Applications of the Reduced Basis Method in Nuclear Physics

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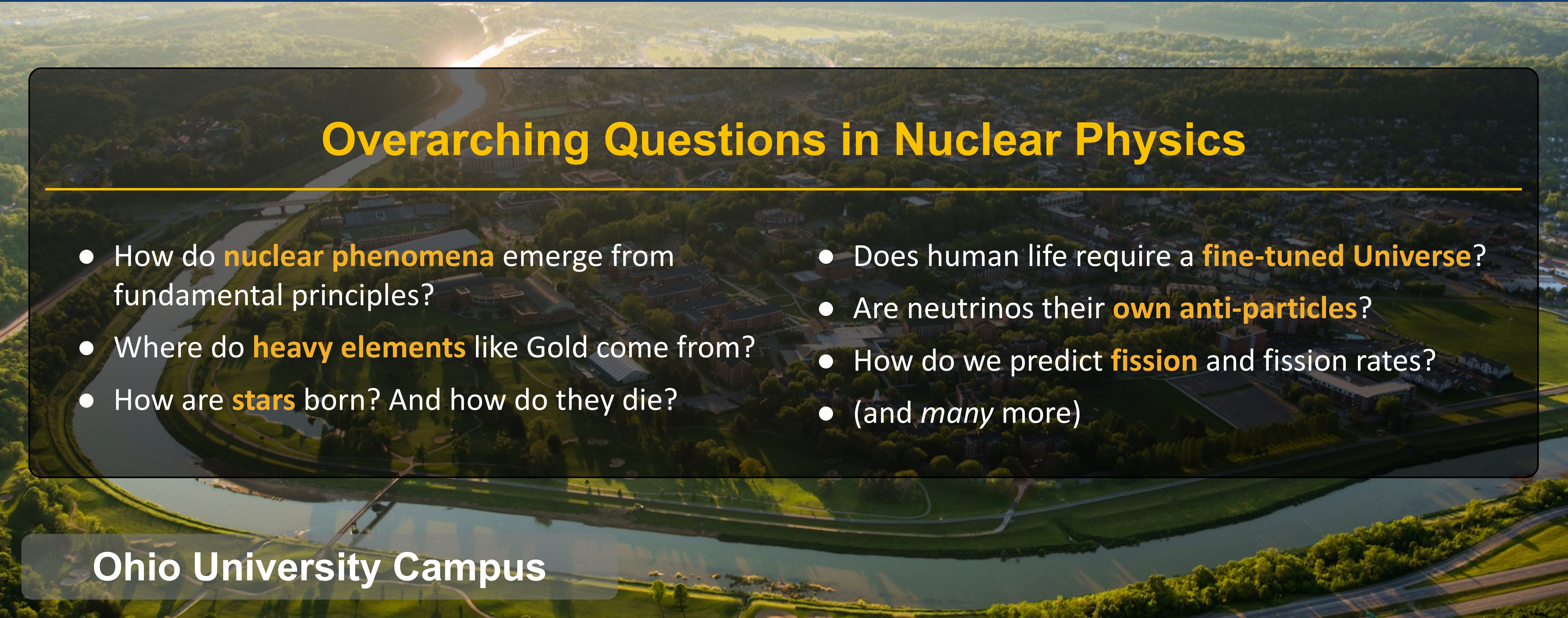
Conference: Nonlinear Model Reduction for Control
May 24, 2023 | Virginia Tech

Overarching Questions in Nuclear Physics

- How do **nuclear phenomena** emerge from fundamental principles?
- Where do **heavy elements** like Gold come from?
- How are **stars** born? And how do they die?
- Does human life require a **fine-tuned Universe**?
- Are neutrinos their **own anti-particles**?
- How do we predict **fission** and fission rates?
- (and *many* more)



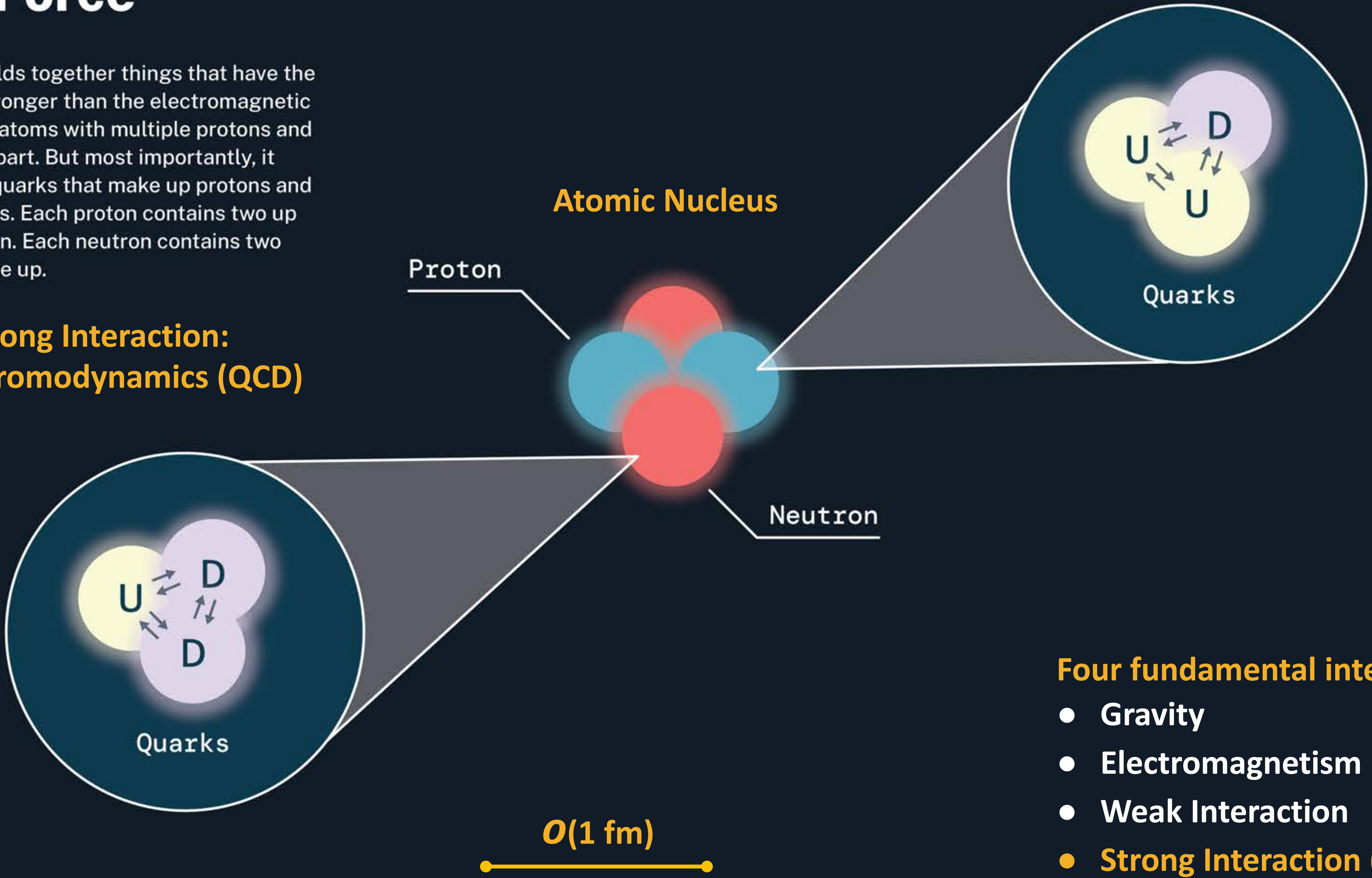
Ohio University Campus

Color Confinement | Asymptotic Freedom | Chiral Symmetry Breaking

Strong Force

The strong force holds together things that have the same charge. It's stronger than the electromagnetic force, so that's why atoms with multiple protons and neutrons don't fly apart. But most importantly, it holds together the quarks that make up protons and neutrons themselves. Each proton contains two up quarks and one down. Each neutron contains two down quarks and one up.

Theory of Strong Interaction: Quantum Chromodynamics (QCD)

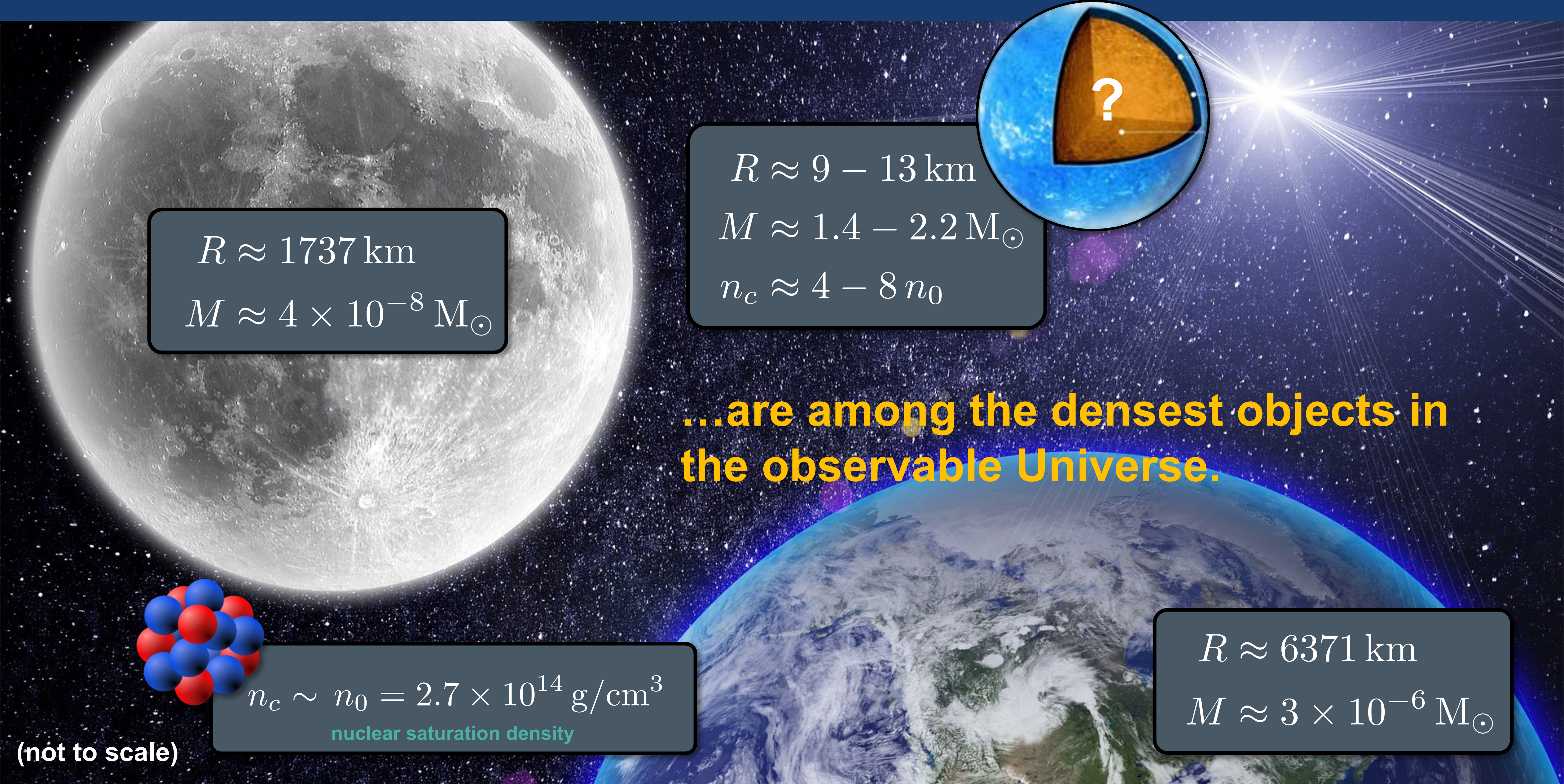


Four fundamental interactions:

- Gravity
- Electromagnetism
- Weak Interaction
- Strong Interaction (or Force)

[NASA]

