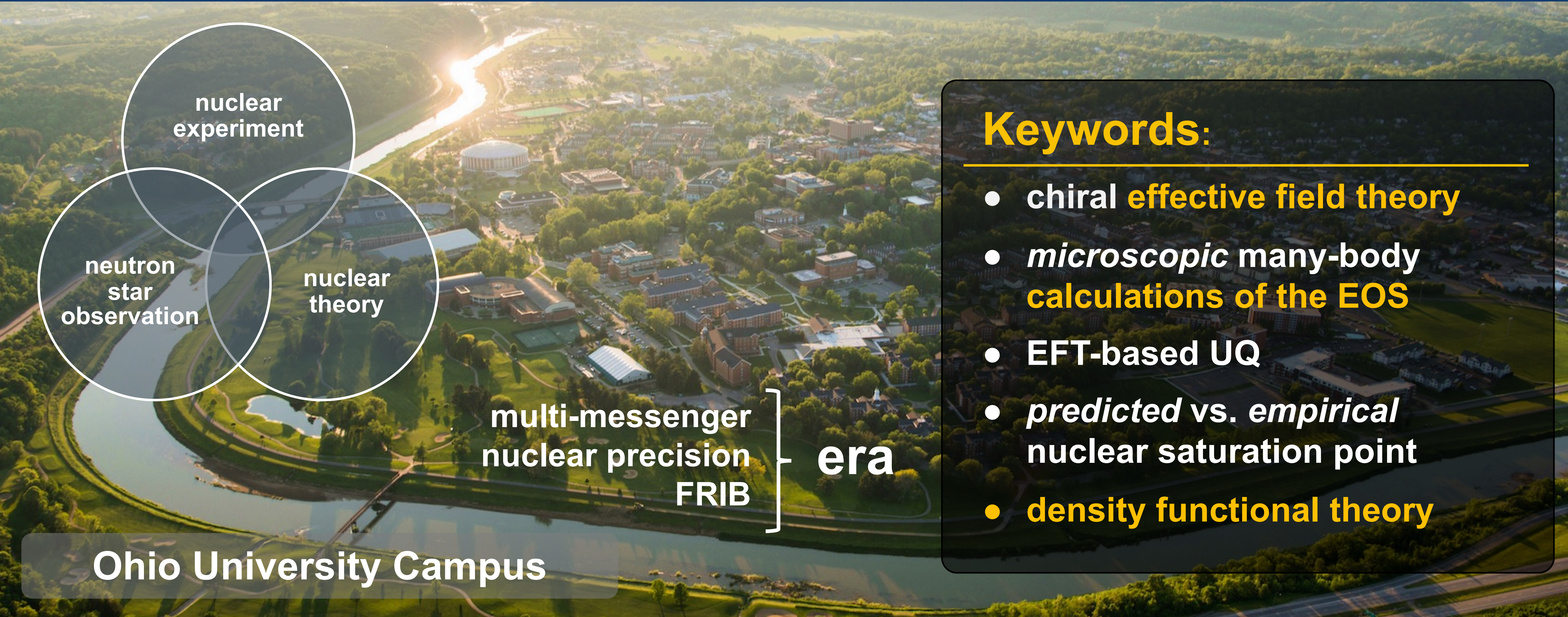
How well do we know the nuclear saturation point? Insights from EFT & DFT with Bayesian UQ

Christian Drischler (drischler@ohio.edu)

INT Workshop INT-22r-2a: Neutron-Rich Matter on Heaven and Earth
June 30, 2023

BUQEYE Collaboration



nuclear experiment

neutron star observation

nuclear theory

multi-messenger
nuclear precision
FRIB

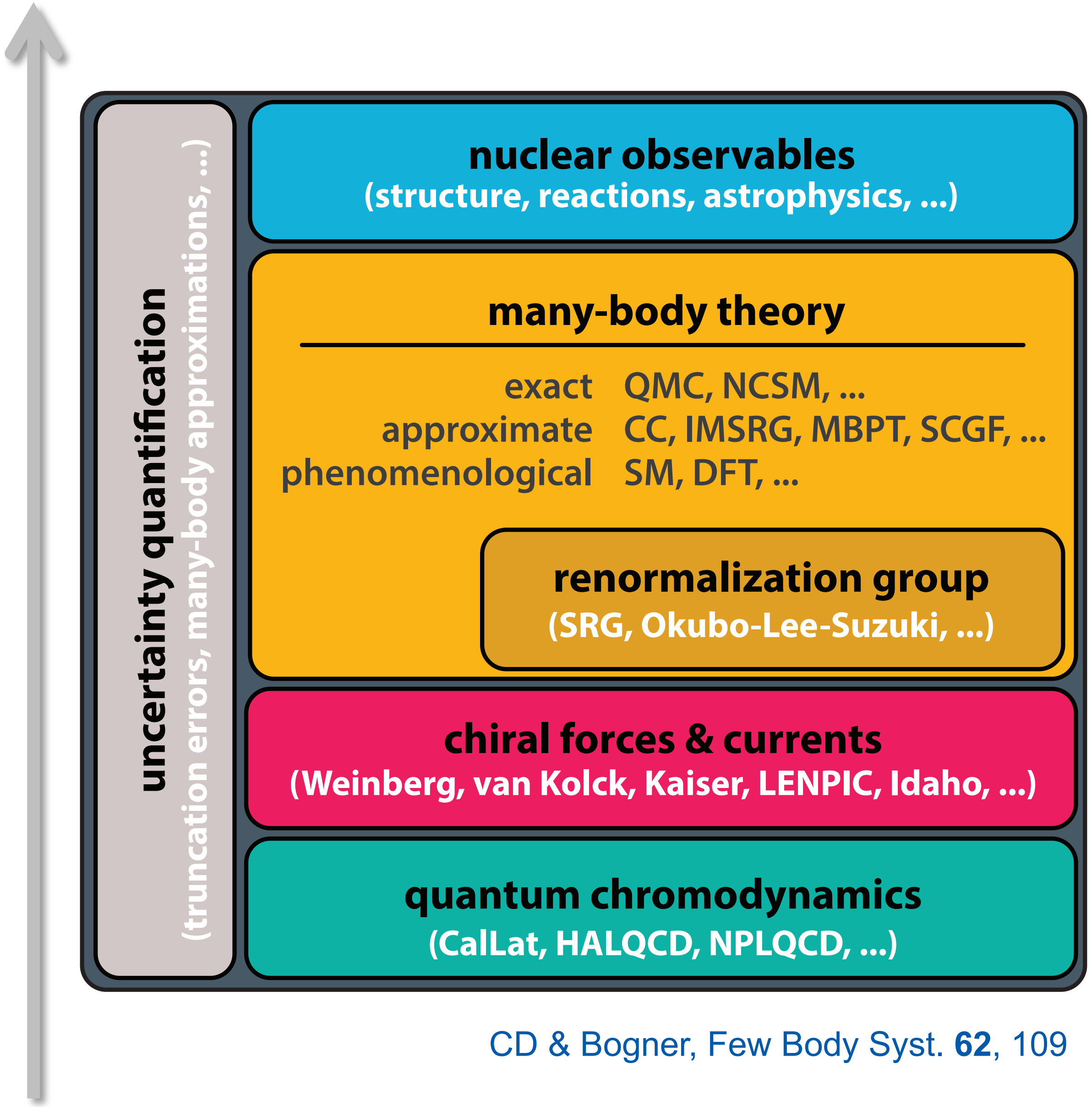
} era

Keywords:

- chiral effective field theory
- *microscopic* many-body calculations of the EOS
- EFT-based UQ
- *predicted* vs. *empirical* nuclear saturation point
- density functional theory

Ohio University Campus

Ab initio workflow (idealized)



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, ...)

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

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

Here: nuclear equation of state (EOS)
energy per particle (and related quantities)

See also Rahul Somasundaram's talk (QMC):
Constraining the neutron star equation of state from gravitational wave detections

Here: many-body perturbation theory (MBPT)

automated, computationally efficient method
allows to estimate many-body uncertainties

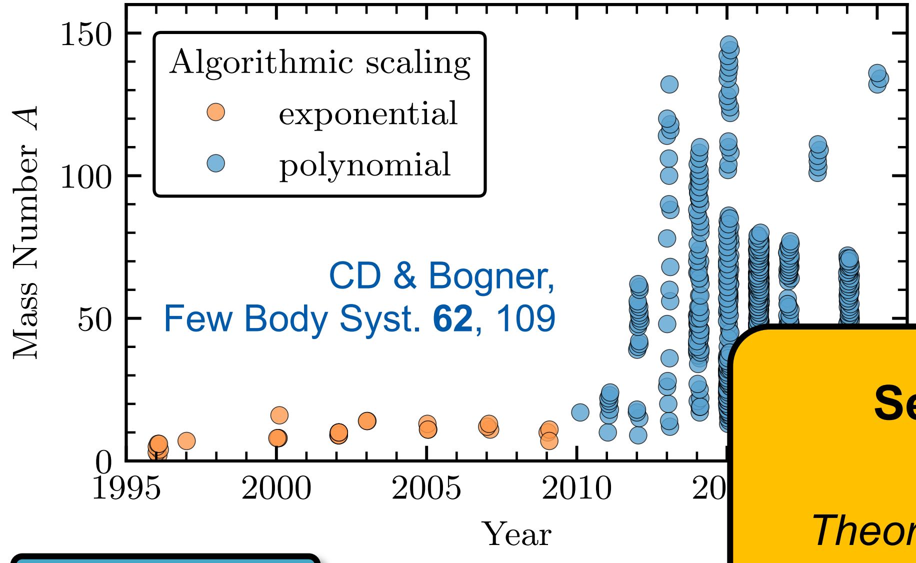
Widely applicable:

- ✓ arbitrary proton fractions
- ✓ finite temperature
- ✓ optical potentials, linear response, nuclei, …

Other frameworks include **quantum Monte Carlo**, coupled cluster, and self-consistent Green's functions

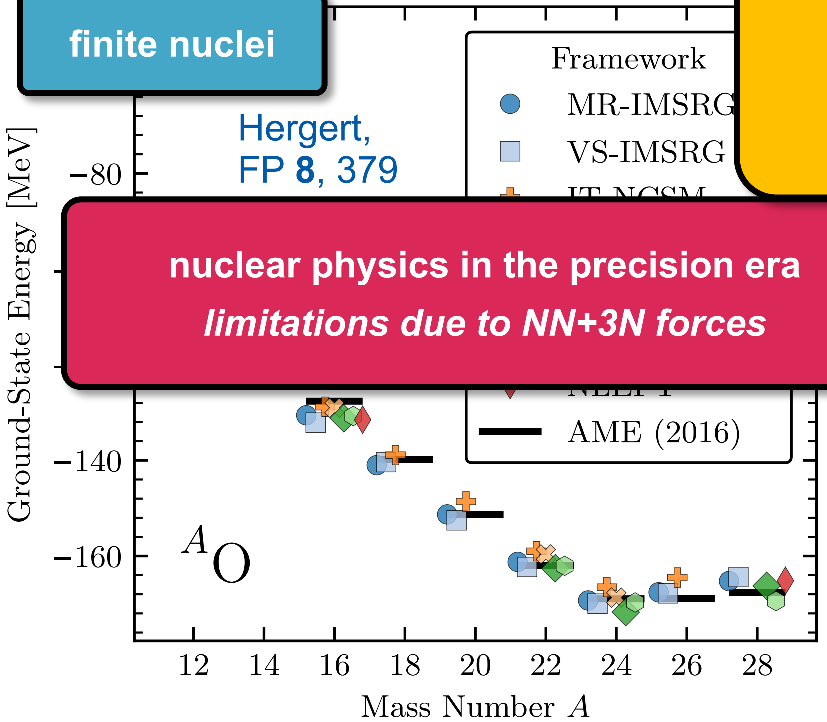
CD, Haxton, McElvain, Mereghetti *et al.*, PPNP **121**, 103888

