Applications of Bayesian Uncertainty Quantification to Microscopic Nuclear Matter Calculations

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Theory Seminar at Jefferson Lab
March 18, 2024

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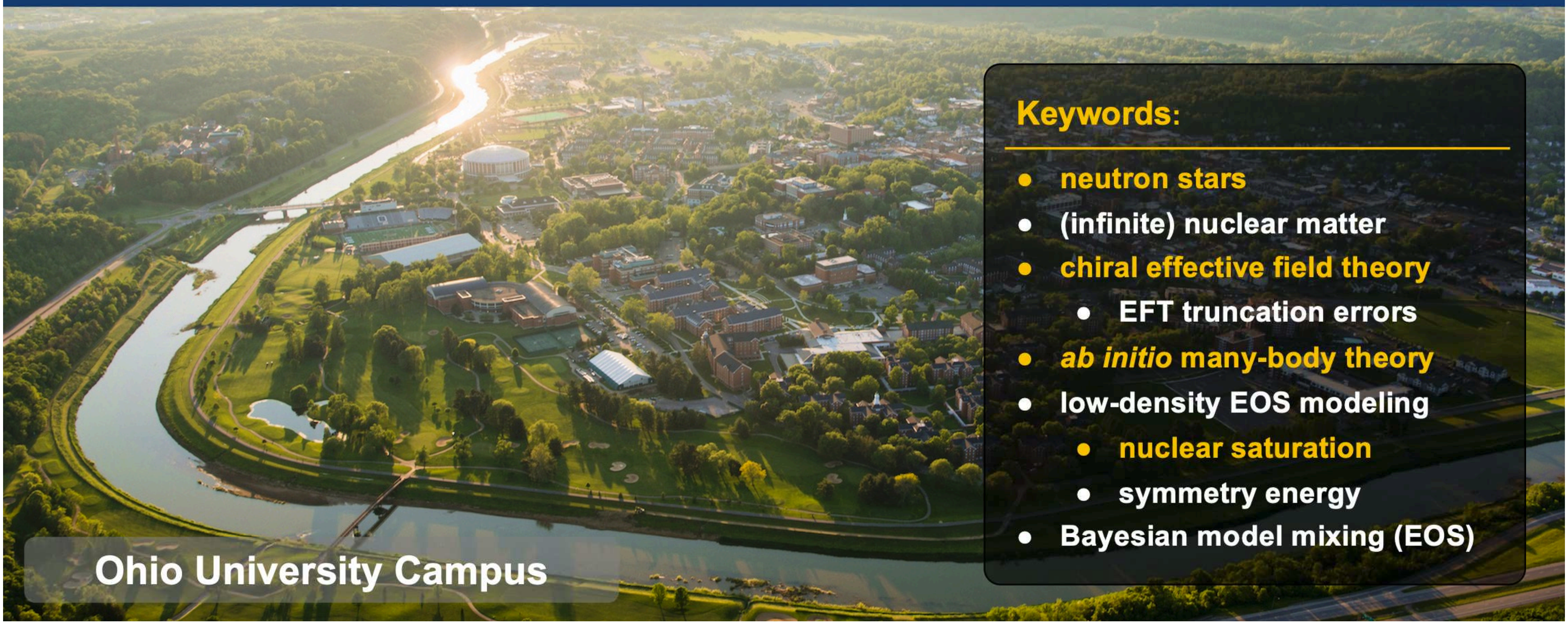
STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

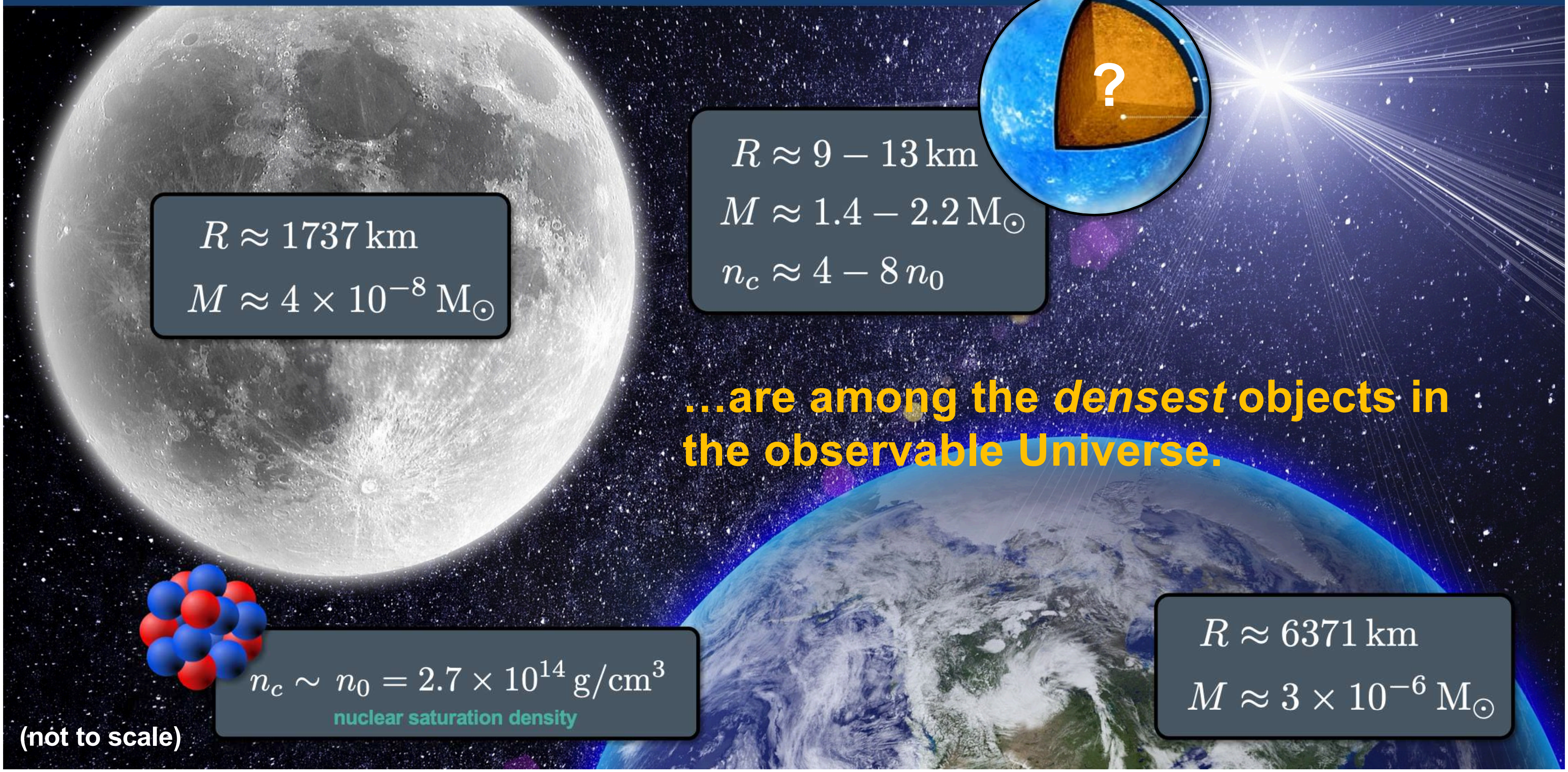
BUQEYE Collaboration

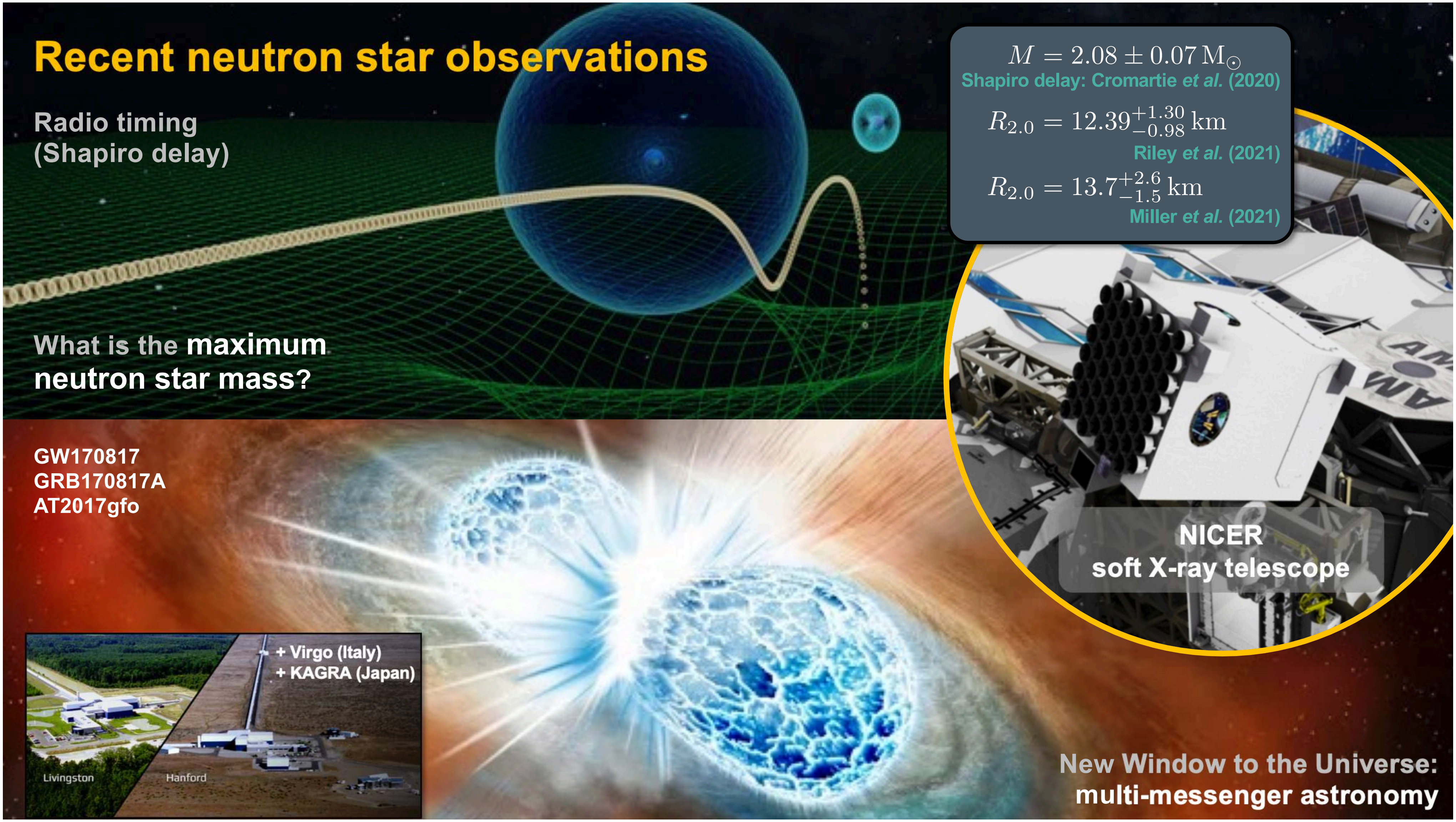


Keywords:

- neutron stars
- (infinite) nuclear matter
- chiral effective field theory
    - EFT truncation errors
- *ab initio* many-body theory
- low-density EOS modeling
    - nuclear saturation
    - symmetry energy
- Bayesian model mixing (EOS)

Neutron stars…




Recent neutron star observations
Radio timing
(Shapiro delay)
What is the maximum neutron star mass?
$M = 2.08 \pm 0.07\,\mathrm{M}_\odot$
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)
NICER
soft X-ray telescope
GW170817
GRB170817A
AT2017gfo
+ Virgo (Italy)
+ KAGRA (Japan)
Livingston
Hanford
New Window to the Universe:
multi-messenger astronomy

FRIB and FRIB Science

Facility for Rare Isotope Beams
at Michigan State University

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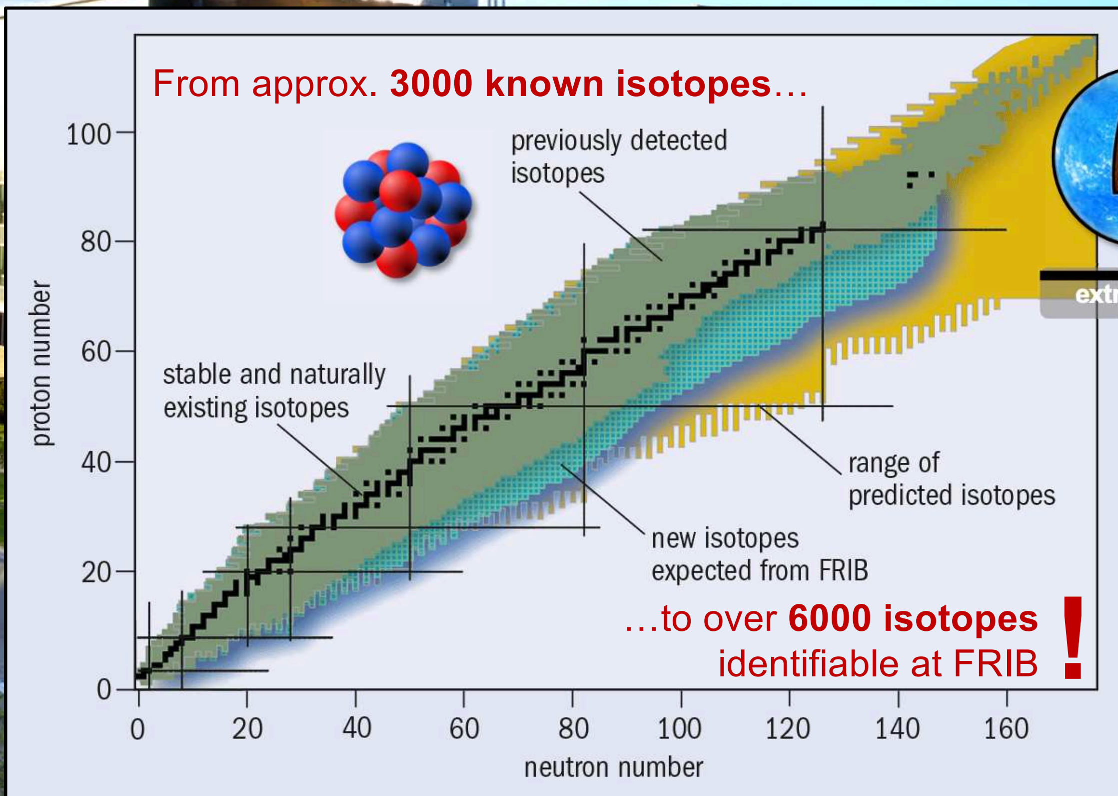
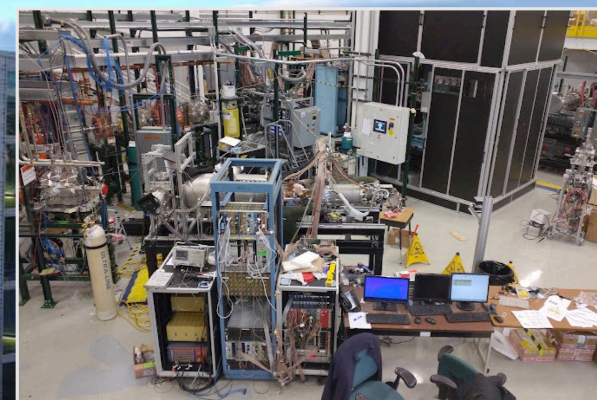