Neutron stars…



GW170817: first binary neutron star merger observed

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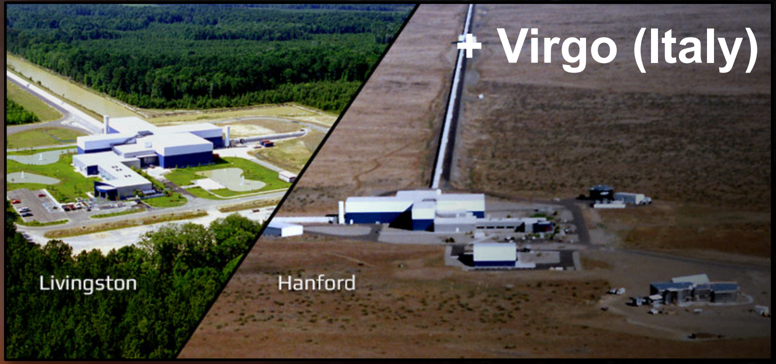
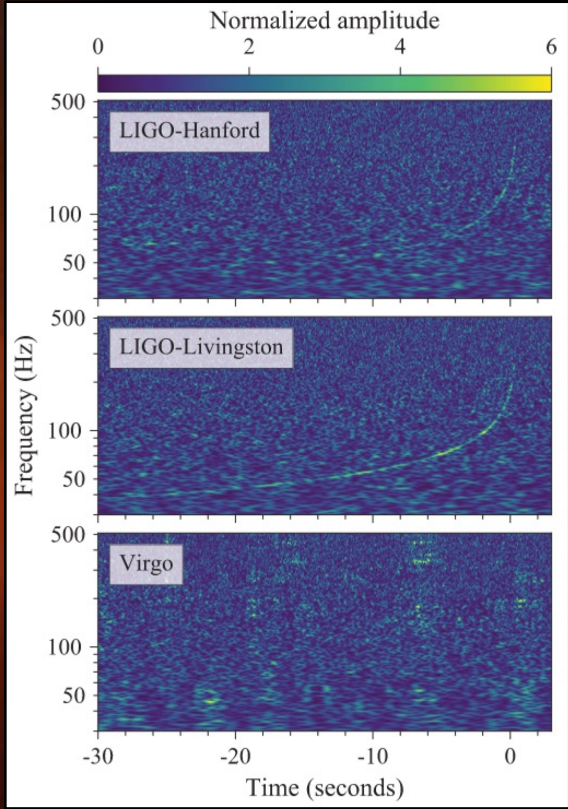
Nobel Prize 2017

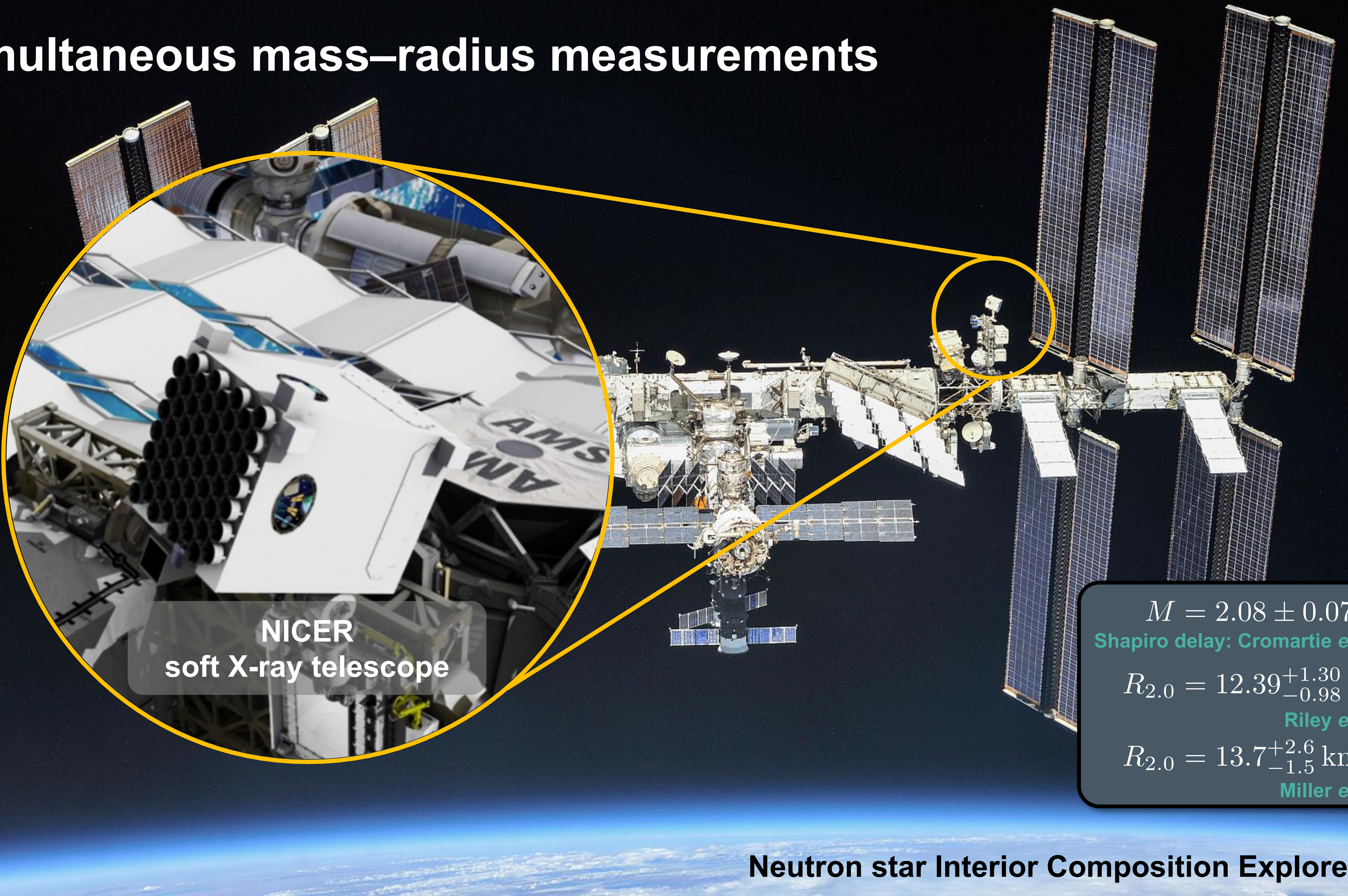


Multi-messenger event:
- gravitational waves
- electromagnetic signals
  - GRB170817A
  - AT2017gfo



Multi-Messenger Astronomy has opened a **new window** to the Universe

Simultaneous mass–radius measurements



$$M = 2.08 \pm 0.07\,\mathrm{M}_\odot$$

Shapiro delay: Cromartie *et al.* (2020)

$$R_{2.0} = 12.39^{+1.30}_{-0.98}\,\mathrm{km}$$

Riley *et al.* (2021)

$$R_{2.0} = 13.7^{+2.6}_{-1.5}\,\mathrm{km}$$

Miller *et al.* (2021)

Neutron star Interior Composition ExploreR @ ISS

FRIB and FRIB Science

Facility for Rare Isotope Beams
at Michigan State University

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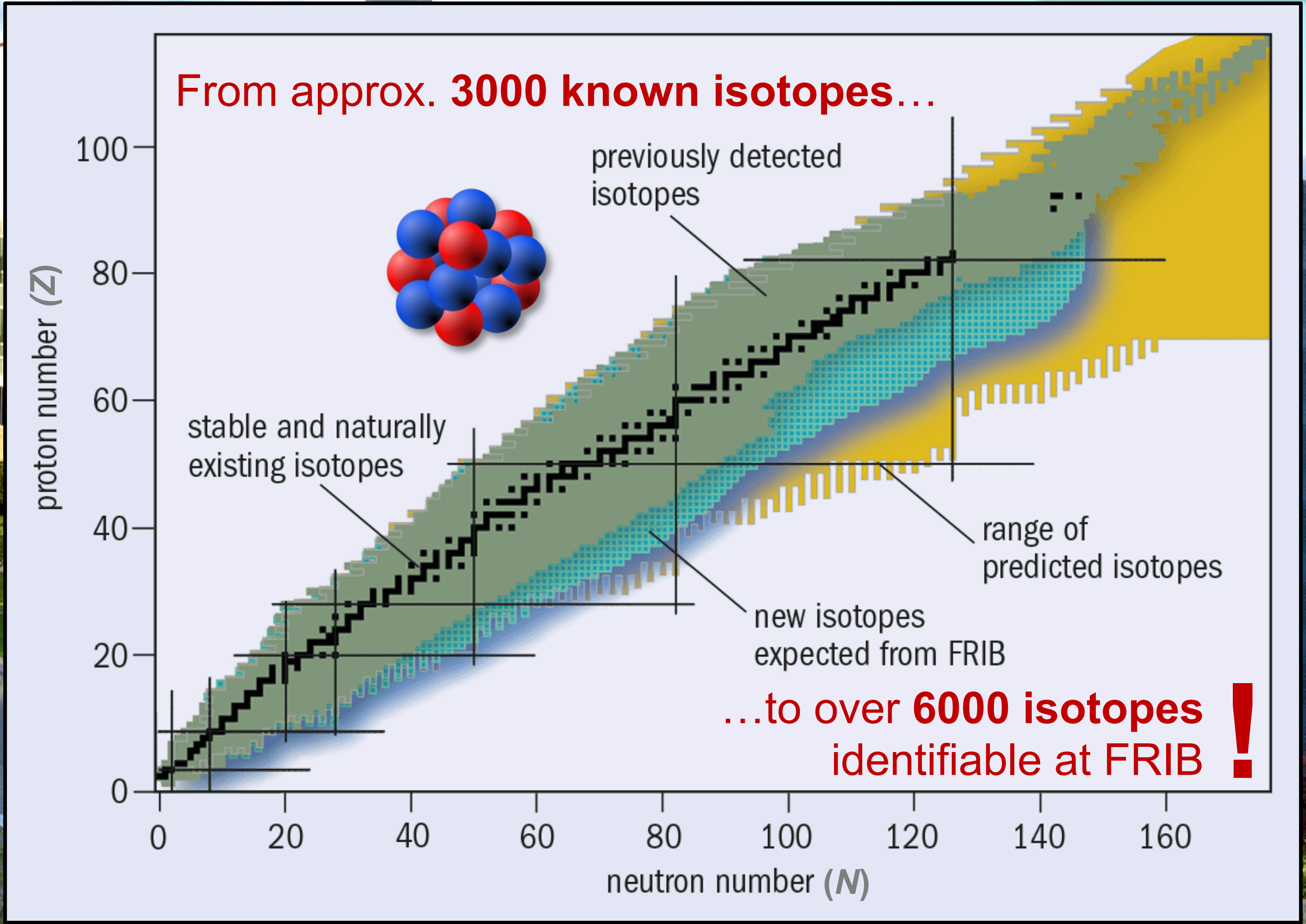
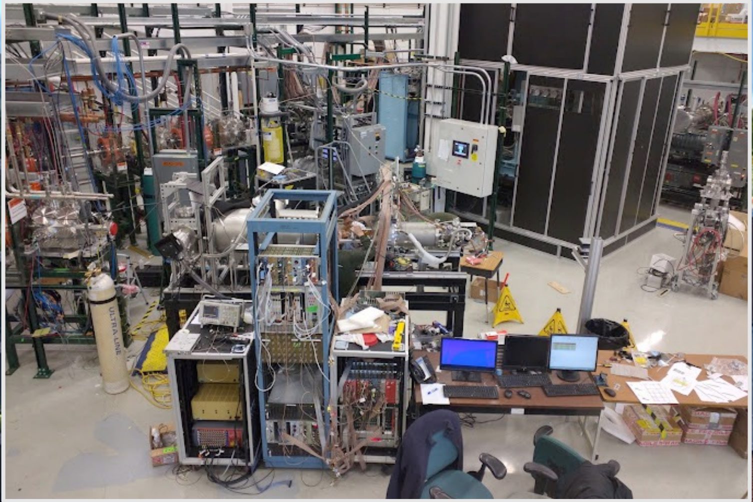
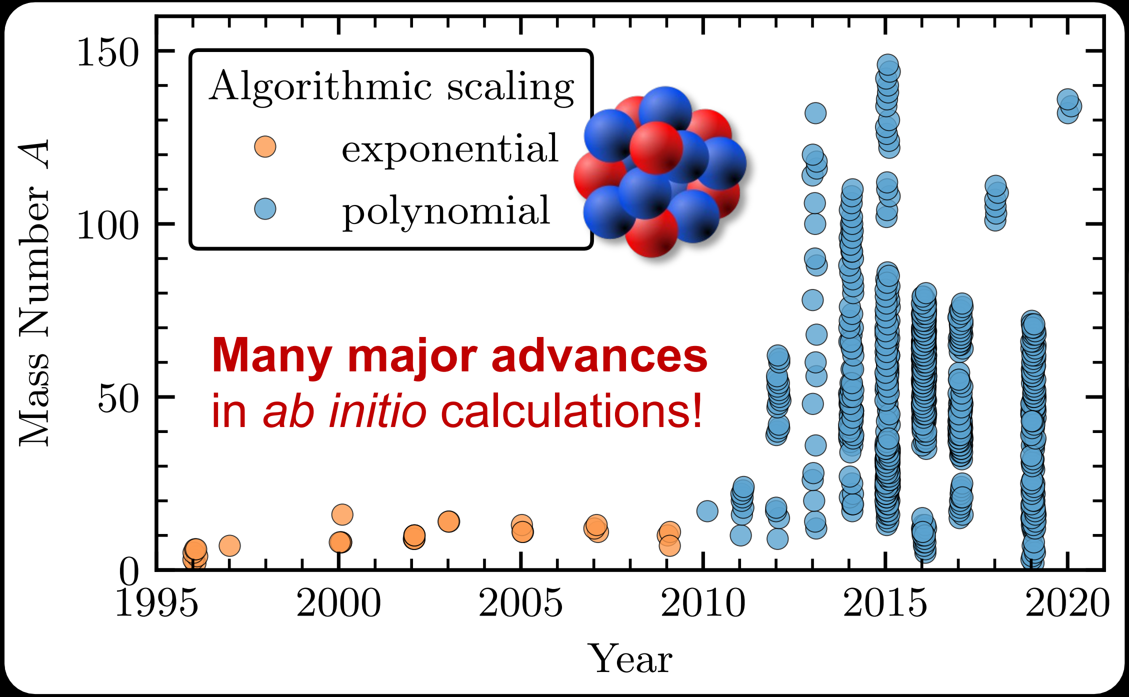
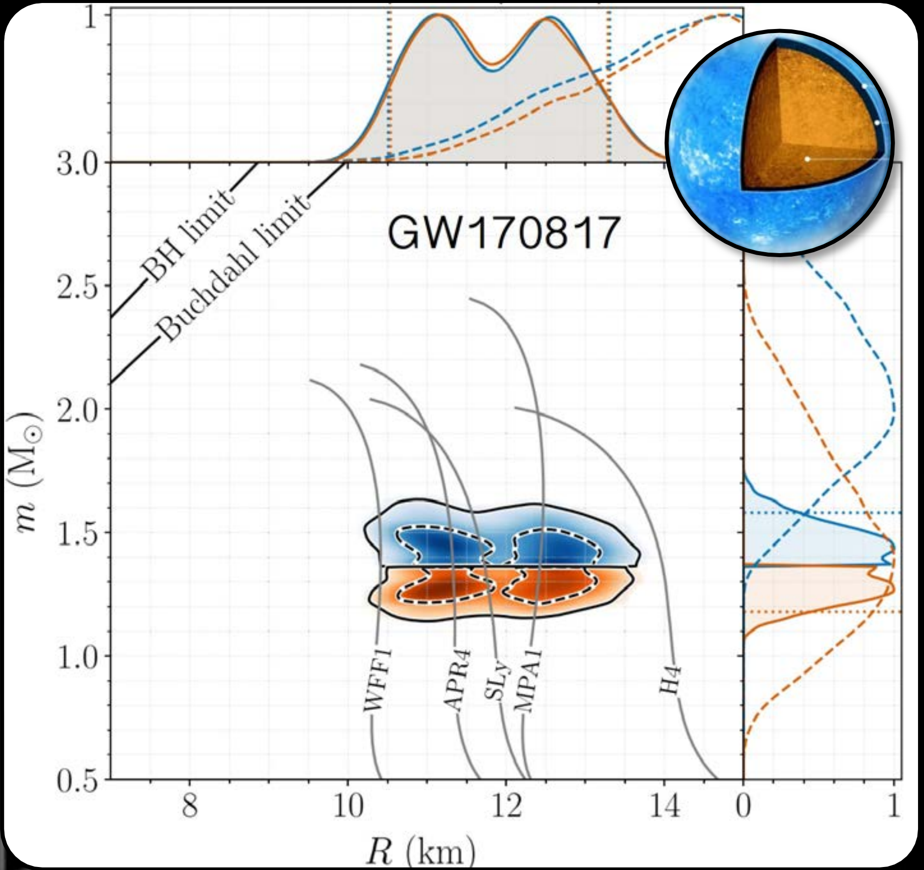