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

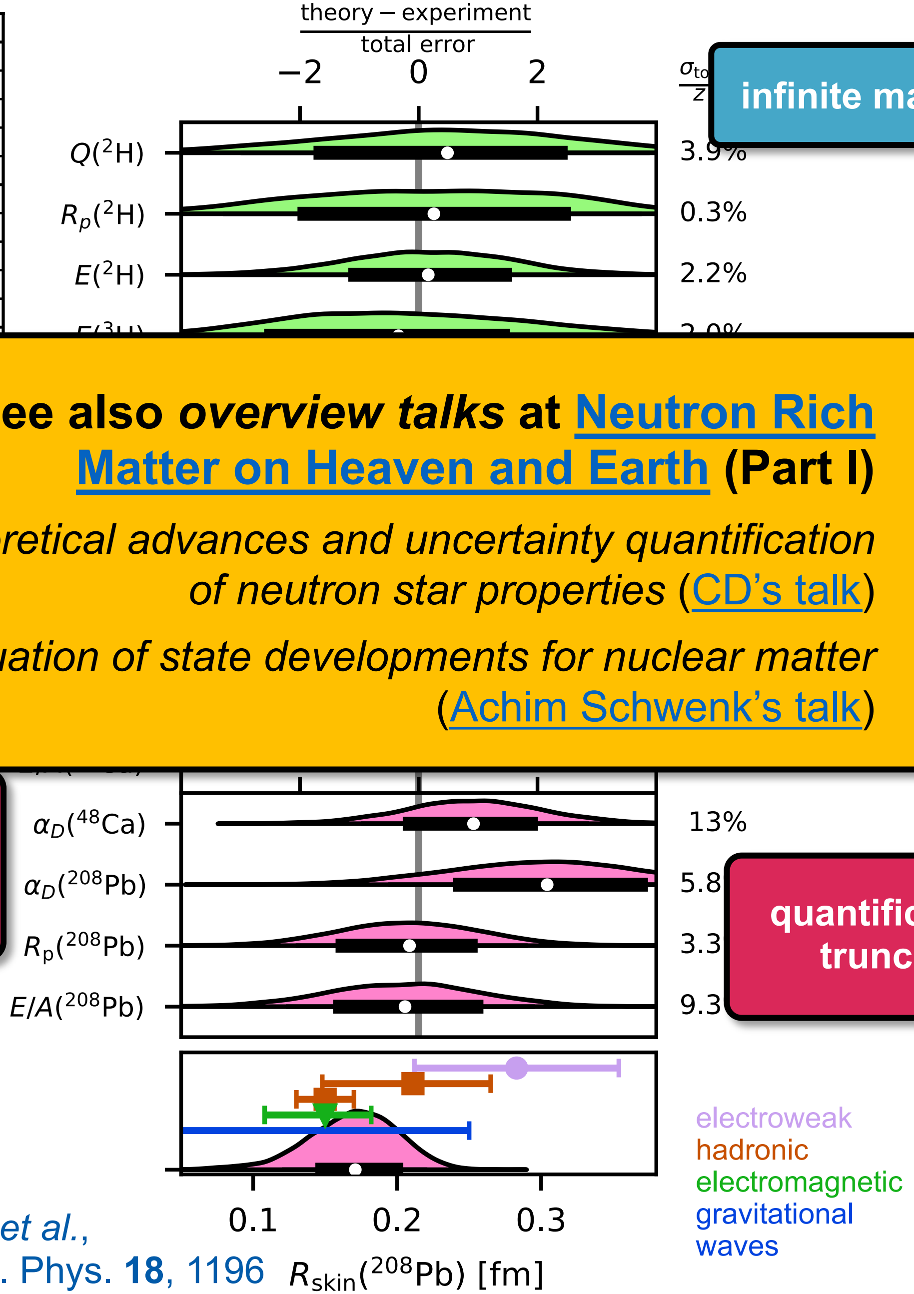


CD & Bogner, Few Body Syst. **62**, 109

finite nuclei

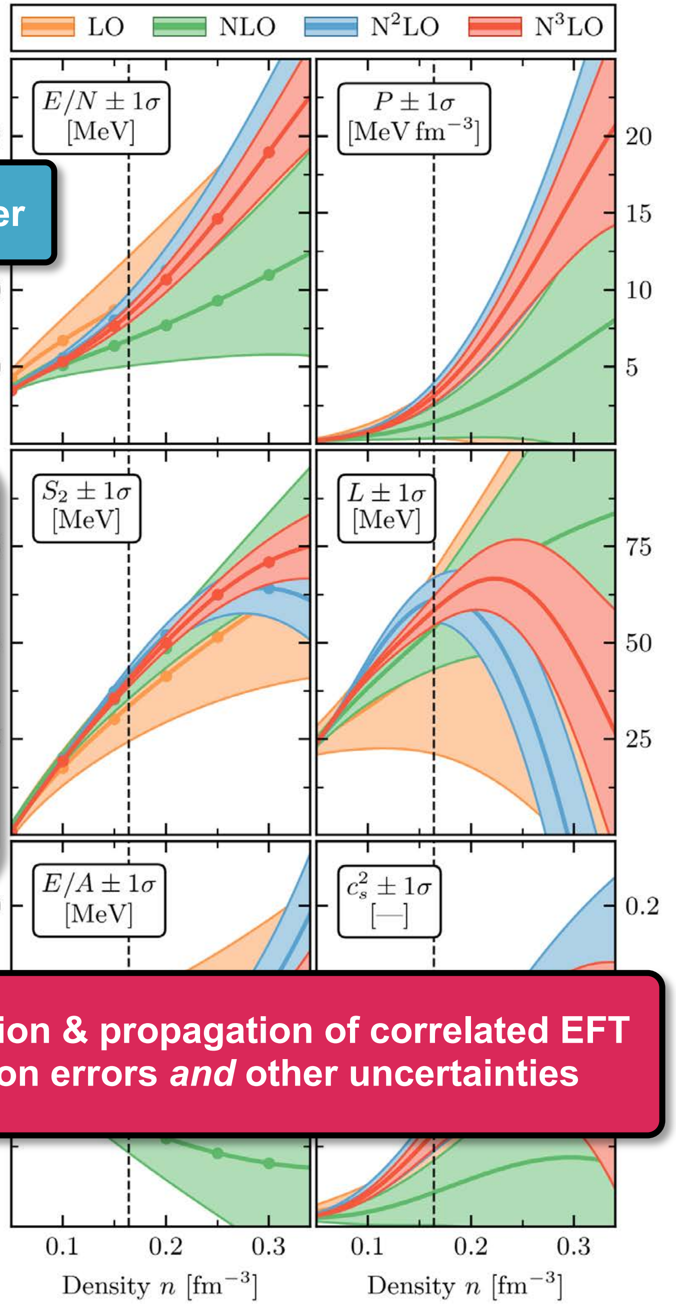


Hergert, FP **8**, 379



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

infinite matter



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

See also *overview talks* at Neutron Rich Matter on Heaven and Earth (Part I)

Theoretical advances and uncertainty quantification of neutron star properties (CD's talk)

Equation of state developments for nuclear matter (Achim Schwenk's talk)

nuclear physics in the precision era

limitations due to NN+3N forces

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

Chiral nuclear forces

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

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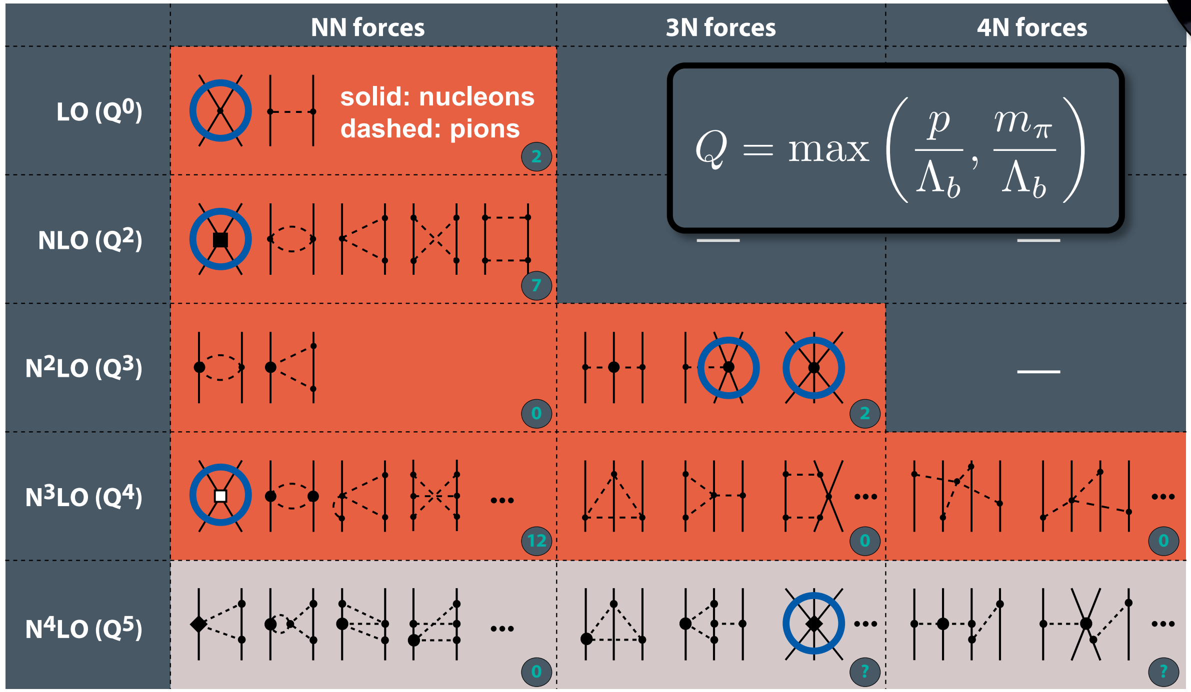


$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

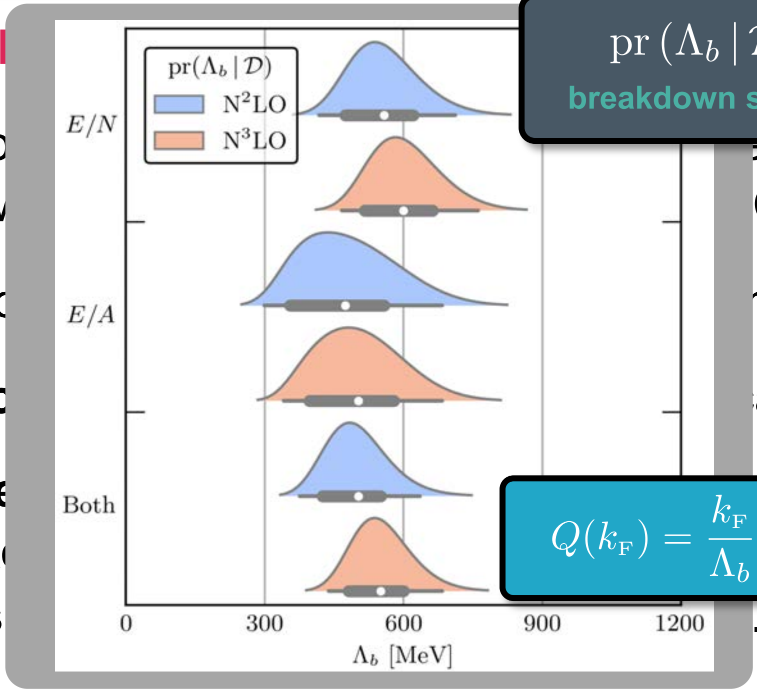
Cl … pions)

dominant ap … eractions
consistent w … CD

three- and fo … n N^{3}LO

enables **unc** … ation)

parameter e … **ergy)**
couplings t … as
phase shifts … .



$\mathrm{pr}\,(\Lambda_b \mid \mathcal{D})$
breakdown scale

$$Q(k_F) = \frac{k_F}{\Lambda_b}$$

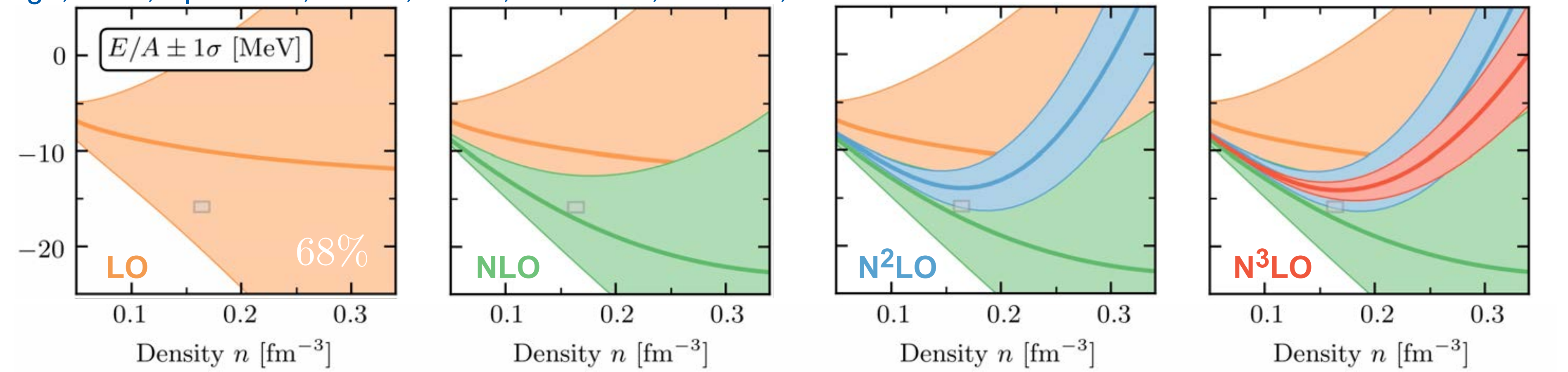
Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Krebs, Machleidt, Meißner, ...

An example:
symmetric matter

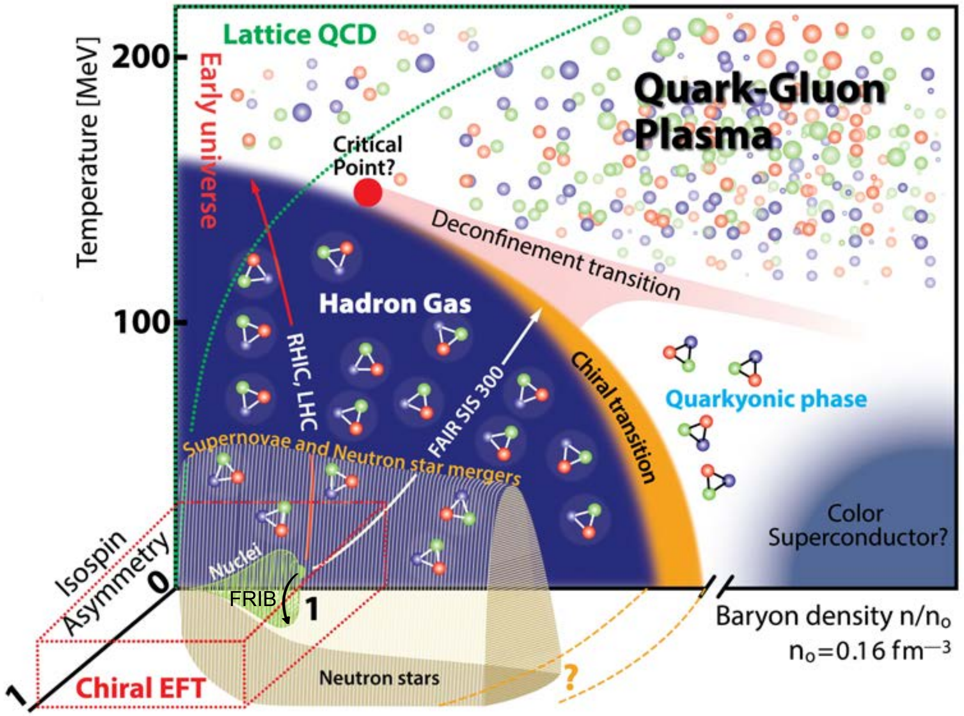
$$y = \frac{E}{A}, \quad k = 4 \quad (\mathrm{N^3LO})$$