extrapolate



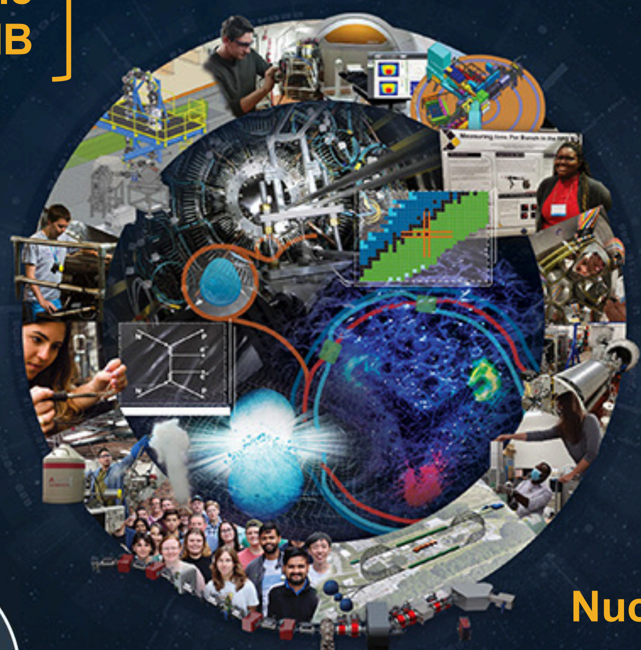
+ other beam facilities: ARIEL, CEBAF, FAIR, GANIL, RHIC, ...

nuclear precision
multi-messenger
exascale
FRIB
era

How do **nuclear phenomena** emerge from fundamental principles?

How are **stars** born? And how do they die?

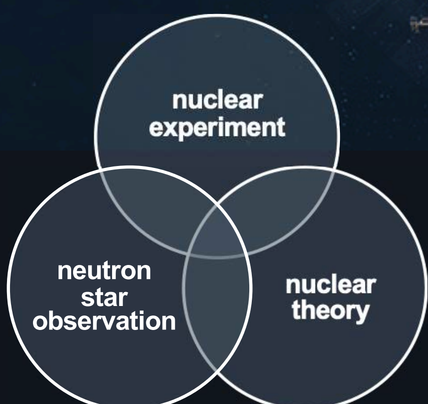
…



A NEW ERA OF DISCOVERY

THE 2023 LONG RANGE PLAN FOR NUCLEAR SCIENCE

https://nuclearsciencefuture.org/



Nuclear theory:

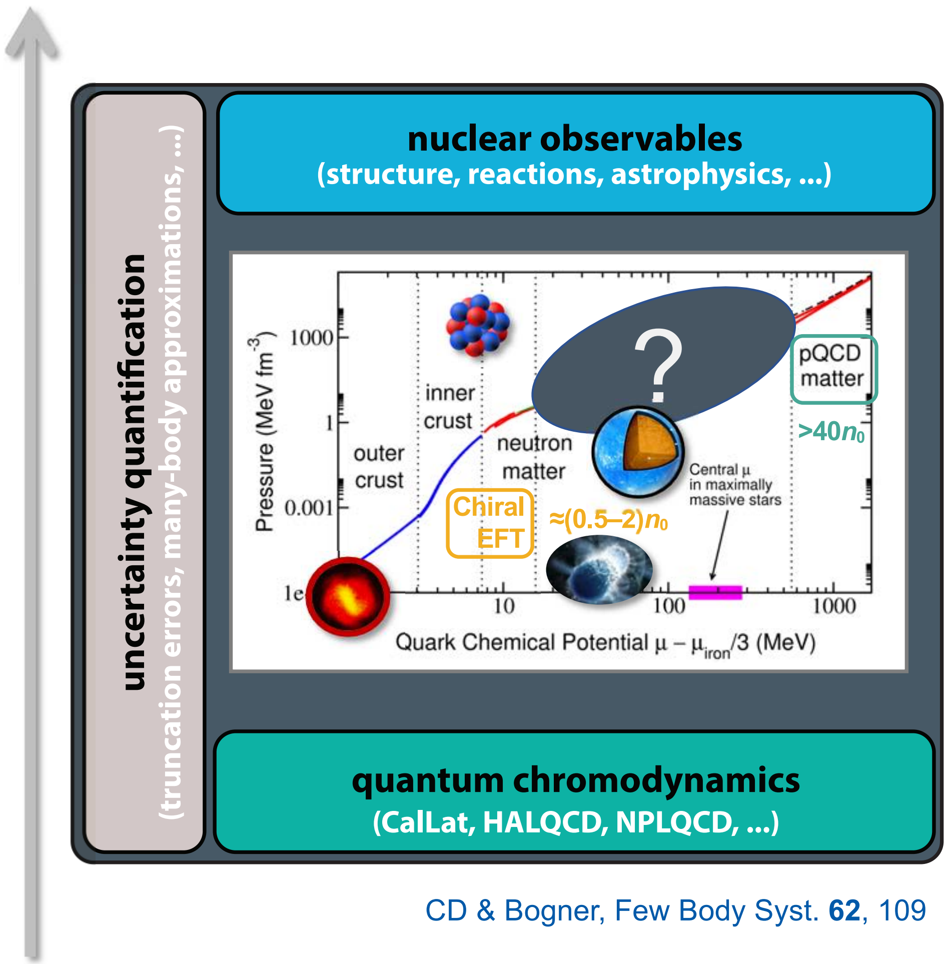
- **interpret** these observations & experiments *microscopically*
- **predict** outcomes when experiments are *not* feasible
- **quantify & propagate** our **theoretical uncertainties**

Major efforts:

Bayesian methods for calibration, UQ and propagation, EOS inference, experimental design, sensitivity studies, fast & accurate emulators …

Boehnlein *et al.*, RMP **94**, 031003

Ab initio workflow (idealized)



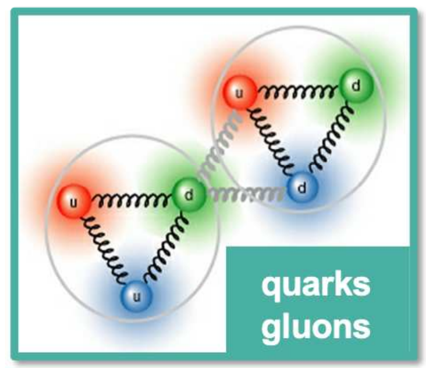
CD & Bogner, Few Body Syst. **62**, 109

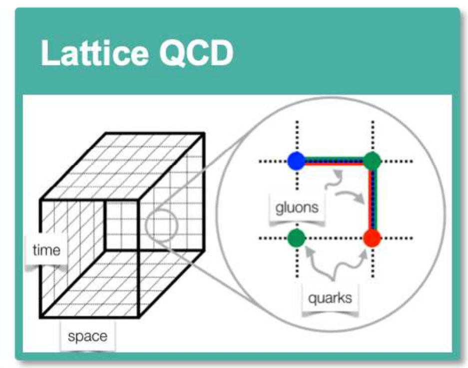
Here: nuclear equation of state (EOS)

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)

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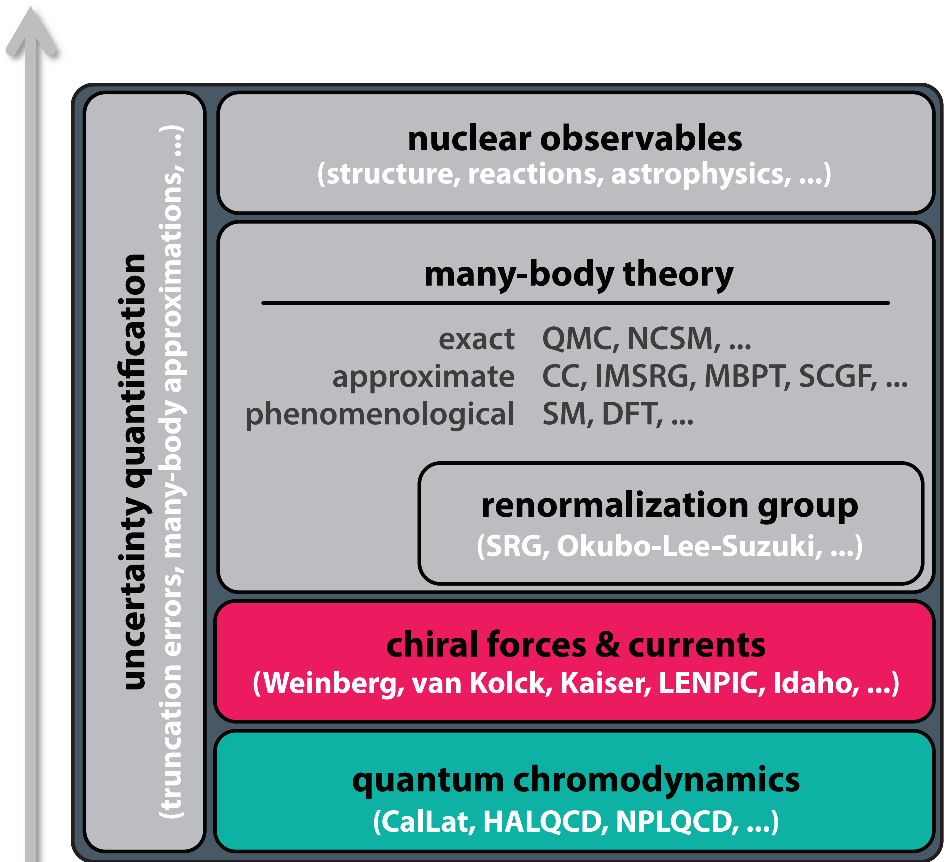

CD & Bogner, Few Body Syst. **62**, 109

Here: nuclear equation of state (EOS)
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$$\frac{E}{A}(n, \delta, T)$$

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neutron excess δ
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)

Modern theory of nuclear forces

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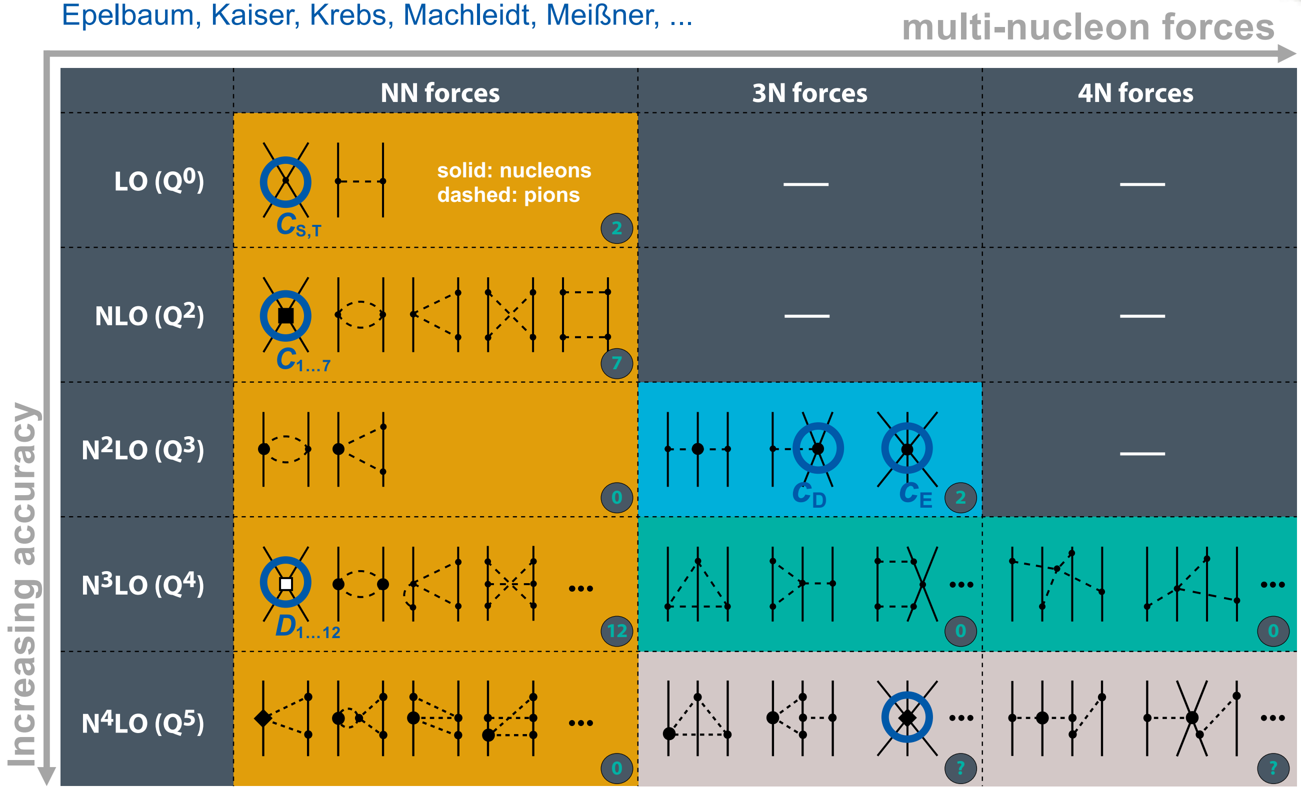
Hierarchy of chiral nuclear forces up to N^{4}LO