World's leading rare isotope research facility





1.1 Exaflops

700 Petabytes

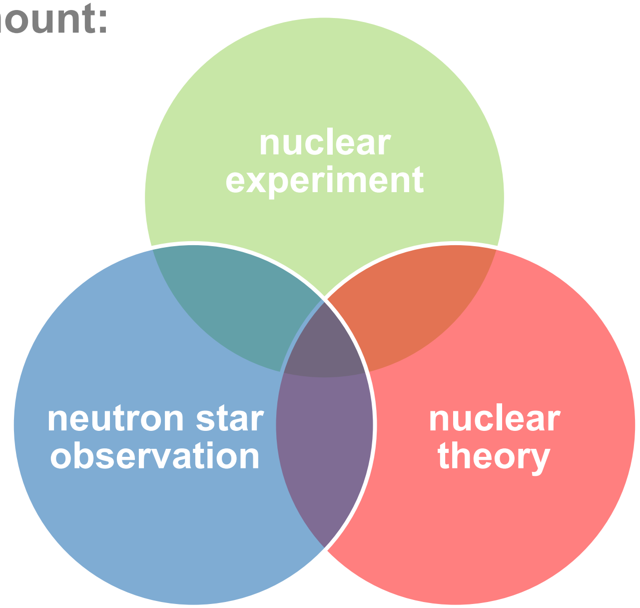
40 Megawatts

#1 Supercomputer

Frontier @ Oak Ridge Leadership Computing Facility

Opportunity & challenge for nuclear theory

Coordinated efforts are paramount:



We just entered a **Golden Era for Nuclear Physics & Astrophysics**

unique opportunity to obtain a **fundamental understanding** of strongly interacting matter, with great **potential for discovery**

Nuclear theory: How do we

- **interpret** these experiments & observations *microscopically*
- **predict** outcomes when experiments are *not* feasible
- **quantify & propagate** our **theoretical uncertainties**

Major efforts:

Bayesian methods for calibration, uncertainty quantification and propagation, experimental design, sensitivity studies, …

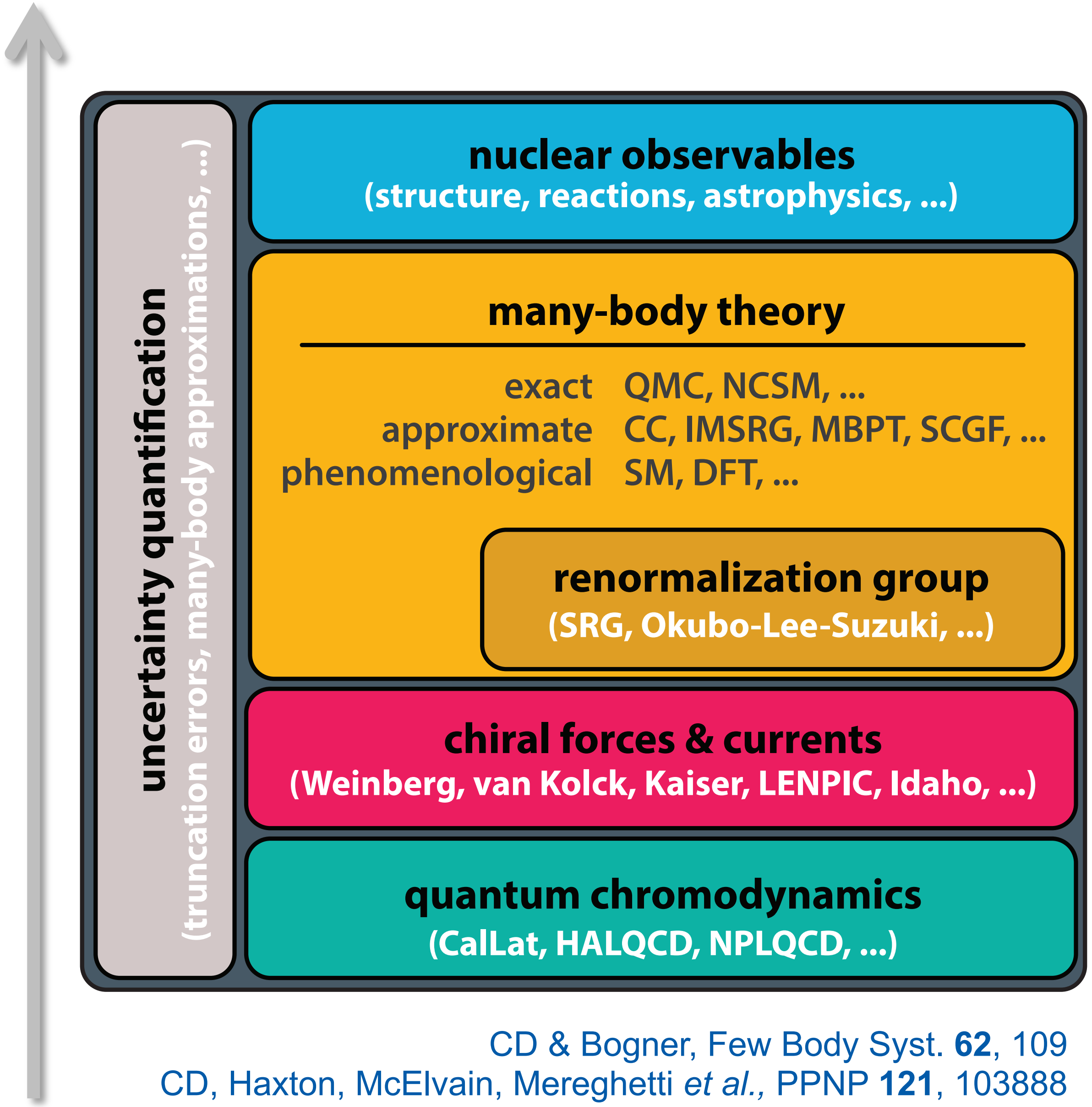
Requires **expensive calculations (HPC)**, repeated millions of times with different model parameters (MC sampling)

Reduced Order Modeling (ROM) is a *game changer* in making all of that possible.