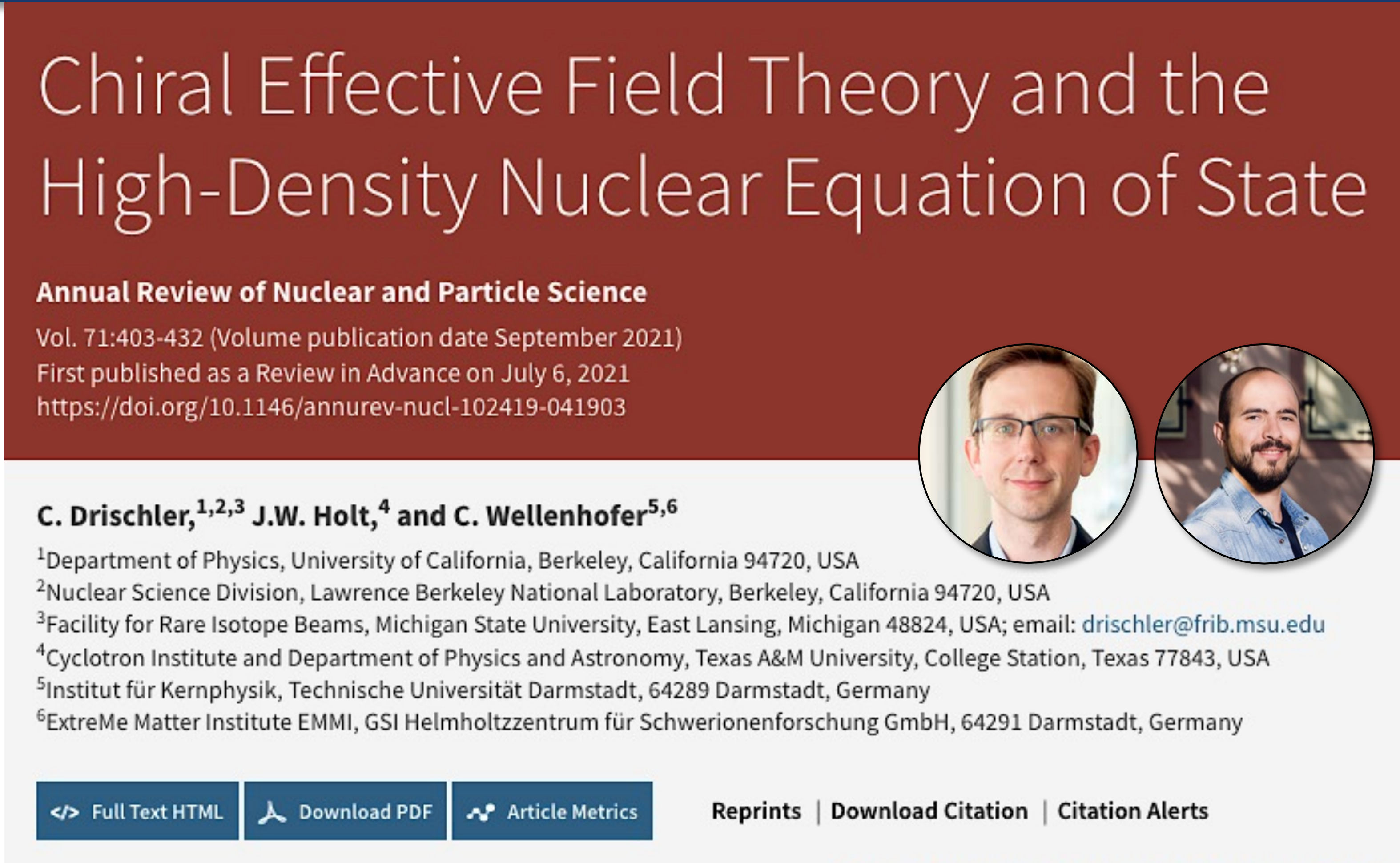
Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$



More details? Recent review article





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

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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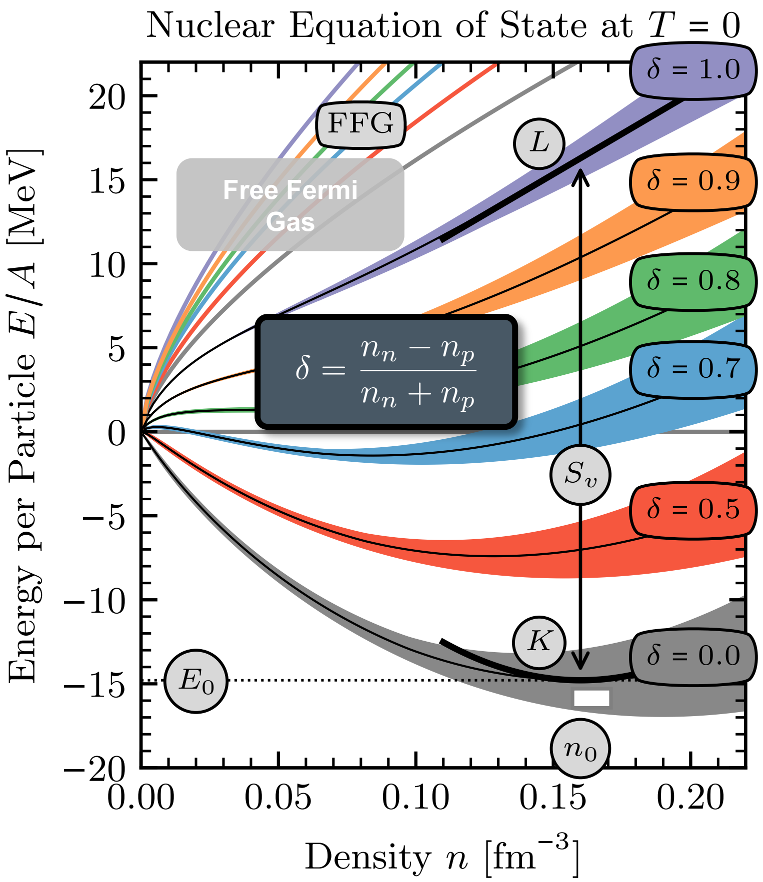
Keywords:

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

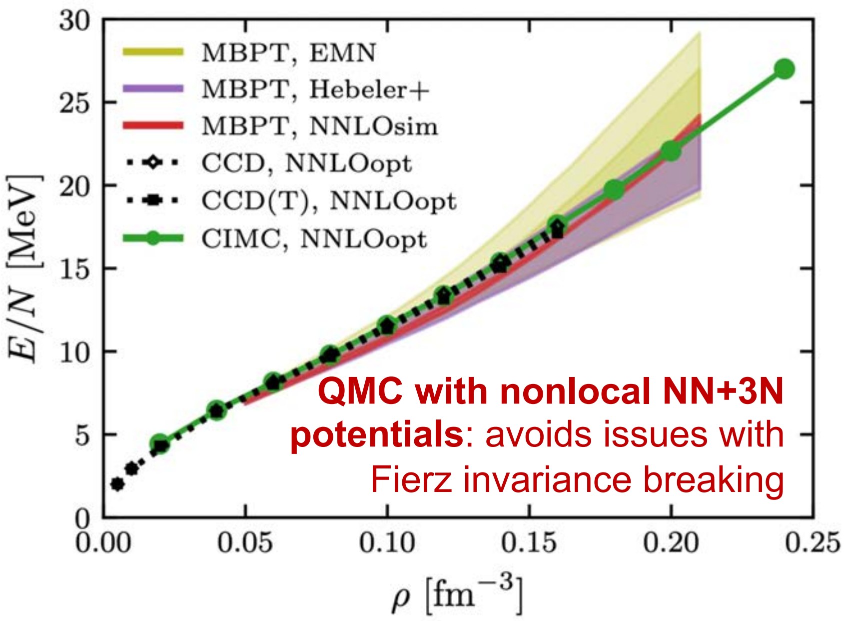
Open Access

Isospin asymmetric nuclear matter

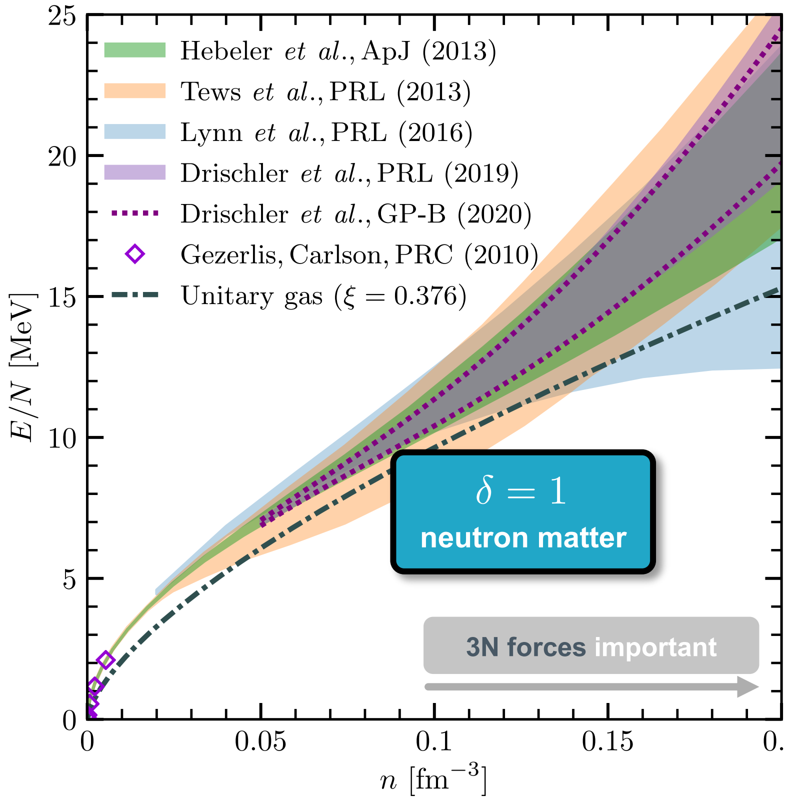


Free Fermi Gas

$$\delta = \frac{n_n - n_p}{n_n + n_p}$$



QMC with nonlocal NN+3N potentials: avoids issues with Fierz invariance breaking



$\delta = 1$
neutron matter

3N forces important

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

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

saturation point: **fine-tuned cancellation**
betw
cont

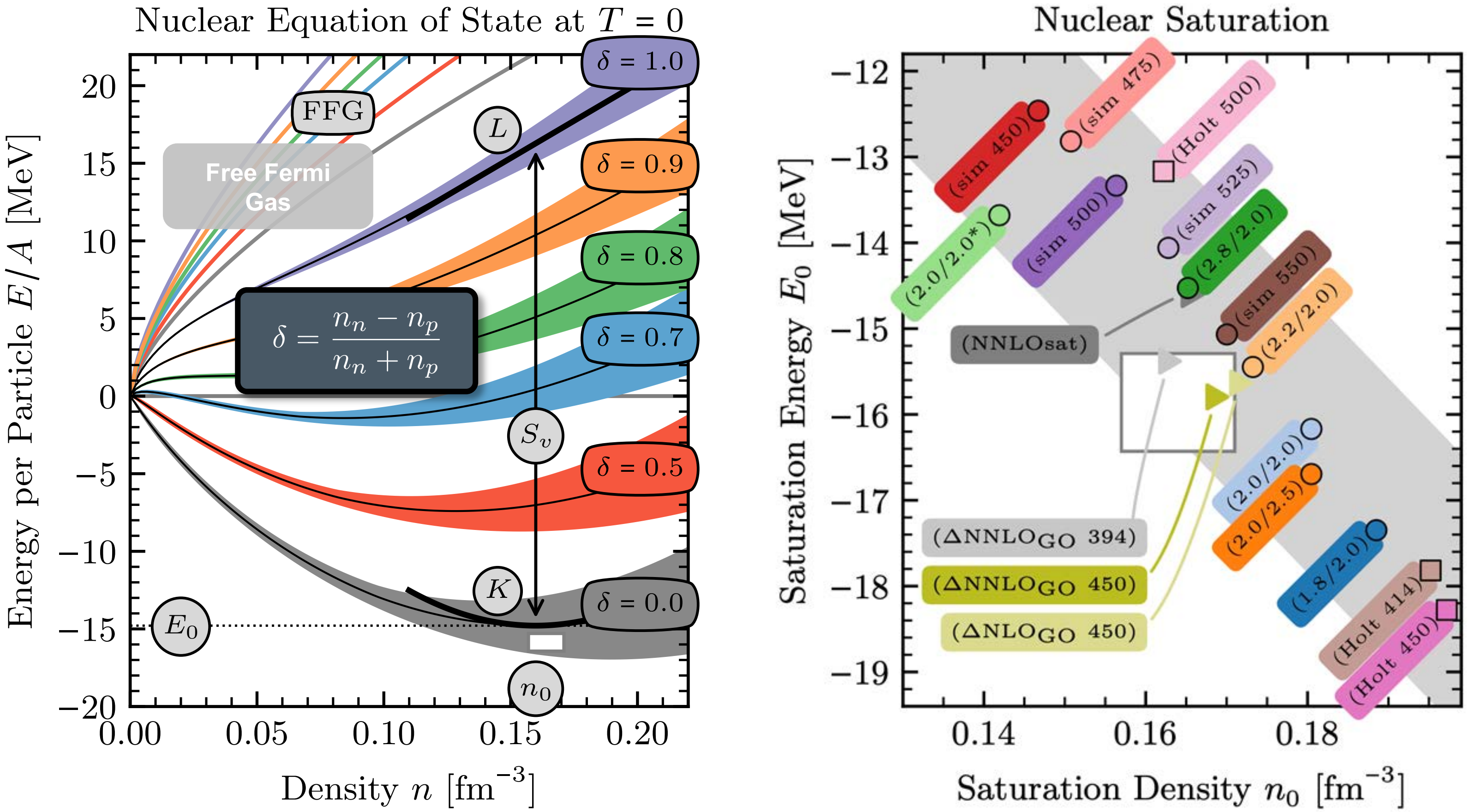
See also Marc Salinas's talk:
Bayesian Refinement of RMF Models

CD, H Simonis, Stroberg *et al.*, PRC **96**, 014303; Ekström *et al.*, PRC **97**, 024332; Atkinson *et al.*, PRC **102**, 044333; and many more

