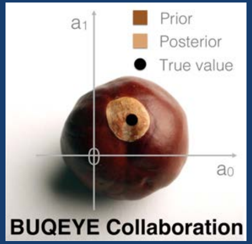
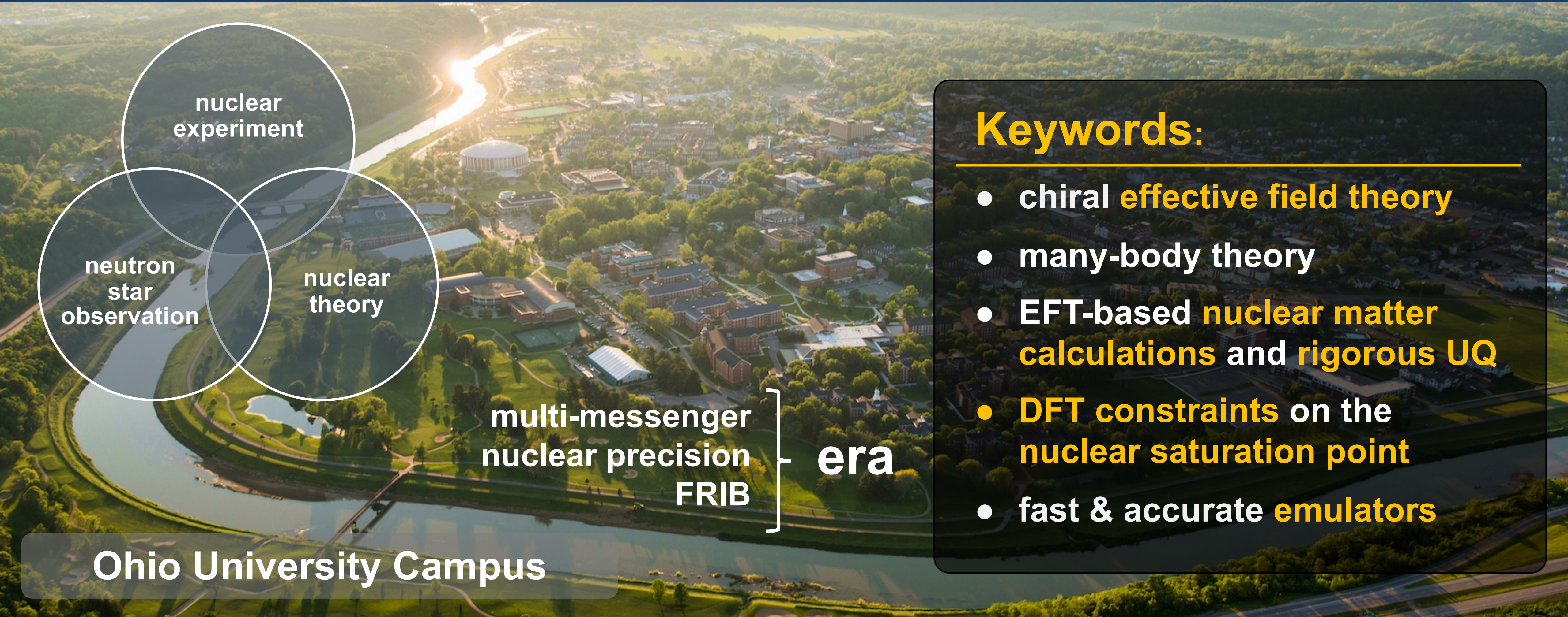
Microscopic and empirical constraints of the nuclear equation of state

Christian Drischler (drischler@ohio.edu)

INT-23-1a: Intersection of nuclear structure & high-energy nuclear collisions
February 6, 2023



BUQEYE Collaboration



nuclear experiment

neutron star observation

nuclear theory

multi-messenger
nuclear precision
FRIB

era

Ohio University Campus

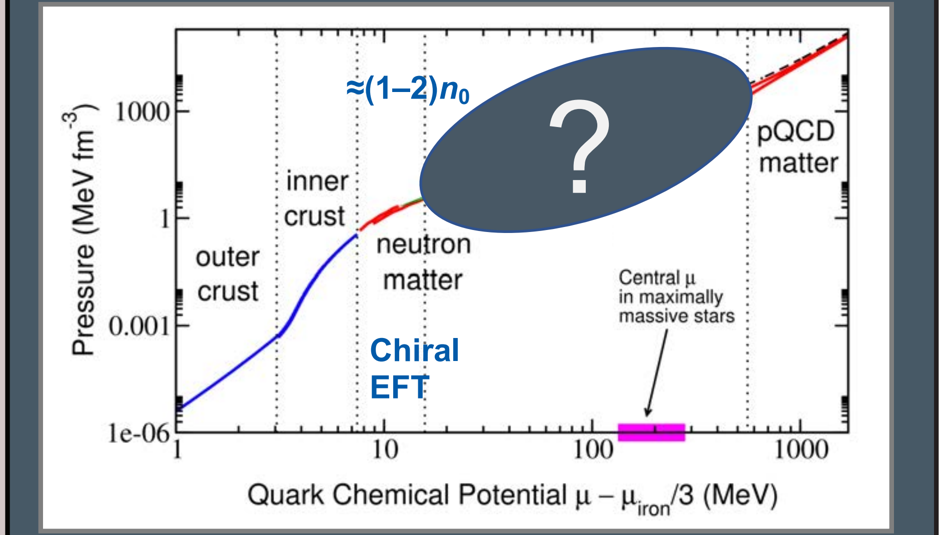
Keywords:

- chiral effective field theory
- many-body theory
- EFT-based nuclear matter calculations and rigorous UQ
- DFT constraints on the nuclear saturation point
- fast & accurate emulators

Ab initio workflow (idealized)

uncertainty quantification
(truncation errors, many-body approximations, ...)

nuclear observables
(structure, reactions, astrophysics, ...)



quantum chromodynamics
(CalLat, HALQCD, NPLQCD, ...)

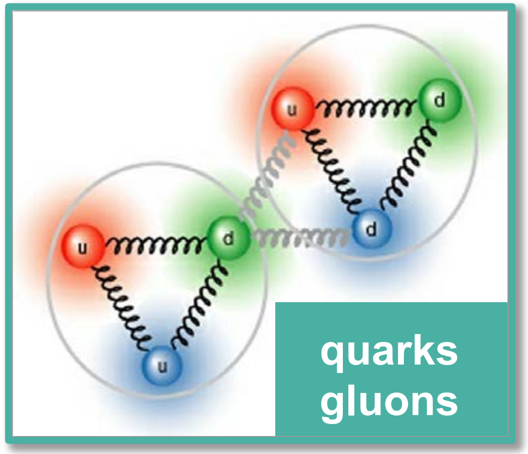
CD & Bogner, Few Body Syst. **62**, 109

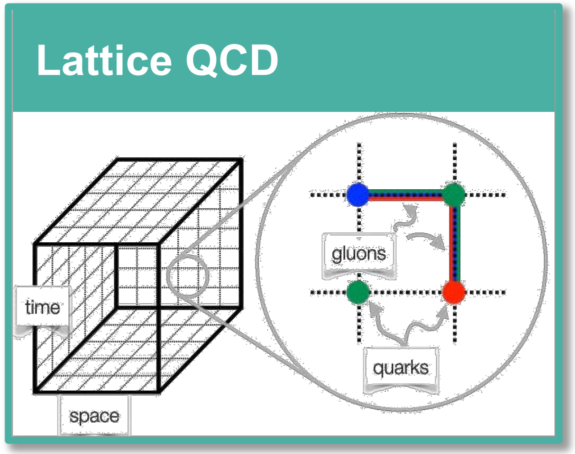
Here: nuclear equation of state (EOS)

energy per particle (and derived quantities)

$$\frac{E}{A}(n, \delta, T)$$

baryon density *n*
neutron excess *δ*
temperature *T*



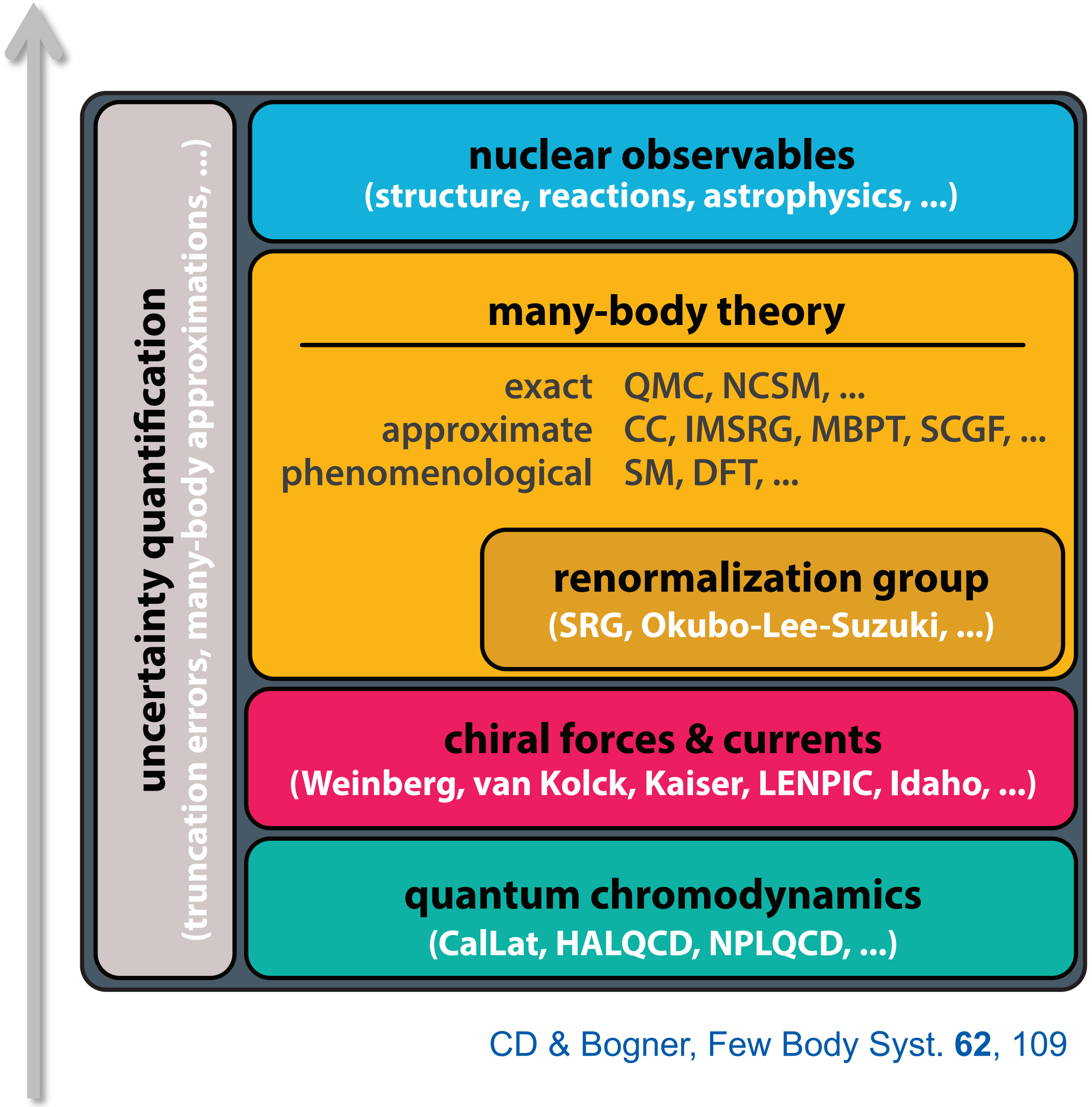


theory of strong interactions

QCD is nonperturbative at the low energies relevant for nuclear physics (cf. pQCD & LQCD)

CD, Haxton, McElvain, Mereghetti *et al.*, PPNP **121**, 103888

Ab initio workflow (idealized)



uncertainty quantification
(truncation errors, many-body approximations, ...)

nuclear observables
(structure, reactions, astrophysics, ...)

many-body theory

exact	QMC, NCSM, ...
approximate	CC, IMSRG, MBPT, SCGF, ...
phenomenological	SM, DFT, ...

renormalization group
(SRG, Okubo-Lee-Suzuki, ...)

chiral forces & currents
(Weinberg, van Kolck, Kaiser, LENPIC, Idaho, ...)

quantum chromodynamics
(CalLat, HALQCD, NPLQCD, ...)