Only applied *recently* to many nuclear theory problems but **known in the MOR community for years!**

RBM for eigenvalue problems reinvented in the last five years, coined **Eigenvector Continuation (EC)** Frame *et al.*, PRL **121**, 032501 (2017)

Ab initio workflow (idealized)



CD & Bogner, Few Body Syst. **62**, 109
CD, Haxton, McElvain, Mereghetti *et al.*, PPNP **121**, 103888

$$H(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle$$

Schrödinger Equation

computational framework

Seek eigenvalues (energies) and eigenvectors (wave functions) of nuclear Hamiltonians **(from chiral EFT)**

Many complementary high-fidelity methods:

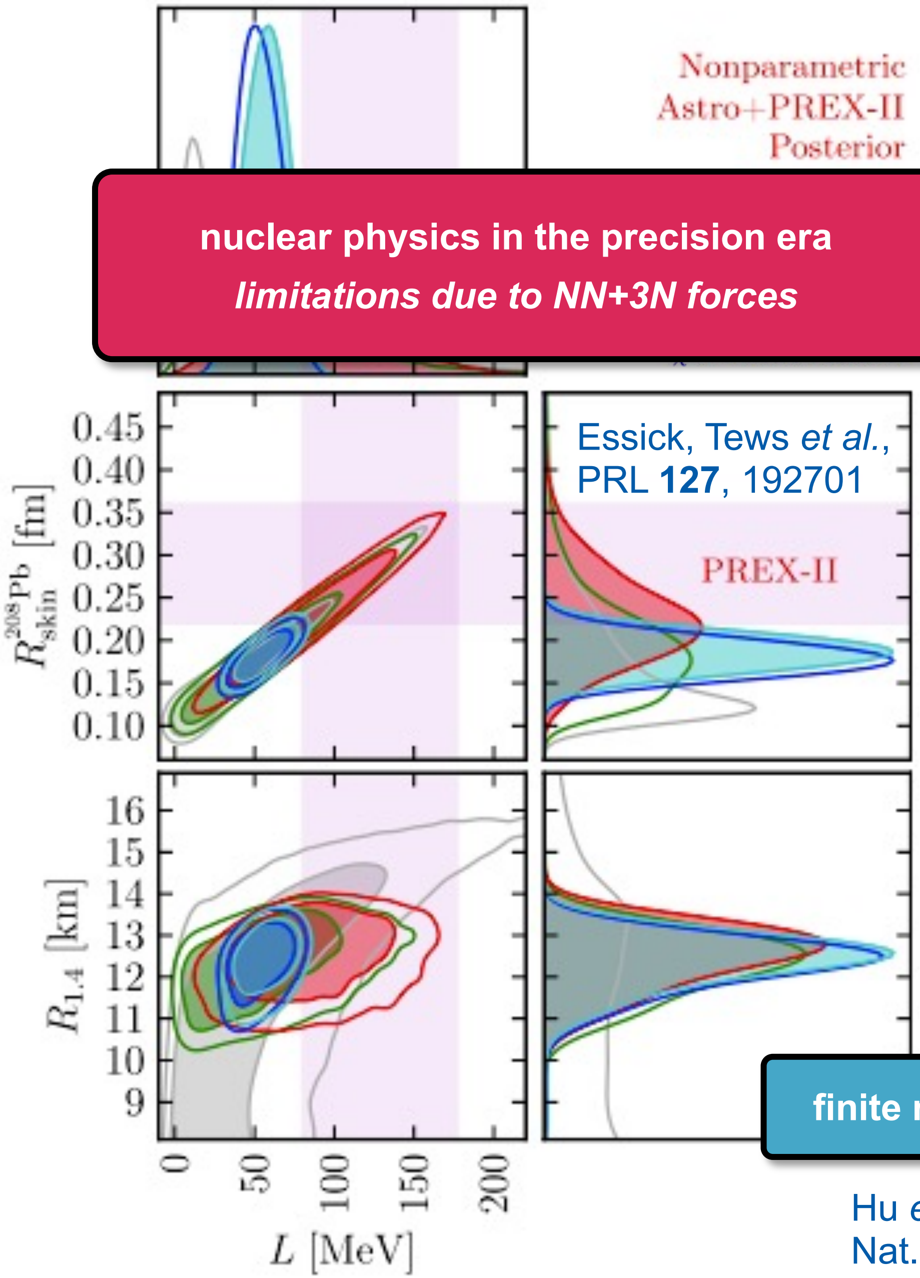
- Large-scale matrix diagonalization (up to 10^{10}) but only need lowest few eigenvalues/vectors (NCSM)
- Solving nonlinear equations (CC)
- PDEs and coupled ODEs (IM-SRG, Faddeev)
- Integral equations (SCGF)
- Stochastic (MC) methods (NLEFT, GFMC, VMC)

***e.g.*, "Volume extrapolation via eigenvector continuation,"**
Yapa & König, PRC **106**, 014309

chiral effective field theory (EFT)

provides microscopic Hamiltonians (Hermitian) consistent with the symmetries of *low-energy* QCD

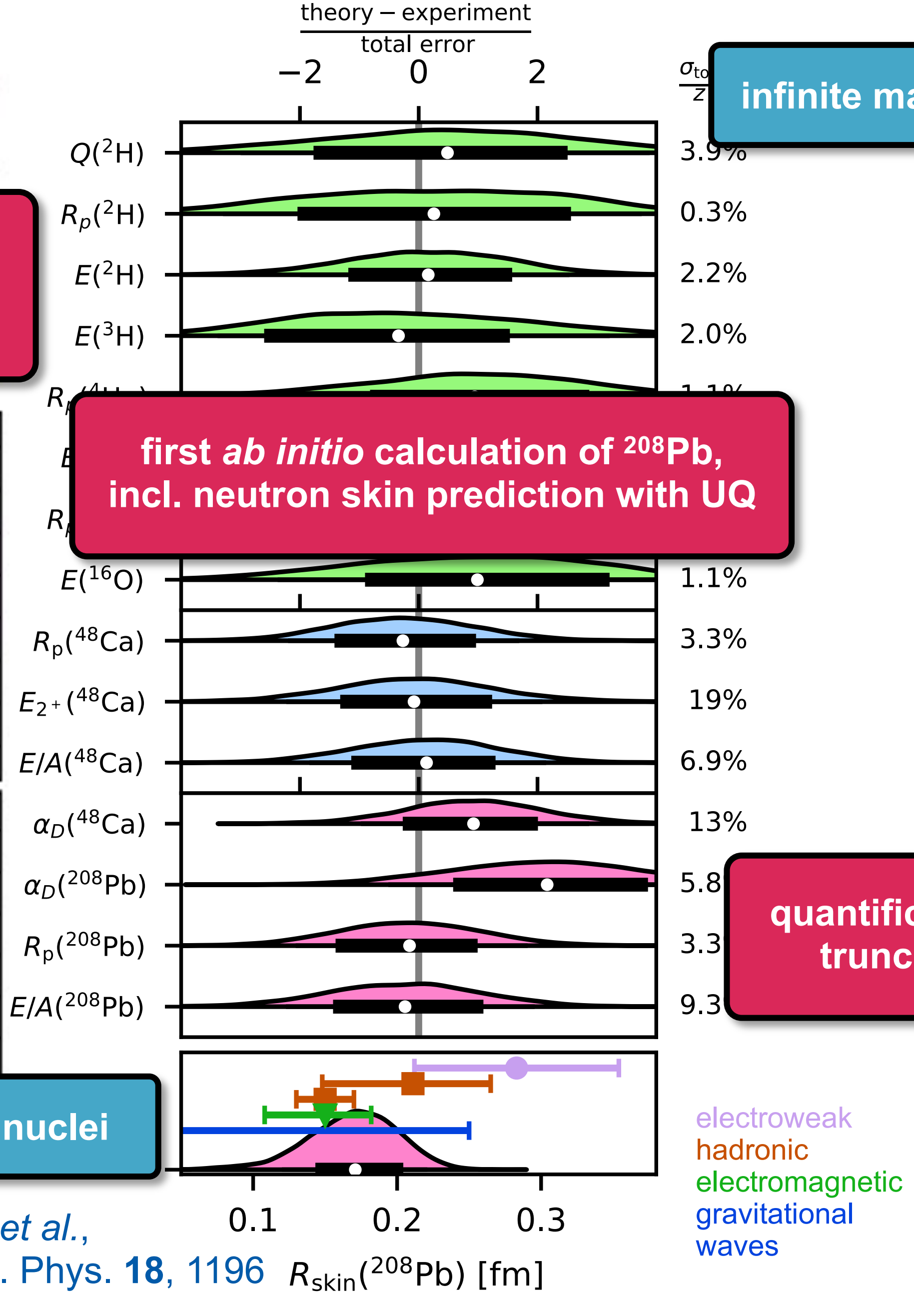
Major process: CEFT, many-body theory, and UQ!



nuclear physics in the precision era

limitations due to NN+3N forces

Essick, Tews *et al.*, PRL **127**, 192701

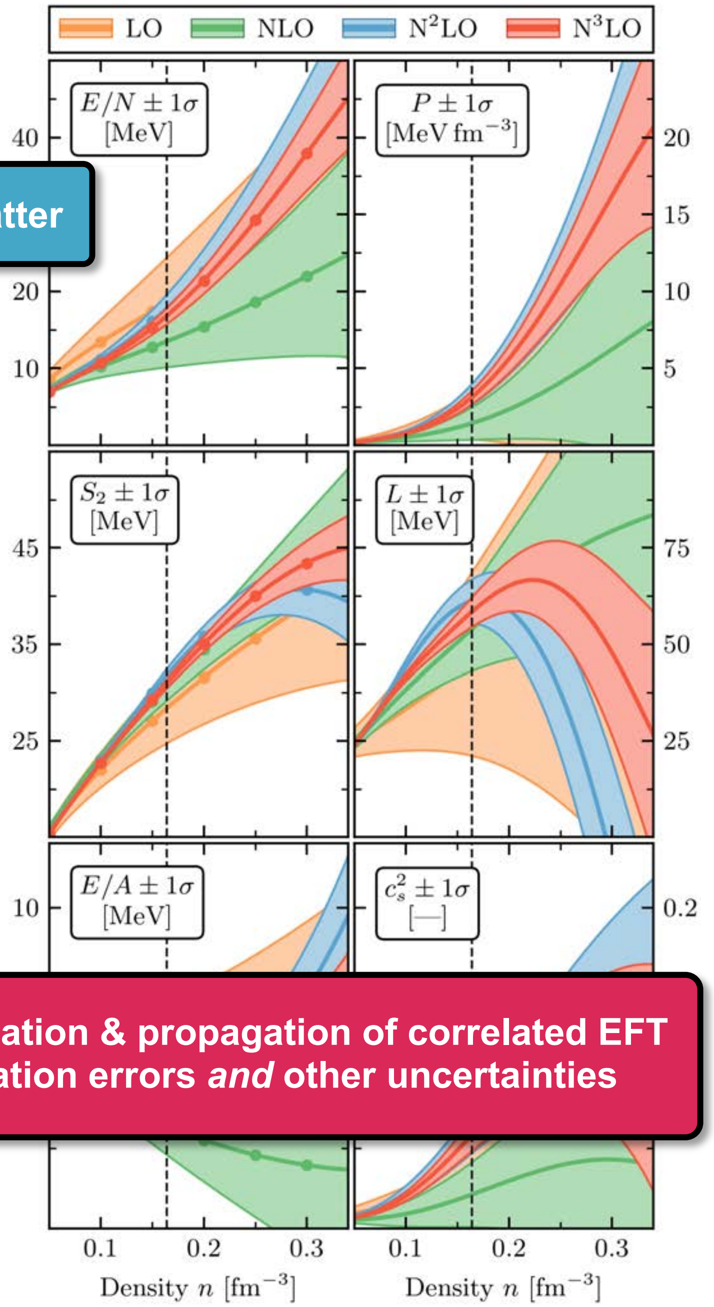


first *ab initio* calculation of ^{208}Pb, incl. neutron skin prediction with UQ

finite nuclei

electroweak
hadronic
electromagnetic
gravitational waves

Hu *et al.*, Nat. Phys. **18**, 1196



infinite matter

quantification & propagation of correlated EFT truncation errors *and* other uncertainties

CD, Furnstahl, Melendez, Phillips, PRL **125**, 202702

Model Reduction for Nuclear Physics

CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

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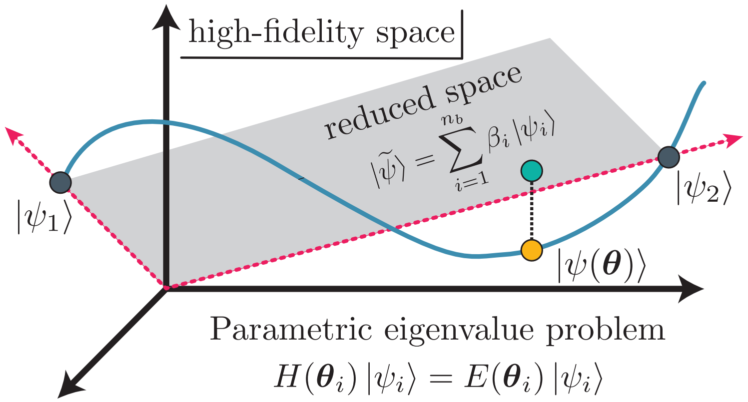
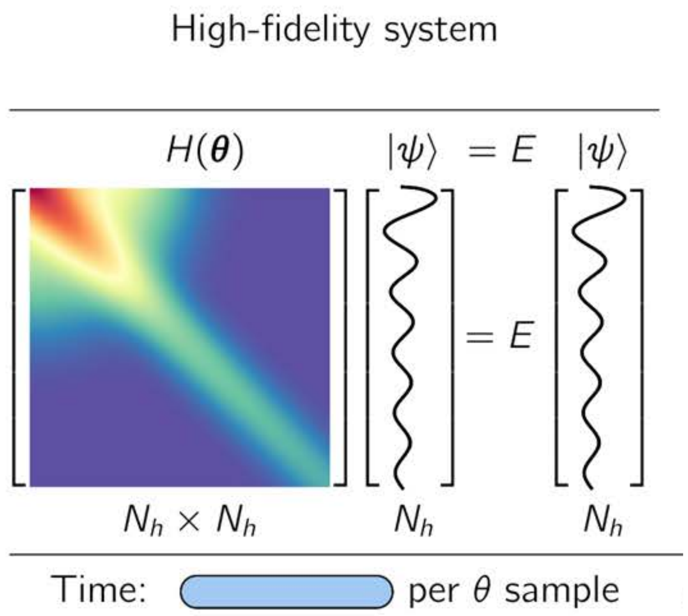
Fast & accurate emulators (a.k.a. Galerkin ROMs)

A fast *surrogate model* capable of approximating high-fidelity model calculations with high accuracy at small computational cost.