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

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



For recent reviews of **delta-full EFT**, see, *e.g.*:
Piarulli & Tews, Front. Phys. **7**, 245; Piarulli & Schiavilla, Few Body Syst. **62**, 10

Chiral effective field theory

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

degrees of freedom: **nucleons** & **pions**

EFT expansion enables **uncertainty quantification** (EFT truncation errors)

fit the unknown couplings to experimental (or lattice) data

- NN: phase shifts & deuteron
- 3N: binding energies, charge radii (only 2 couplings through N^{3}LO)

Correlated EFT truncation error model

Melendez, Furnstahl *et al.*,
PRC **100**, 044001

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your EFT

Increasing accuracy

LO (Q^0)	y_0
NLO (Q^2)	y_1
N²LO (Q^3)	y_2
N³LO (Q^4)	y_3
N⁴LO (Q^5)	y_4 (unknown)

$$y_k = y_{\rm ref}\sum_{n=0}^{k} c_n Q^n$$

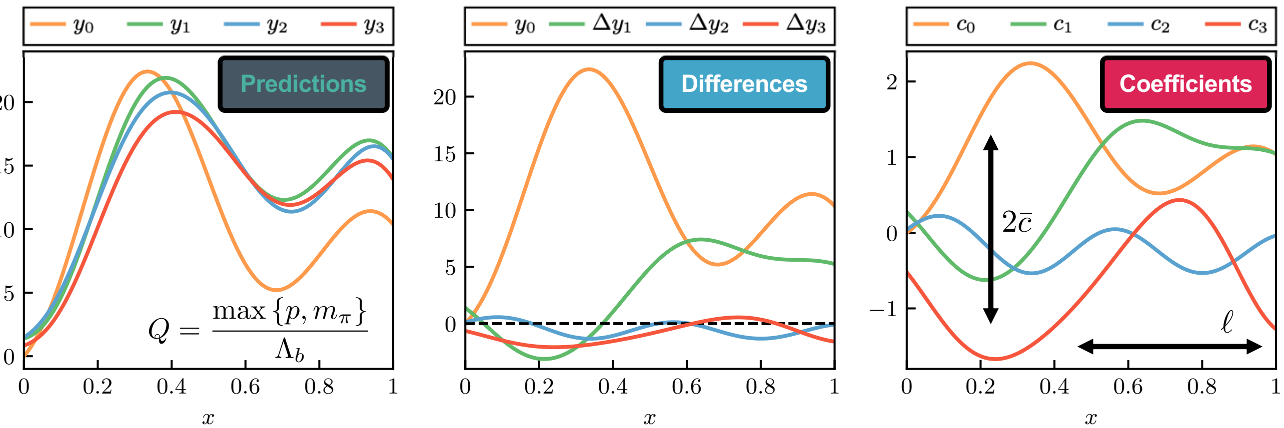
EFT prediction at $k^{\rm th}$ order

want full prediction: $y = y_k + \delta y_k$

need to infer theory uncertainty from the *computed* EFT orders

$$\delta y_k = y_{\rm ref}\sum_{n=k+1}^{\infty} c_n Q^n$$

to-all-orders truncation error



$$\mathcal{GP}\left[0, \bar{c}^2\, r(x, x'; l)\right]$$

***natural* coefficients**

Bayesian estimation of the **kernel** hyper-parameters (guided by prior information)

Here: **RBF** (stationary)

predict observable y_k order by order in EFT

$$\Delta y_n = y_n - y_{n-1}$$

differences

model all coefficients as independent draws from a *single* Gaussian Process

Note: c_n are *not* the EFT's LEC

Accounts for **correlations** in the observable $y(x)$

Model checking diagnostics (*e.g.*, Mahalanobis distance)

https://github.com/buqeye/gsum

First rigorous uncertainty quantification

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

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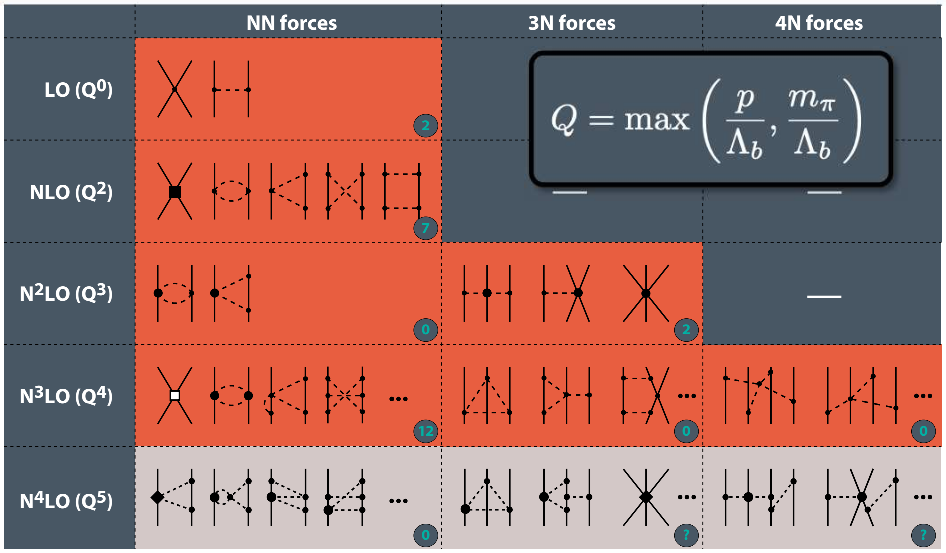
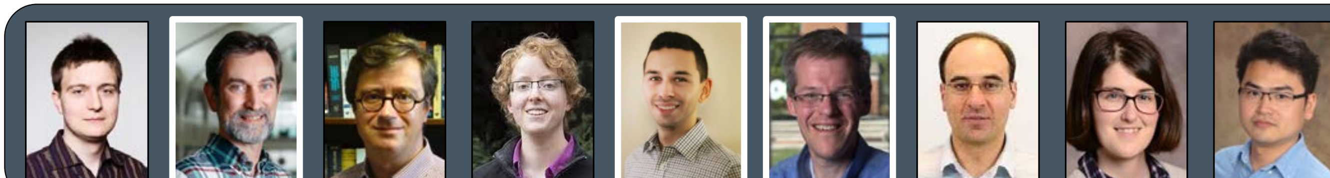
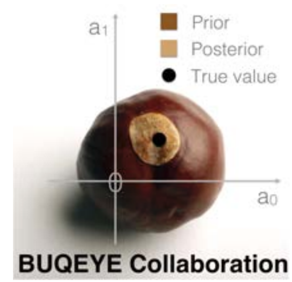


$\{y_0, y_2, y_3, \ldots, y_k\}$	**predict observable *y* order by order in the chiral expansion**
$y_k = y_{\text{ref}} \sum_{n=0}^{k} c_n Q^n$	**make a *falsifiable* model assumption for the convergence pattern**
$\mathcal{GP}\left[0, \bar{c}^2\, r(x, x'; l)\right]$	**model all c_n as independent draws from a single Gaussian Process**
$\delta y_k = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$	**learn hyperparameters of that GP & compute to-all-orders truncation error**



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



Bayesian
Uncertainty
Quantification:
Errors for
Your
EFT

First rigorous uncertainty quantification

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

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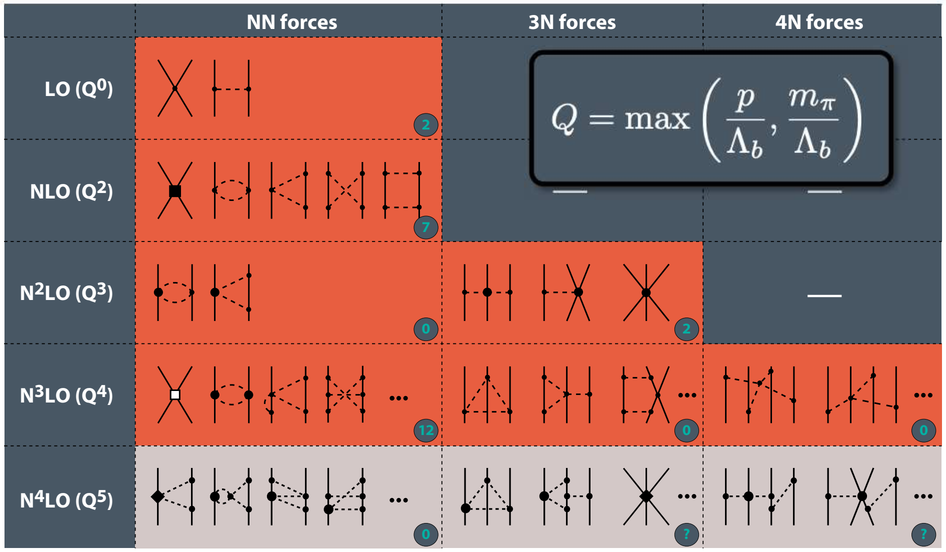

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

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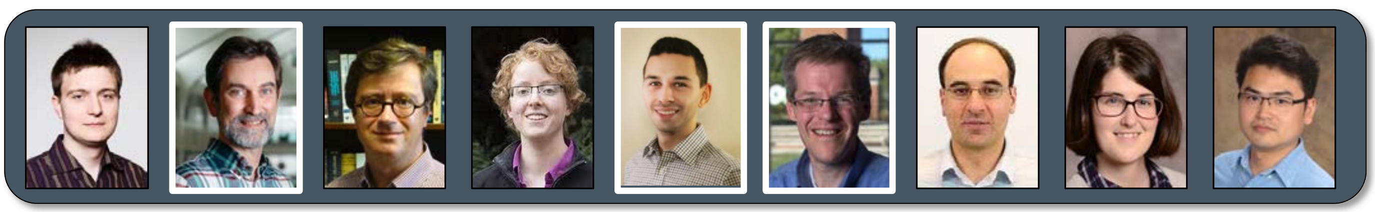

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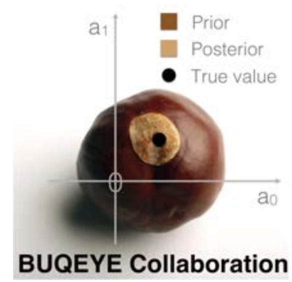

Bayesian **U**ncertainty **Q**uantification: **E**rrors for **Y**our **EFT**

First rigorous uncertainty quantification

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

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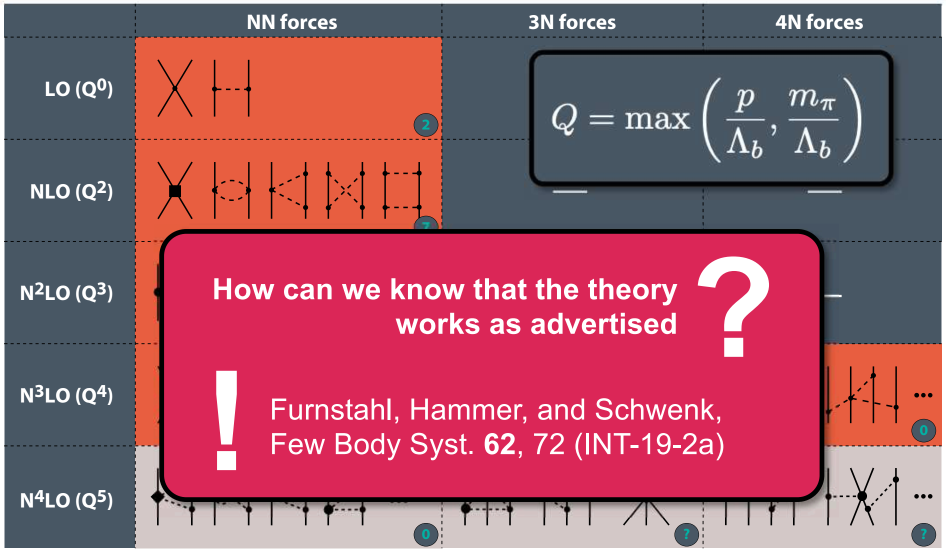

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

How can we know that the theory works as advertised ?

! Furnstahl, Hammer, and Schwenk, Few Body Syst. **62**, 72 (INT-19-2a)

$\{y_0, y_2, y_3, \ldots, y_k\}$	**predict observable *y* order by order in the chiral expansion**
$y_k = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$	**make a *falsifiable* model assumption for the convergence pattern**
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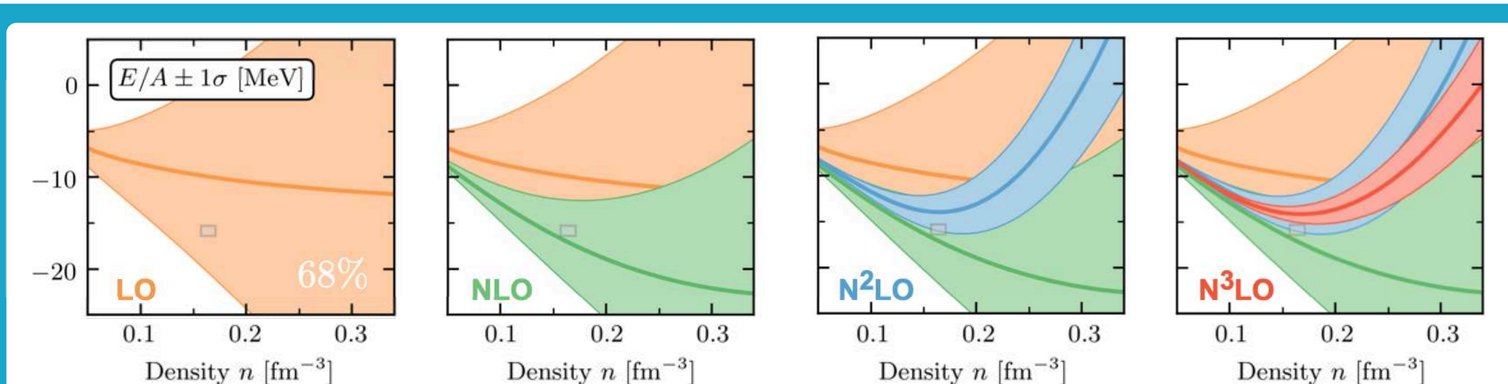
An example: symmetric matter