CD & Bogner, Few Body Syst. **62**, 109

Here: nuclear equation of state (EOS)

energy per particle (and derived quantities)

$$\frac{E}{A}(n, \delta, T)$$

baryon density *n*
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temperature *T*

computational framework

solves the (many-body) Schrödinger equation requires a nuclear potential as input

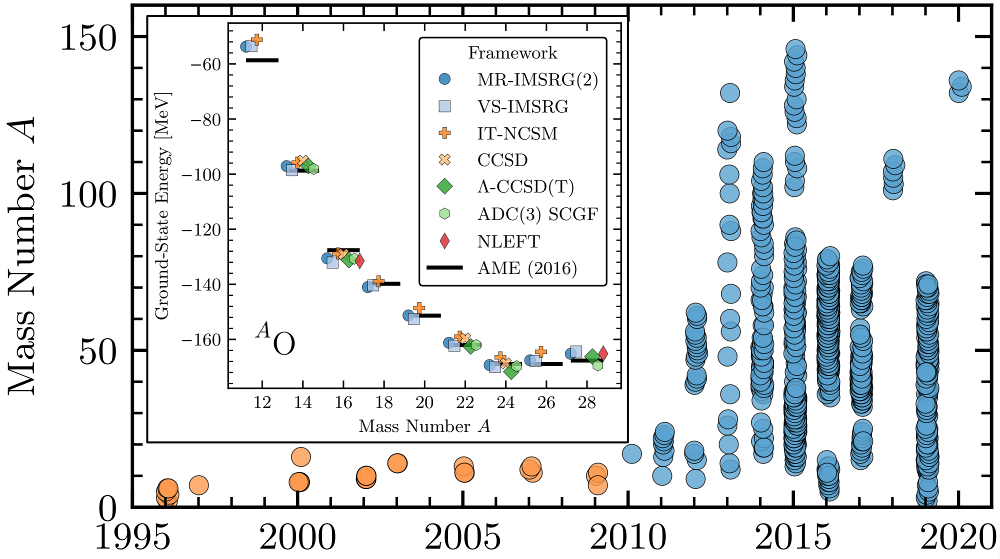
chiral effective field theory

provides microscopic interactions consistent with the symmetries of *low-energy* QCD

theory of strong interactions

QCD is nonperturbative at the low energies relevant for nuclear physics (cf. pQCD & LQCD)

nuclear physics in the *precision* era:
limitations due to NN+3N forces

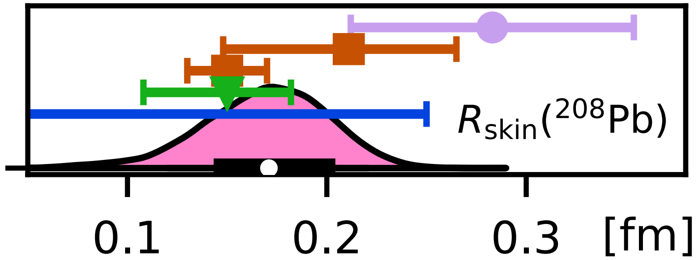


finite nuclei

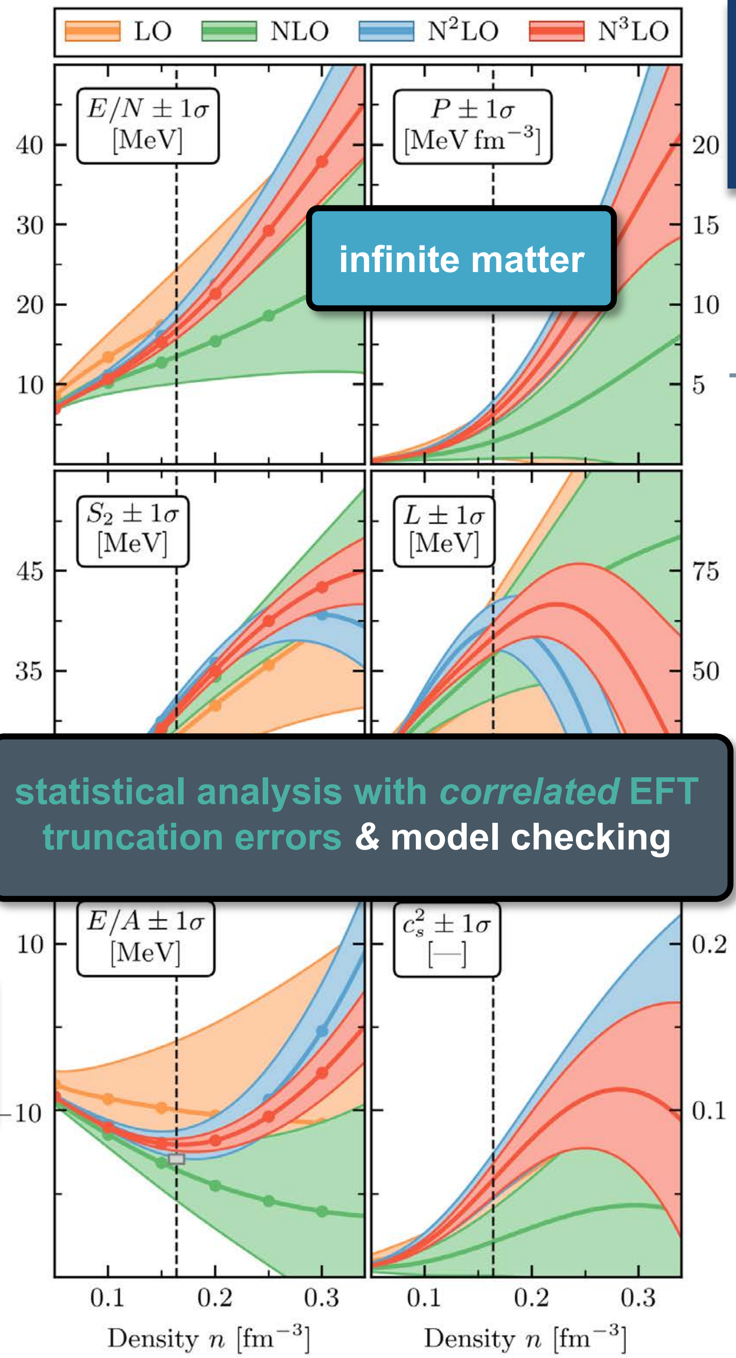
Hergert, Front. in Phys. **8**, 379
CD & Bogner, Few Body Syst. **62**, 109

Hu, Jiang *et al.*,
Nature Phys.
18, 1196

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



Constraints from:
electroweak
hadronic
electromagnetic
gravitational
waves



infinite matter

statistical analysis with *correlated* EFT truncation errors & model checking

CD, Furnstahl, Melendez, Phillips, PRL **125**, 202702
CD, Hebeler, Schwenk, PRL **122**, 042501

CD, Holt & Wellenhofer,
Ann. Rev. NPS **71**, 403

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Tremendous progress

in CEFT, many-body theory, UQ & HPC

CEFT enables *ab initio* calculations of **finite nuclei** & **nuclear matter** at $T \geq 0$ and arbitrary proton fractions ($n \lesssim 2n_{\mathrm{sat}}$)

Computational & algorithmic advances in *all* many-body frameworks

Many-Body Perturbation Theory

- fully automated | GPU-accelerated
- full N^{3}LO calculations

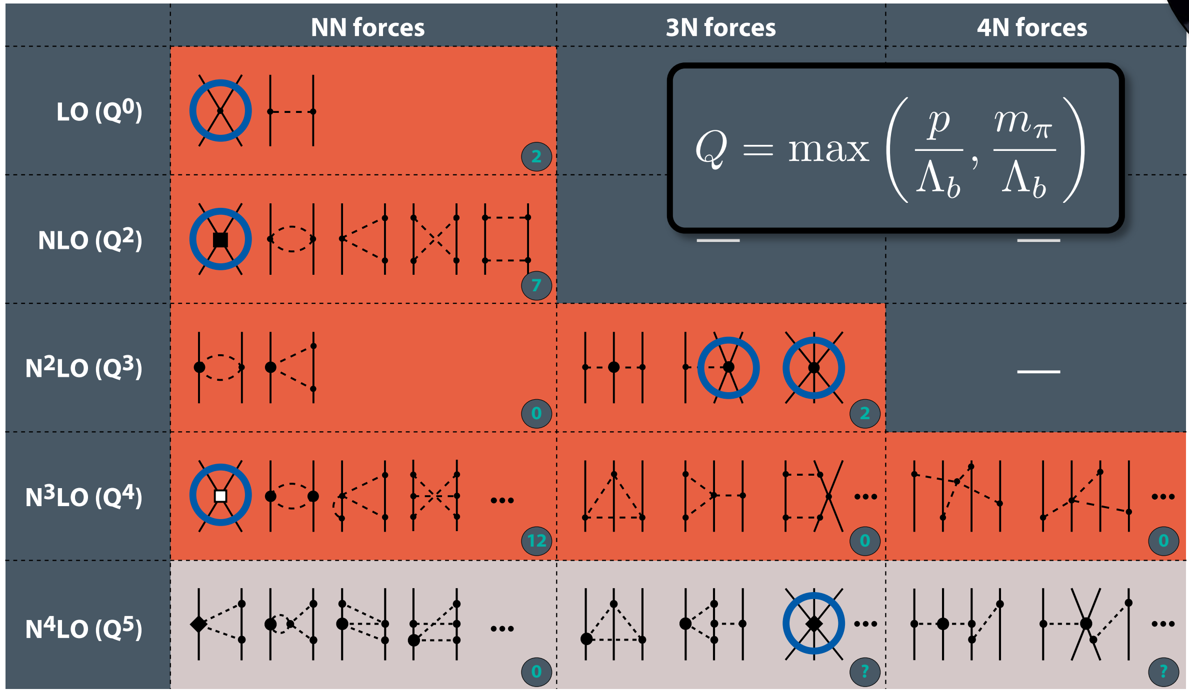
Quantum Monte Carlo with local CEFT interactions: Lonardoni, Tews, Gandolfi, Carlson, PRR **2**, 022033(R)

Bayesian statistics allows for **rigorous UQ & propagation** in EFT-based calculations (use emulators!)

At what density does CEFT break down and why ?

Rigorous UQ for nuclear matter

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



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

Chiral Effective Field Theory (nucleons & pions)

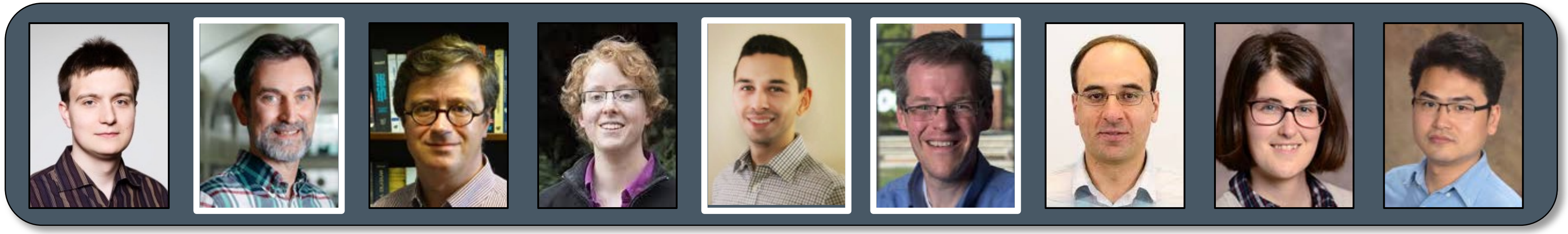
dominant approach for deriving *microscopic* interactions consistent with the symmetries of *low-energy* QCD

three- and four-*neutron* forces predicted through N^{3}LO

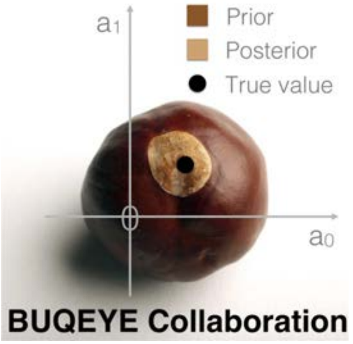
Correlated EFT truncation errors from **order-by-order calculations** & physics-informed GP truncation error model

model checking is important (”trust but verify”)

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



Open-source software & tutorials (Jupyter): https://buqeye.github.io



Bayesian
Uncertainty
Quantification:
Errors for
our
EFT

Rigorous UQ for nuclear matter

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

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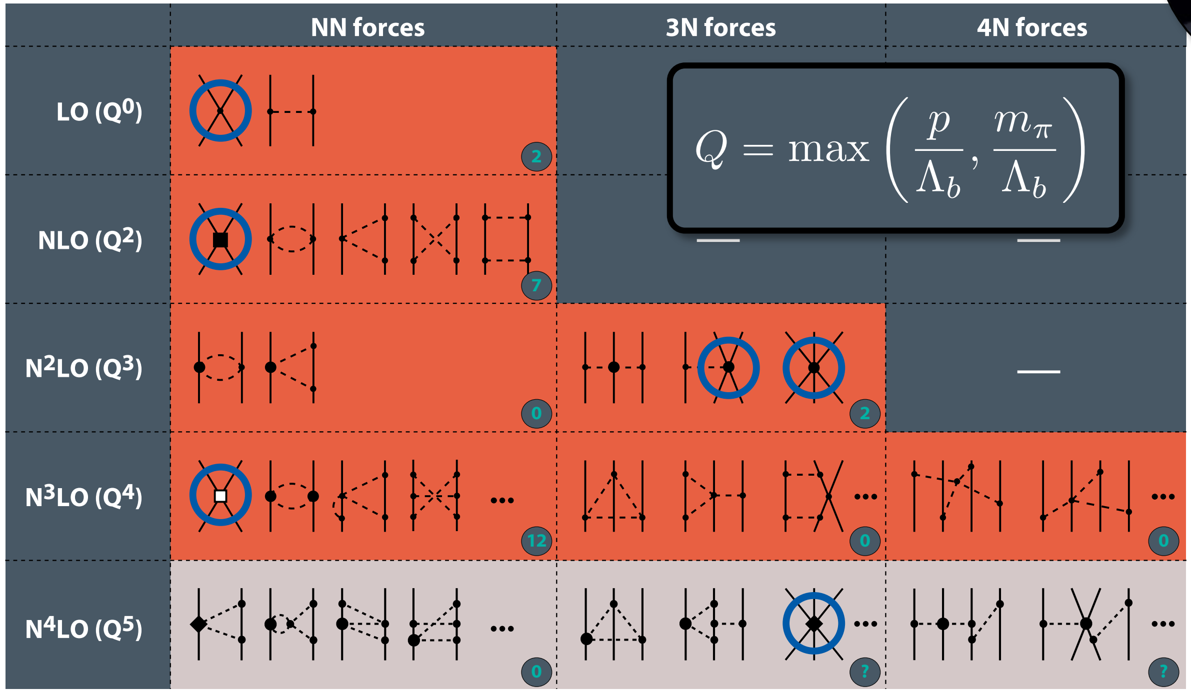