Here: many-body Schrödinger Equation for bound states (E < 0)





Construct **reduced order models (snapshot based)** by systematically removing superfluous information in high-fidelity models

Other methods currently being studied in nuclear physics include: Dynamic Mode Decomposition (DMD), Sparse Identification of Nonlinear Dynamics (SINDy), low-rank approximations, and many more.

CPU time scales with the length of

Model Reduction for Nuclear Physics

CD, Melendez, Garcia, Furnstahl, and Zhang, Front. Phys. **10**, 92931

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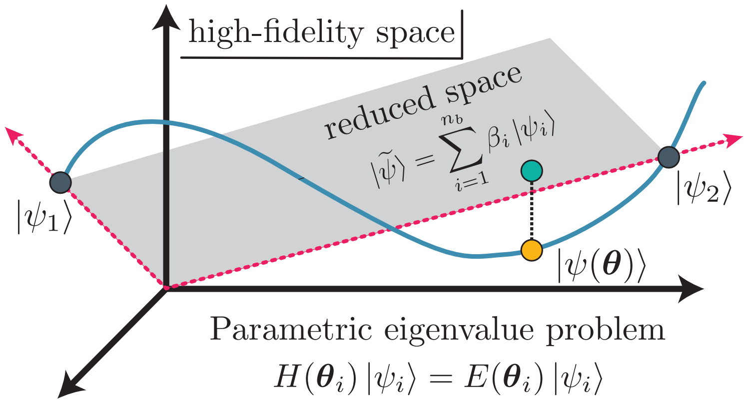

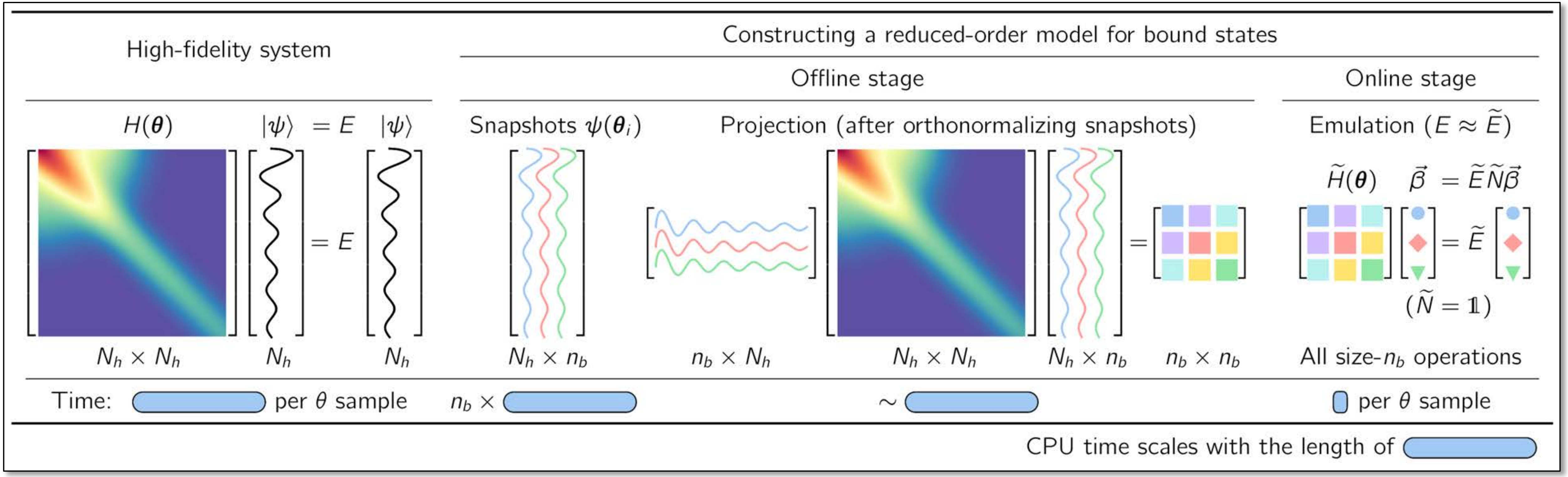

Example: Bayesian parameter estimation

Other applications:
modeling nuclear properties & simulating reactions, accelerator physics, …

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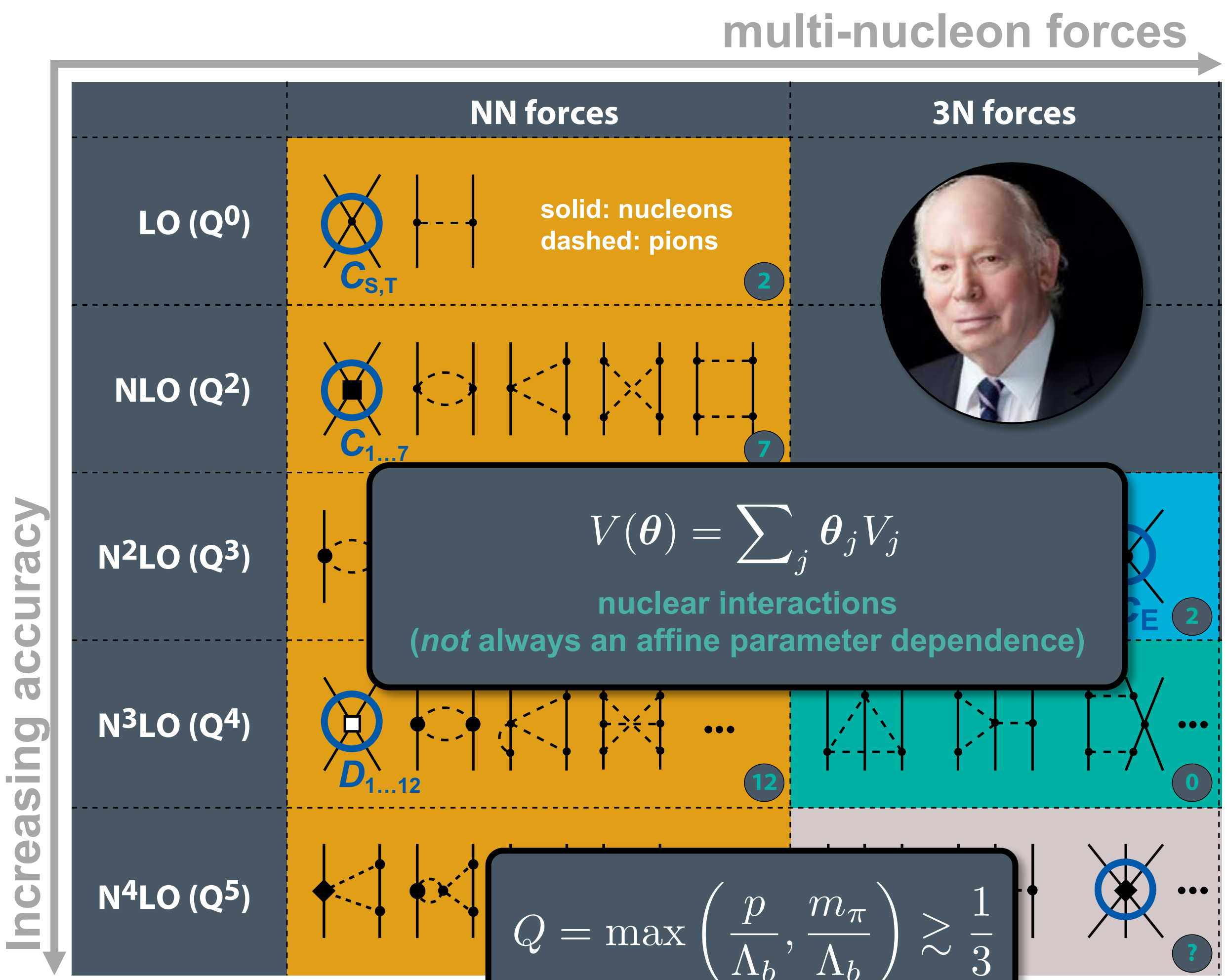
Hierarchy of chiral nuclear forces up to N^{4}LO



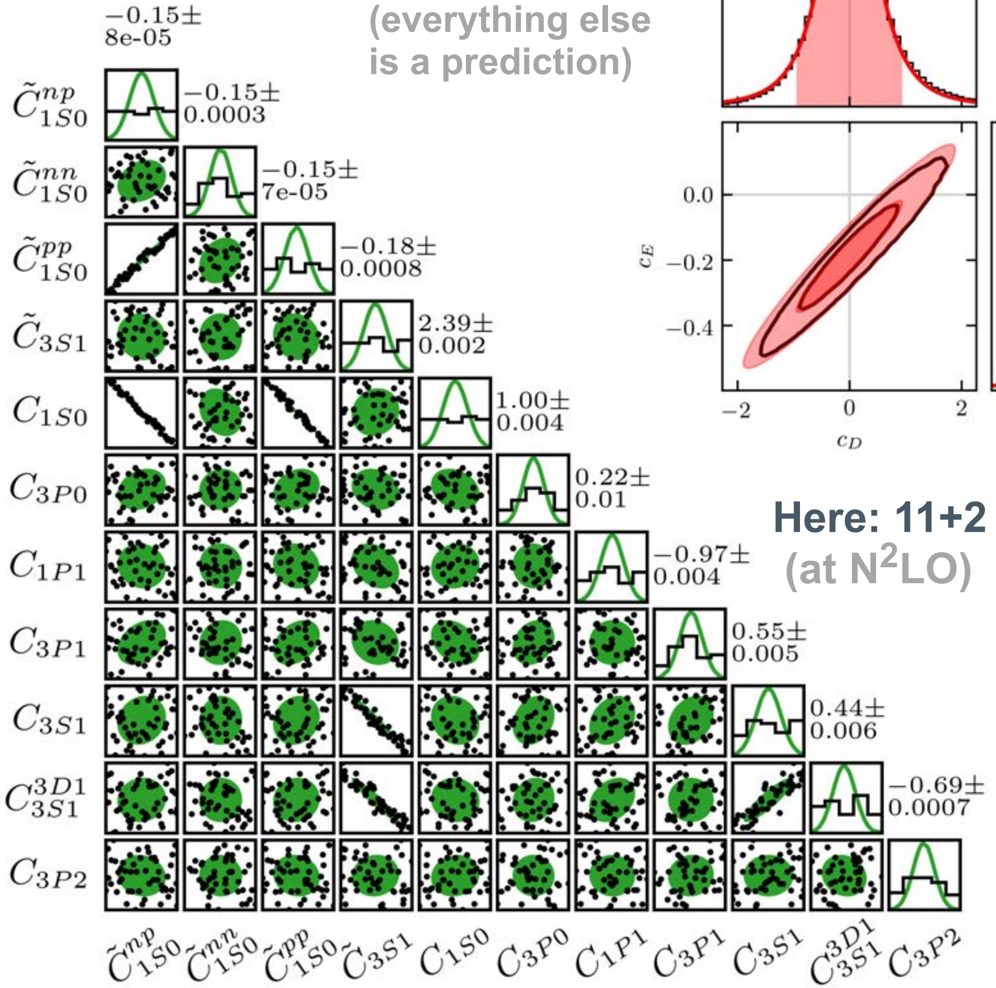
$$V(\boldsymbol{\theta}) = \sum_j \theta_j V_j$$