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

Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$



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

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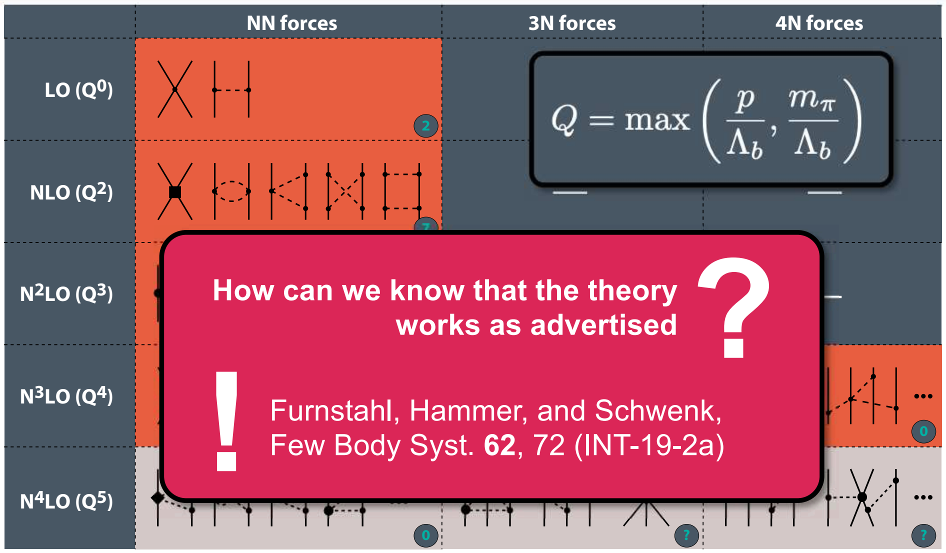

$\{y_0, y_2, y_3, \ldots, y_k\}$ — **predict observable *y* order by order in the chiral expansion**

$y_k = y_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n$ — **make a *falsifiable* model assumption for the convergence pattern**

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$\delta y_k = y_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$ — **learn hyperparameters of that GP & compute to-all-orders truncation error**

Recent applications of BUQEYE's EFT truncation error model:

Bayesian analysis of muon capture on deuteron in chiral effective field theory
Gnech, Marcucci, and Viviani, arXiv:2305.07568

Gaussian process error modeling for chiral EFT calculations of np ↔ dγ at low energies
Acharya & Bacca, Phys. Lett. B **827**, 137011

***Ab initio* predictions link the neutron skin of ^{208}Pb to nuclear forces**
Hu, Jiang, Miyagi *et al.*, Nat. Phys. **18**, 1196

***Ab initio* nucleon-nucleus elastic scattering with chiral EFT uncertainties**
Baker, McClung, Elster *et al.*, Phys. Rev. C **106**, 064605

Ab initio workflow (idealized)

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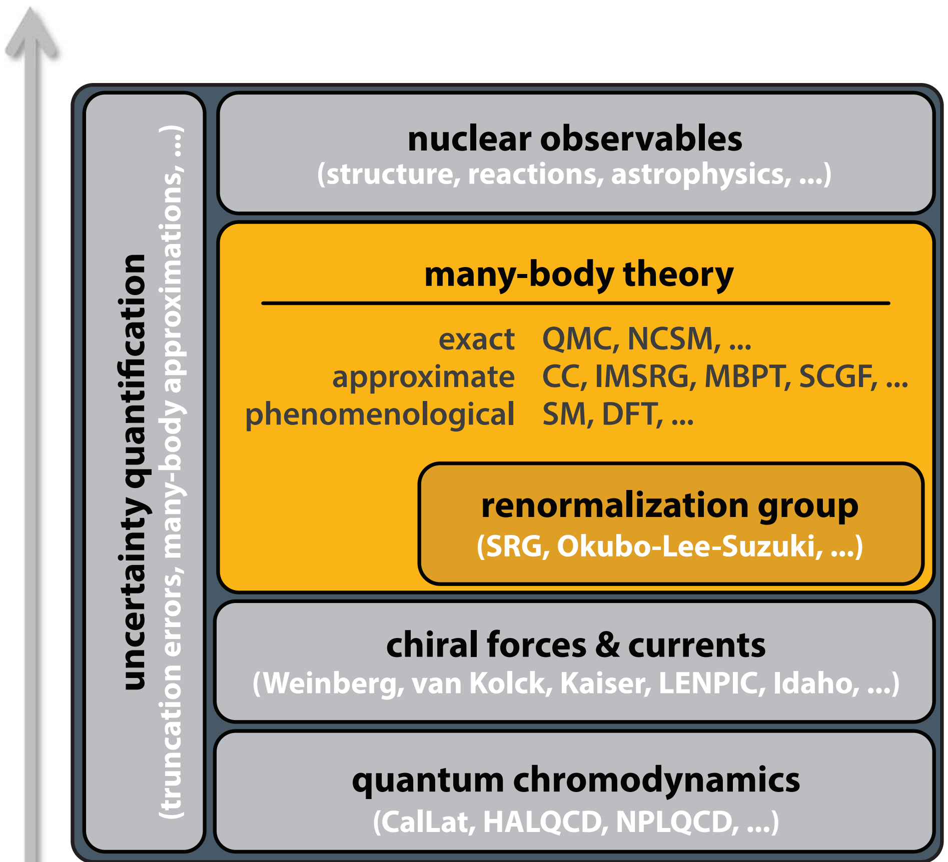
$$H(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta})\,|\psi(\boldsymbol{\theta})\rangle$$

Schrödinger Equation



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

Here: Many-Body Perturbation Theory (MBPT)

computationally efficient
allows estimating many-body uncertainties
accelerated by RG-softening of nuclear interactions

Widely applicable:

- ✓ arbitrary neutron excesses
- ✓ finite temperature
- ✓ finite nuclei
- ✓ optical potentials, …

Other frameworks include Quantum Monte Carlo and Coupled Cluster theory

Many-body perturbation theory (MBPT) in a nutshell

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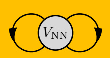
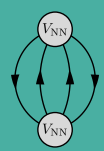


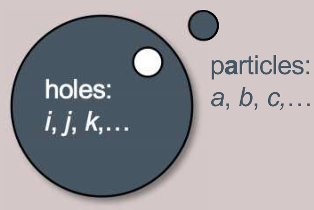
$$\frac{E^{(0)}}{V} = +\frac{1}{2}\sum_{ij} \langle ij \,|\, \overline{V}_{\rm NN} \,|\, ij \rangle$$

Hartree-Fock



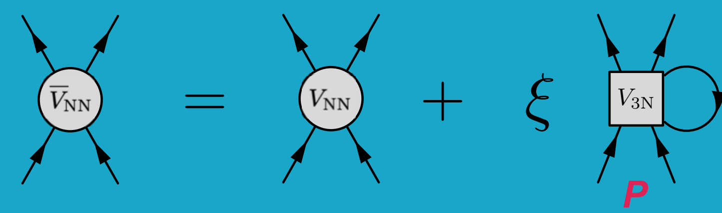
$$\frac{E^{(2)}}{V} = \frac{1}{4}\sum_{\substack{ij\\ab}} \frac{|\langle ij|\overline{V}_{\rm NN}|ab\rangle|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}$$

second order

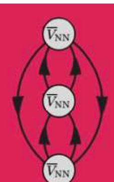


$$|i\rangle = |\mathbf{k}_i \sigma_i \tau_i\rangle$$

effective potential | genuine NN forces | normal-ordered 3N forces

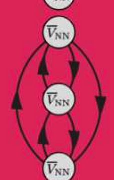


required uncontrolled approximations | involved at N^3LO



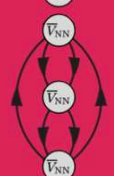
$$\frac{E^{(3)}_{hh}}{V} = +\frac{1}{8}\sum_{\substack{ab\\ijkl}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab \rangle \langle kl \,|\, \overline{V}_{\rm NN} \,|\, ij \rangle \langle ab \,|\, \overline{V}_{\rm NN} \,|\, kl \rangle}{D_{ijab} D_{klab}}$$

involved partial-wave decomposition



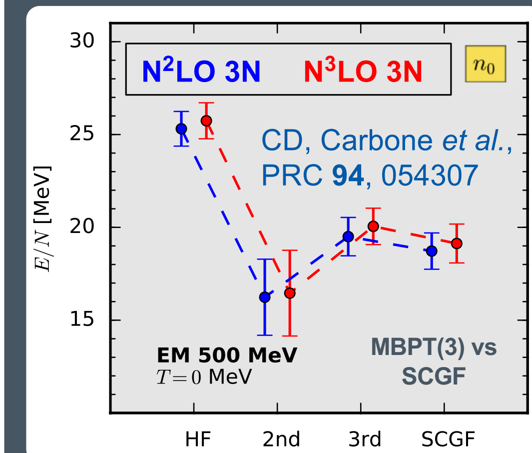
$$\frac{E^{(3)}_{ph}}{V} = +\sum_{\substack{abc\\ijk}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab \rangle \langle ak \,|\, \overline{V}_{\rm NN} \,|\, ic \rangle \langle bc \,|\, \overline{V}_{\rm NN} \,|\, jk \rangle}{D_{ijab} D_{jkbc}}$$

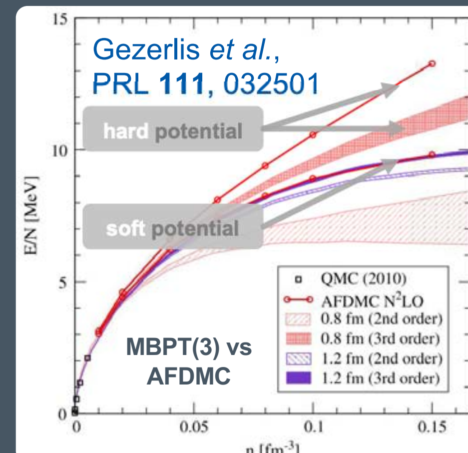
see Coraggio, Holt *et al.*, PRC **89**, 044321



$$\frac{E^{(3)}_{pp}}{V} = +\frac{1}{8}\sum_{\substack{abcd\\ij}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab \rangle \langle ab \,|\, \overline{V}_{\rm NN} \,|\, cd \rangle \langle cd \,|\, \overline{V}_{\rm NN} \,|\, ij \rangle}{D_{ijab} D_{ijcd}}$$

third order





nonperturbative benchmarks in neutron matter

Renaissance of MBPT

CD, Hebeler, Schwenk, PRL **122**, 042501
CD, McElvain *et al.*, in prep.

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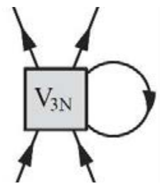

efficient evaluation of MBPT diagrams

with **NN**, **3N**, and **4N forces**

- **implementation of arbitrary MBPT diagrams** has become **straightforward** (numerically exact)
- multi-dimensional momentum integrals: improved VEGAS
- GPU-accelerated normal ordering of **3N interactions**
- propagation of importance sampling distributions
- **controlled evaluation of 1000s of MBPT diagrams**

Ground-state energy of the dilute Fermi gas at fourth order (complete):
Wellenhofer, CD, Schwenk, PRC **104**, 014003 & PLB **802**, 135247

Arthuis *et al.*,
Comput. Phys. **240**, 202

high-order MBPT calculations of the EOS

automated code generation

analytic expressions interaction & MBPT diagrams

automated diagram generation

High-order MBPT for nuclear matter

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The number of diagrams increases rapidly!

	1,	**3,**	**39,**	**840,**	**27 300,**	**1 232 280,**	**…**
n =	2	3	4	5	6	7	

Integer sequence A064732:
Number of labeled Hugenholtz diagrams with n nodes.

with automated diagram generation

Stevenson, Int. J. Mod. Phys. C **14**, 1135
Arthuis *et al.*, Comput. Phys. **240**, 202

automated approach to MBPT for nuclear matter

for residual 3N contributions, see Xu, Li, and Xu, arXiv:1810.08804

Ab initio workflow (idealized)

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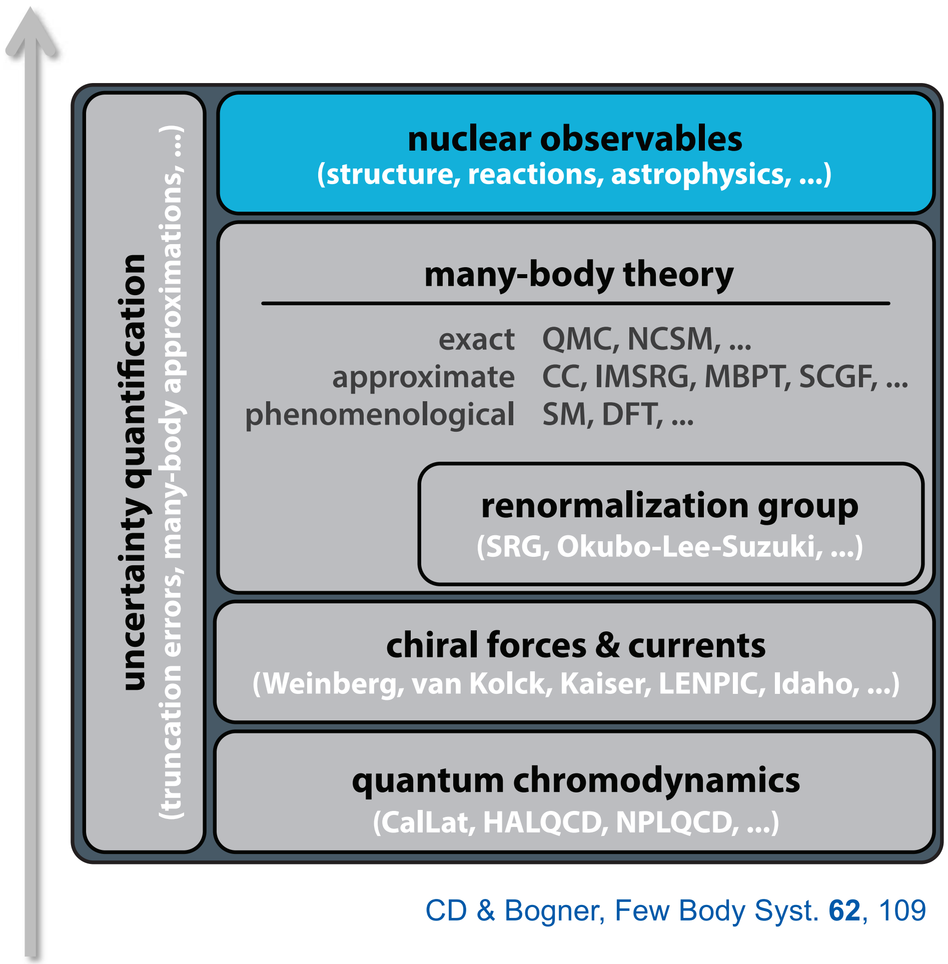