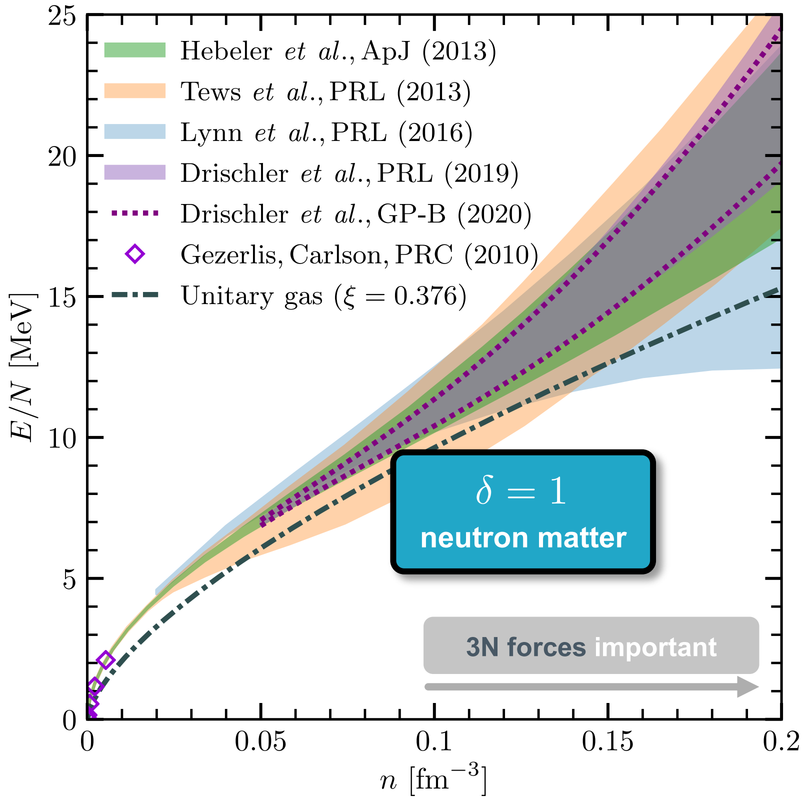
neutron matter below saturation density is **well-constrained** by NN scattering phase shifts

see also Configuration-Interaction Monte Carlo, Arthuis *et al.*, arXiv:2203.16167

Isospin asymmetric nuclear matter



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



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

saturation point: **fine-tuned cancellation**
betw
cont

empirical constraints provide **important**
s of chiral interactions, esp. 3NF
(λ / Λ$_{3N}$) in fm^{-1} or (Λ) in MeV

See also Marc Salinas's talk:
Bayesian Refinement of RMF Models

CD, H Simonis, Stroberg *et al.*, PRC **96**, 014303; Ekström *et al.*, PRC **97**, 024332; Atkinson *et al.*, PRC **102**, 044333; and many more

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

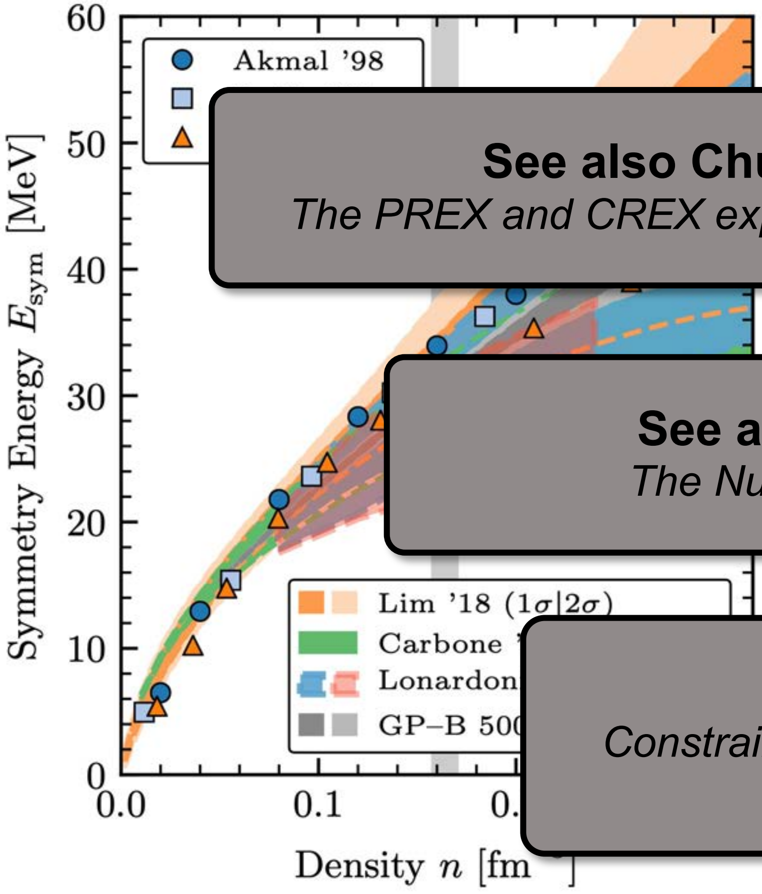
see also Configuration-Interaction Monte Carlo, Arthuis *et al.*, arXiv:2203.16167

Nuclear symmetry energy

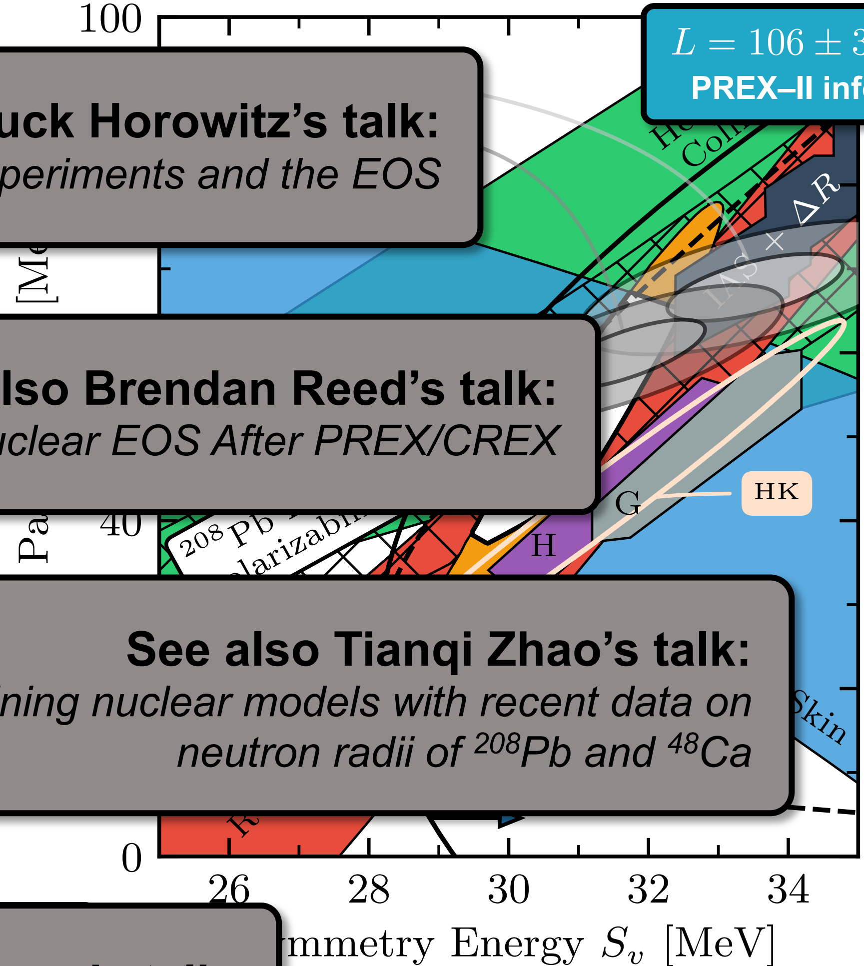
agreement between various constraints

(be careful: probe different densities)

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



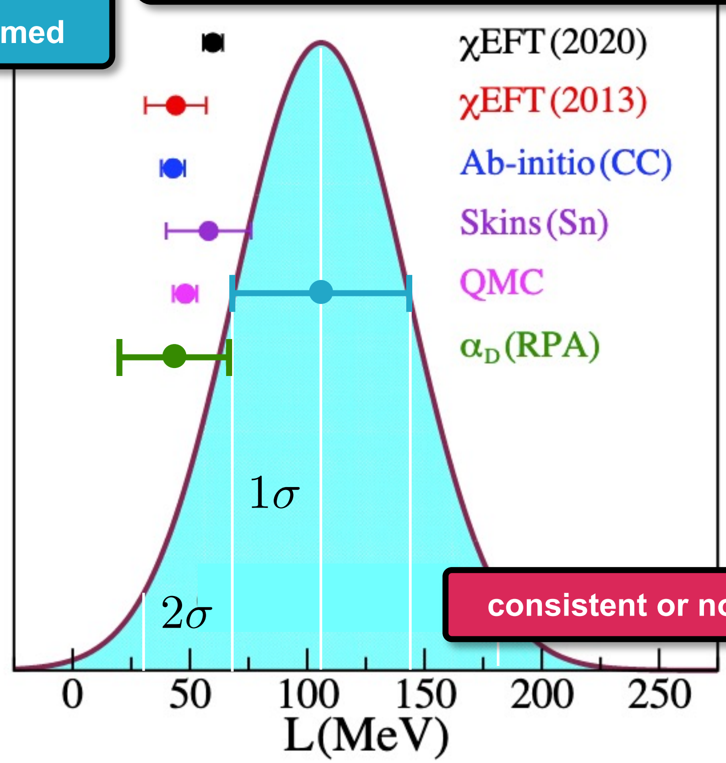
See also Chuck Horowitz's talk:
The PREX and CREX experiments and the EOS



$L = 106 \pm 37\,\mathrm{MeV}$
PREX–II informed

See also Brendan Reed's talk:
The Nuclear EOS After PREX/CREX

See also Tianqi Zhao's talk:
Constraining nuclear models with recent data on neutron radii of ^{208}Pb and ^{48}Ca



consistent or not?

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

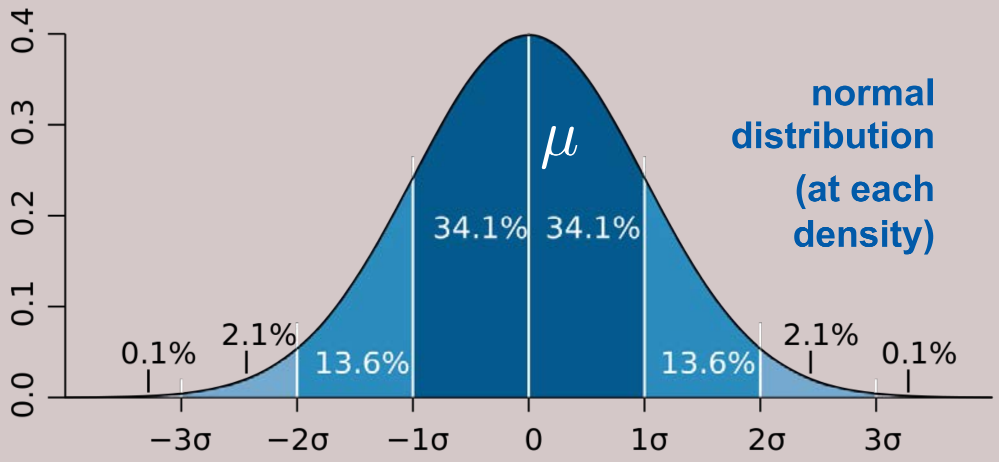
See also David Tsang's talk:
Probing nuclear physics with neutron star mergers

t *et al.*, ARNPS **71**, 403
er & Lim, APJ **771**, 51

Neutron skin constraints with **±0.03 fm or better** are needed: **MREX @ MESA** (~2030)

Why correlations are important: symmetry energy

Reminder: Statistics 101



normal distribution (at each density)

$$S_2 \sim \mathcal{N}\left(\mu_{S_2}, \sigma^2_{S_2}\right)$$

$$\mu_{S_2} = \mu_{\mathrm{PNM}} - \mu_{\mathrm{SNM}}$$

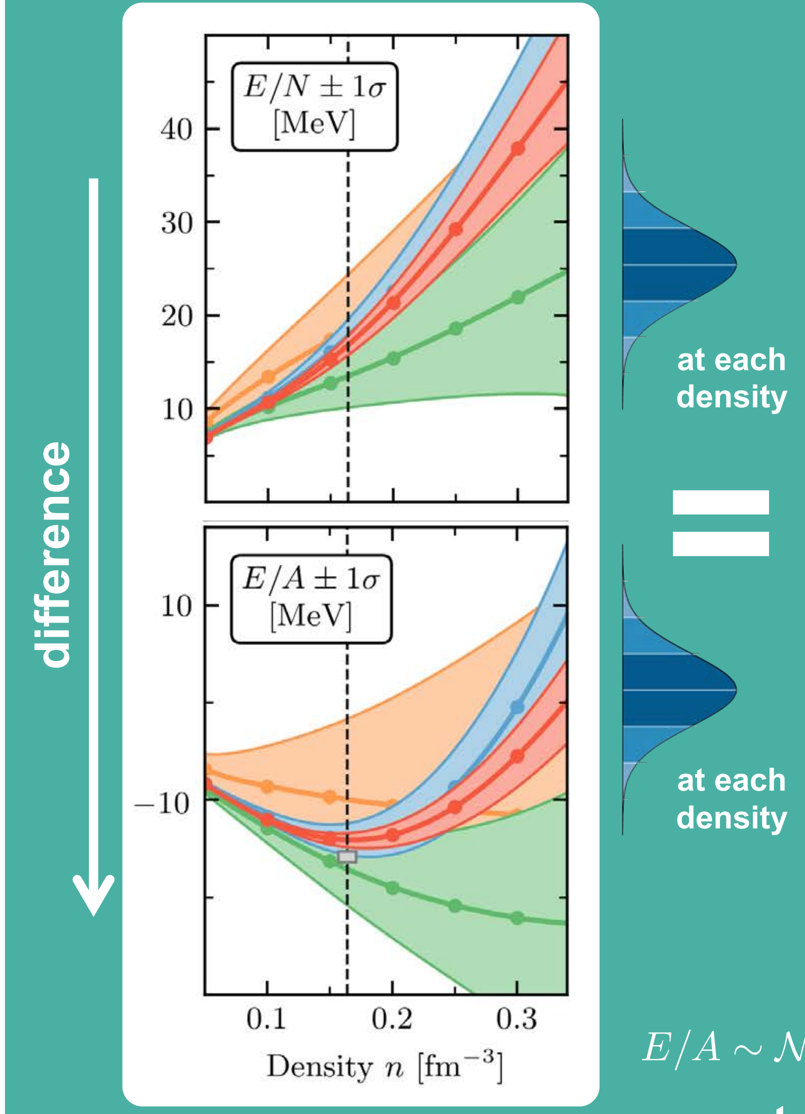
$$\sigma^2_{S_2} = \sigma^2_{\mathrm{PNM}} + \sigma^2_{\mathrm{SNM}} - 2\sigma_{\mathrm{PNM}}\sigma_{\mathrm{SNM}}\boxed{\rho}$$