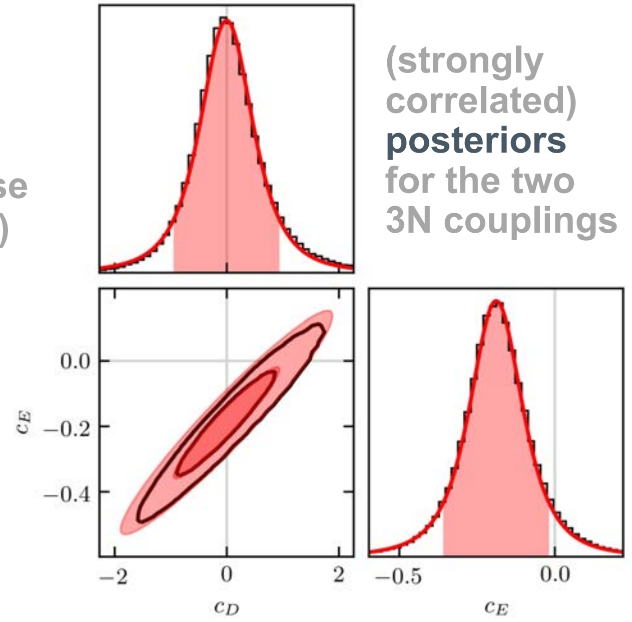
nuclear interactions
(*not* always an affine parameter dependence)

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right) \gtrsim \frac{1}{3}$$

Fit model parameters to few-body observables

(everything else is a prediction)





(strongly correlated) **posteriors** for the two 3N couplings

Here: 11+2 parameters (at N^{2}LO)

but typically closer to 30 parameters

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Krebs, Machleidt, Meißner, …

Wesolowski, Svensson *et al.*, PRC **104**, 064001

Emulators for bound-state calculations

$$H(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle$$

Schrödinger Equation

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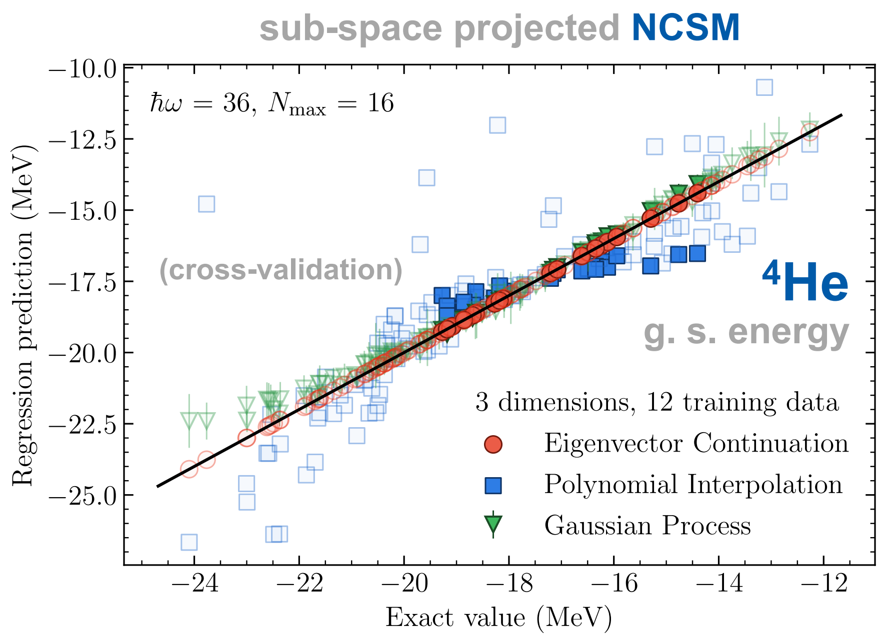
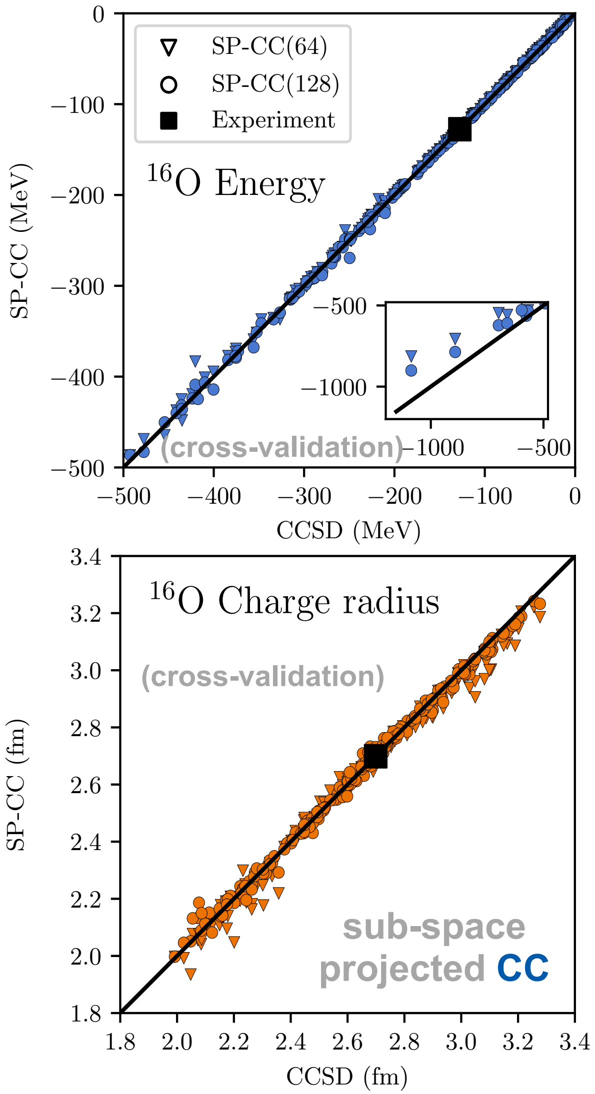


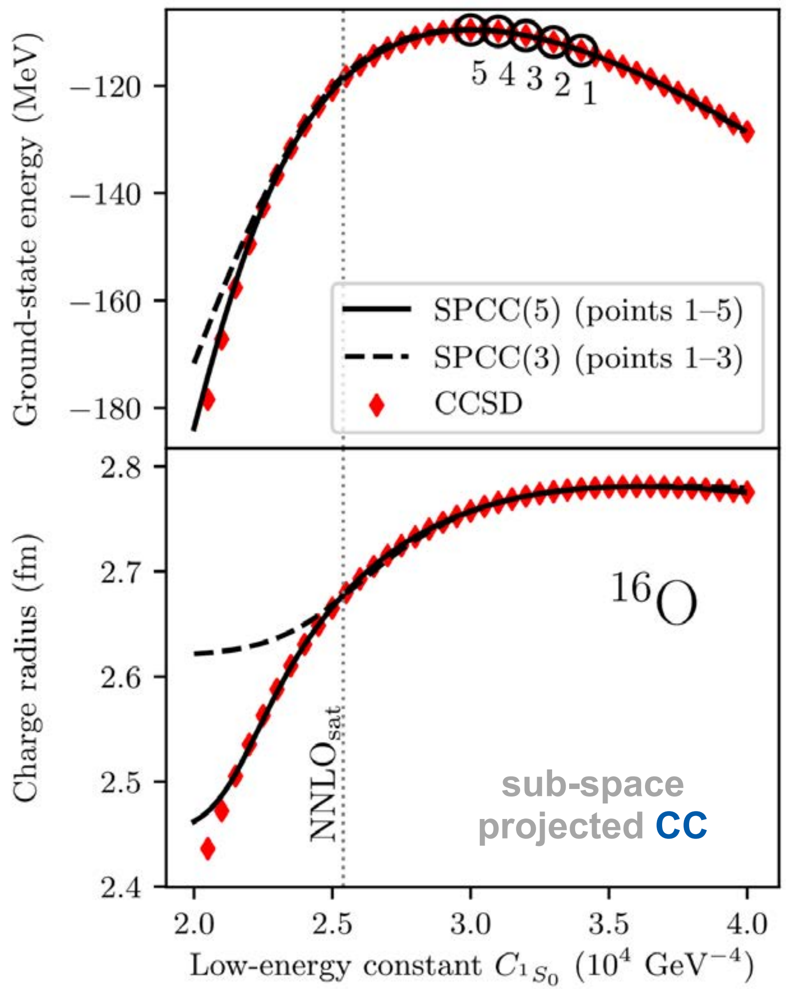
interpolation (solid symbols)
extrapolation (semitransparent symbols)

König, Ekström *et al.*, PLB **810**, 135814

Fast & accurate emulation via subspace projection methods (RBM)

RBM-driven emulators have **accurately approximated g. s. properties** binding energies & charge radii, beating GPs





Ekström & Hagen, PRL **123**, 252501

Sensitivity analysis: millions of points sampled in 1h on a standard laptop.

An equivalent set of exact CC computations would require 20 years.

Similarity Renormalization Group (SRG)

Hergert *et al.*, Phys. Rep. **621**, 165
Bogner *et al.*, Prog. Part. Nucl. Phys. **65**

Basic idea behind the SRG is to **render the Hamiltonian *H*(*s*) diagonal** w.r.t. a given basis via a continuous unitary transformation

$$H(s) = U(s)H(0)U^{\dagger}(s)$$

initial Hamiltonian $H(s = 0)$
flow parameter s

Applied to pre-diagonalize the Hamiltonian or as a many-body framework on its own.

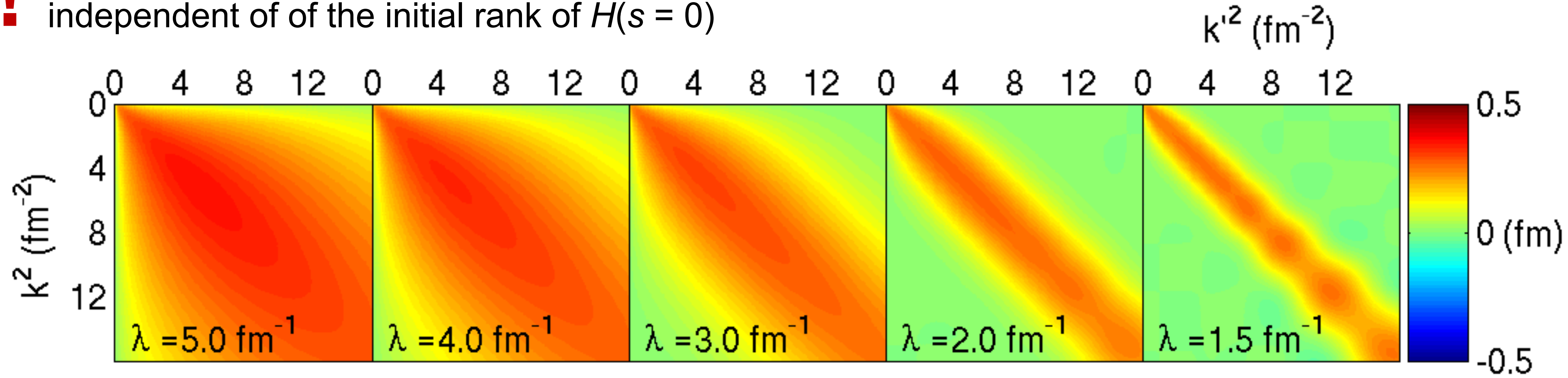
Taking the derivatives w.r.t. *s*, results in the SRG flow equation

$$\frac{d}{ds}H(s) = [\eta(s), H(s)] \,,$$

With some chosen (antihermitian) generator

$$\eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s) \,.$$

! **No free lunch:** commutator increases the particle rank of *H*(*s*), independent of of the initial rank of *H*(*s* = 0)



$$s \propto \frac{1}{\lambda^4}$$

***s* increases**

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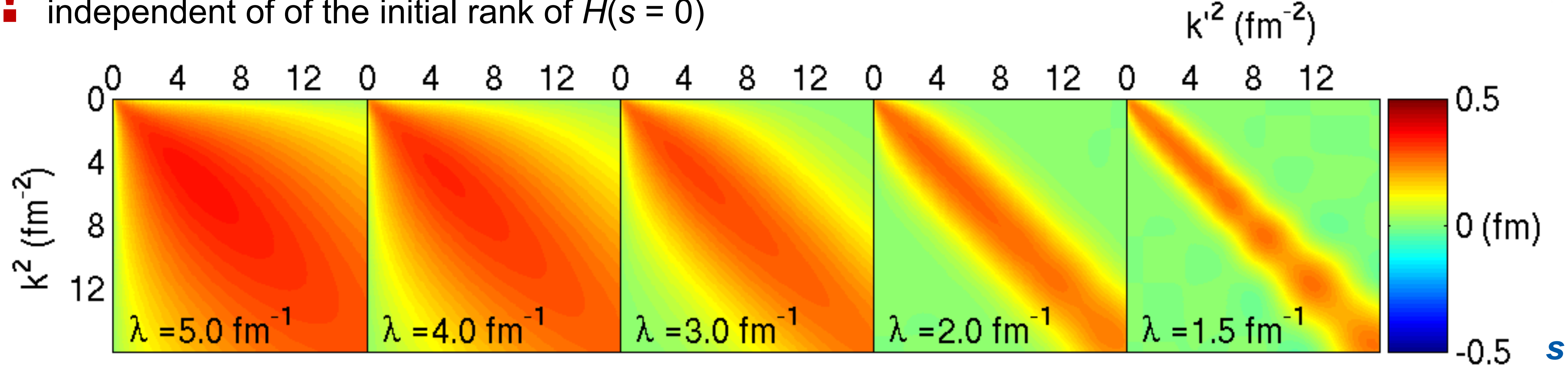
Taking the derivatives w.r.t. *s*, results in the SRG flow equation

$$\frac{dV_s(k,k')}{ds} = -(k^2-k'^2)^2\,V_s(k,k') + \frac{2}{\pi}\int_0^\infty q^2\,dq\,(k^2+k'^2-2q^2) \times V_s(k,q)\,V_s(q,k')\ .$$