CD & Bogner, Few Body Syst. **62**, 109

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Uncertainty quantification

robust estimates of theoretical uncertainties using Bayesian machine learning via Gaussian Processes

uncertainties in EFT-based calculations due to:

- **truncating the EFT expansion**
- **applying many-body (and other) approximations**
- **fitting LECs to experimental data (*not* included)**

e.g., see CD, Melendez *et al.*, PRC **102**, 054315
Furnstahl, Natalie Klco *et al.*, PRC **92**, 024005
Cacciari & Houdeau, JHEP **1109**, 039
Bagnaschi, Cacciari *et al.*, JHEP **1502**, 133

Isospin asymmetric nuclear matter

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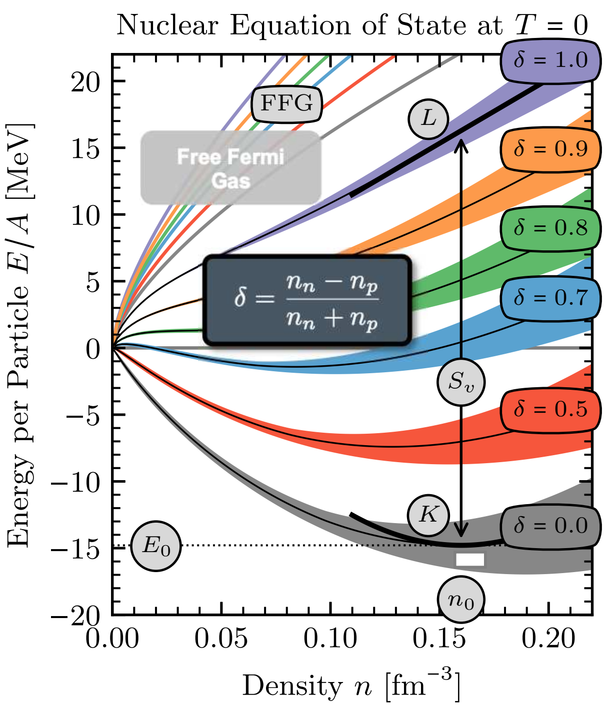
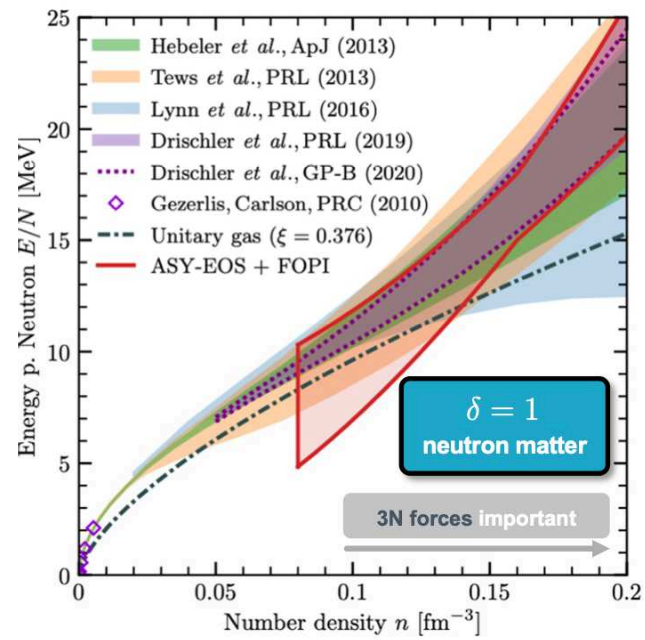


CD, Holt, and Wellenhofer, Annu. Rev. Nucl. Part. Sci. **71**, 403



Huth, Pang *et al.*, Nature **606**, 276

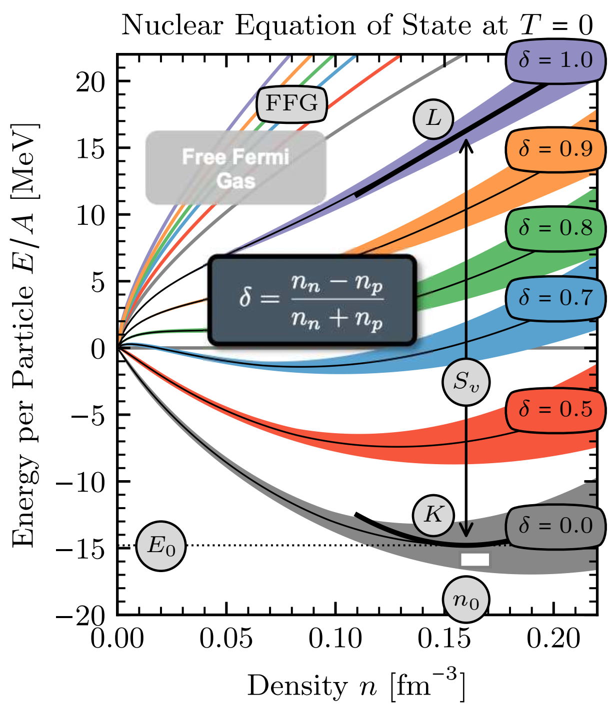
Great progress in **microscopic EOS calculations** at densities $\lesssim 2n_0$ and neutron star EOS modeling

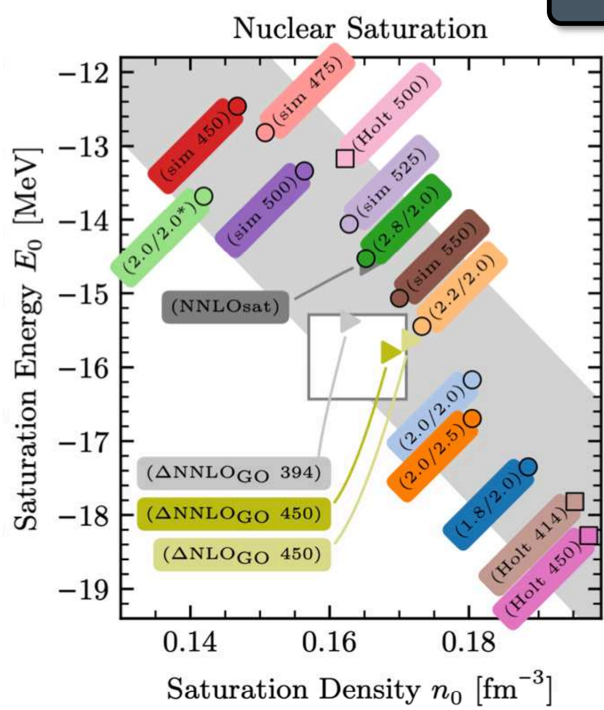
Pure neutron matter $\lesssim n_0$ is well-constrained by scattering data

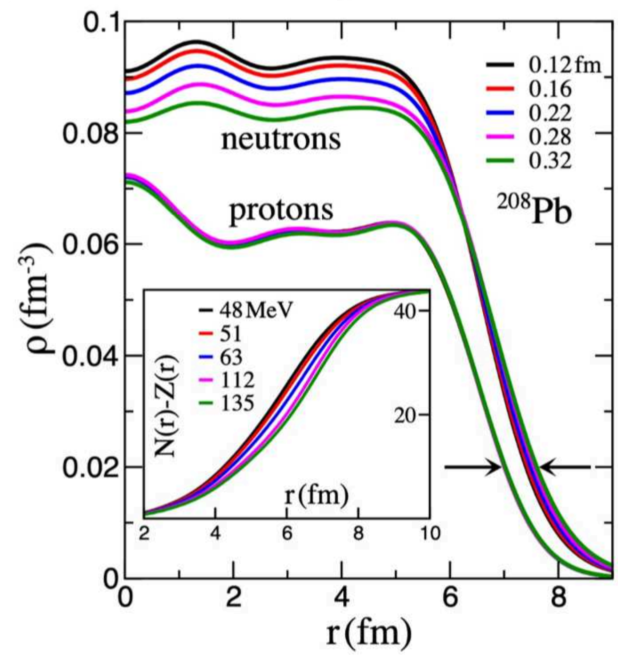
3N forces are weaker than in SNM

Isospin asymmetric nuclear matter

$$\frac{\mathrm{d}}{\mathrm{d}n}\frac{E}{A}(n,0)\Big|_{n=n_0} = 0$$







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

Piekarewicz & Fattoyev, Phys. Today **72**, 7

Great progress in **microscopic EOS calculations** at densities $\lesssim 2n_0$ and neutron star EOS modeling

Saturation: **fine-tuned cancellation** in the nuclear interactions (ideal for benchmarks)
Annotations: (λ / Λ_{3N}) in fm^{-1} or (Λ) in MeV

Needed: improved NN+3N interactions with good saturation properties and robust UQ

Nuclear saturation point: EFT predictions

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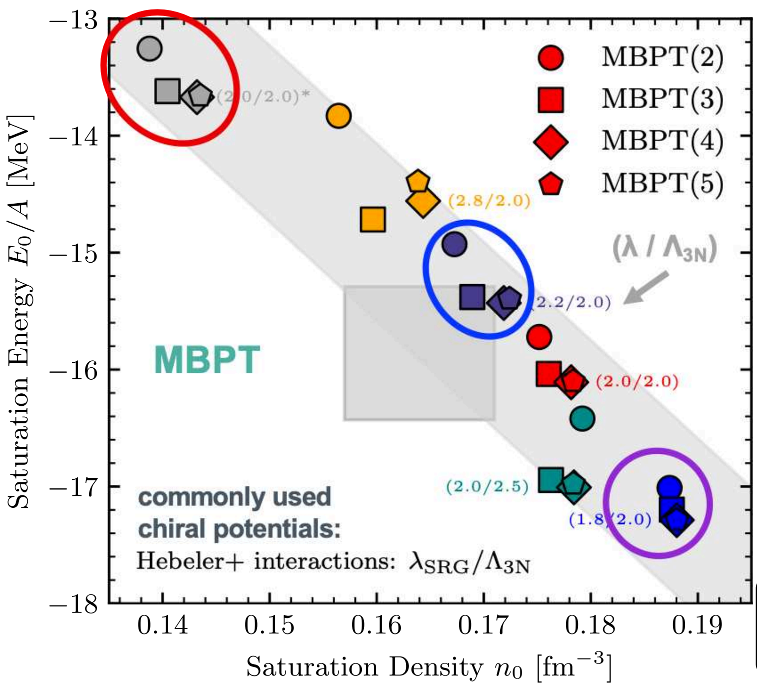
MBPT(*n*)	2	3	4	5
NN+3N	[illegible]	[illegible]	[illegible] N)	✓
residual 3N	[illegible]	[illegible]	✗	✗

Excellent MBPT convergence (with these soft chiral potentials)



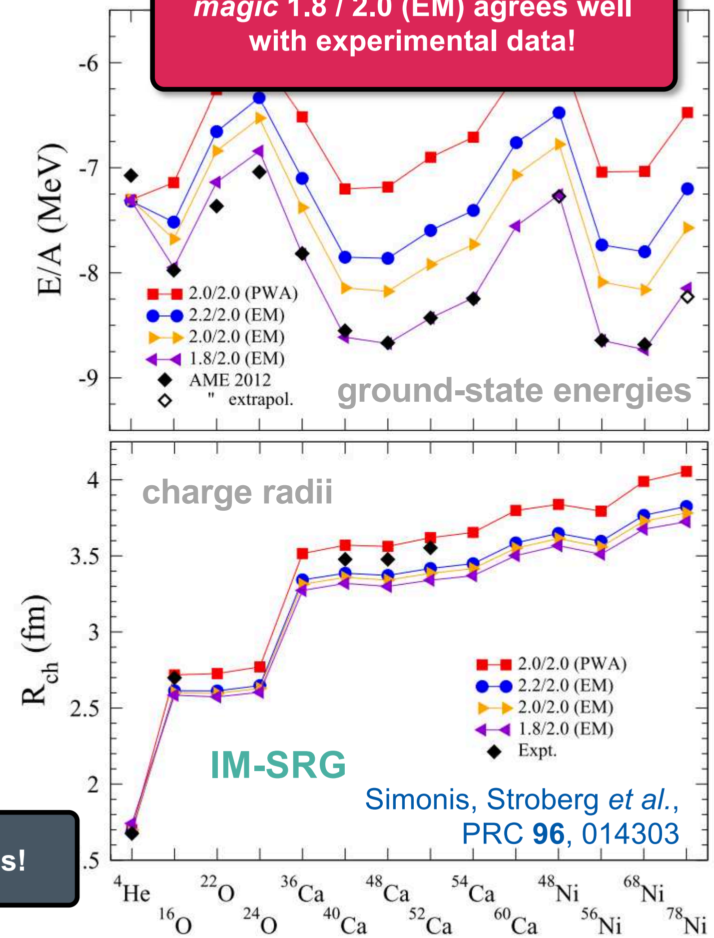
(new)

Infinite Matter

chiral EFT: constrained by two- and few-body data *only*

Same interactions!