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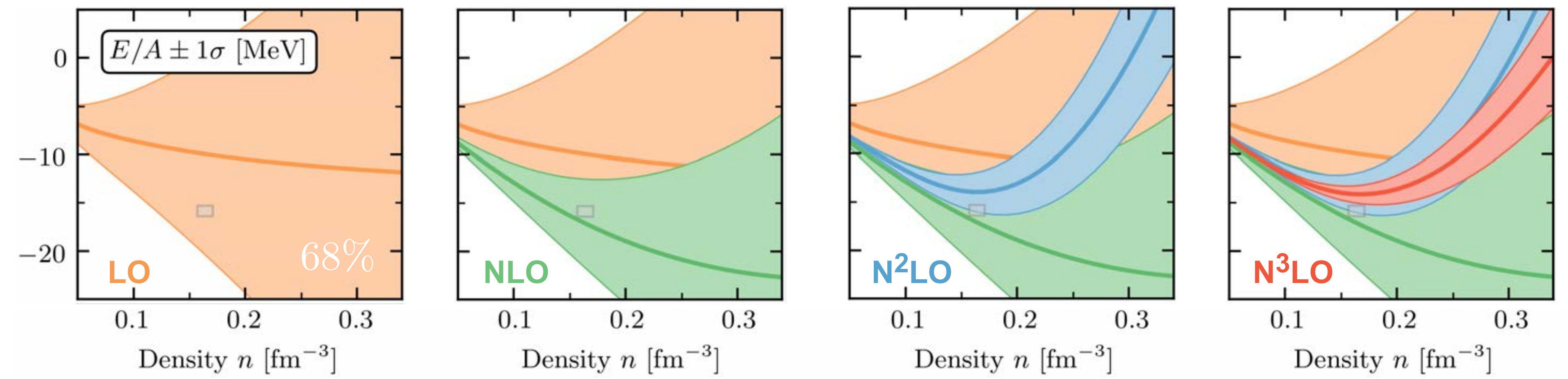
An example: symmetric matter

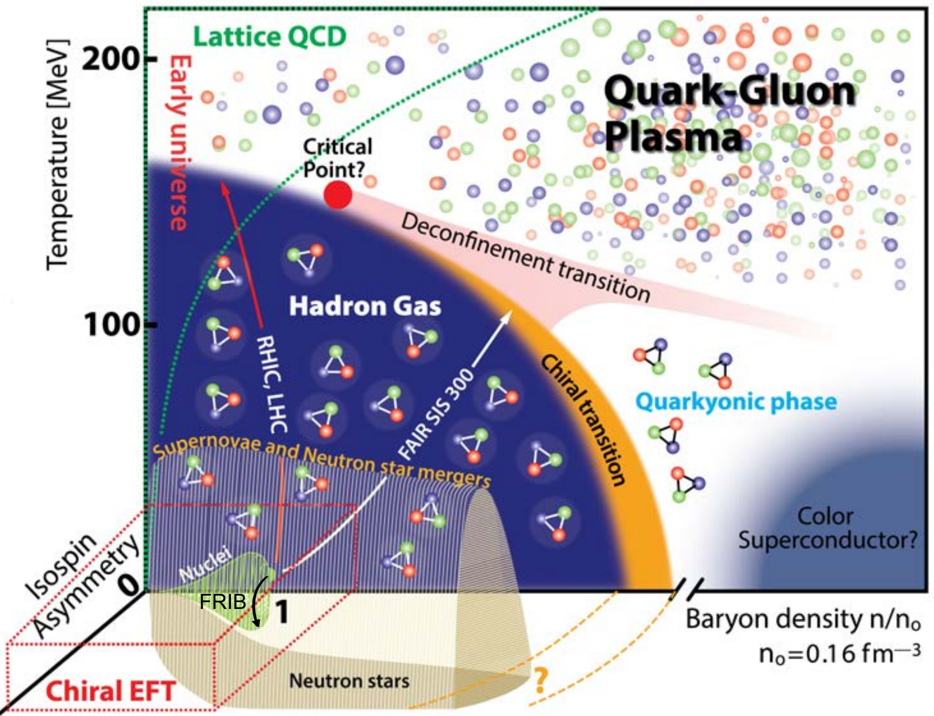
$$y = \frac{E}{A}, \quad k = 4 \quad (\mathrm{N^3LO})$$

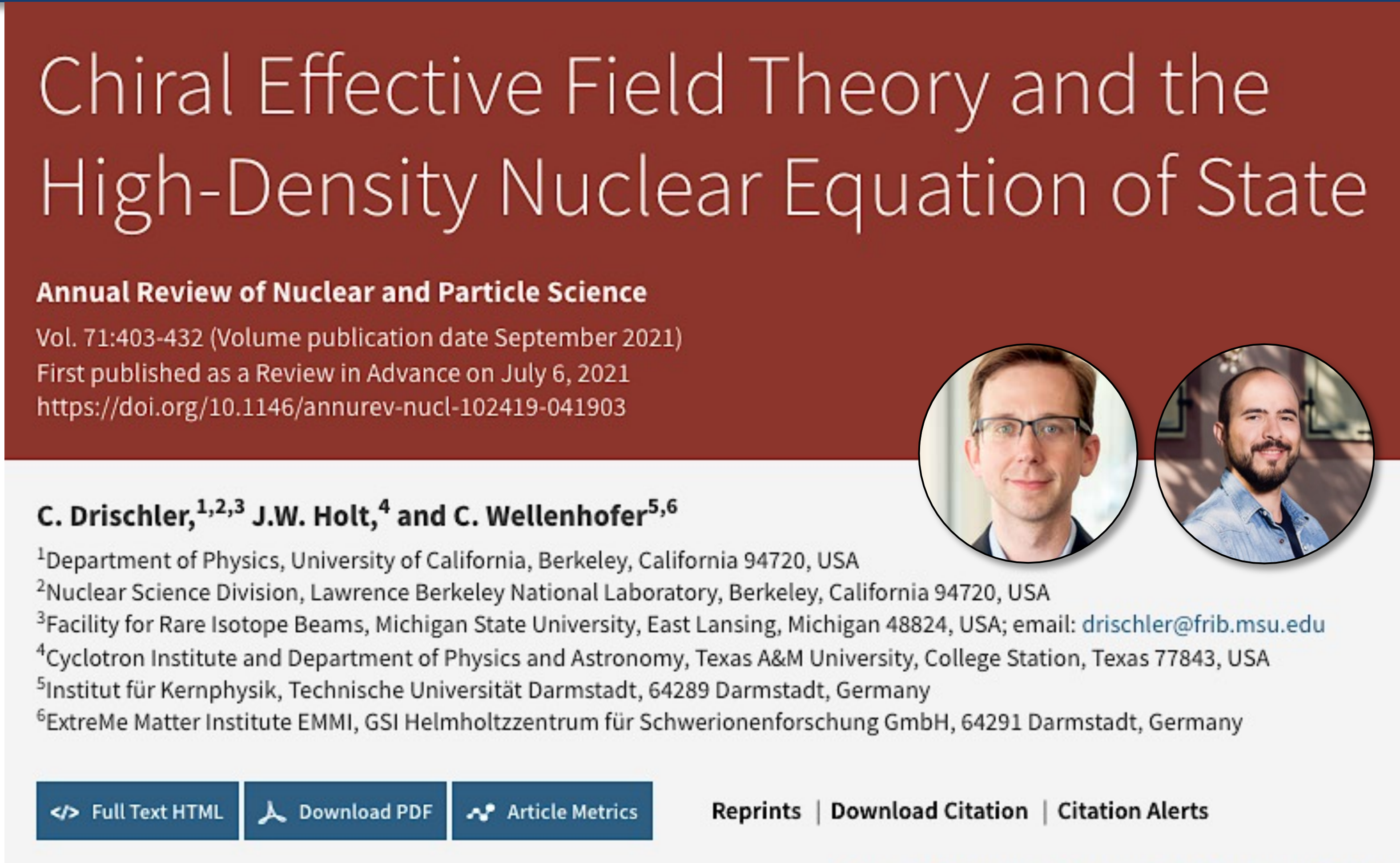
Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$



More details? Recent review article





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

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Keywords:

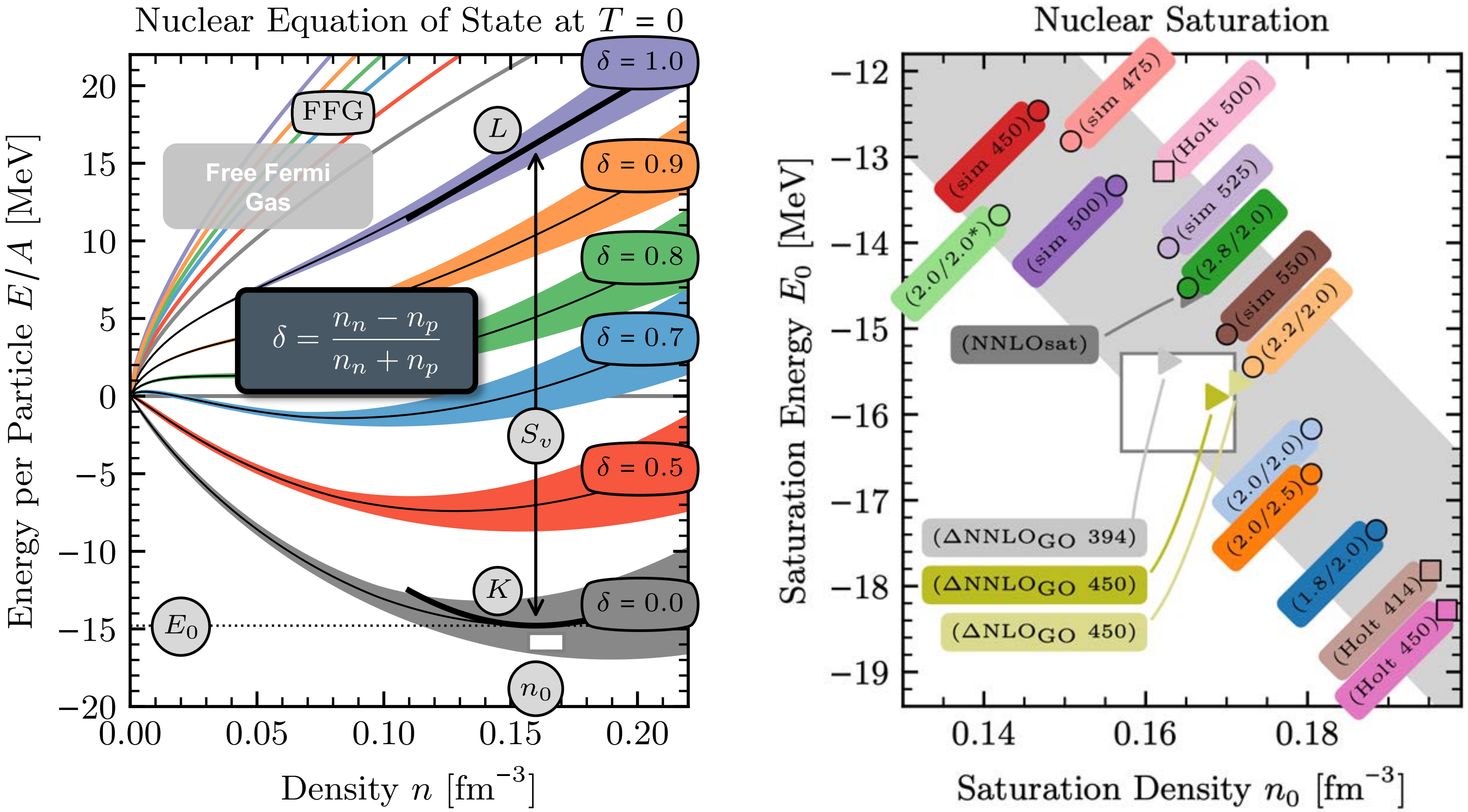
Chiral EFT | neutron stars | MBPT
nuclear matter at zero and finite temperature
Bayesian uncertainty quantification
recent neutron star observations

see also in the same journal:
James Lattimer, Annu. Rev. Nucl. Part. Sci. **71**, 433

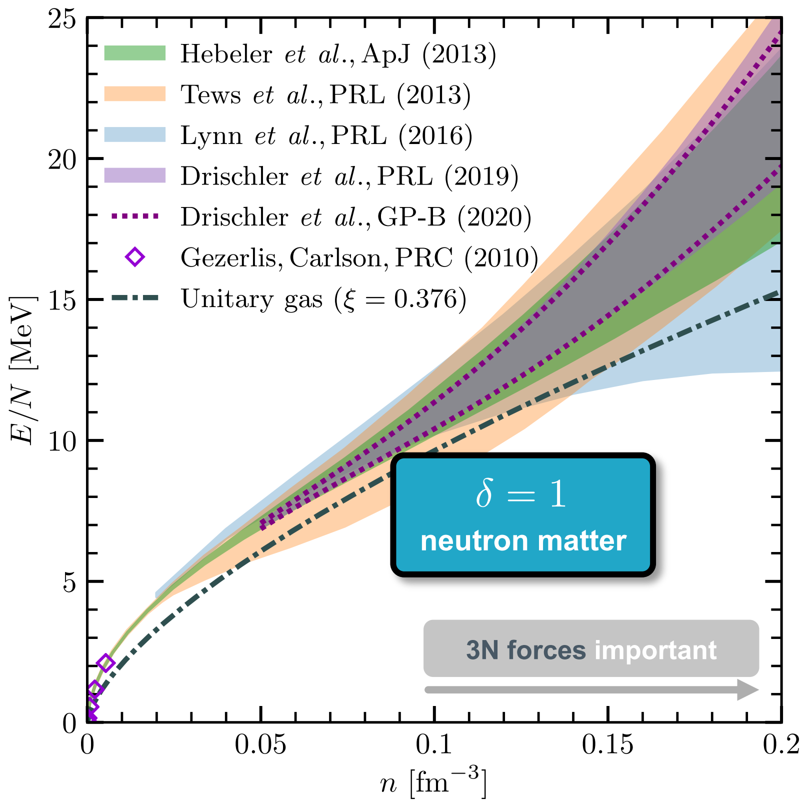
see also Sorensen *et al.*, arXiv:2301.13253