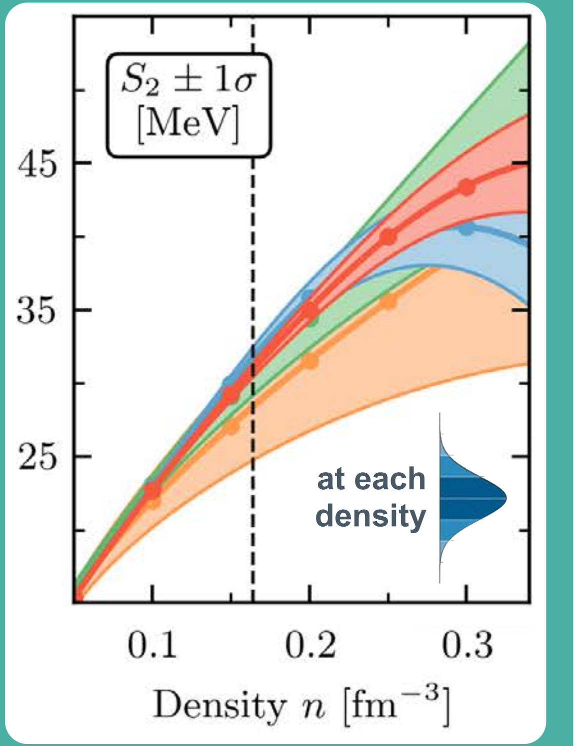
correlation coefficient $-1 \leqslant \rho \leqslant +1$

---

may result in smaller uncertainties than one might *naively* expect

$$S_2(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$



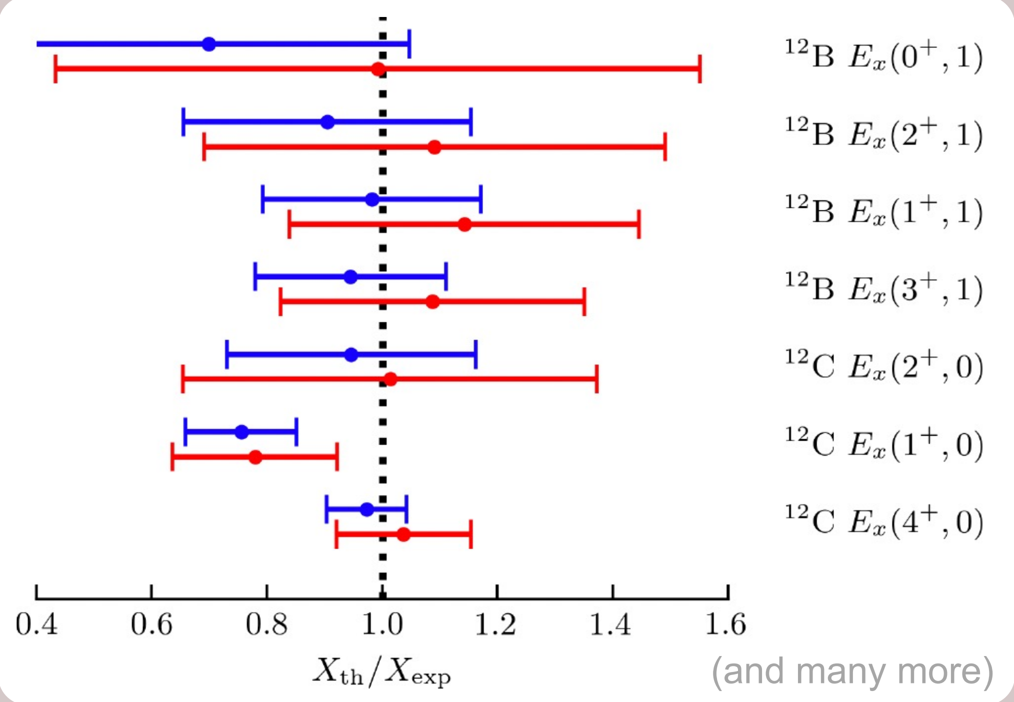


$E/A \sim \mathcal{N}\left(\mu, \sigma^2\right)$

symmetry energy | multi-task GPs

Why correlations are important: symmetry energy

Similar idea: excitation energies in light nuclei



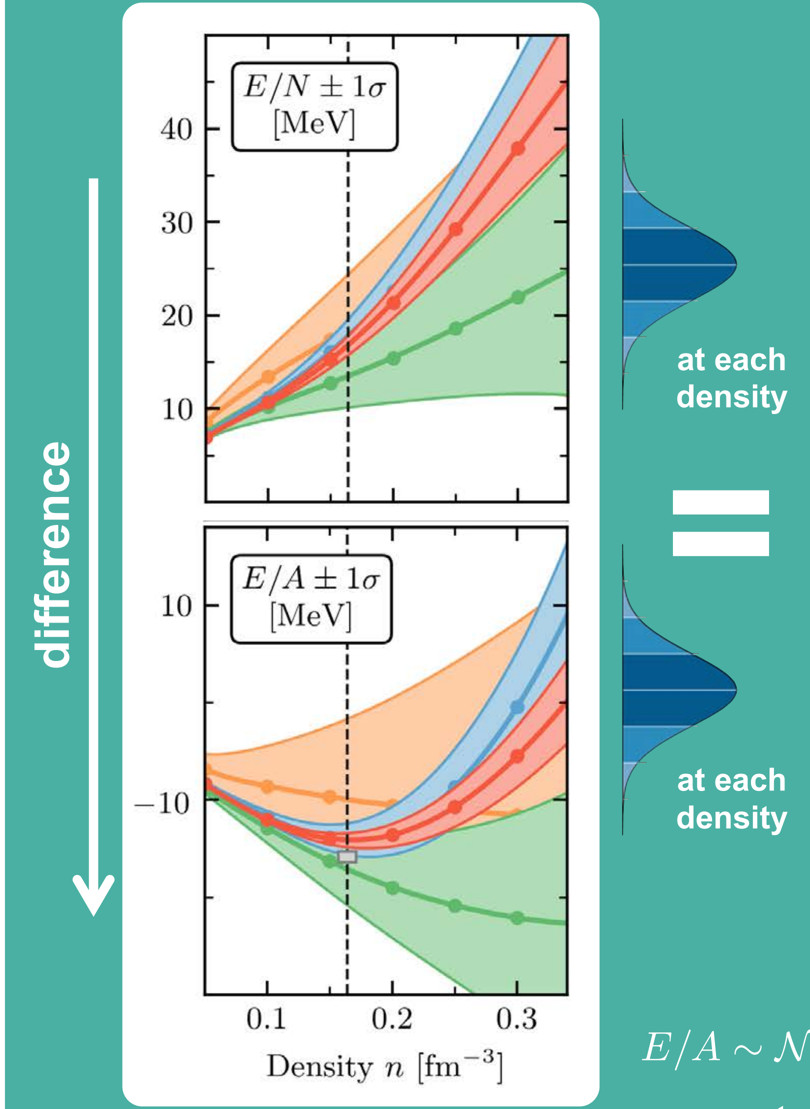
(and many more)

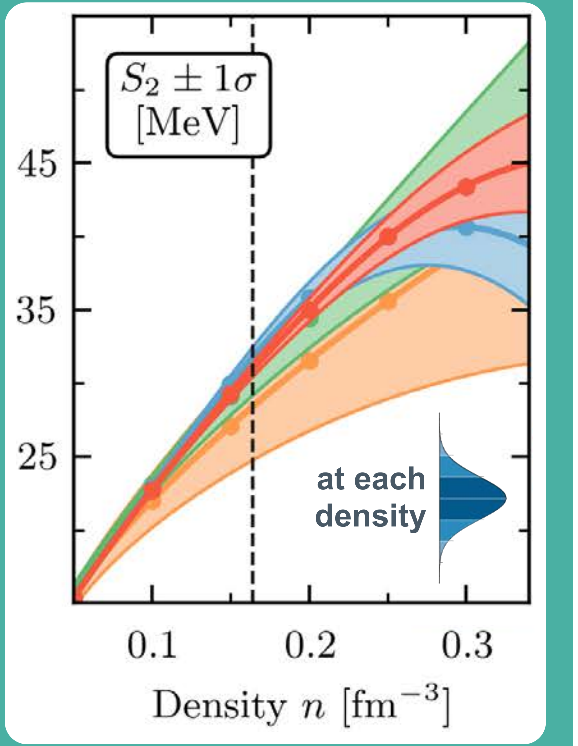
Correlated EFT truncation errors are **2 to 3x smaller** than when summed in quadrature

LENPIC, PRC **103**, 054001; PRC **106**, 064002

How can we exploit correlations? Are there observables we have not looked at?

$$S_2(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$

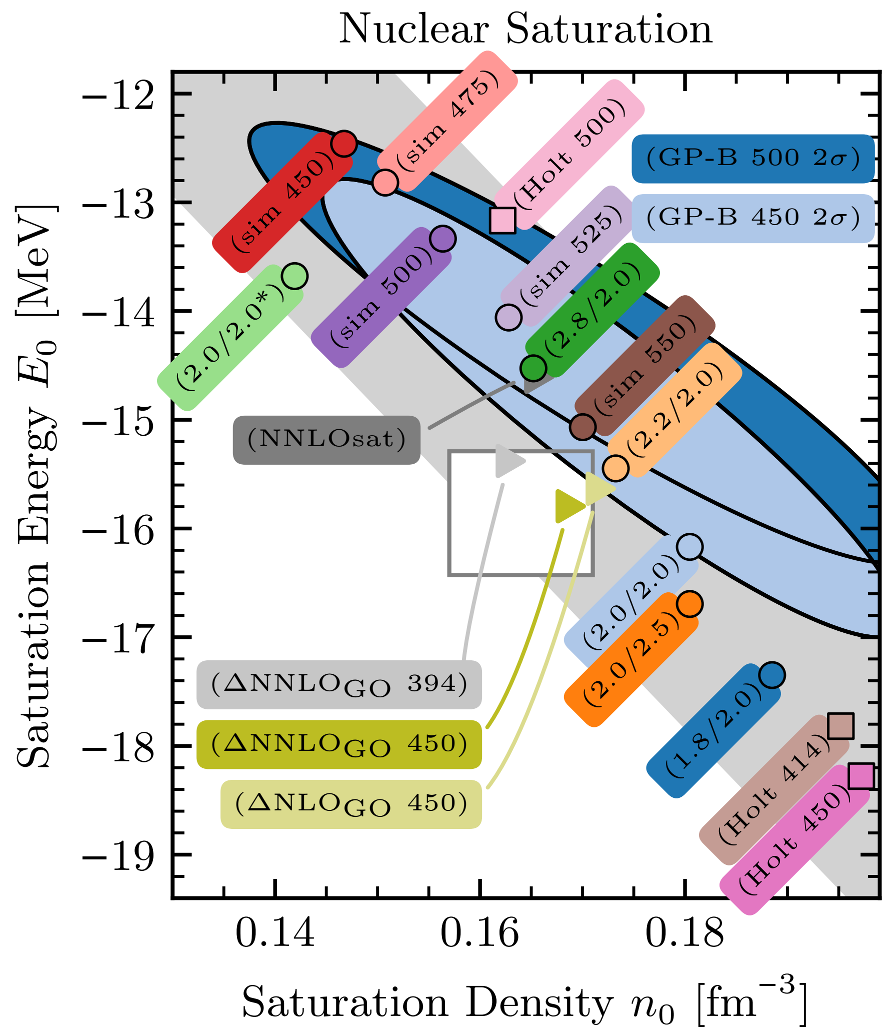




$E/A \sim \mathcal{N}(\mu, \sigma^2)$

symmetry energy | multi-task GPs

Empirical saturation box (overview)



