup> P. McKee,<sup>3</sup> D. G. Meekins,<sup>8</sup> H. Mkrtchyan,<sup>5</sup> T. Navasardyan,<sup>5</sup> G. Niculescu,<sup>19</sup> A. K. Opper,<sup>20</sup>
C. Perdrisat,<sup>21</sup> D. H. Potterveld,<sup>4</sup> V. Punjabi,<sup>22</sup> X. Qian,<sup>13</sup> P. E. Reimer,<sup>4</sup> J. Roche,<sup>20,8</sup> V. M. Rodriguez,<sup>9</sup> O. Rondon,<sup>3</sup>
E. Schulte,<sup>4</sup> J. Seely,<sup>10</sup> E. Segbefia,<sup>18</sup> K. Slifer,<sup>3</sup> G. R. Smith,<sup>8</sup> P. Solvignon,<sup>8</sup> V. Tadevosyan,<sup>5</sup> S. Tajima,<sup>3</sup> L. Tang,<sup>8,18</sup>
G. Testa,<sup>17</sup> R. Trojer,<sup>17</sup> V. Tvaskis,<sup>18</sup> W. F. Vulcan,<sup>8</sup> C. Wasko,<sup>3</sup> F. R. Wesselmann,<sup>22</sup> S. A. Wood,<sup>8</sup>
J. Wright,<sup>3</sup> and X. Zheng<sup>3,4</sup>



FIG. 2. Pernucleon cross section ratios vs x at  $\theta_e = 18^\circ$ .



FIG. 3 (color online). The  ${}^{4}\text{He}/{}^{3}\text{He}$  ratios from E02-019  $(Q^{2} \approx 2.9 \text{ GeV}^{2})$  and CLAS  $(\langle Q^{2} \rangle \approx 1.6 \text{ GeV}^{2})$ ; errors are combined statistical and systematic uncertainties. For x > 2.2, the uncertainties in the  ${}^{3}\text{He}$  cross section are large enough that a one-sigma variation of these results yields an asymmetric error band in the ratio. The error bars shown for this region represent the central 68% confidence level region.

#### DIS in the quark cluster model

$$\frac{v}{\sigma_{M}} \frac{d^{2}\sigma}{d\Omega dE'} = vW_{2}(v,Q^{2}) + vW_{1}(v,Q^{2})\tan^{2}(\theta/2)$$

$$vW_{2}(v,Q^{2}) = vW_{2}^{in}(v,Q^{2}) + vW_{2}^{q-el}(v,Q^{2})$$

$$vW_{2}^{in}(v,Q^{2}) = \sum_{quarks-j} e_{j}^{2}\xi P(\xi)$$

$$P(\xi) = \sum_{clusters-i} p_{i}\overline{P}_{i}(\xi)$$

$$\overline{P}_{i}(\xi) = \int_{0}^{\xi_{i/A}^{ih}} dy \int_{0}^{\xi_{q/i}^{ih}} du \ \overline{n}_{q/i}(u) N_{i/A}(y) \delta(uy - \xi)$$

$$\xi_{i/A}^{th} = \left\{ \left(1 + \frac{m_{i}^{2}}{M^{2}} \frac{Q^{2}}{v^{2}}\right)^{1/2} + 1\right\} / \left\{ \left(1 + \frac{Q^{2}}{v^{2}}\right)^{1/2} + 1\right\}$$

$$\xi_{q/i}^{th} = 2 / \left\{ \left(1 + \frac{4m_{i}^{2}}{Q^{2}}\right)^{1/2} + 1\right\}$$

 $\overline{n}_{q/i}$  from Regge behavior and counting rules (phase space)  $N_{i/A}$  from non-relativistic wave functions (NRWFs)  $p_i$  quark cluster probabilities evaluated from NRWFs based on critical separation of  $2R_c \sim 1 fm$ 

#### DIS in the quark cluster model







J.P. Vary, Proc. VII Int'l Seminar on High Energy Physics Problems, "Quark Cluster Model of Nuclei and Lepton Scattering Results," Multiquark Interactions and Quantum Chromodynamics, V.V. Burov, Ed., Dubna #D-1, 2-84-599 (1984) 186 [staircase function for x > 1]

See also: Proceedings of HUGS at CEBAF1992, & many conf. proceedings

#### DIS in the quark cluster model

#### Selected references:

H.J. Pirner and J.P. Vary, "Deep-Inelastic Electron Scattering and the Quark Structure of <sup>3</sup>He," Phys. Rev. Lett. **46**, 1376 (1981)

J.P. Vary, Proc. VII Int'l Seminar on High Energy Physics Problems, "Quark Cluster Model of Nuclei and Lepton Scattering Results," Multiquark Interactions and Quantum Chromodynamics, V.V. Burov, Ed., Dubna #D-1, 2-84-599 (1984) 186 [staircase function for x > 1]

M. Sato, S.A. Coon, H.J. Pirner and J.P. Vary, "Quark Cluster Probabilities in Nuclei," Phys. Rev. C **33**, 1062 (1986)

A. Harindranath and J. P. Vary, "Quark Cluster Model Predictions for the Nuclear Drell-Yan Process," Phys. Rev. D **34**, 3378 (1986) [staircase function for x > 1 in DY]

G. Yen, J. P. Vary, A. Harindranath, and H. J. Pirner, "Quark Cluster Model for Deep-Inelastic Lepton-Deuteron Scattering," Phys. Rev. C **42**, 1665 (1990)