Open Access

Neutron matter & symmetric matter



CD, Holt, and Wellenhofer, Annu. Rev. Nucl. Part. Sci. **71**, 403



Huth *et al.*, PRC **103**, 025803

saturation point: **fine-tuned cancellation** between the kinetic and interaction contributions (ideal testbed for chiral EFT)

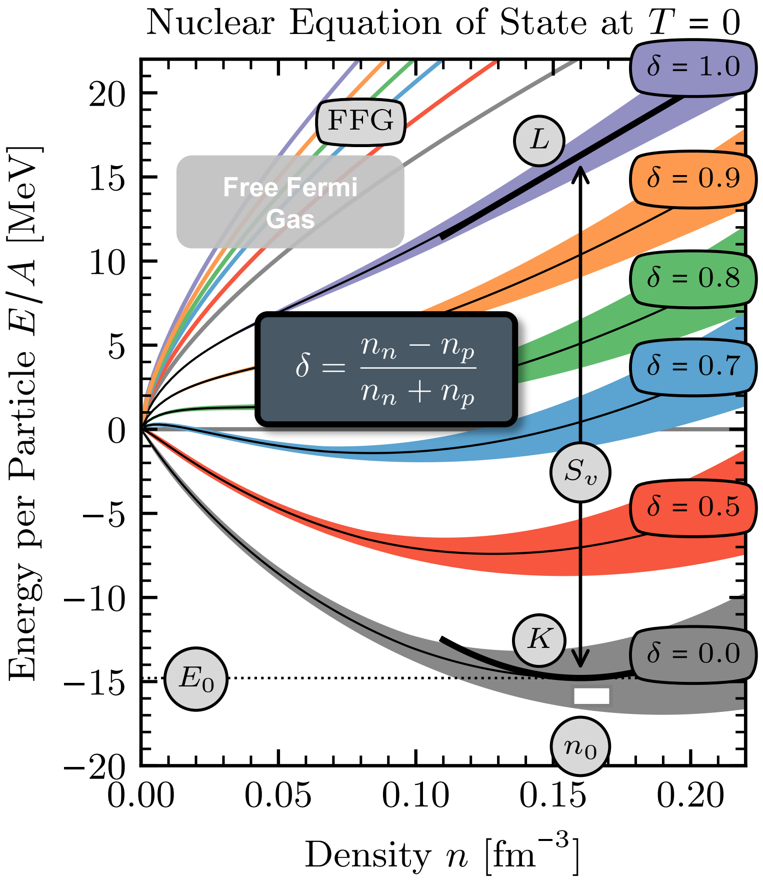
empirical constraints provide **important benchmarks** of chiral interactions, esp. 3NF

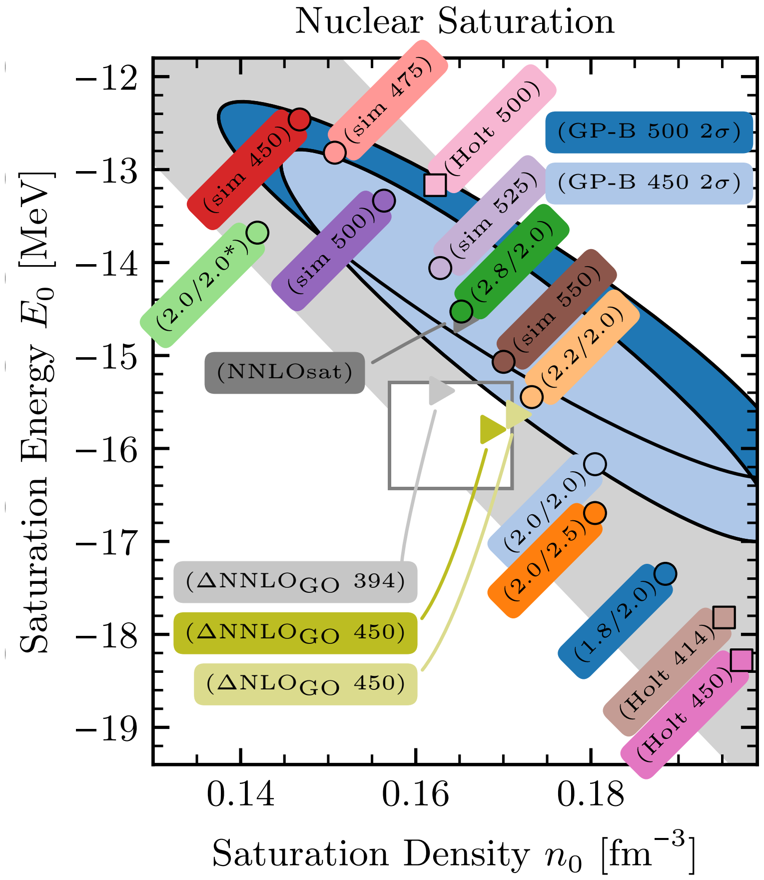
Annotations: (λ / Λ_{3N}) in fm^{-1} or (Λ) in MeV

neutron matter below saturation density is **well-constrained** by NN scattering phase shifts

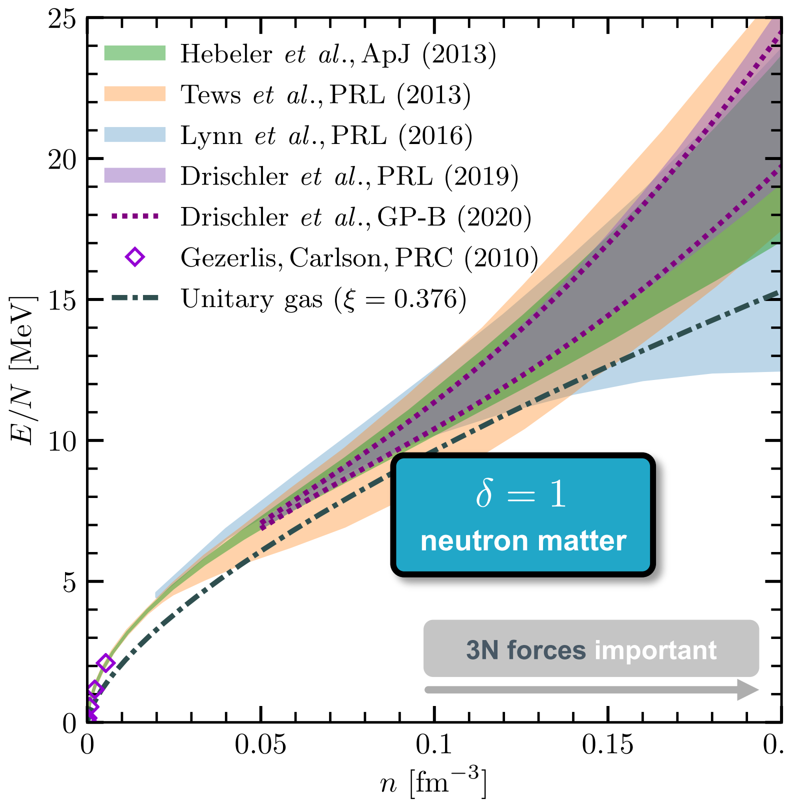
CD, Hebeler *et al.*, PRL **122**, 042501; Hoppe, CD *et al.*, PRC **100**, 024318; Simonis, Stroberg *et al.*, PRC **96**, 014303; Ekström *et al.*, PRC **97**, 024332; Atkinson *et al.*, PRC **102**, 044333; and many more

Neutron matter & symmetric matter





CD, Holt, and Wellenhofer, Annu. Rev. Nucl. Part. Sci. **71**, 403



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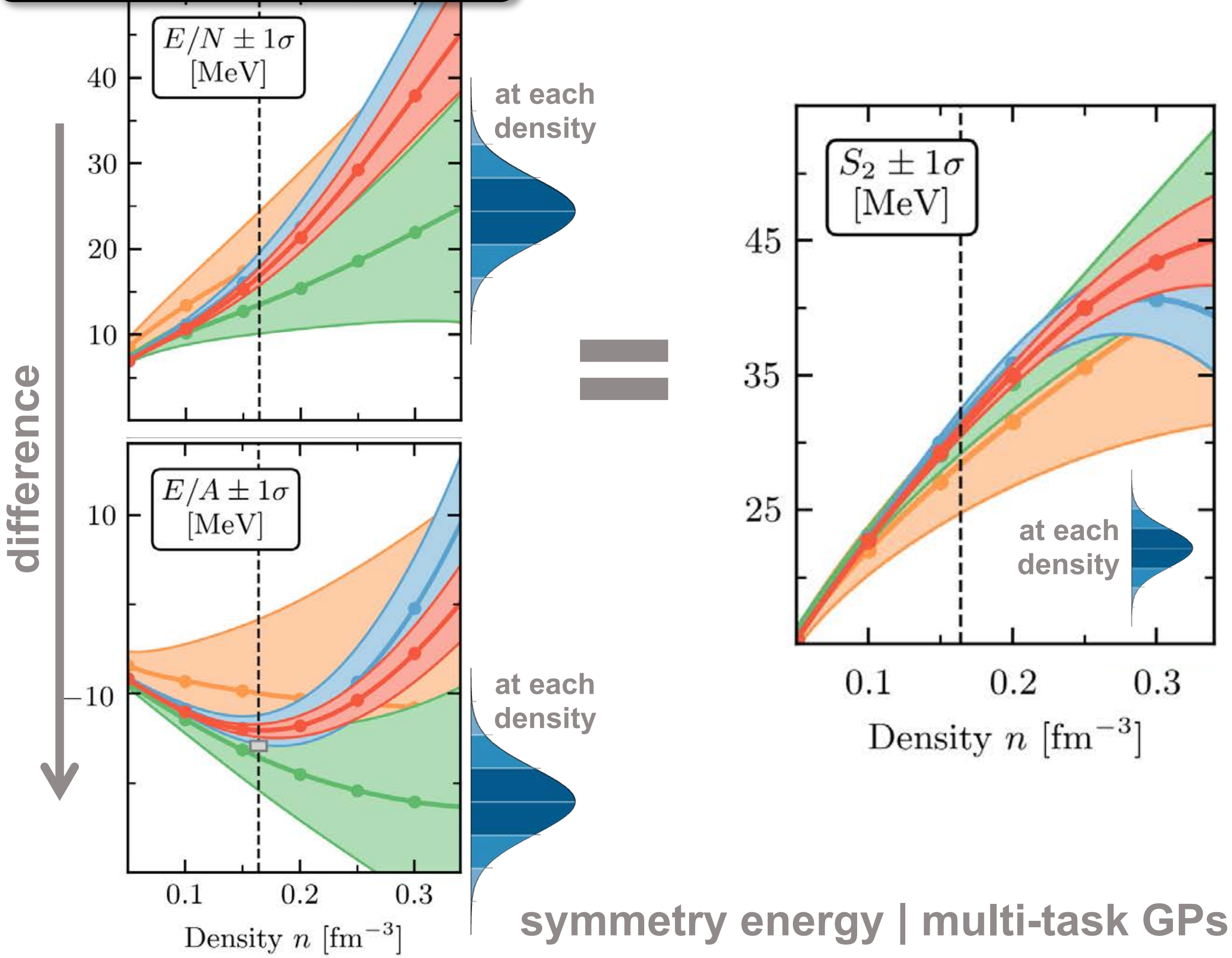
Nuclear symmetry energy

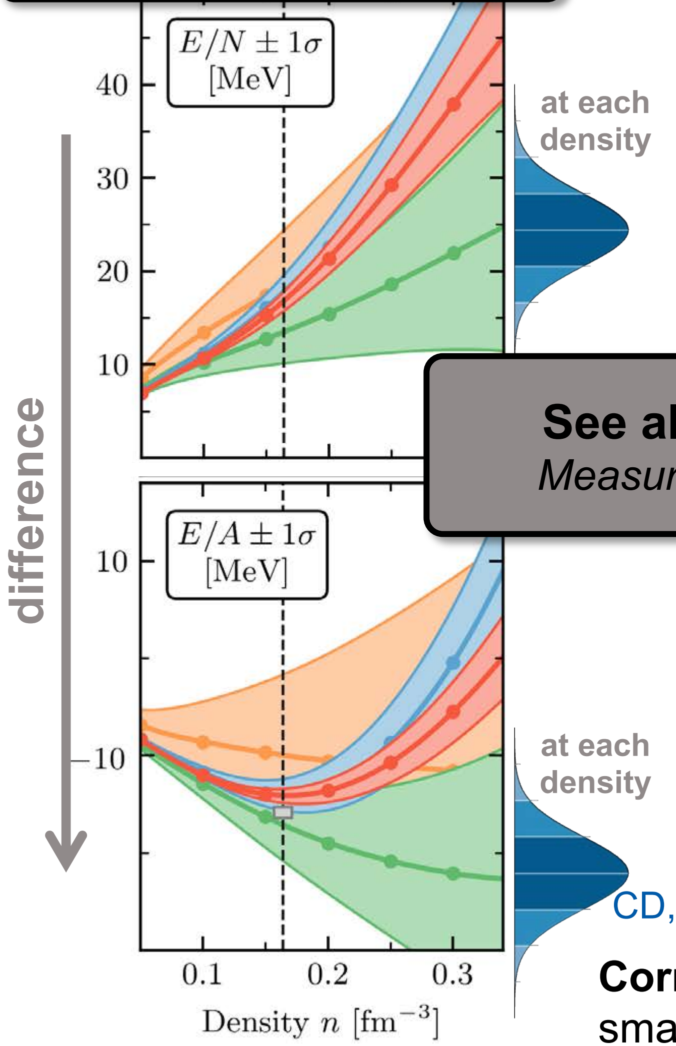
$$E_{\rm sym}(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$