With some chosen (antihermitian) generator

! **No free lunch:** commutator increases the particle rank of $H(s)$, independent of of the initial rank of $H(s=0)$

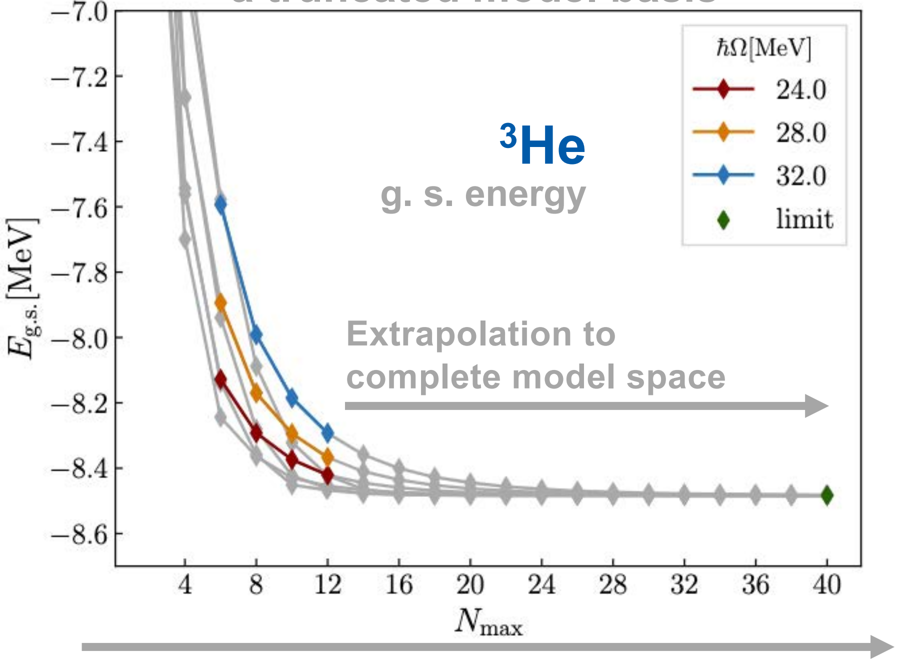


$$s \propto \frac{1}{\lambda^4}$$

s increases

Example: large extrapolations

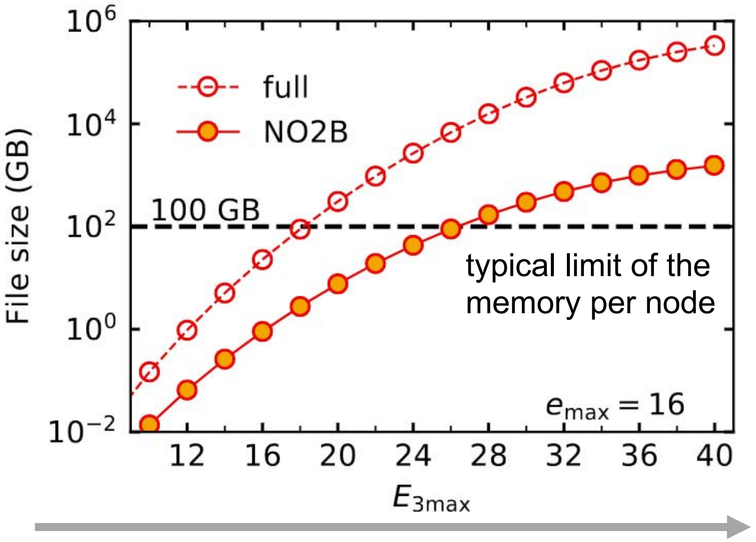
Direct diagonalization in a truncated model basis



model space truncation

Knöll, Wolfgruber *et al.*, PLB **839**, 137781

File size of 3N matrix elements (single precision)

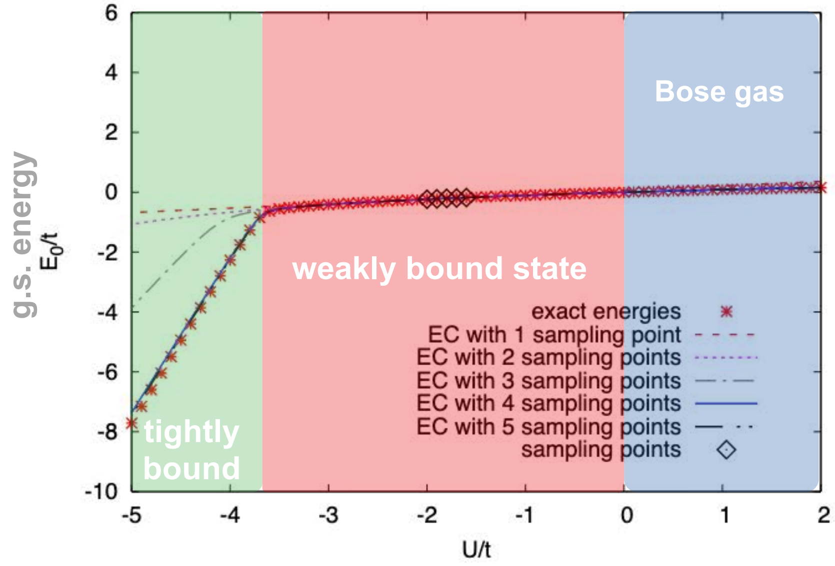


model space truncation

3N contributions are important!

Miyagi, Stroberg *et al.*, PRC **105**, 014302

3D Bose-Hubbard model (4 bosons)



coupling

PT converges rapidly for $U/t > -3.8$

Frame *et al.*, PRL **121**, 032501
Sarkar & Lee, PRR **4**, 023214

Needed: **extrapolation** of observables to infinite Hilbert spaces along with uncertainty estimates

Artificial Neutral Networks are being studied to extract converged results

Needed: **tensor compression** methods to mitigate computational costs of storing and evaluating 3N forces (tensor trains?)

Novel storage scheme allows for E_{3max} = 28, as needed for heavy nuclei such as ^{132}Sn

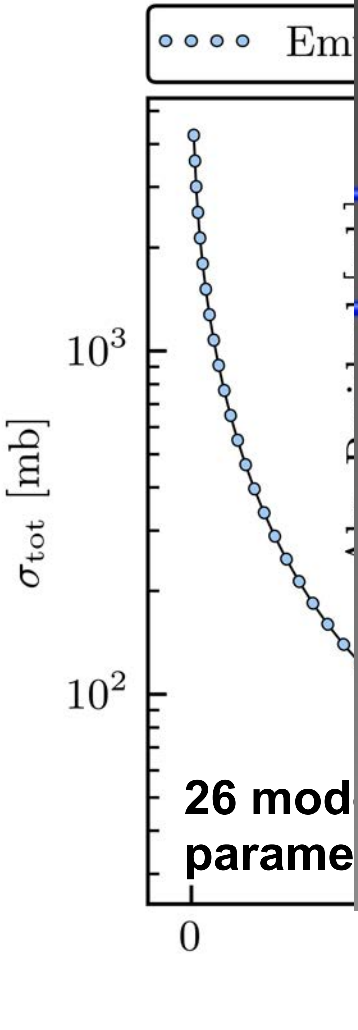
Needed: MOR-driven extrapolations to regions where current methods are not efficient or experiments are not feasible

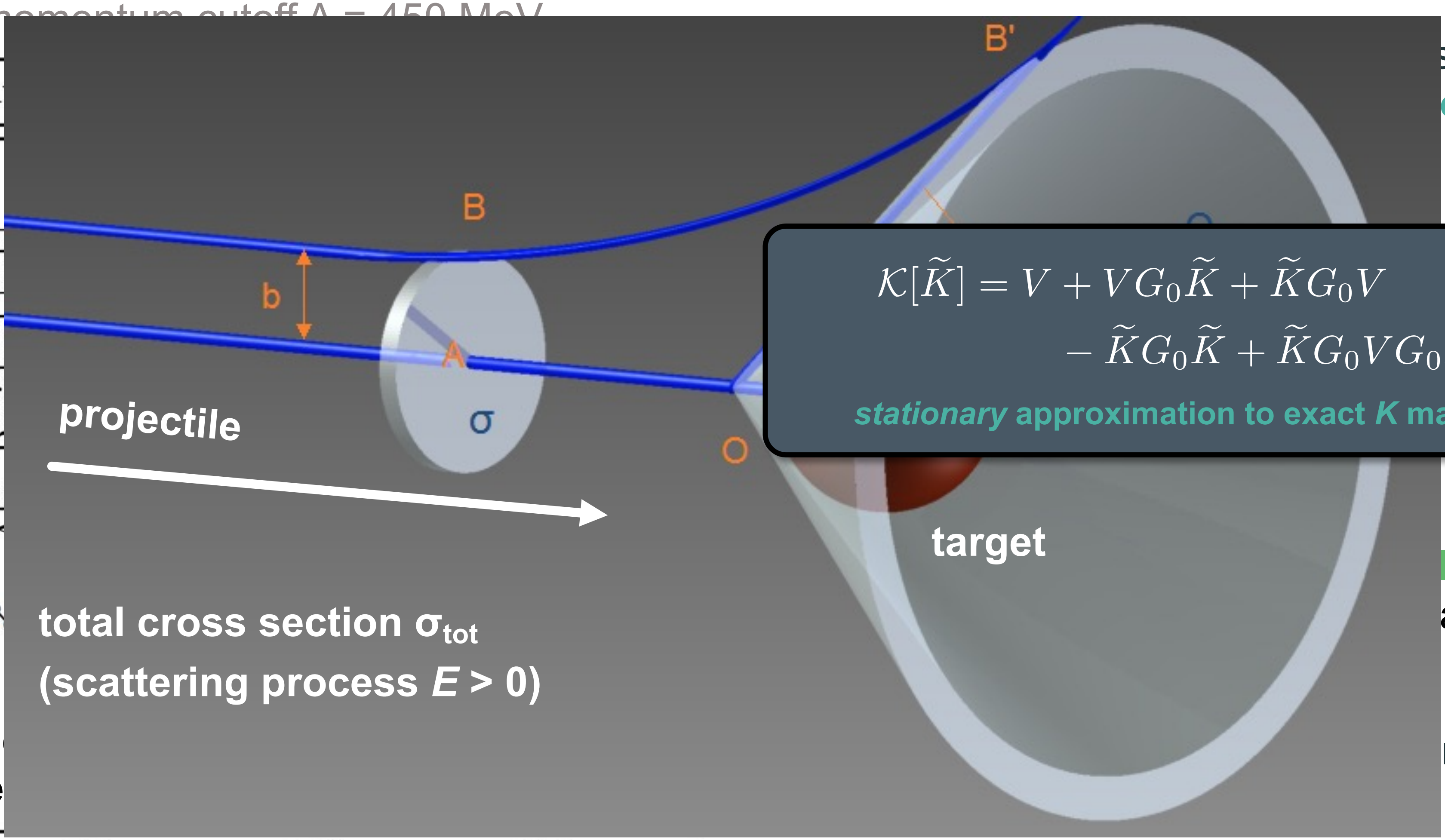
Needed: **emulator uncertainties**, convergence analyses, active learning