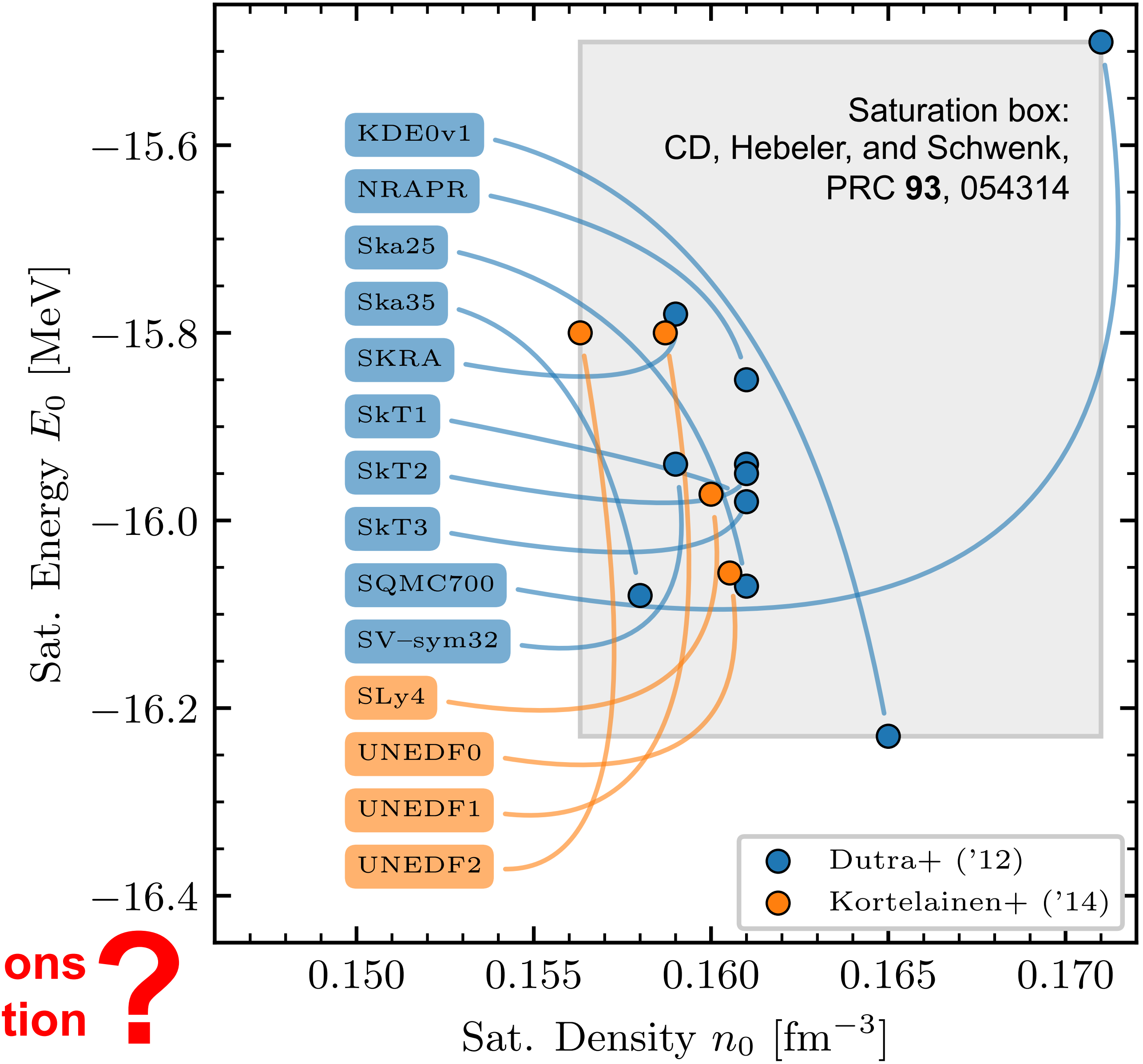
Empirical saturation box (overview)

OHIO UNIVERSITY

Empirical saturation box (2016):

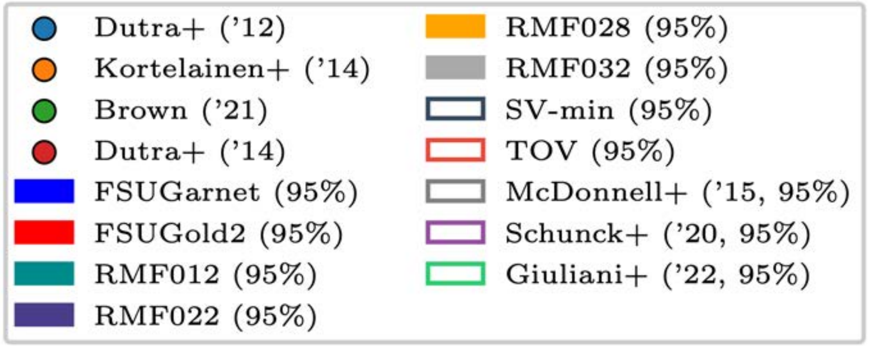
- based on 14 (out of 240+) functionals that reproduce well selected nuclear properties
- often used to benchmark chiral interactions
- **limited *statistical* meaning at best**

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



How can we benchmark chiral NN+3N interactions *rigorously* in terms of nuclear saturation?

Select empirical constraints from DFT



Significant progress in UQ for DFT:

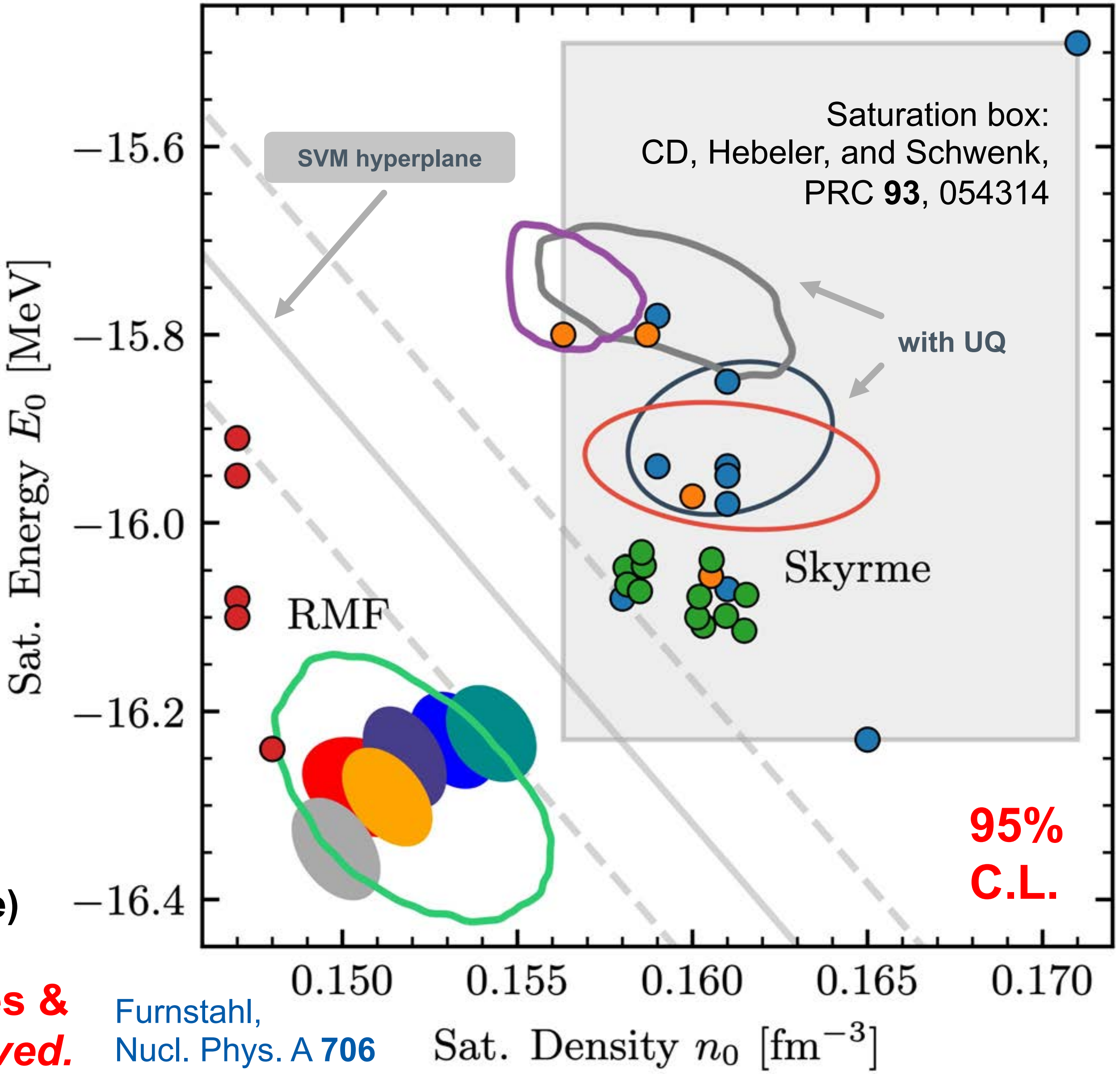
Schunck, O'Neal, Grosskopf, Lawrence, Wild, JPG: NP **47**, 074001
McDonnell, Schunck, Higdon, Sarich, Wild, Nazarewicz, PRL **114**, 12250
Neufcourt, Cao, Nazarewicz, Olsen, Viens, PRL **122**, 062502
Chen & Piekarewicz, PRC **90**, 044305; **and more**

Recently: UQ is driven by emulators (game changers!)

Bonilla, Giuliani, Godbey, Lee, PRC **106**, 054322
Giuliani, Godbey, Bonilla, Viens, Piekarewicz, Front. Phys. **10**

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

Skyrme models: *systematically lower* binding energies & larger saturation densities. *This has been long observed.*

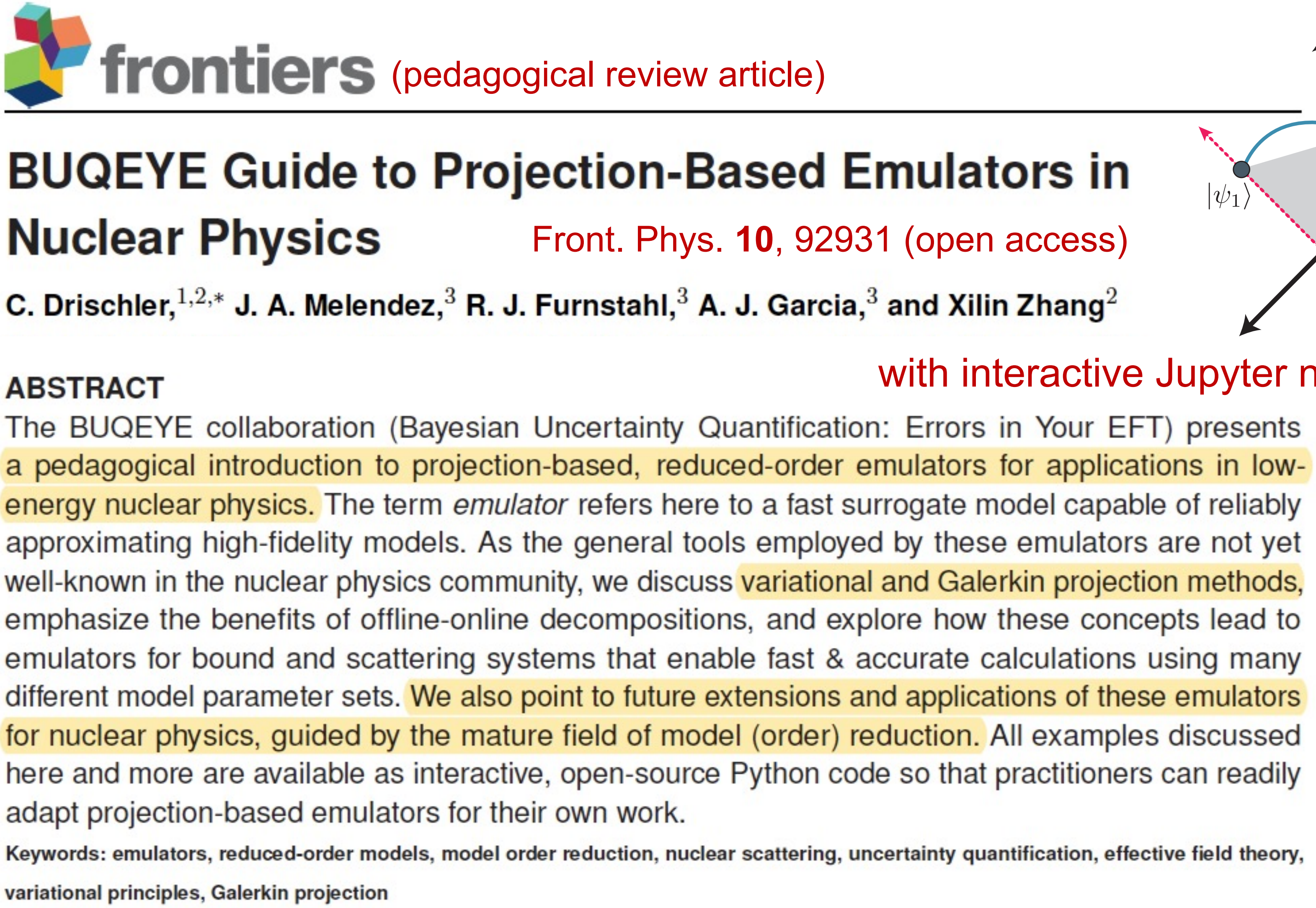


Saturation box:
CD, Hebeler, and Schwenk,
PRC **93**, 054314

95% C.L.

Furnstahl,
Nucl. Phys. A **706**

Emulators: game changers in nuclear physics!



frontiers (pedagogical review article)

BUQEYE Guide to Projection-Based Emulators in Nuclear Physics

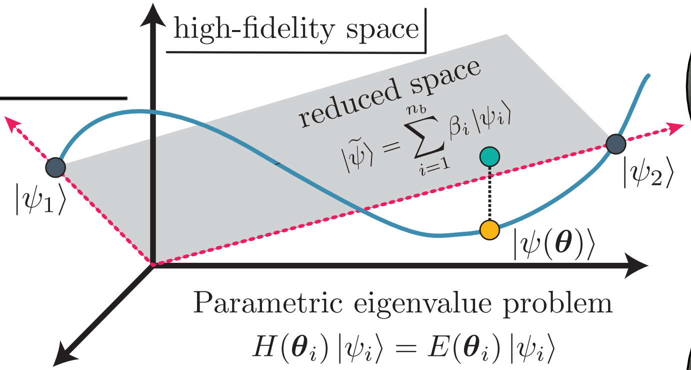
Front. Phys. **10**, 92931 (open access)

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

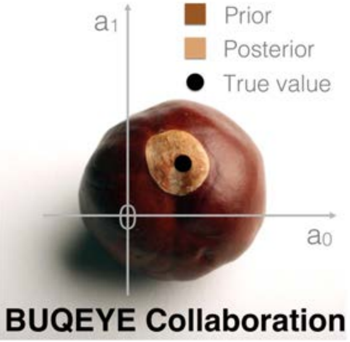


Parametric eigenvalue problem

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

with interactive Jupyter notebooks on GitHub!