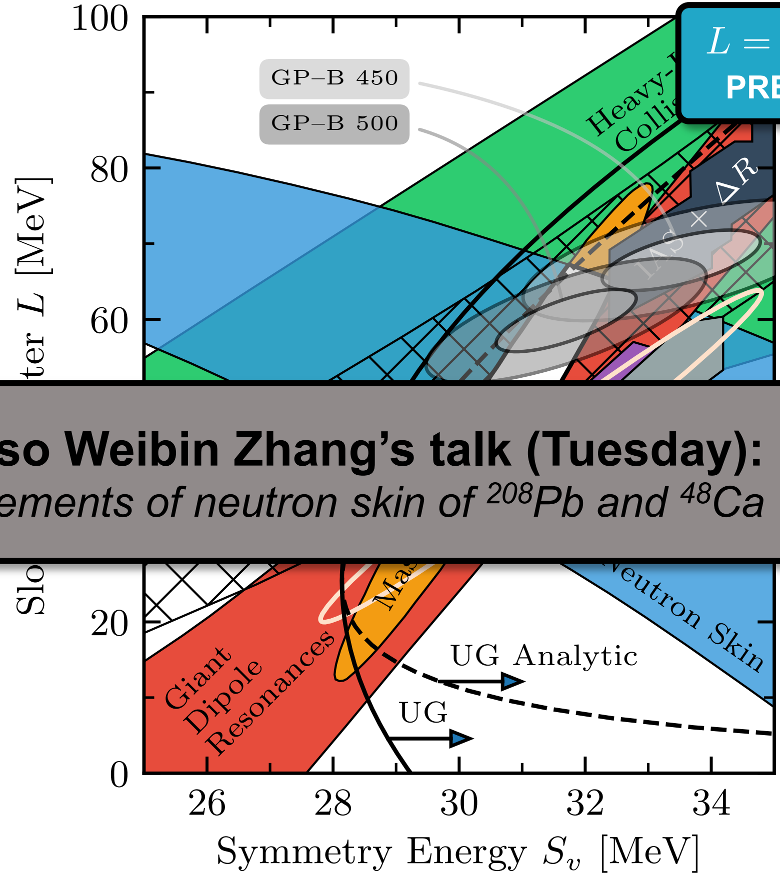
symmetry energy | multi-task GPs

Nuclear symmetry energy (at saturation density)

$$E_{\mathrm{sym}}(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$



excellent agreement between various constraints (note: probe different densities)



$L = 106 \pm 37\,\mathrm{MeV}$

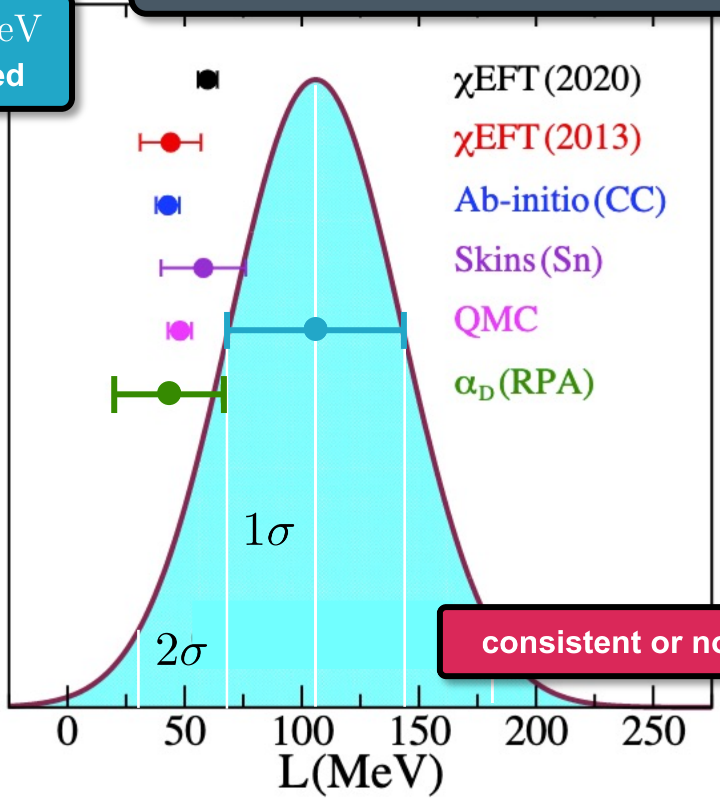
PREX–II informed

See also Weibin Zhang's talk (Tuesday):

Measurements of neutron skin of ^{208}Pb and ^{48}Ca

CD, Holt *et al.*, ARNPS **71**, 403; Lattimer & Lim, APJ **771**, 51

$$S_2(n) \equiv S_v + \frac{L}{3}\left(\frac{n-n_0}{n_0}\right) + \ldots$$



consistent or not?

Reinhard *et al.*, PRL **127**, 232501
Reed, Fattoyev *et al.*, PRL **126**, 172503
Piekarewicz, PRC **104**, 024329

Correlations are important: uncertainties can be smaller than one *might* naively think

"Tension" between PREX-II and different theoretical approaches at the ~68-95% level

Select empirical constraints from DFT (overview)

Empirical saturation box (2016):

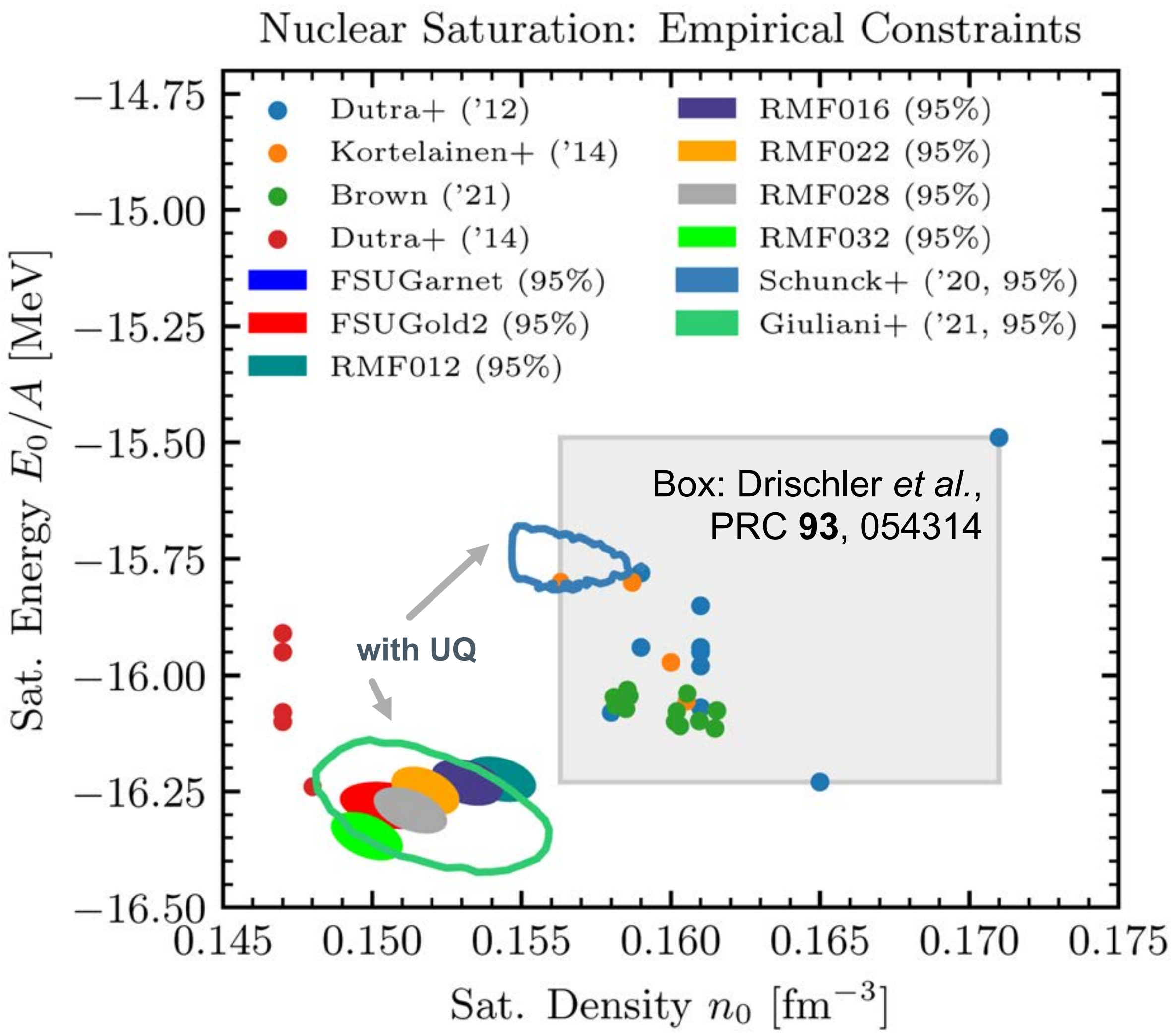
- based on 14 (out of 240) functionals that reproduce well selected nuclear properties
- often used to benchmark chiral interactions
- **limited *statistical* meaning at best**

Significant progress in UQ for DFT:

Schunck, O'Neal, Grosskopf, Lawrence, Wild, JPG: NP **47**, 074001
McDonnell, Schunck, Higdon, Sarich, Wild, Nazarewicz, PRL **114**, 122501
Neufcourt, Cao, Nazarewicz, Olsen, Viens, PRL **122**, 062502
Chen & Piekarewicz, PRC **90**, 044305; **and more**

Recently: UQ driven by projection-based emulators (promising!)

Bonilla, Giuliani, Godbey, Lee, PRC **106**, 054322
Giuliani, Godbey, Bonilla, Viens, Piekarewicz, arXiv:2209.13039

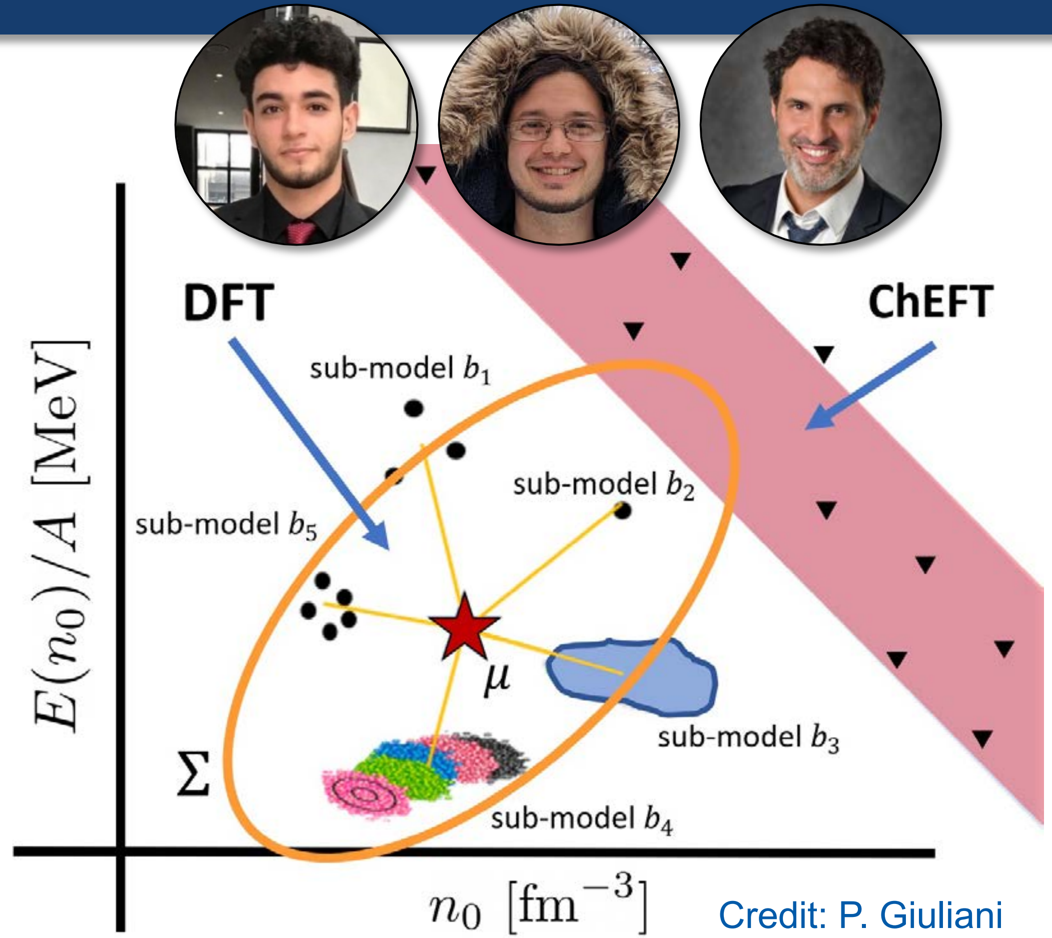


Empirical constraints are *precise* but *not very accurate* **(systematic uncertainties are *difficult* to estimate)**

Unclear how to use these scattered DFT constraints to benchmark saturation properties of chiral interactions rigorously

Dutra *et al.*, PRC **85**, 035201
Kortelainen *et al.*, PRC **89**, 054314
Brown & Schwenk, PRC C **89**, 011307

Bayesian inference: empirical saturation point



Credit: P. Giuliani

Model assumption: DFT samples are random draws from a bivariate normal distribution with *unknown* mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$