H.J. Pirner and J.P. Vary, "Boundary between hadron and quark/gluon structure of nuclei," Phys. Rev. C **84**, 015201 (2011); nucl-th/1008.4962 Under what conditions do we require a quark-based description on nuclear structure? "Quark Percolation in Cold and Hot Nuclei"



Comparison between Quark-Cluster Model and JLAB data



Data: K.S. Egiyan, et al., Phys. Rev. Lett. 96, 082501 (2006)
Theory: H.J. Pirner and J.P. Vary, Phys. Rev. Lett. 46, 1376 (1981) and Phys. Rev. C 84, 015201 (2011); nucl-th/1008.4962;
M. Sato, S.A. Coon, H.J. Pirner and J.P. Vary, Phys. Rev. C 33, 1062 (1986) VOLUME 34, NUMBER 11

#### Quark-cluster-model predictions for the nuclear Drell-Yan process

A. Harindranath and J. P. Vary

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We evaluate the quark-cluster-model predictions for lepton pair production in proton-nucleus, pion-nucleus, and nucleus-nucleus interactions. We examine the issue of a possible ambiguity between the K factor and the probability of six-quark clusters in nuclei. We present predictions for cross sections and cross-section ratios which show substantial sensitivity to different features of the model. The model compares well with the existing data.

#### I. DY CROSS SECTION

In the hadron-hadron center-of-momentum frame we denote the total energy by  $\sqrt{s}$ . For hadrons A and B the four-momenta are  $P_A = (\sqrt{s}/2, 0, 0, \sqrt{s}/2)$  and  $P_B = (\sqrt{s}/2, 0, 0, -\sqrt{s}/2)$ . Let  $x_1 (x_2)$  denote the fraction of longitudinal momentum carried by quark 1 (2) in hadron A (B). Then the longitudinal momentum of the lepton pair with invariant mass M is given by

$$P_L = p_1 + p_2 = (x_1 - x_2) \frac{\sqrt{s}}{2}$$
.

$$\frac{d^2\sigma}{dx_1 dx_2} = \frac{4\pi\alpha^2}{9sx_1 x_2} \sum e_a^2 F_a(x_1, x_2)$$



FIG. 7. QCM prediction for the ratio of DY cross sections for Fe and D as a function of  $x_2$  (for  $x_1=0.1$ ) in the region  $0.1 \le x_2 \le 1.9$ .



Comparison of quark percolation with RHIC data

Theory: H.J. Pirner and J.P. Vary, Phys. Rev. C 84, 015201 (2011); nucl-th/1008.4962

## BLFQ study of QCD bound states - Yang Li, ISU PhD student

Hadrons are QCD bound states. In this study, we'll focus on  $\Lambda$  baryon. Setup the problem:

- We adopt the previous symmetries and constraints;
- **2** Fock space truncation:  $|uds\rangle + |udsg\rangle$ ;
- sector dependent renormalization, which has shown success in many-body computing [18].

Basic procedures:

- Enumerate Fock space, within constraints and truncation;
- Onstruct Hamiltonian matrix;
- Oiagonalize Hamiltonian, regularization and renormalization are essential for convergence;

Compute experimental observables

## Vertices



Renormalization is performed in  $|uds\rangle$  sector.

## some preliminary results

At continuum, physical observables should be independent to all regulators and HO natural length. We renormalize the ground state to physical mass of  $\Lambda(1116)$ , and study the convergence of first excited state.



Colorlines: convergence of first excited state energy with different HO lengths  $1/\sqrt{M_{\rm HO}\Omega_{\rm HO}}$ .

Colorlines: convergence of first excited state energy with with odd/even  $N_{\text{max}}$ .  $(1/\sqrt{M_{\text{HO}}\Omega_{\text{HO}}}=1 \text{ fm})$ 

## some preliminary results



# 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 <sup>6</sup>Li
- Established need for NNN potentials to explain neutrino -<sup>12</sup>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 <sup>10</sup>B by including chiral NNN potentials
- Successful prediction of low-lying <sup>14</sup>F spectrum (resonances) before experiment
- Developed/applied methods to extract phase shifts (J-matrix, external trap)
- Explained the anomalous long lifetime of <sup>14</sup>C with chiral NN+NNN potentials
- Solved systems of trapped neutrons for improved density functionals in isospin extremes

### **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

Applications underway to Light Front QCD and strong time-dependent QED

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

#### **Nuclear Physics**

#### Recent Collaborators

**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 Notre Dame: Mark Caprio ANL: Harry Lee, Steve Pieper LANL: Joe Carlson, Stefano Gandolfi UA: Bruce Barrett, Sid Coon, Bira van Kolck, Michael Kruse, Matthew Avetian LSU: Jerry Draayer, Tomas Dytrych, Kristina Sviratcheva, Chairul Bahri UW: Martin Savage, Ionel Stetcu ISU: Heli Honkanen, Xingbo Zhao, Pieter Maris, Paul Wiecki, Yang Li, Quantum Field **Kirill Tuchin** 

Theory Stanford: Stan Brodsky

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

International

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

Germany: Hans-Juergen Pirner Costa Rica: Guy de Teramond India: Avaroth Harindranath, Usha Kulshreshtha, Daya Kulshreshtha, Asmita Mukherjee