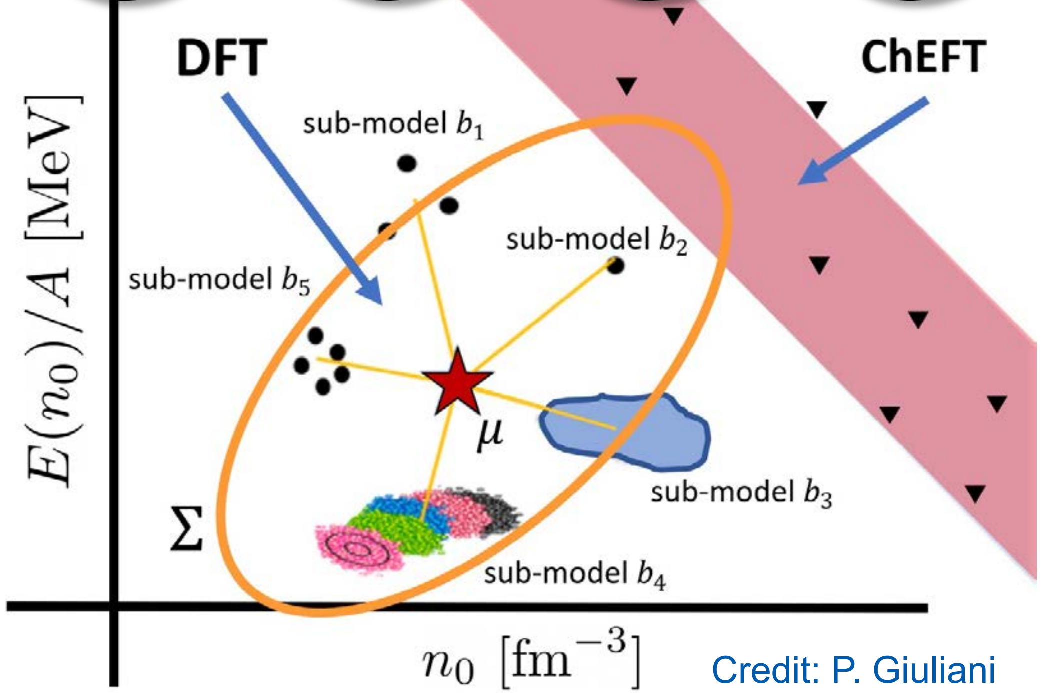
see also
our Literature Guide
Melendez, CD *et al.*,
J. Phys. G **49**, 102001



BUQEYE Collaboration

Companion website with lots of pedagogical material: https://github.com/buqeye/frontiers-emulator-review
see also Godbey Giuliani *et al.*, https://github.com/kylegodbey/nuclear-rbm

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)

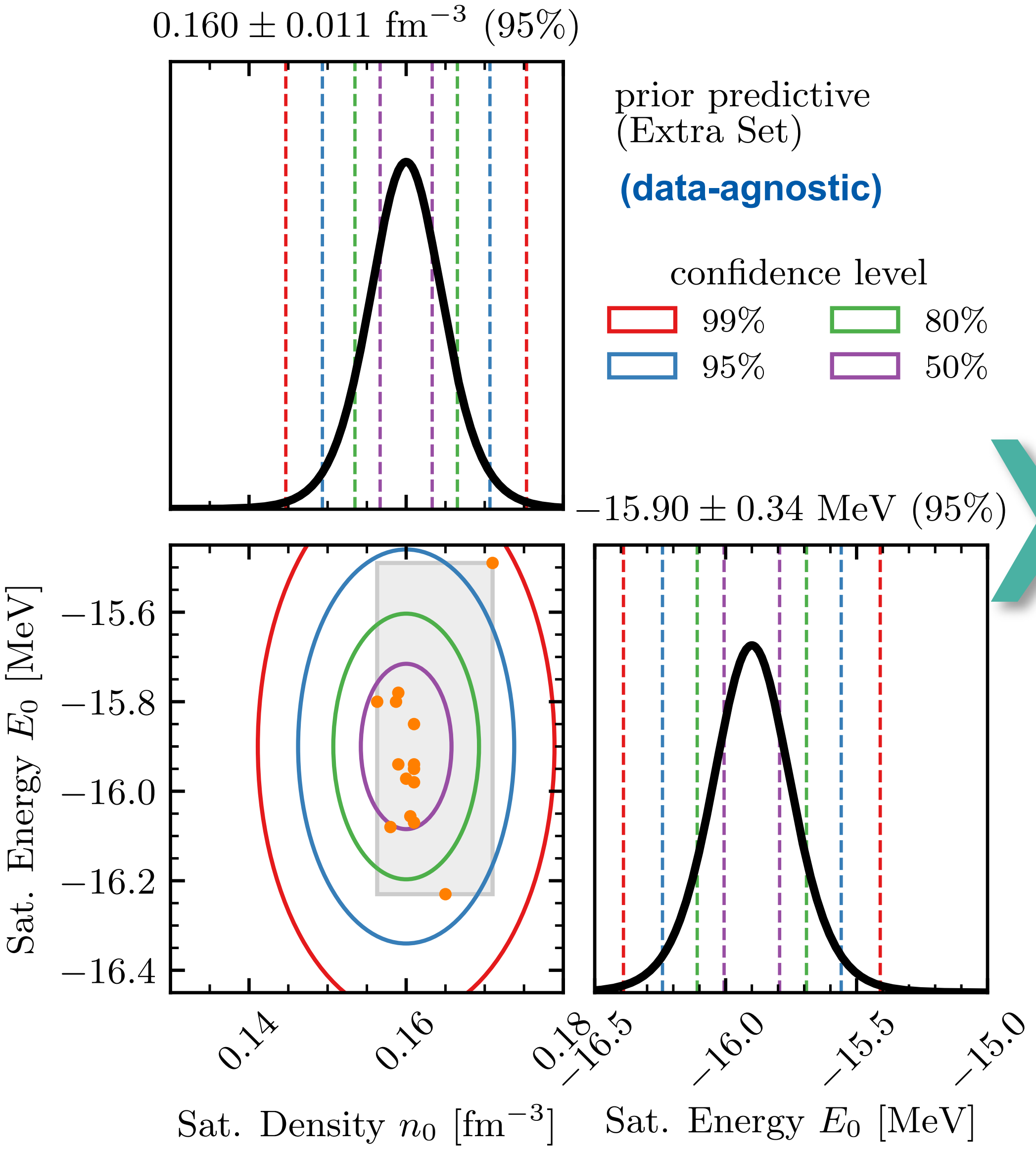
posterior predictive (marginalization)

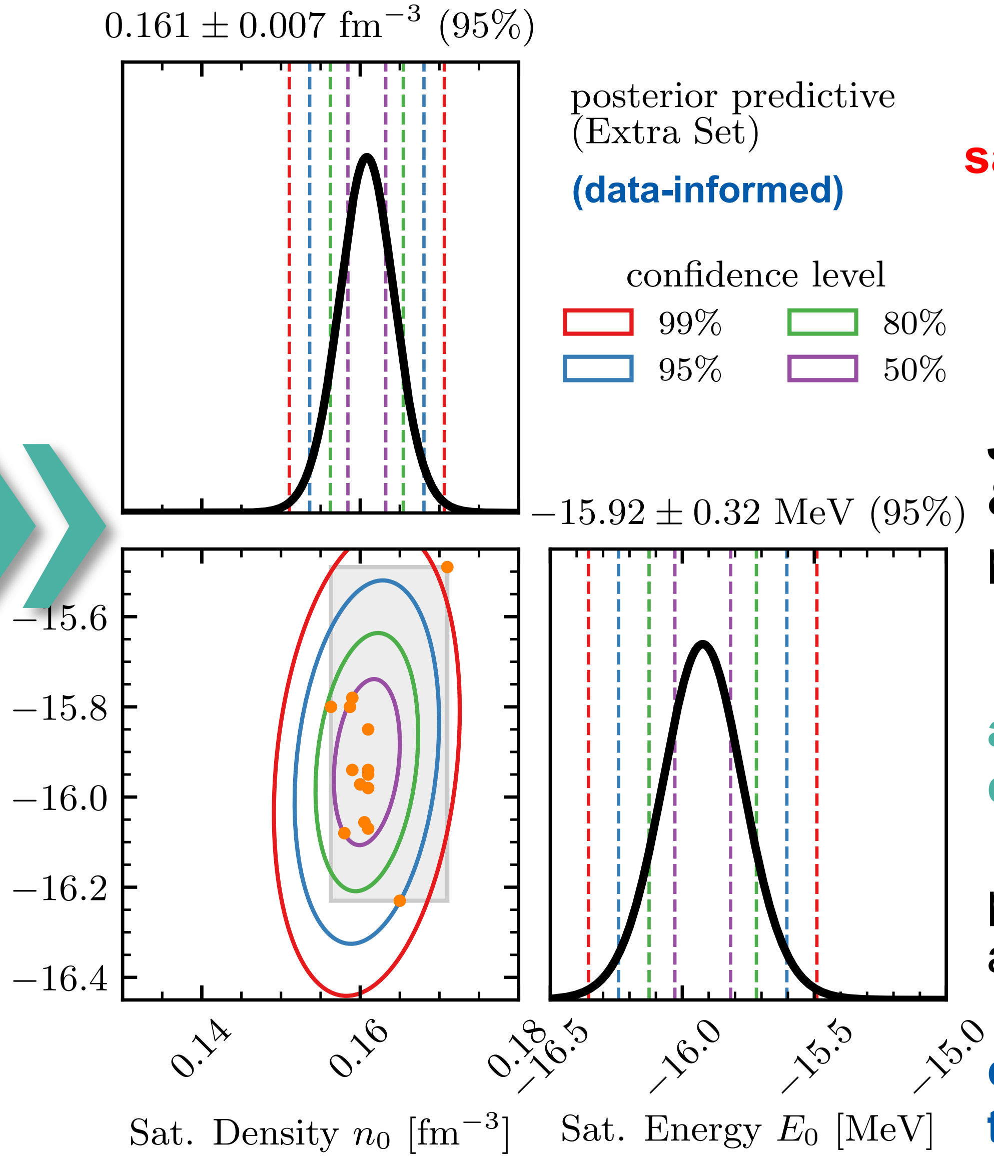
$$P(\mathbf{y}^*|\mathcal{D}) \propto \int \mathrm{d}\boldsymbol{\mu}\, \mathrm{d}\boldsymbol{\Sigma}\; \underbrace{P(\mathbf{y}^*|\boldsymbol{\mu}, \boldsymbol{\Sigma})}_{\text{model}} \; \underbrace{P(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathcal{D})}_{\text{posterior}}$$

(evaluates to a bivariate *t*-distribution)

Analysis: Saturation box (2016)

(preliminary)





Only data used to construct the **saturation box** are considered !

Jupyter notebooks & tutorials will be publicly available

analytic calculations due to conjugacy

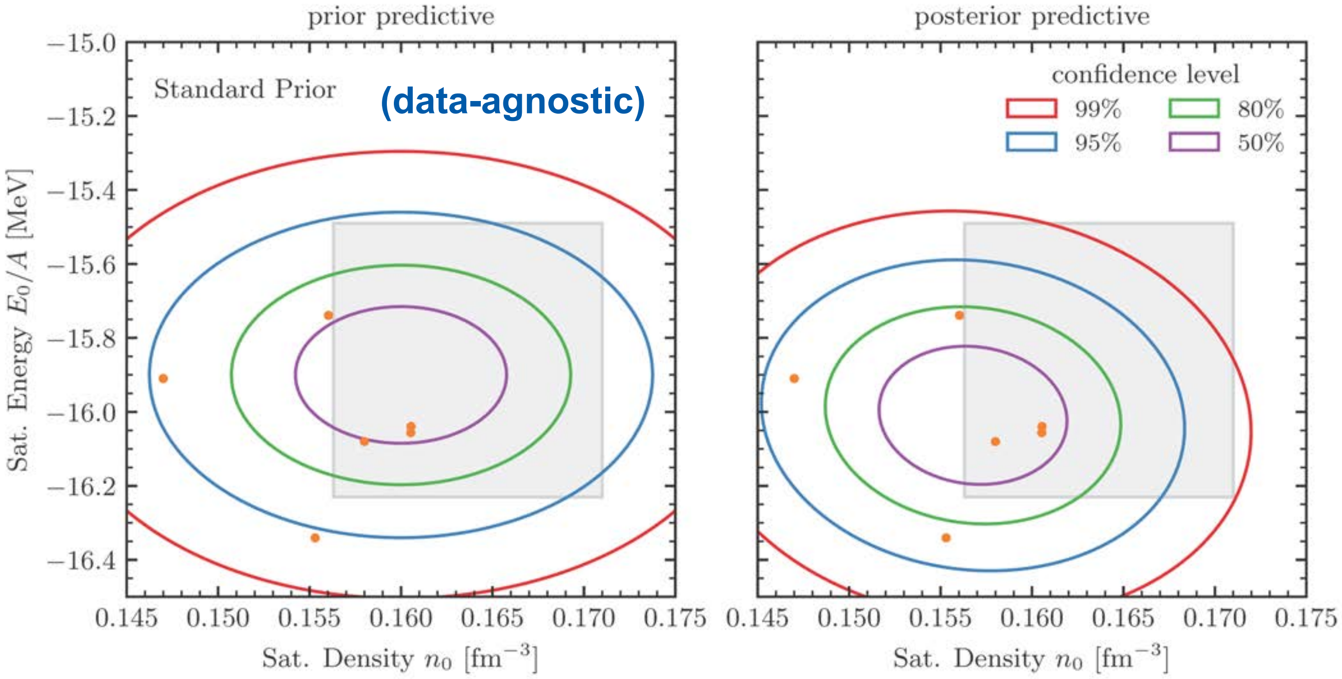
predictives & marginals are ***t*-distributions**