» $\mathbf{y}^* = [n_0, E(n_0)/A] \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Bayes' theorem

$$\underbrace{P(\boldsymbol{\mu}, \boldsymbol{\Sigma} | \mathcal{D})}_{\text{posterior}} \propto \underbrace{P(\mathcal{D} | \boldsymbol{\mu}, \boldsymbol{\Sigma})}_{\text{likelihood}} \; \underbrace{P(\boldsymbol{\mu}, \boldsymbol{\Sigma})}_{\text{prior}}$$

prior

$$P(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathrm{NIW}_{\nu_0}(\boldsymbol{\mu}, \Sigma)$$

$$\boldsymbol{\mu} | \boldsymbol{\mu}_0, \kappa, \boldsymbol{\Sigma} \sim \mathcal{N}\left(\boldsymbol{\mu} \middle| \boldsymbol{\mu}_0, \frac{1}{\kappa}\boldsymbol{\Sigma}\right)$$

$$\boldsymbol{\Sigma} | \boldsymbol{\Psi}, \nu \sim \mathcal{W}^{-1}(\boldsymbol{\Sigma} | \boldsymbol{\Psi}, \nu)$$

likelihood

$$P(\mathcal{D} | \boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto |\Sigma|^{-\frac{n}{2}} \exp\left[-\frac{1}{2}\sum_{i=1}^{n}(\mathbf{y}_i - \boldsymbol{\mu})\boldsymbol{\Sigma}^{-1}(\mathbf{y}_i - \boldsymbol{\mu})\right]$$

posterior

same as the conjugate prior but with updated hyperparameters (analytic expression)

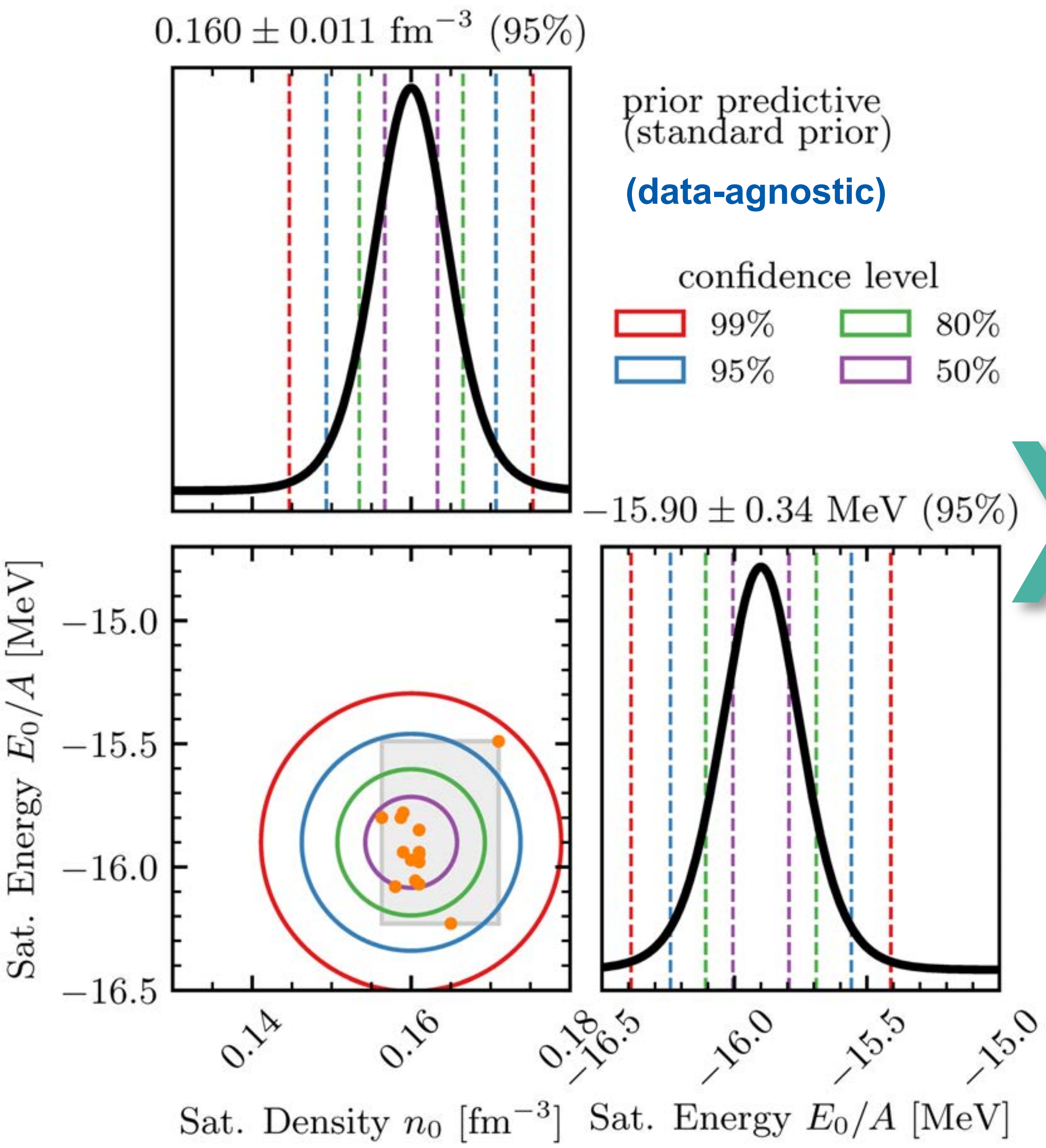
posterior predictive (marginalization)

$$P(\mathbf{y}^* | \mathcal{D}) \propto \int \mathrm{d}\boldsymbol{\mu}\, \mathrm{d}\boldsymbol{\Sigma}\; \underbrace{P(\mathbf{y}^* | \boldsymbol{\mu}, \boldsymbol{\Sigma})}_{\text{model}} \; \underbrace{P(\boldsymbol{\mu}, \boldsymbol{\Sigma} | \mathcal{D})}_{\text{posterior}}$$

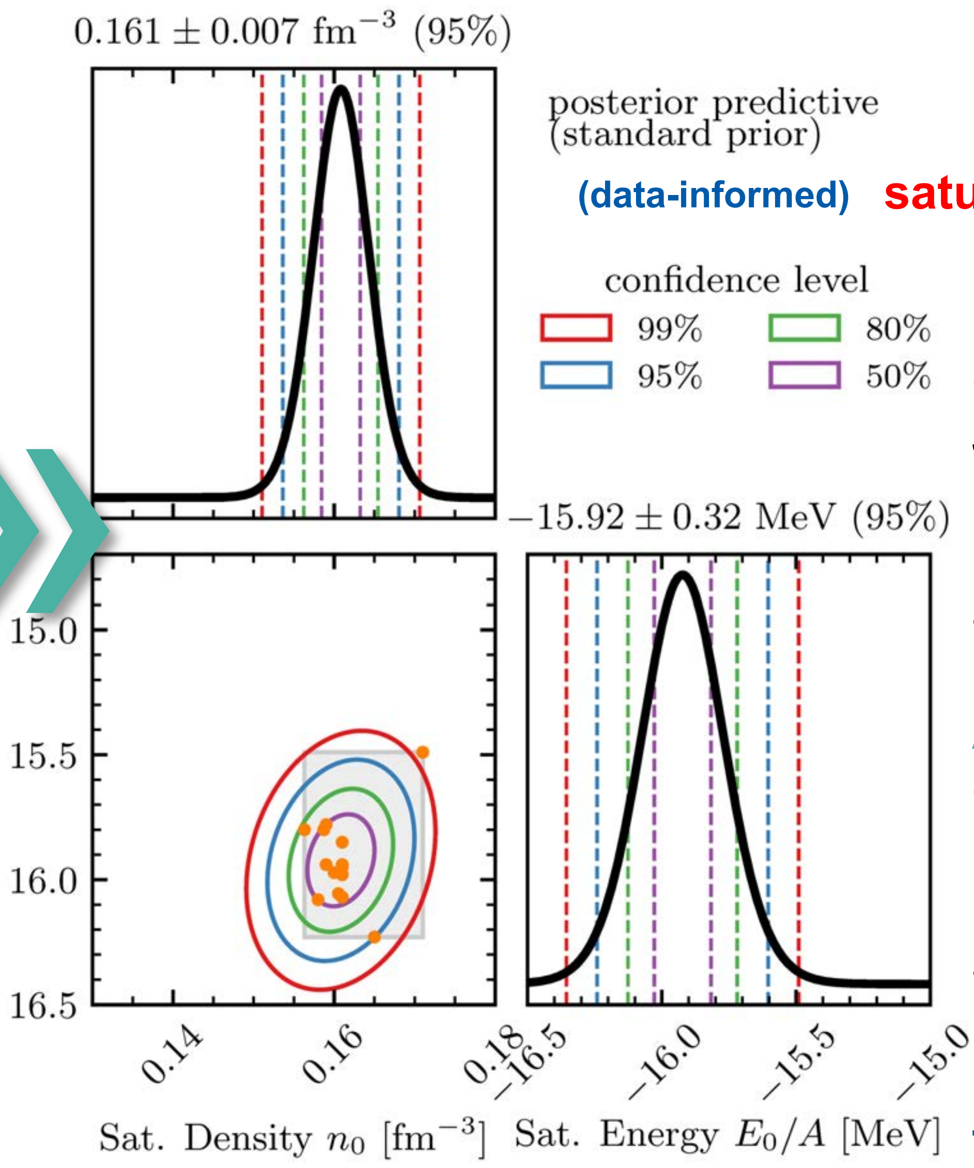
(evaluates to a bivariate t-distribution)

Analysis: Saturation Box (2016)

(preliminary)



(data-agnostic)



(data-informed)

Only data used for **saturation box (2016)** are considered **!**

Open-source Jupyter notebooks & tutorials will be provided to extend and use the results

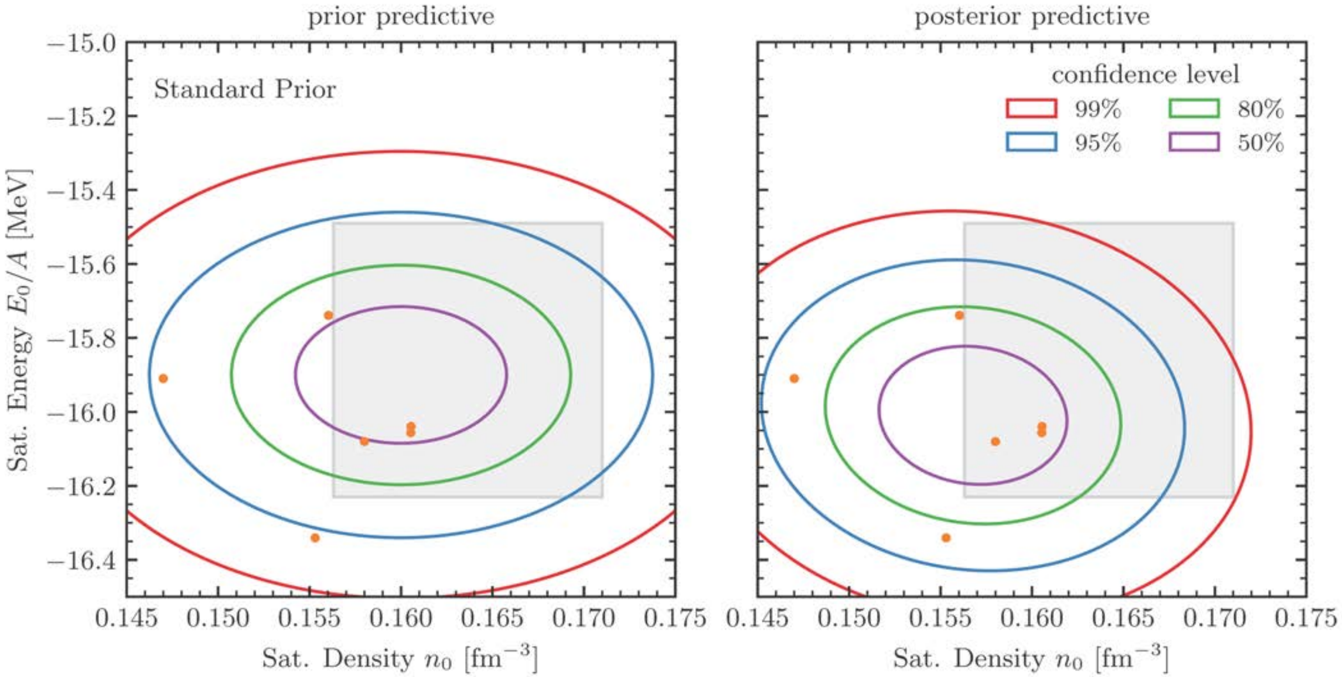
Analytic calculations due to conjugacy

predictives & marginals are **t-distributions**

Can easily investigate the prior sensitivity

All DFT constraint: joint MC analysis (preliminary)