***magic* 1.8 / 2.0 (EM) agrees well with experimental data!**

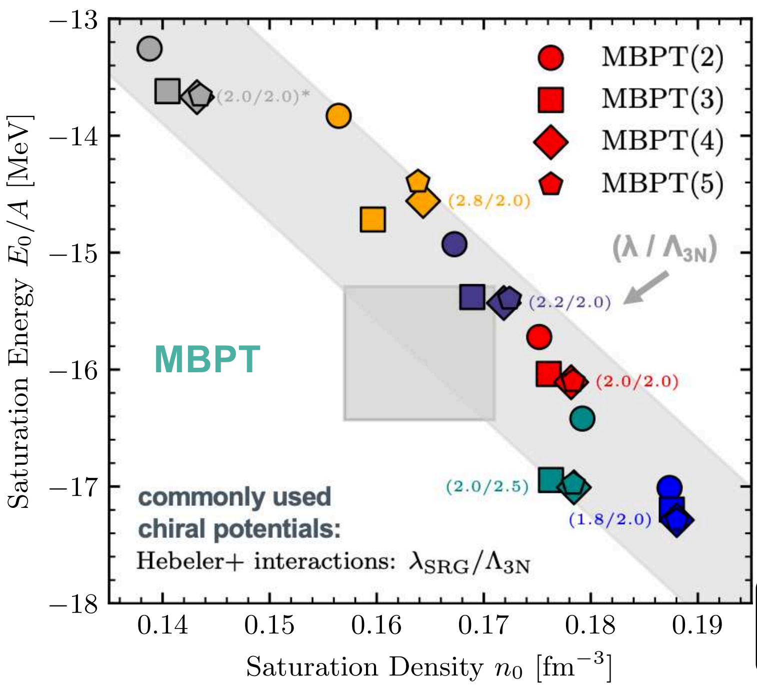


Finite Nuclei (closed-shell)

Nuclear saturation point: EFT vs DFT

MBPT(*n*)	2	3	4	5
NN+3N	[illegible]	[illegible]	…N)	✓
residual 3N	✓ (1)	✓ (…)	✗	✗

Excellent MBPT convergence (with these soft chiral potentials)

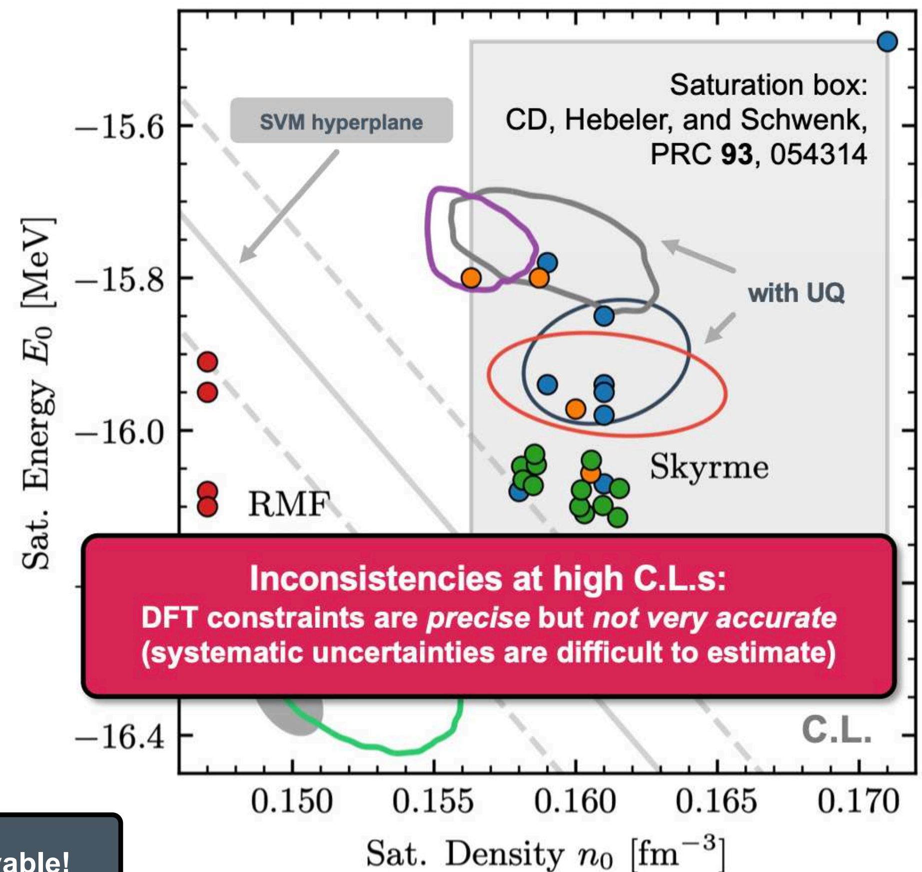


(new)

Infinite Matter

***Not* an observable!**

chiral EFT: constrained by two- and few-body data *only*



Inconsistencies at high C.L.s:
DFT constraints are *precise* but *not very accurate*
(systematic uncertainties are difficult to estimate)

DFT: calibrated to nuclear *observables* and extrapolated to infinite matter

Nuclear saturation point: Skyrme vs RMF models

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Skyrme models systematically predict (n_0, E_0) *higher* than RMF models, causing a *distinct* separation between the two model classes. *This has been long observed.*

e.g., see Furnstahl, NPA **706**

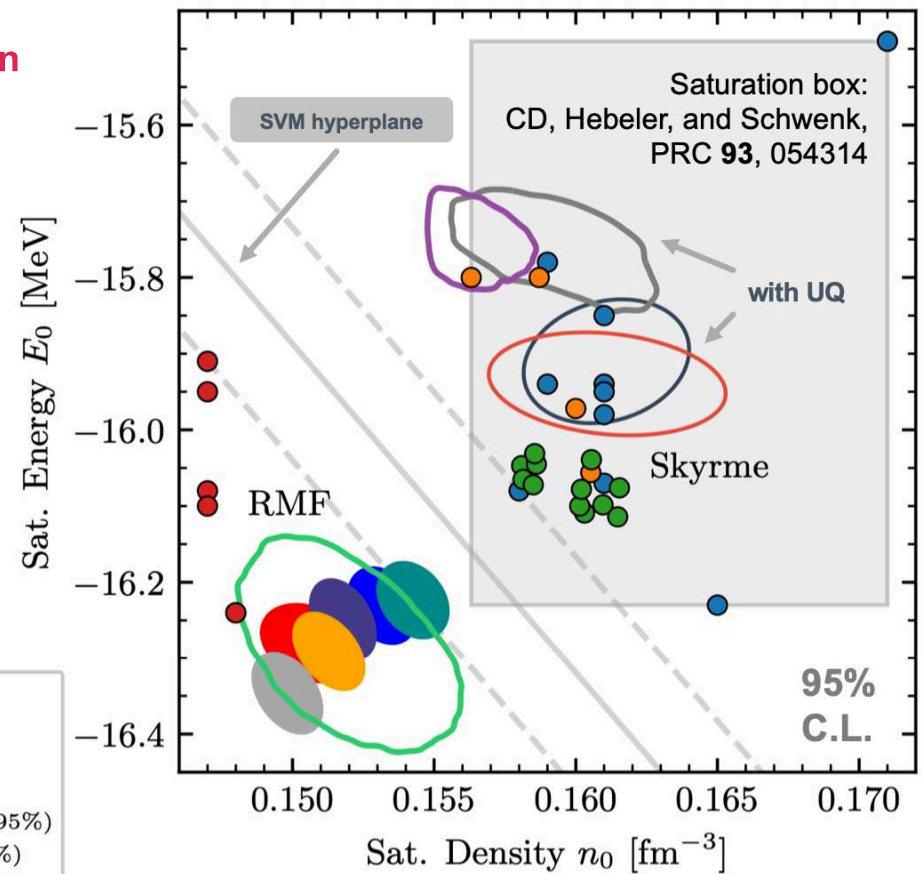
Inconsistency may be due to the different functional forms and/or the parameter estimation protocols

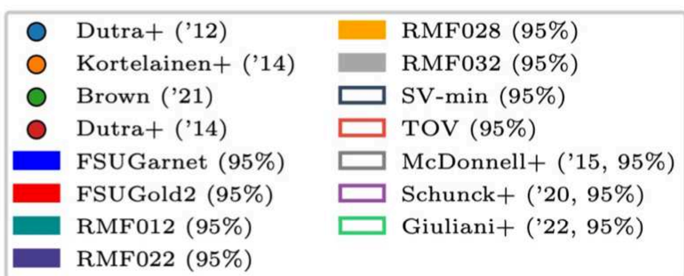
Significant progress in UQ for DFT:

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 is driven by emulators

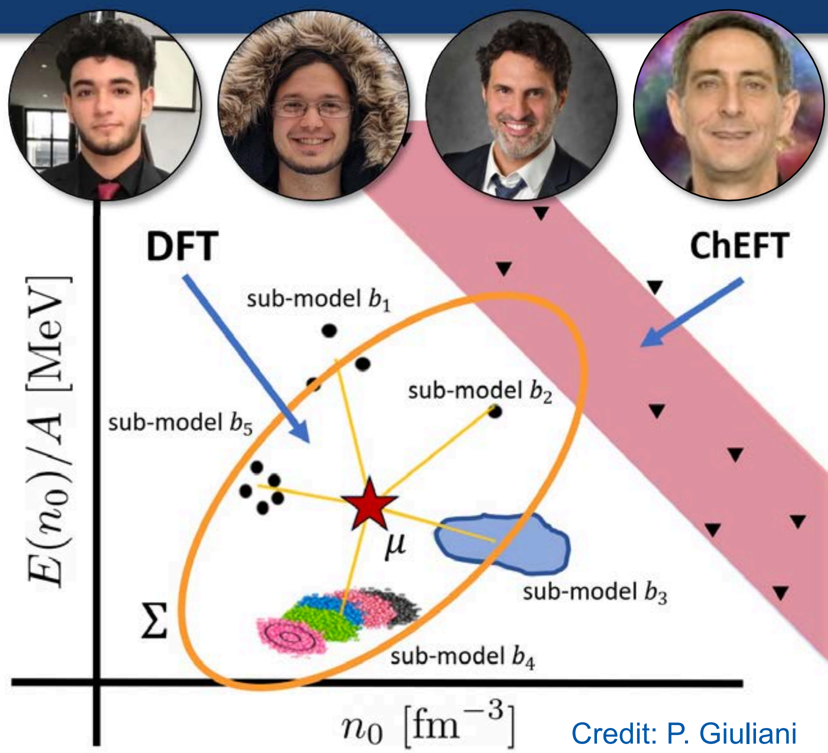
Bonilla, Giuliani, Godbey, Lee, PRC **106**, 054322
Giuliani, Godbey, Bonilla, Viens, Piekarewicz, Front. Phys. **10**





DFT: calibrated to nuclear *observables* and extrapolated to infinite matter

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

$$P(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathcal{D}) \propto P(\mathcal{D}|\boldsymbol{\mu}, \boldsymbol{\Sigma})\ P(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

posterior — likelihood — 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 expressions)

posterior predictive (marginalization)

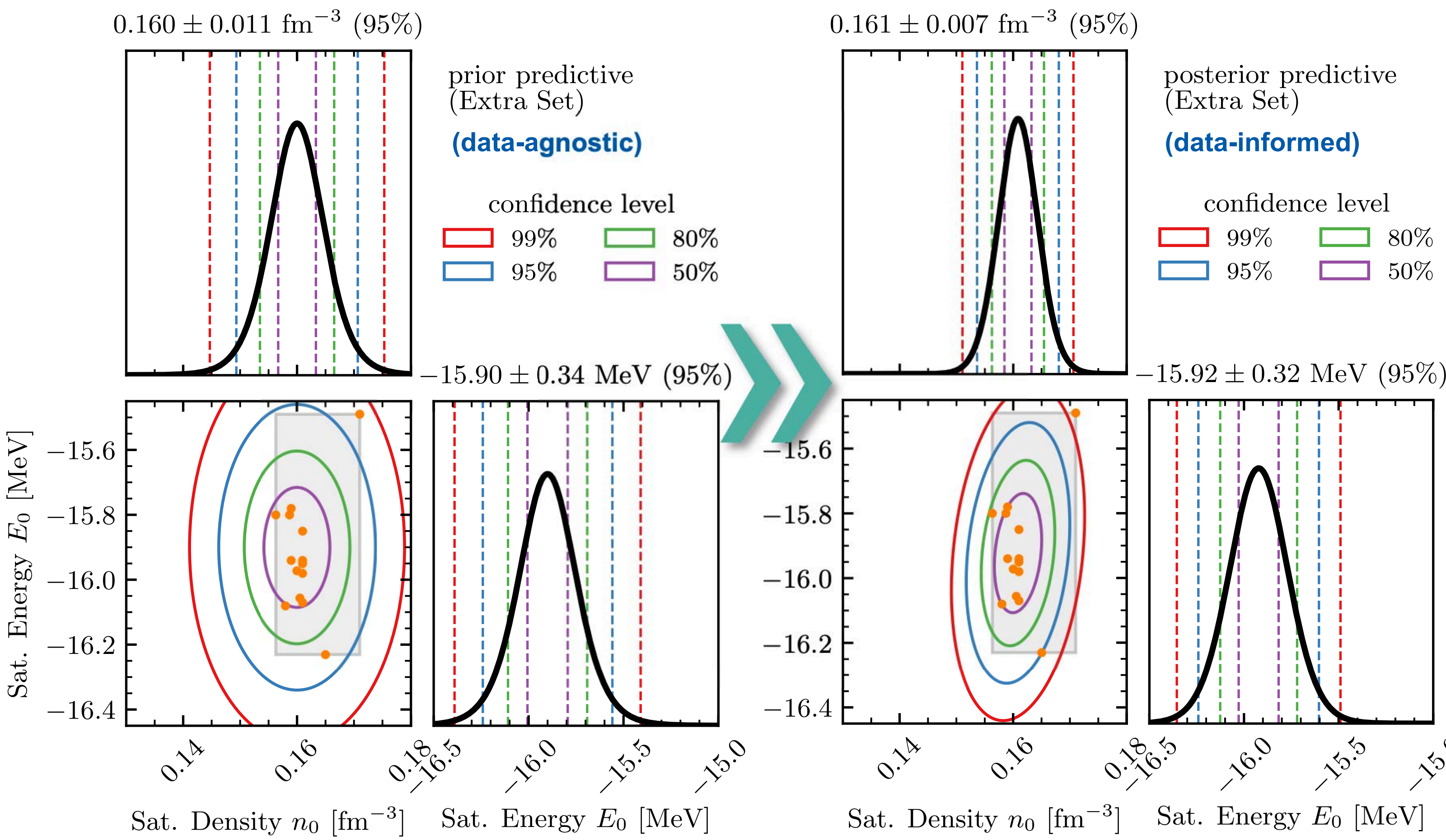
$$P(\mathbf{y}^*|\mathcal{D}) \propto \int \mathrm{d}\boldsymbol{\mu}\,\mathrm{d}\boldsymbol{\Sigma}\ P(\mathbf{y}^*|\boldsymbol{\mu}, \boldsymbol{\Sigma})\, P(\boldsymbol{\mu}, \boldsymbol{\Sigma}|\mathcal{D})$$

model — posterior

(evaluates to a bivariate *t*-distribution)

Analysis: Saturation box (2016)

(preliminary)



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

analytic calculations due to conjugated distributions

predictive & marginal distributions are ***t*-distributions**

Only a mild prior sensitivity despite the data-limited case

Jupyter notebooks will be provided

All DFT constraints: joint MC analysis (preliminary)

MICHIGAN STATE UNIVERSITY SROP SUMMER RESEARCH OPPORTUNITIES PROGRAM

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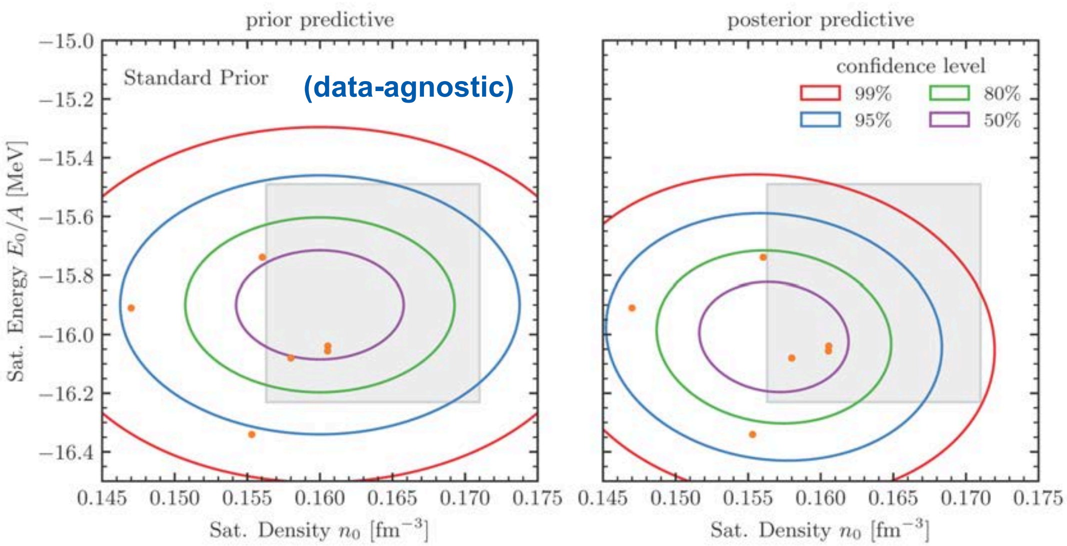
Uncertainties in the DFT constraints break conjugacy!