can easily investigate the prior sensitivity

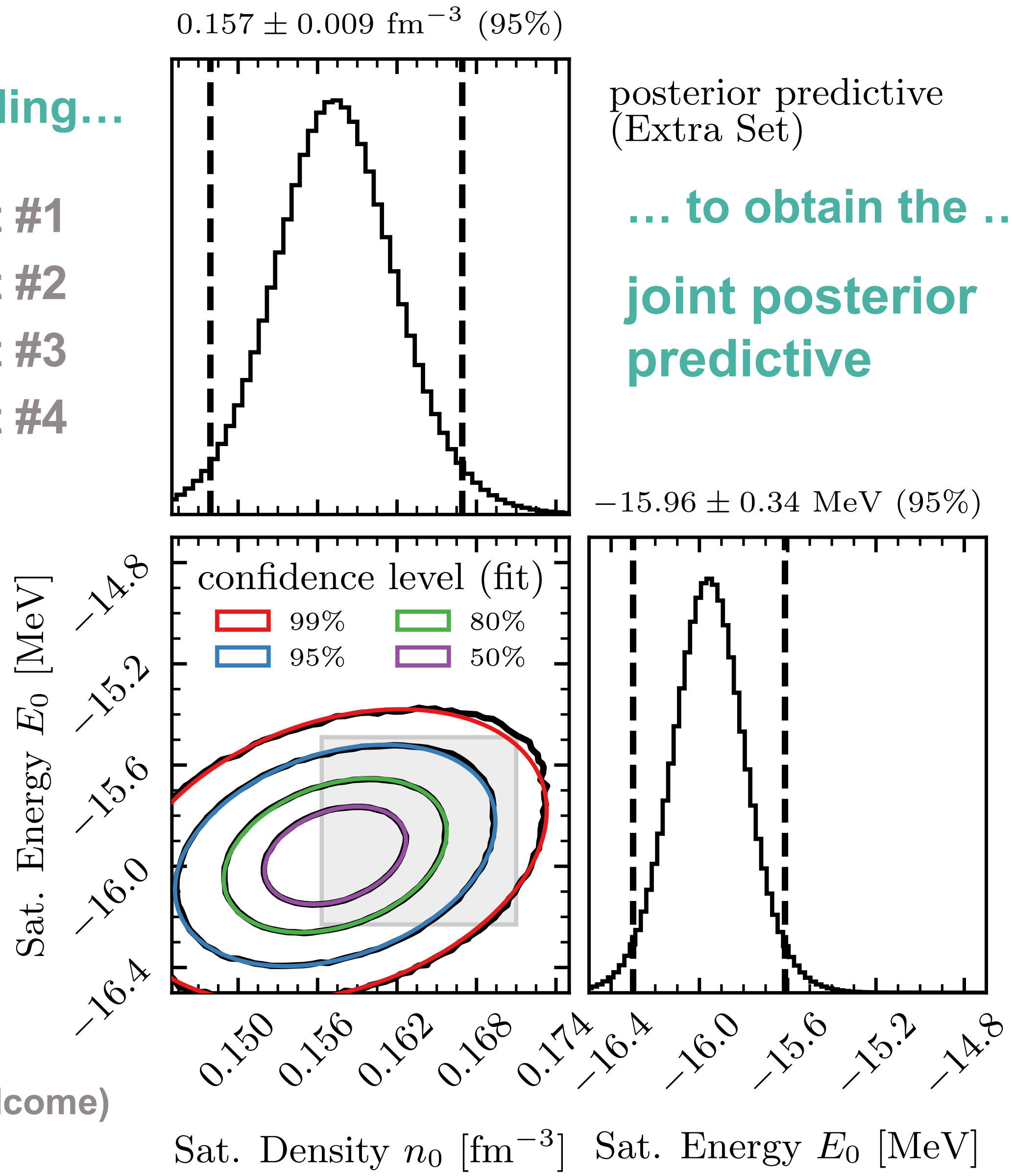
All DFT constraints: joint MC analysis (preliminary)

Uncertainties in the DFT constraints break conjugacy!

Mixture modeling comes to the rescue! Use simple MC sampling…



set #1
set #2
set #3
set #4
…



… to obtain the …

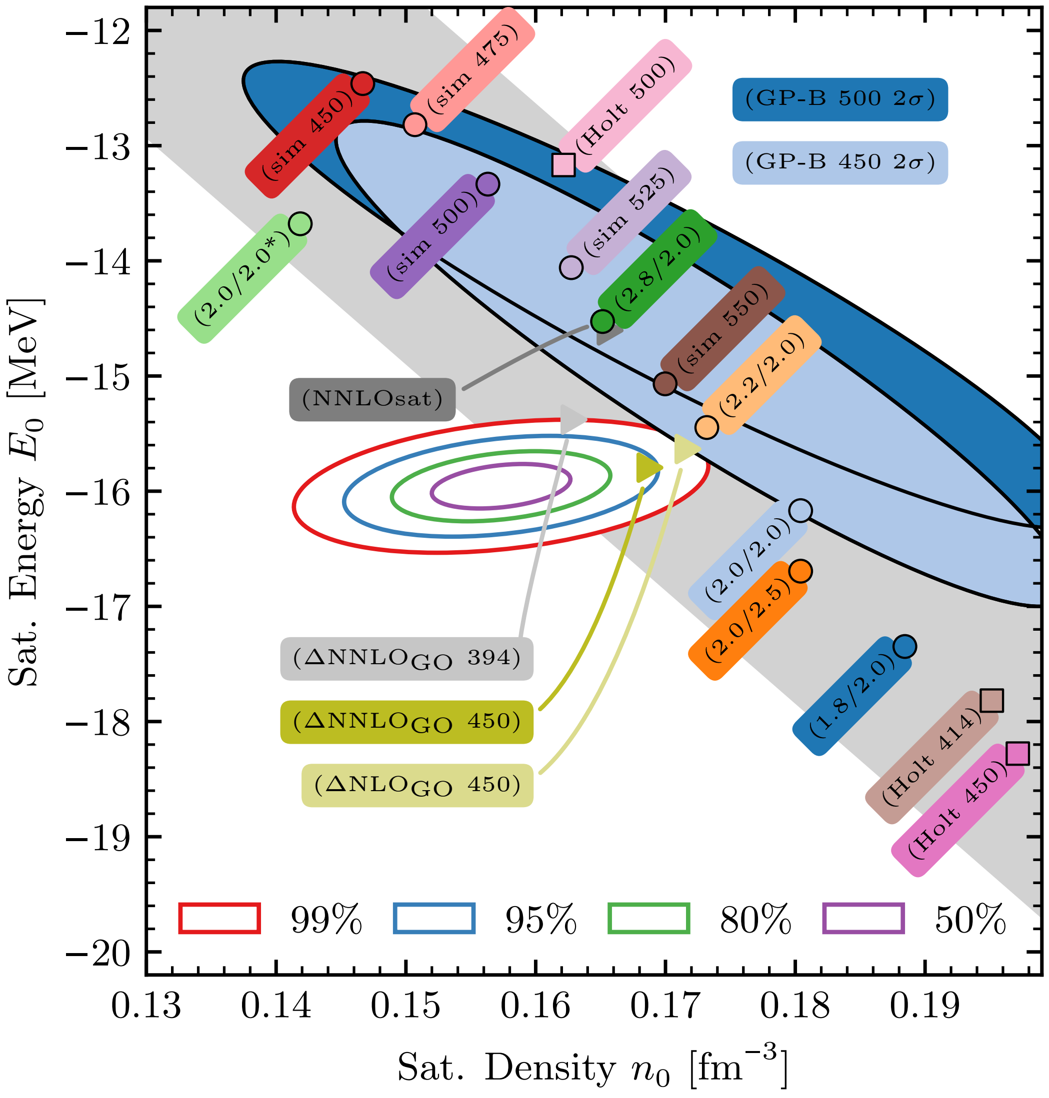
joint posterior predictive

Joint DFT constraint has approx. a *t*-distribution and is *consistent* with the commonly 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)

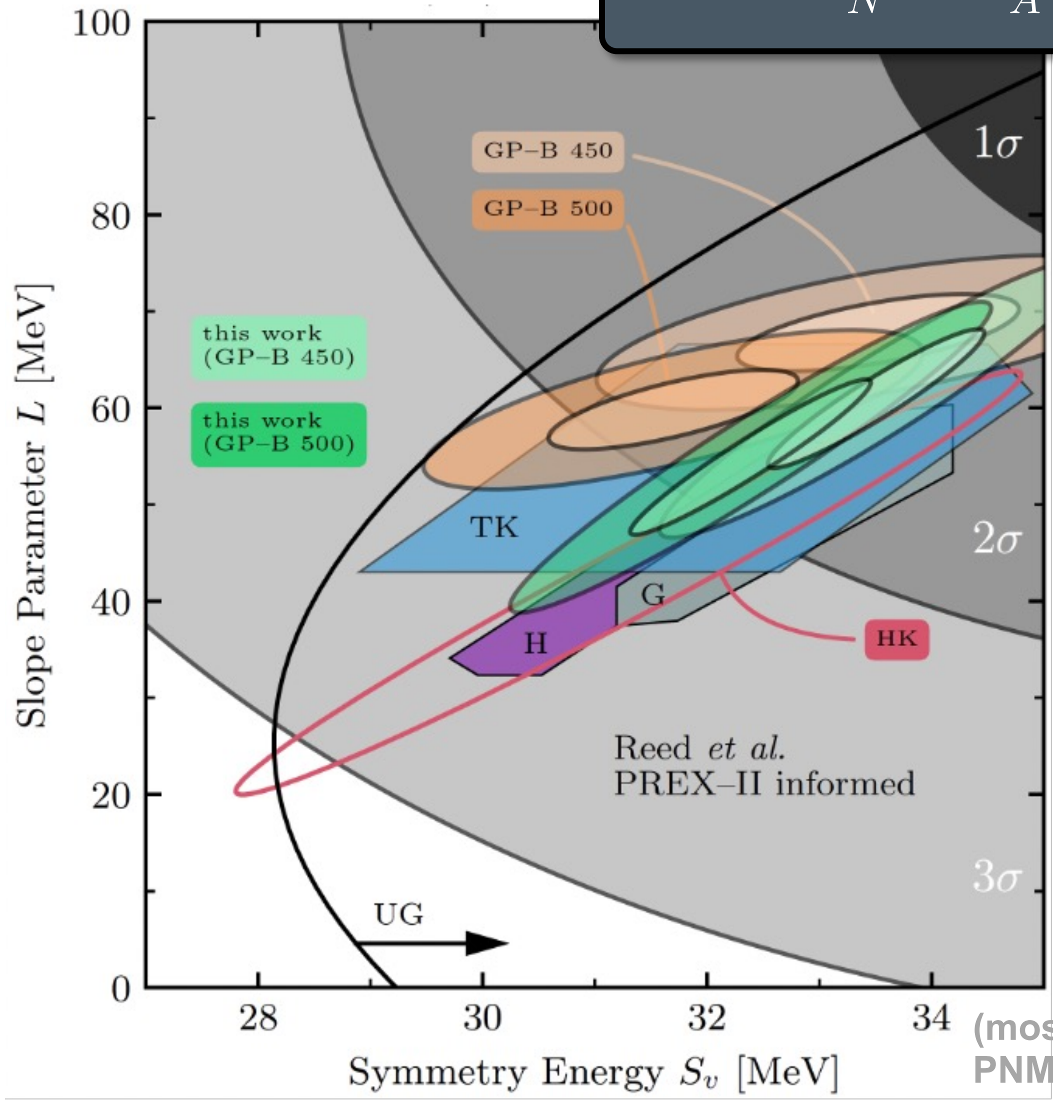
Nuclear saturation | symmetry energy (preliminary)



Inferred *empirical* saturation point is not well reproduced by a wide range of chiral NN+3N interactions (high C.L.)

Combined with microscopic PNM calculations at N^{3}LO:

$$S_2(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$

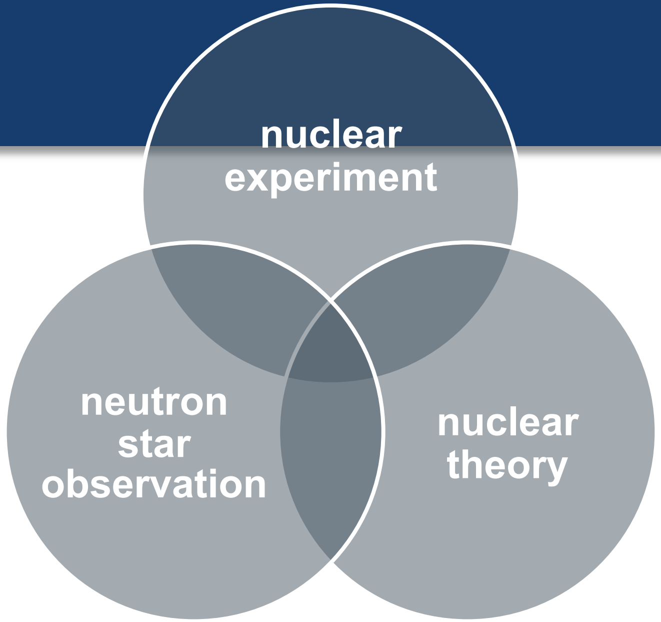


(mostly PNM-based)

Take-away points

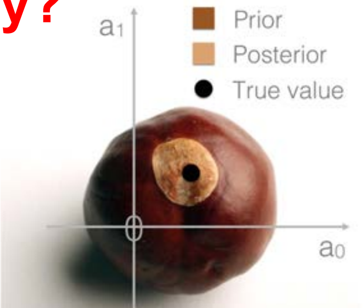
multi-messenger
nuclear precision
FRIB

} 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 ($n \lesssim 2n_{\mathrm{sat}}$). Where does it break down *and* why?
2. Bayesian statistics allows for rigorous UQ in EFT-based calculations (facilitated by new emulators!). EFT predictions *statistically* consistent?
3. Need for improved constraints on the nuclear matter EOS in the density regime $1 \lesssim n/n_{\mathrm{sat}} \lesssim 2$. How can these constraints help guide or validate nuclear theory?
4. Our *preliminary* analysis suggests for the empirical saturation point: $n_0 \approx 0.157 \pm 0.009\ \mathrm{fm}^{-3}$, with $E_0/A \approx -15.96 \pm 0.34$ MeV (95%, correlated!)



BUQEYE Collaboration

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