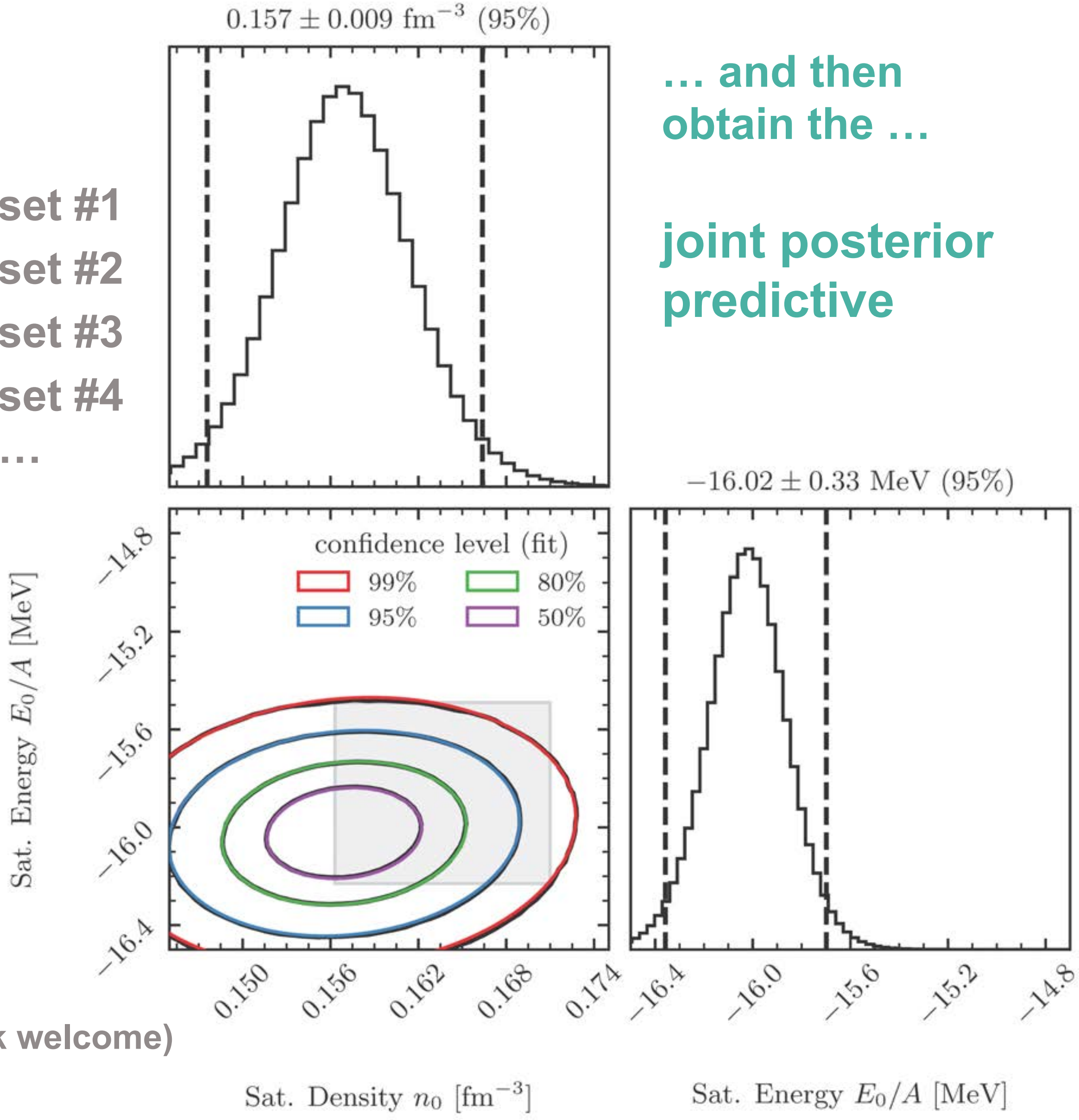
Strategy: treat data sets as empirical distributions and Monte Carlo sample from each DFT distribution …



set #1
set #2
set #3
set #4
…

… and then obtain the …

joint posterior predictive

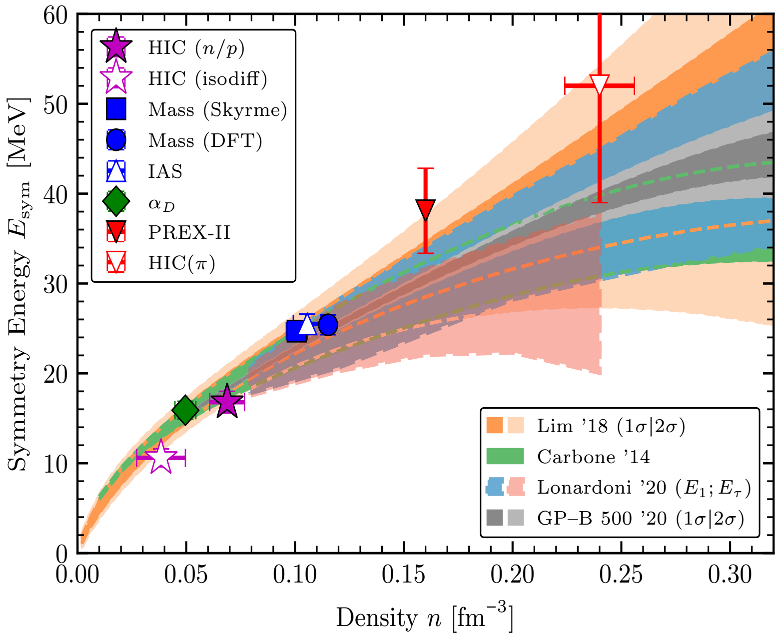


Joint DFT constraint is *consistent* with the widely used box estimate (95% C.L.) **but shifted toward lower (n_0, E_0/A)**

What other constraints should we consider?
What is our prior knowledge of saturation?

(feedback welcome)

Exploring the limits of chiral EFT



CD, Holt *et al.*, ARNPS **71**, 403
exp. constraints compiled by B. Tsang

experimental & observational constraints are important for testing and improving chiral EFT interactions

needed: improved predictions with **novel NN+3N interactions** and robust uncertainty quantification

See also Betty Tsang's talk (tomorrow)
Nuclear structure constraints on EOS

See also Bill Lynch's talk (Thursday)
The role of Nuclear structure in reaction experiments

Exploring the limits of chiral EFT

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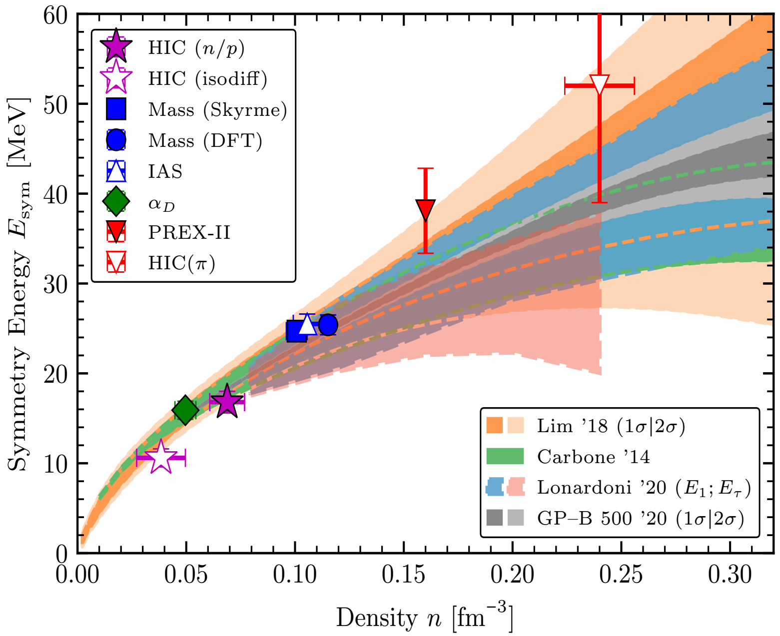

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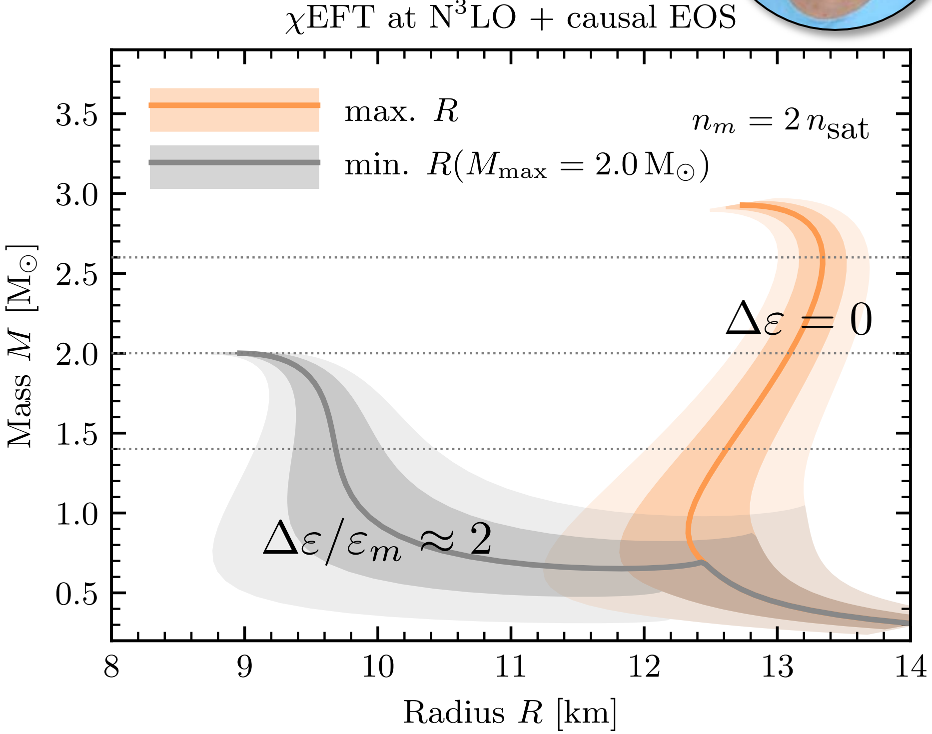
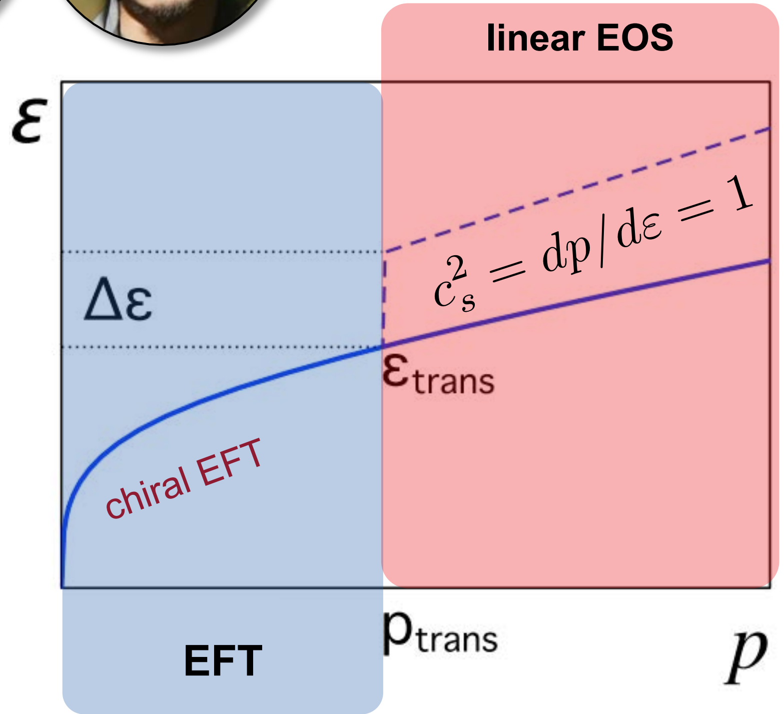


CD, Han, Lattimer *et al.*, PRC **103**, 045808
CD, Han, and Reddy, PRC **105**, 035808



Han & Prakash, APJ **899**, 2
Alford *et al.*, JPG: NPP **46**, 114001

experimental & observational constraints are important for testing and improving chiral EFT interactions

needed: improved predictions with **novel NN+3N interactions** and robust uncertainty quantification

derived **bounds on the neutron star radius** (and sound speed) assuming chiral EFT is valid up to a given critical density (here: $2n_0$)

could already be challenged by NICER

$R_{2.0} = (11.4 - 16.1)$ km

Riley *et al.*, AJL **918**, L27
Miller *et al.*, AJL **918**, L28

extend EFT EOS at n_{m} to linear EoS with finite discontinuity (softening)

continuous match sets upper bound

use **lower limit on $M_{\max}$** from observation to adjust **$\Delta\varepsilon$** and constrain $R_{\min}$

Emulators: mining scattering & reaction data

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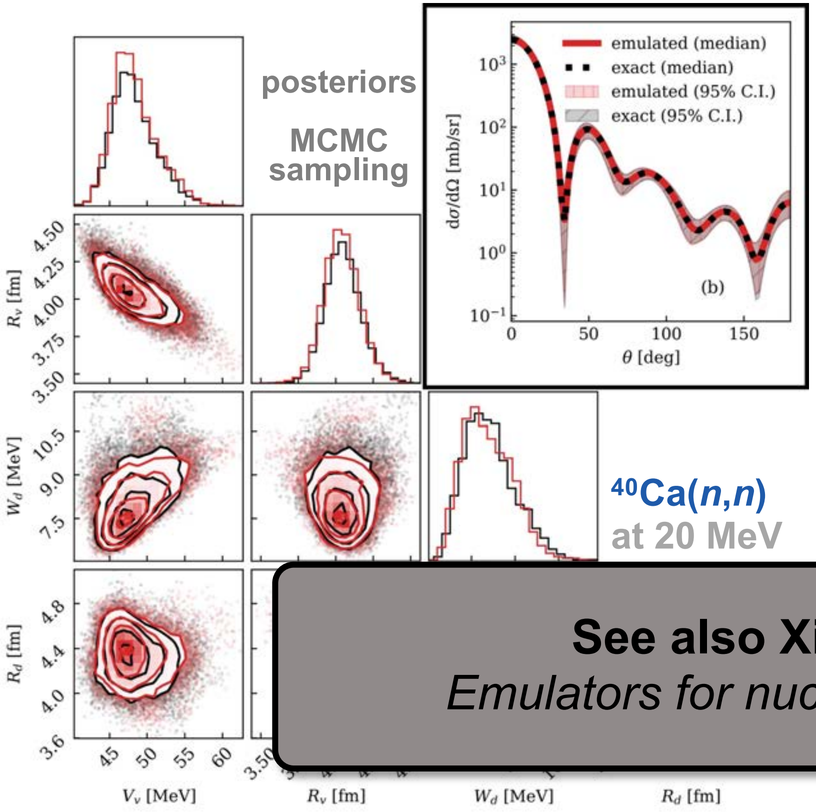