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

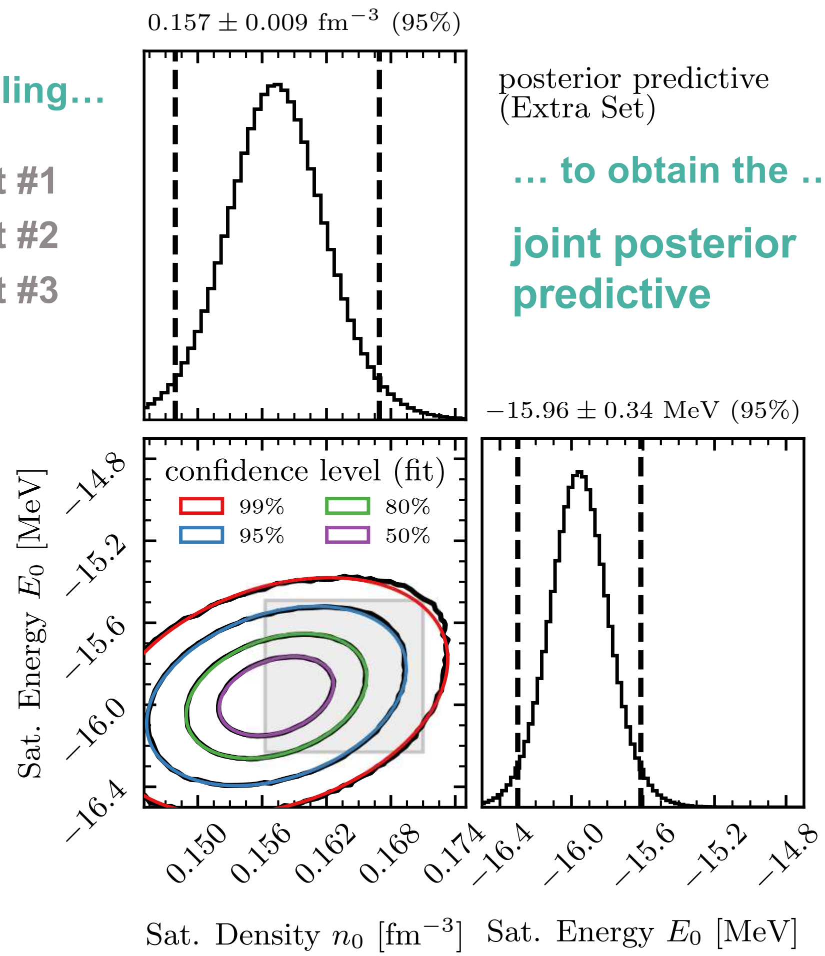


set #1

set #2

set #3

…



… to obtain the …

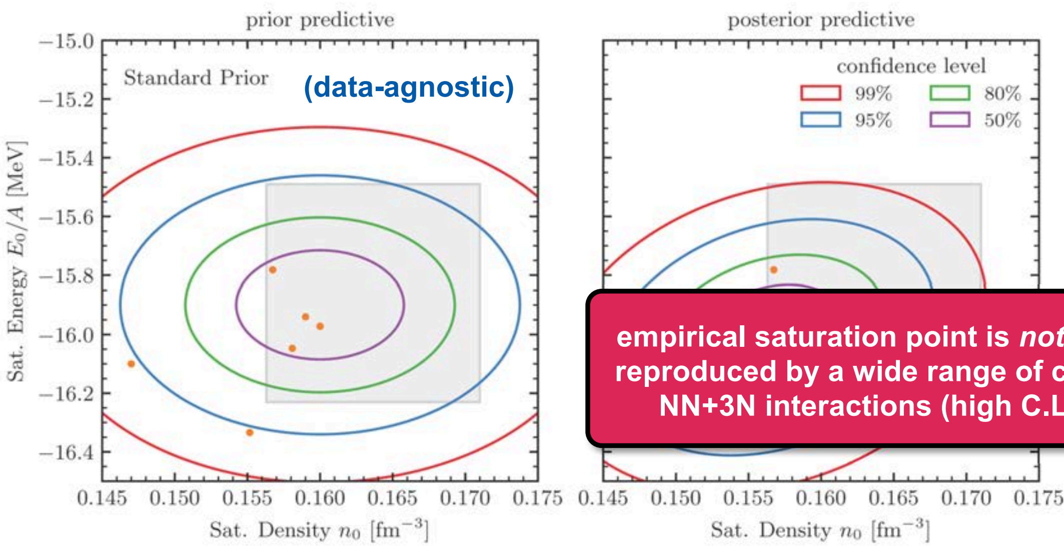
joint posterior predictive

Our constraint is approx. *t*-distributed and *consistent* with the known box estimate **but shifted toward lower (n_0, E_0/A)**

All DFT constraints: joint MC analysis (preliminary)

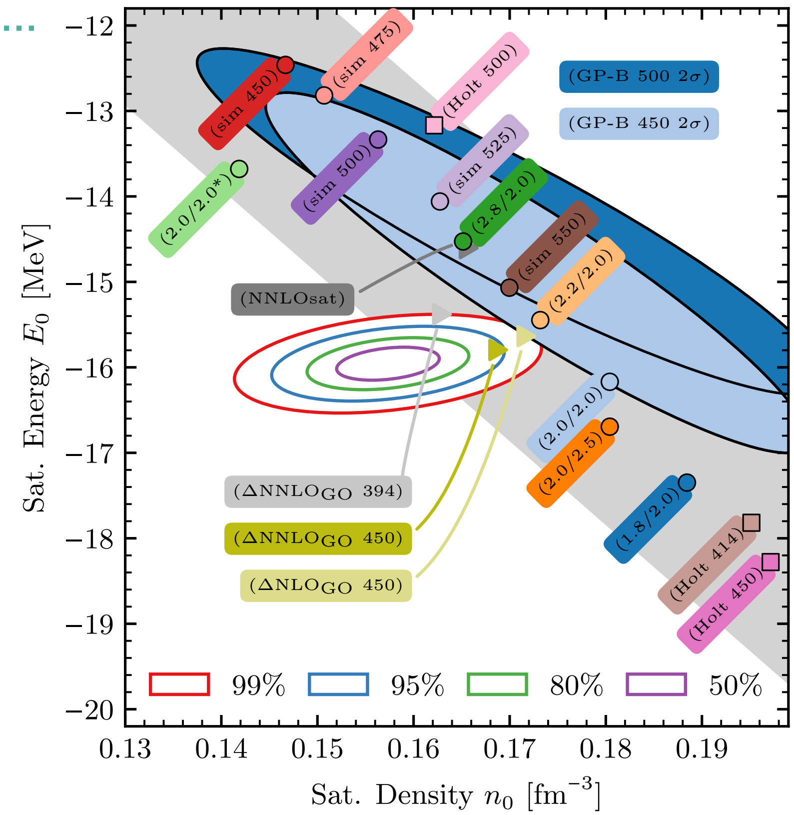
Uncertainties in the DFT constraints break conjugacy!

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



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

EFT vs DFT



Our constraint is approx. *t*-distributed and *consistent* with the known box estimate **but shifted toward lower (n_0, E_0/A)**

Might help construct **chiral NN+3N interactions** that are **predictive** for medium-mass to heavy **nuclei *and* infinite nuclear matter**

for emulators, see:
Jiang, Forssén, Djärv, and Hagen, arXiv:2212.13203; arXiv:2212.13216

CD, Hebeler *et al.*, PRL **122**, 042501; Hoppe, CD *et al.*, PRC **100**, 024318
Simonis *et al.*, PRC **96**, 014303; Ekström *et al.*, PRC **91** 051301; and more

Emulators: game changers for UQ in nuclear physics!

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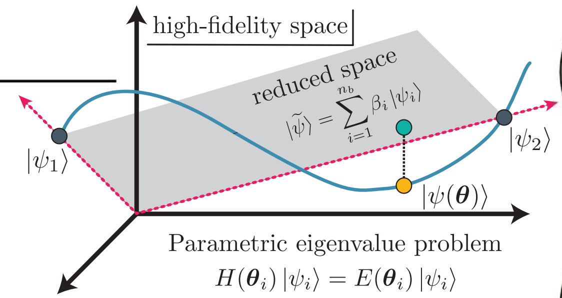
frontiers (pedagogical review article)

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]



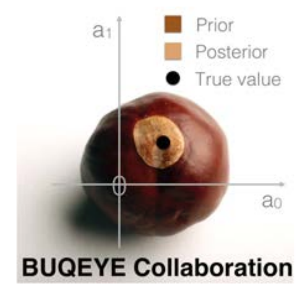
with interactive Jupyter notebooks on GitHub!

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

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
see also Duguet, Ekström, Furnstahl, König, and Lee, arXiv:2310.19419

Nuclear symmetry energy

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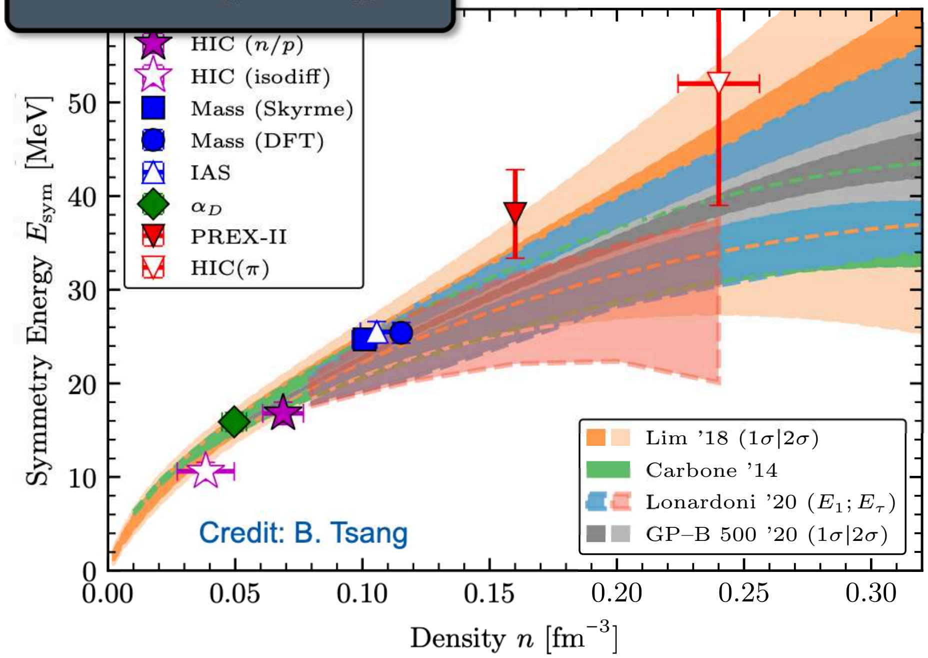
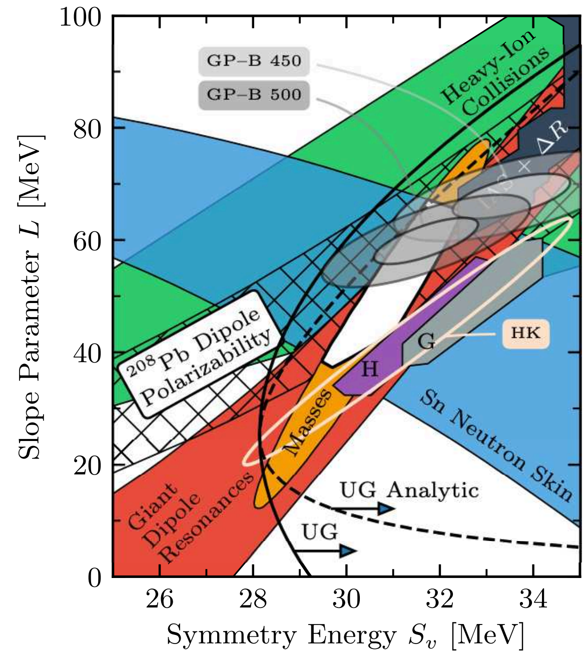
$$E_{\rm sym}(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$



based on CD, Holt *et al.*, ARNPS **71**, 403

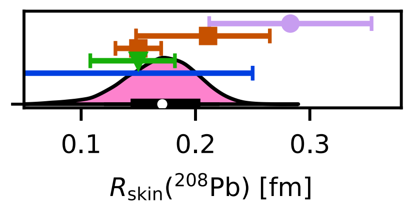
excellent agreement with other constraints
(but: *not* all at the same density)



based on Lattimer & Lim, APJ **771**, 51

ab initio **calculation of ^{208}Pb neutron skin + UQ:**

$$R_{\rm skin}^{208} = 0.14 - 0.20 \text{ fm}$$



electromagnetic electroweak
gravitational waves hadronic

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

matches chiral EFT constraint "H" (PNM)