Emulating nuclear scattering ($E > 0$)

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

SMS chiral NN potential at N^{4}LO+ with
momentum cutoff Λ = 450 MeV





$$\mathcal{K}[\widetilde{K}] = V + VG_0\widetilde{K} + \widetilde{K}G_0V - \widetilde{K}G_0\widetilde{K} + \widetilde{K}G_0VG_0\widetilde{K},$$

stationary **approximation to exact *K* matrix**

total cross section σ_{tot} (scattering process $E > 0$)

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ainties

nd

>300x

faster than the high-fidelity calculation

Emulating nuclear scattering ($E > 0$)

Melendez, CD, Garcia, Furnstahl, and Zhang, PLB **821**, 136608

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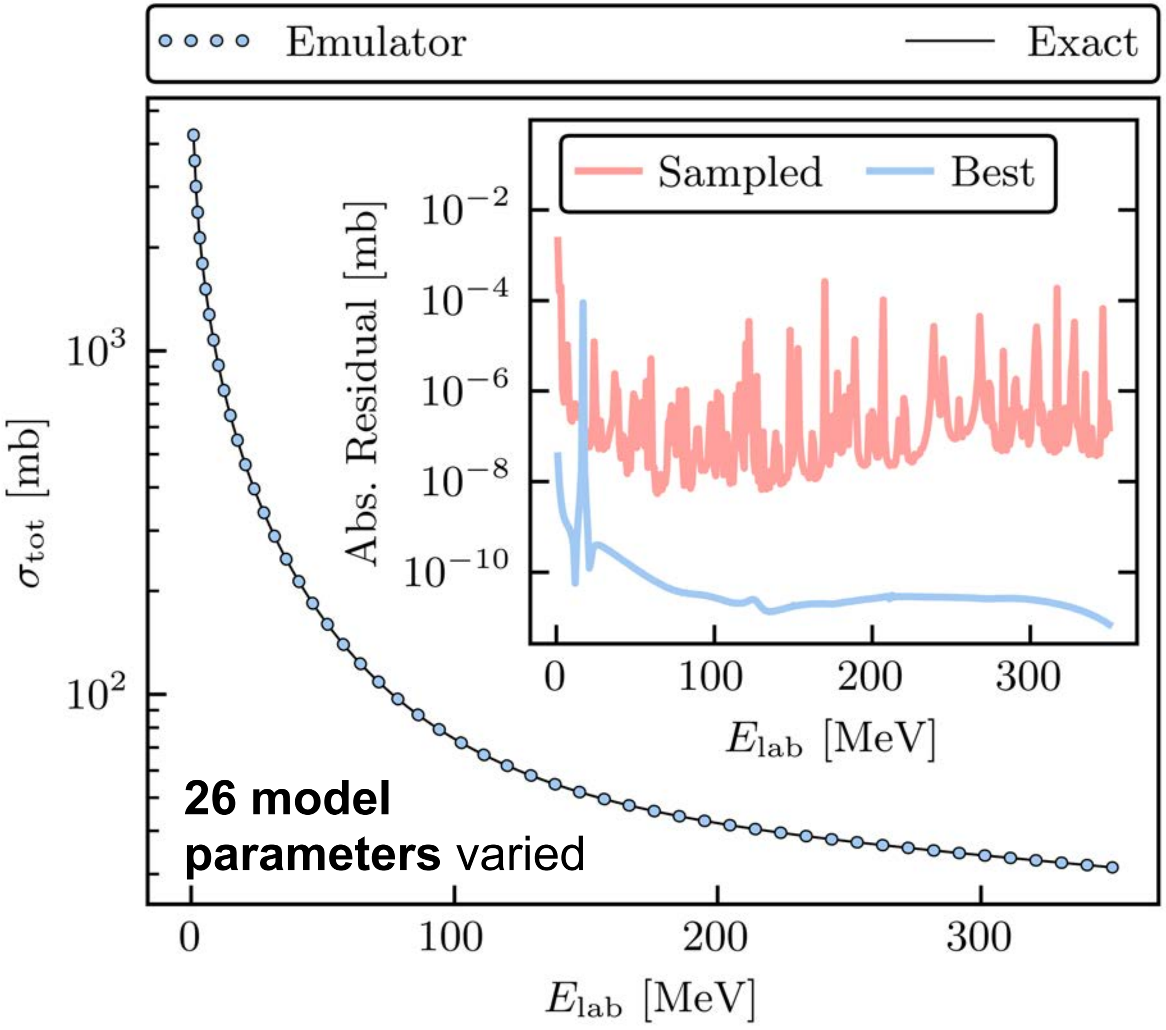

total cross section σ_{tot} (scattering process $E > 0$)

Coefficients of the snapshot basis for the K matrix determined by **Newton's Variational Principle:**

$$\mathcal{K}[\widetilde{K}] = V + VG_0\widetilde{K} + \widetilde{K}G_0V - \widetilde{K}G_0\widetilde{K} + \widetilde{K}G_0VG_0\widetilde{K},$$

***stationary* approximation to exact *K* matrix**

Residuals are vanishingly small compared to experimental uncertainties

Randomly **sample 500 values:** **extrapolation of ±10 [unit]** beyond the range of the training data

>300x

faster than the high-fidelity calculation

Take-away points

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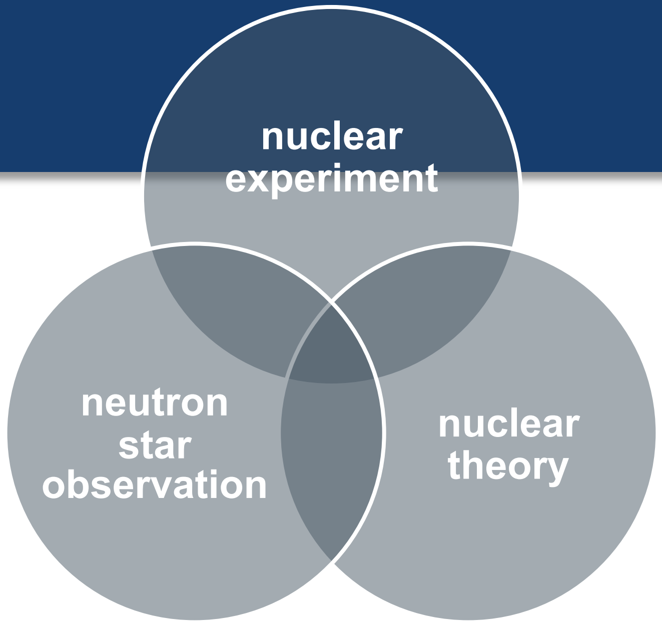
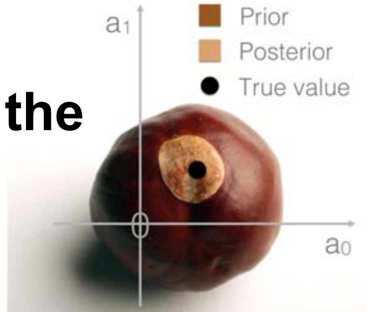
multi-messenger
nuclear precision
FRIB

} era



unique opportunity to obtain a **fundamental understanding** of strongly interacting matter, with great **potential for discovery**

1. **Tremendous progress** in chiral EFT, many-body methods, UQ enables microscopic calculations of atomic nuclei & neutron star matter
2. Upcoming observational & experimental campaigns will provide **stringent constraints** on nuclear matter. Nuclear theory needed for interpretation.
3. Bayesian methods allow for **rigorous UQ & propagation** in EFT-based calculations (facilitated by new emulators for nuclear physics!)
4. Emulators are **game changers in nuclear physics.** Much can be learned from the mature MOR field in Applied Mathematics. **Interest in collaborations!**



BUQEYE Collaboration

Many thanks to: R. Furnstahl A. Garcia P. Giuliani S. Han J. W. Holt J. Lattimer A. Lovell K. McElvain J. Melendez F. Nunes D. Phillips M. Prakash S. Reddy X. Zhang T. Zhao

Model (Order) Reduction for Nuclear Physics

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frontiers (pedagogical review article)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

Front. Phys. **10**, 92931 (open access)

C. Drischler,[1,2,*] J. A. Melendez,[3] R. J. Furnstahl,[3] A. J. Garcia,[3] and Xilin Zhang[2]

ABSTRACT

The BUQEYE collaboration (Bayesian Uncertainty Quantification: Errors in Your EFT) presents a pedagogical introduction to projection-based, reduced-order emulators for applications in low-energy nuclear physics. The term *emulator* refers here to a fast surrogate model capable of reliably approximating high-fidelity models. As the general tools employed by these emulators are not yet well-known in the nuclear physics community, we discuss variational and Galerkin projection methods, emphasize the benefits of offline-online decompositions, and explore how these concepts lead to emulators for bound and scattering systems that enable fast & accurate calculations using many different model parameter sets. We also point to future extensions and applications of these emulators for nuclear physics, guided by the mature field of model (order) reduction. All examples discussed here and more are available as interactive, open-source Python code so that practitioners can readily adapt projection-based emulators for their own work.

Keywords: emulators, reduced-order models, model order reduction, nuclear scattering, uncertainty quantification, effective field theory, variational principles, Galerkin projection

Pedagogical & interactive Jupyter notebooks online!

see also
our Literature Guide
Melendez, CD *et al.*,
J. Phys. G **49**, 102001

Companion website with lots of pedagogical material: https://github.com/buqeye/frontiers-emulator-review

More details? Recent review article

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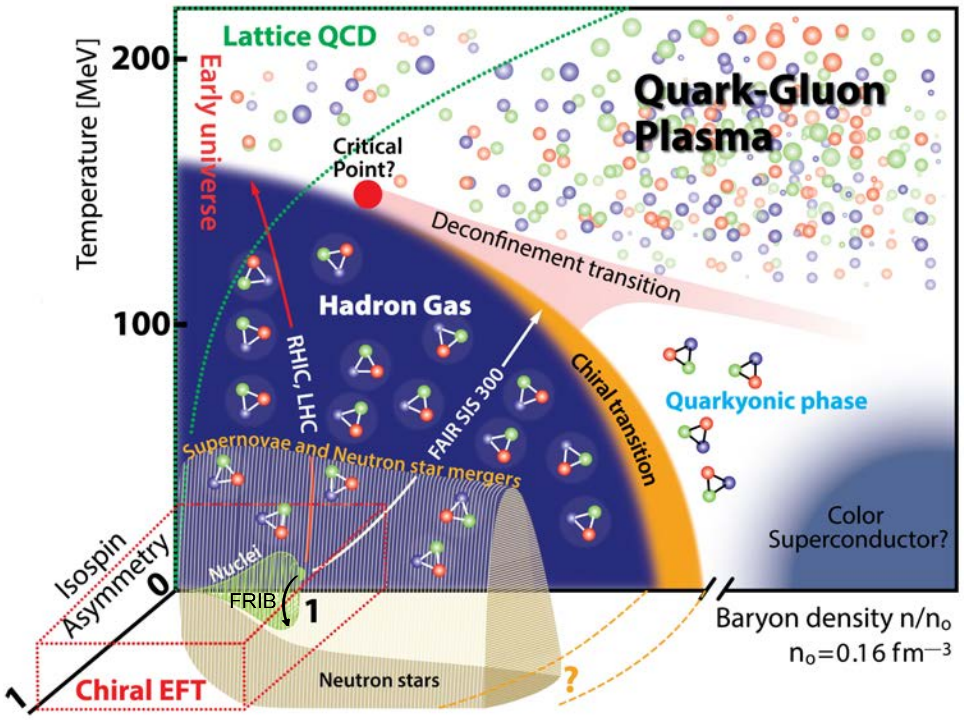

Keywords:

Chiral EFT | neutron stars | MBPT
nuclear matter at zero and finite temperature
Bayesian uncertainty quantification
recent neutron star observations

Chiral Effective Field Theory and the High-Density Nuclear Equation of State

Annual Review of Nuclear and Particle Science

Vol. 71:403-432 (Volume publication date September 2021)
First published as a Review in Advance on July 6, 2021
https://doi.org/10.1146/annurev-nucl-102419-041903

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[4]Cyclotron Institute and Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA
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James Lattimer, Annu. Rev. Nucl. Part. Sci. **71**, 433

see also Sorensen *et al.*, arXiv:2301.13253

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