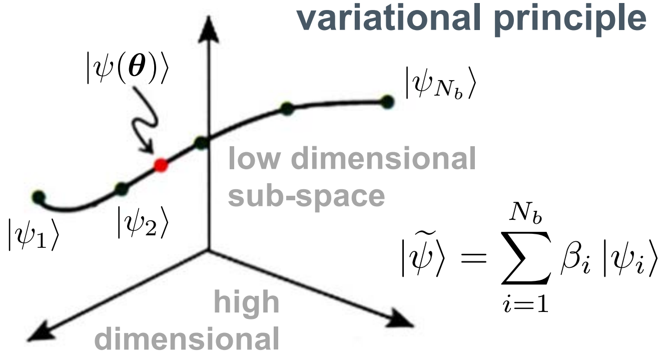
posteriors

MCMC sampling

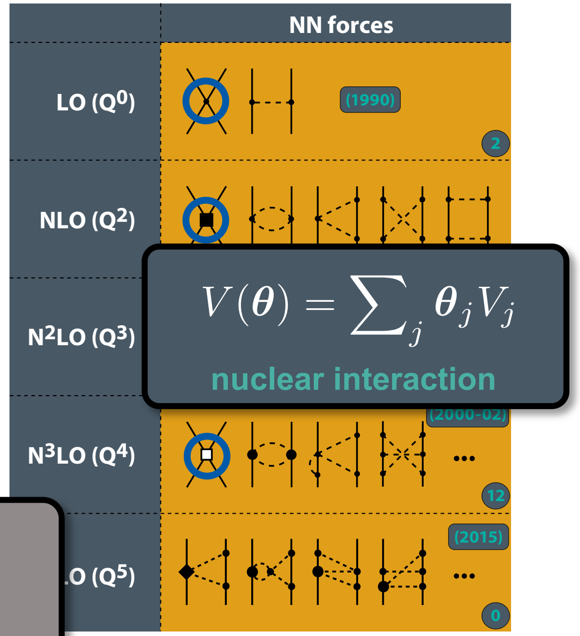
^{40}Ca(n,n) at 20 MeV

CD, Quinonez *et al.*, PLB **823**, 136777

Basis idea of Reduced Basis Methods: **variational principle**



$$|\widetilde{\psi}\rangle = \sum_{i=1}^{N_b} \beta_i\, |\psi_i\rangle$$



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

nuclear interaction

See also Xilin Zhang's talk (next talk)

Emulators for nuclear physics across energy scales

Furnstahl, Garcia *et al.*, PLB **809**, 135719 (Kohn VP)
Melendez, CD *et al.*, PLB **821**, 136608 (Newton VP)
Garcia, CD *et al.*, arXiv:2301.05093 (KVP: coupled channels)

Kohn VP: spurious *singularities* can be mitigated

Proof of principle: fast & accurate emulation of scattering observables for parameter estimation

Goal: improving next-generation optical models & chiral interactions in the FRIB era

Construct **reduced-order models** by removing superfluous information in high-fidelity models

Emulators enable applications *thought* to be prohibitively slow

For bound-state emulators, see Frame *et al.*, PRL **121**, 032501; König, Ekström *et al.*, PLB **810**, 135814; Ekström & Hagen, PRL **123**, 252501, and more

Model (Order) Reduction for nuclear emulators

Emulators
(surrogate models)

data-driven (non-intrusive)
Gaussian Processes, Artificial Neural Networks, etc.

model-driven (intrusive)
reduced-order equations from high-fidelity models

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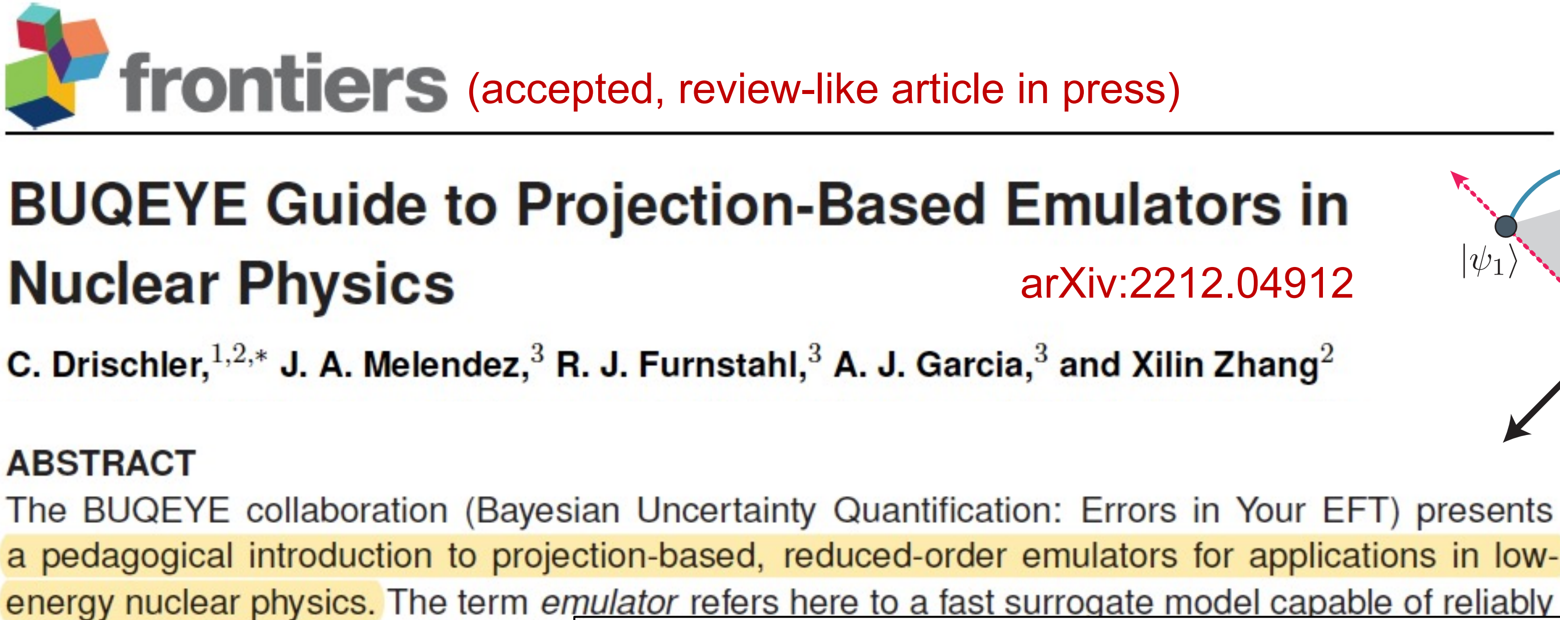
Many pointers to the **model reduction literature** (“Guide”): J. Phys. G **49**, 102001 (2022)

The field of model order reduction (MOR) is growing in importance due to its ability to extract the key insights from complex simulations while discarding computationally burdensome and superfluous information. We provide an overview of MOR methods for the creation of fast & accurate emulators of memory- and compute-intensive nuclear systems. As an example, we describe how “eigenvector continuation” is a special case of a much more general and well-studied MOR formalism for parameterized systems. We continue with an introduction to the Ritz and Galerkin projection methods that underpin many such emulators, while pointing to the relevant MOR theory and its successful applications along the way. We believe that this will open the door to broader applications in nuclear physics and facilitate communication with practitioners in other fields.

see also: CD & Zhang, Chap. 8, pp. 29–36, in Few Body Syst. **63**, 67 (collective pieces of the INT program 21–1b);
for RBMs applied to DFT, see Melendez’s GitHub; Bonilla, Giuliani *et al.*, PRC **106**, 054322; Anderson *et al.*, PRC **106**, L031302

Model (Order) Reduction for nuclear emulators



frontiers (accepted, review-like article in press)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

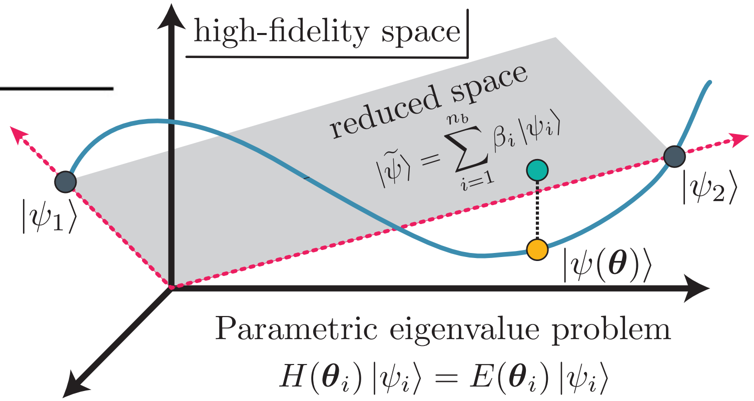
arXiv:2212.04912

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

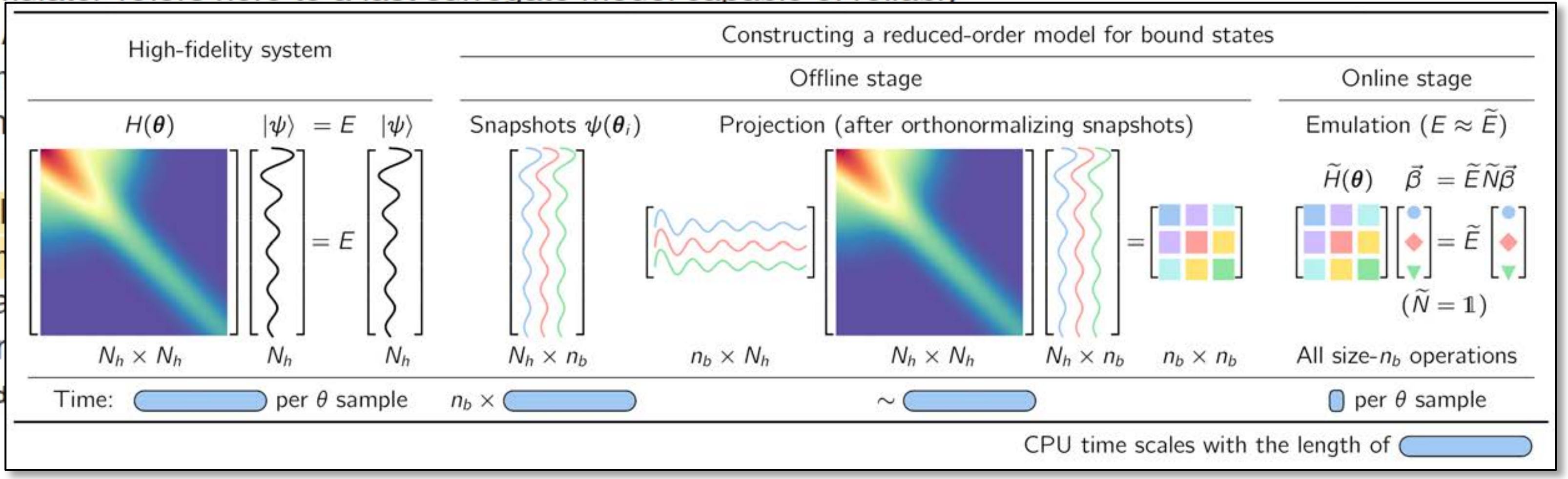
ABSTRACT

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.
well-known in the nuclear physics co
emphasize the benefits of offline-o
emulators for bound and scattering
different model parameter sets. We a
for nuclear physics, guided by the m
here and more are available as intera
adapt projection-based emulators fo

Keywords: emulators, reduced-order models, mod
variational principles, Galerkin projection



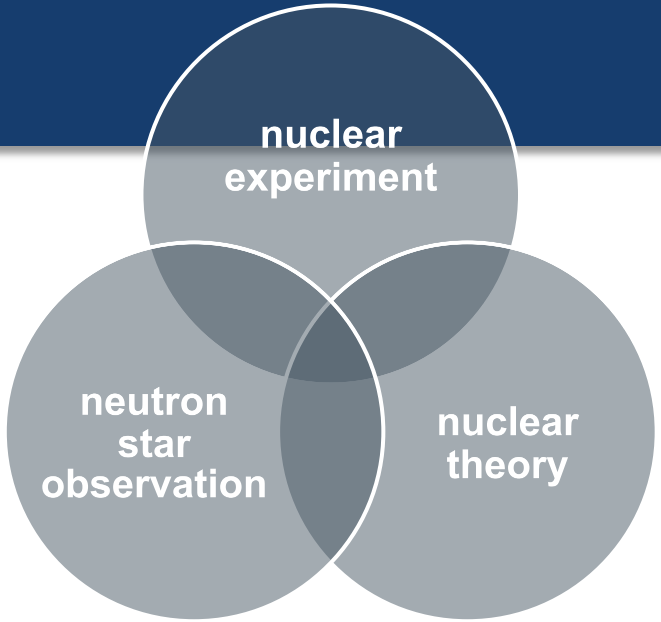
Parametric eigenvalue problem
$H(\boldsymbol{\theta}_i)\,|\psi_i\rangle = E(\boldsymbol{\theta}_i)\,|\psi_i\rangle$



Pedagogical Jupyter notebooks for learning Model (Order) Reduction: https://github.com/buqeye/frontiers-emulator-review

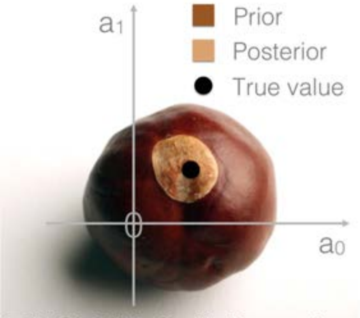
Take-away points

multi-messenger
nuclear precision
FRIB
} era



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

1. **Chiral EFT enables *ab initio* calculations of finite nuclei & nuclear matter at $T \geq 0$ & arbitrary proton fractions ($n \lesssim 2n_{\text{sat}}$). Where does it break down and why?**
2. **Bayesian statistics allows for rigorous UQ & propagation in EFT-based calculations (in many cases facilitated by new emulators!)**
3. **Need for improved constraints of the nuclear matter EOS in the density regime $1 \lesssim n/n_{\text{sat}} \lesssim 2$. Many advances can be expected across multiple disciplines.**
4. **Our *preliminary* analysis suggests for the empirical saturation point: $n_0 \approx 0.157 \pm 0.009$ fm^{-3}, with $E_0/A \approx -16.02 \pm 0.33$ MeV (95%, correlated!)**



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 C. Wellenhofer X. Zhang T. Zhao