Hebeler, Lattimer *et al.*, PRL **105**, 161102

$$\text{pr}(S_v, L\,|\,\mathcal{D}) = \int \text{pr}(S_v, L\,|\,\mathcal{D}, n_0)\,\text{pr}(n_0\,|\,\mathcal{D})\,dn_0$$

$$\text{pr}(n_0\,|\,\mathcal{D}) \approx 0.17 \pm 0.01\,\text{fm}^{-3}$$

Correlations are important: uncertainties can be smaller than one *might* naively think between PNM & SNM

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

Nuclear symmetry energy (at saturation density)

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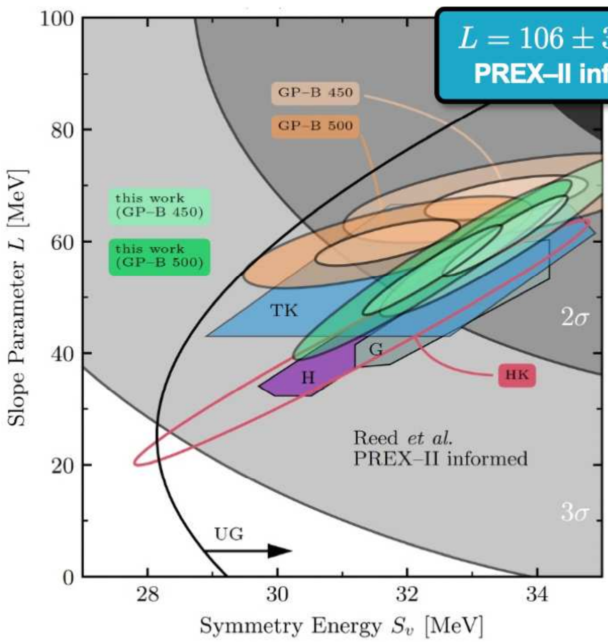
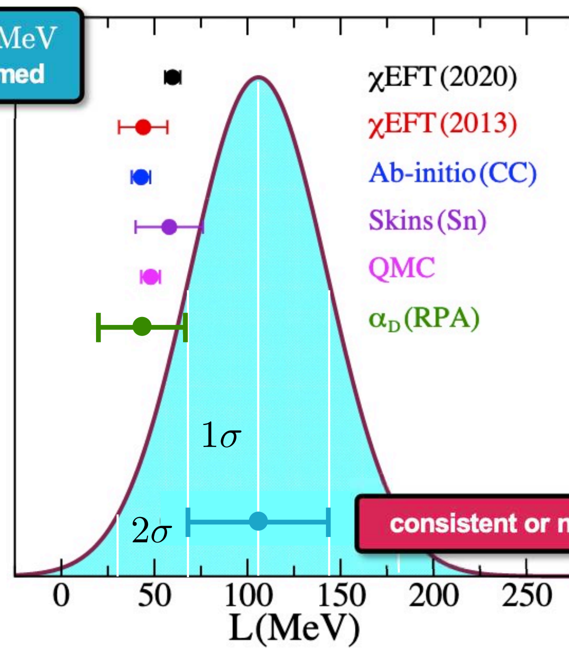
^{208}Pb neutron skin constraints with **±0.03 fm or better** are needed: **MREX @ MESA** (~2030)

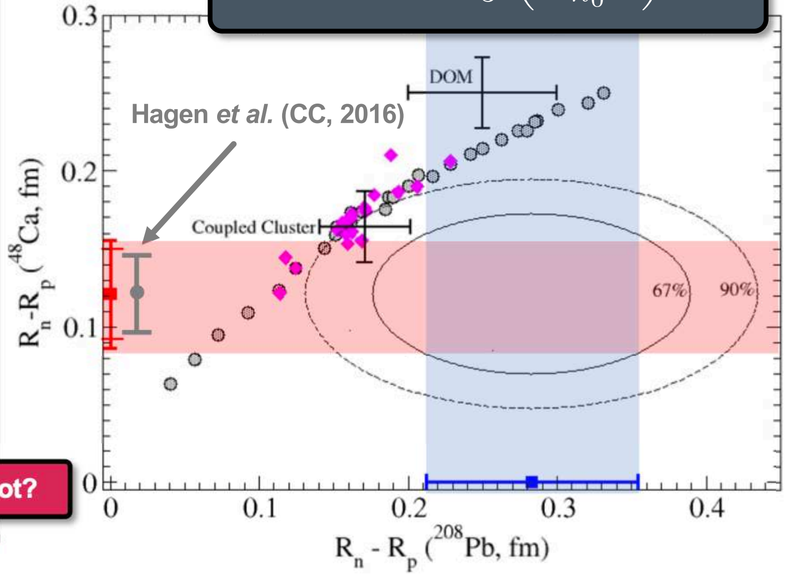
$$E_{\rm sym}(n) \equiv S_v + \frac{L}{3}\left(\frac{n-n_0}{n_0}\right) + \ldots$$



CD, Giuliani, Viens *et al.*, in prep.



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



Adhikari *et al.* (PREX-II), PRL **126**, 172502
Adhikari *et al.* (CREX), PRL **129**, 042501

"Tension" between PREX-II and theory predictions at the ~68-95% level

Current DFT models have difficulties in reproducing CREX *and* PREX-II

Ideas: Salinas *et al.*, PRC **107**, 045802; arXiv:2312.13474; Alford *et al.*, PRC **106**, 055804

***ab initio* calculations predict small ^{48}Ca skin,** in agreement with CREX

predicted dipole polarizability also agrees with experiment (RCNP)

Birkhan *et al.*, PRL **118**, 252501

Exploring the limits of chiral EFT

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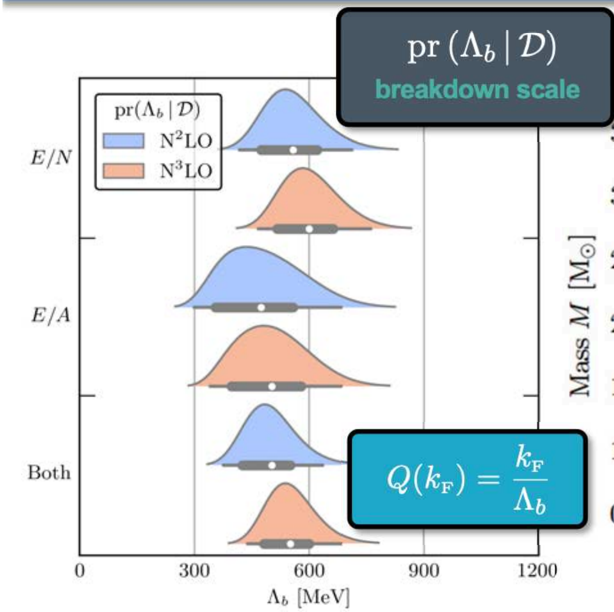

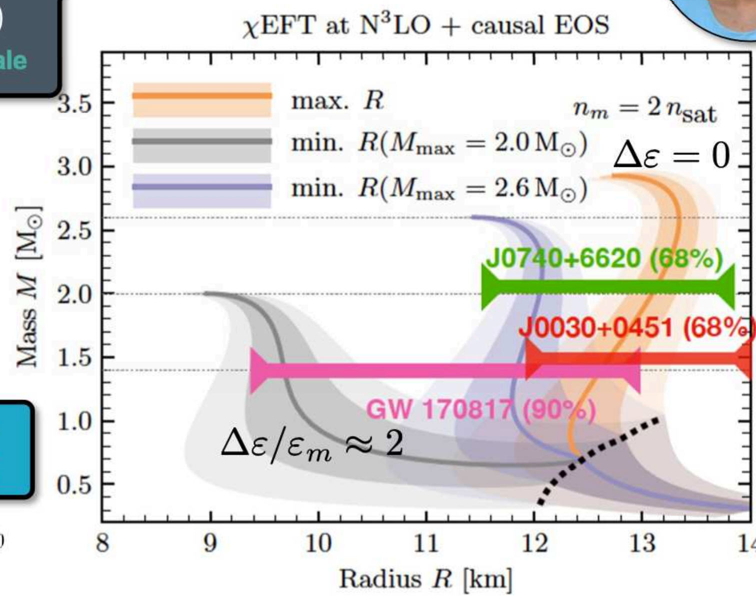

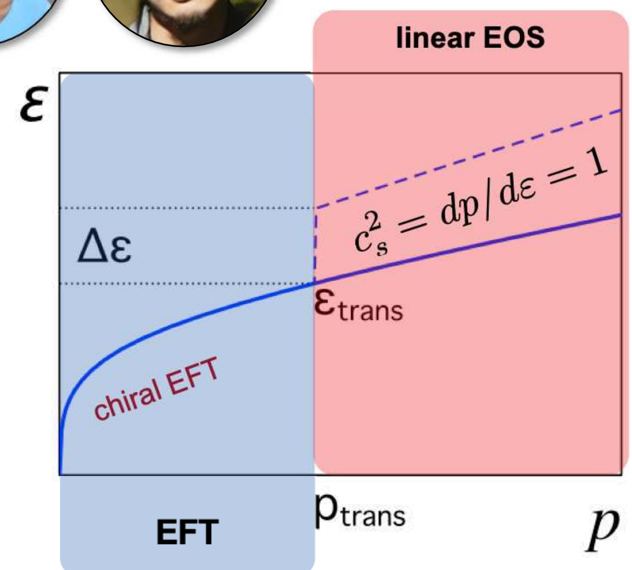

CD, Melendez *et al.*, PRC **102**, 054315

Bayesian inference of the in-medium breakdown scale

But: at what *density* does chiral EFT break down?

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

derived **bounds on the neutron star radius** (and sound speed), assuming chiral EFT breaks down at a given 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

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

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}

New SNM predictions at intermediate densities

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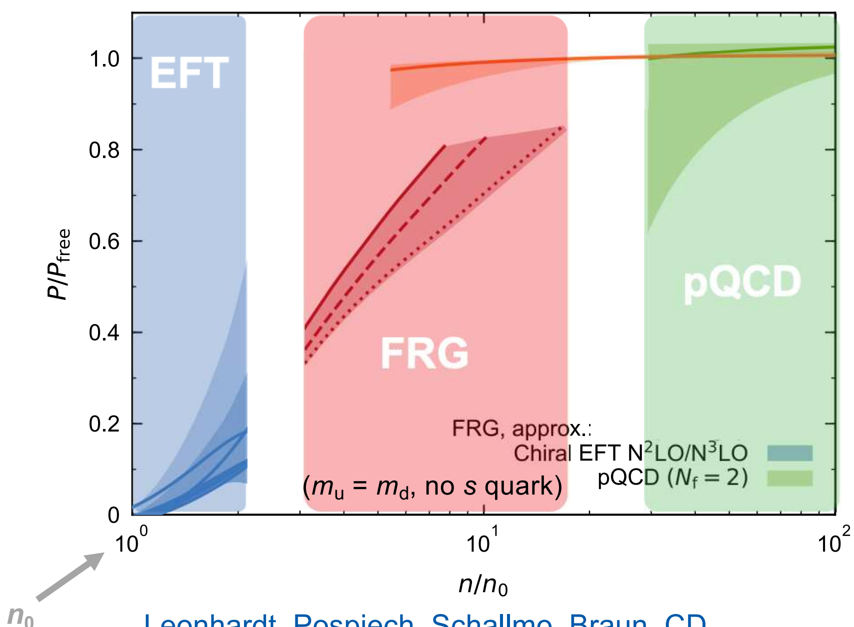
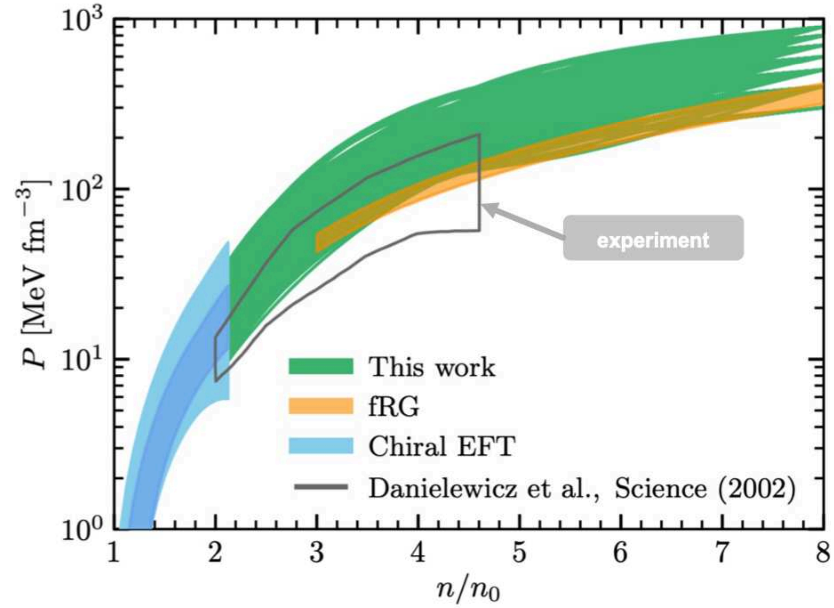


Leonhardt, Pospiech, Schallmo, Braun, CD, Hebeler, and Schwenk, PRL **125**, 142502



Huth, Wellenhofer, and Schwenk, PRC **103**, 025803

functional Renormalization Group (fRG):
ab initio constraints at intermediate densities (~3—10n_0)

major advances in pQCD calculations of cold strongly interacting matter: all but one term at O(α_s^3) calculated

remarkable consistency between theory predictions, experiment, and astrophysics

Goal: global QCD-based EOS models with fully quantified uncertainties

For pQCD, see: Gorda, Kurkela, Vuorinen *et al.*, PRL **131**, 181902; PRL **121**, 202701; ApJ **950**, 107; PRD **104**, 074015; and more

Correlated EFT truncation error model (revisited)

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your EFT

Increasing accuracy

- LO (Q^0)
- NLO (Q^2)
- N^2LO (Q^3)
- N^3LO (Q^4)
- N^4LO (Q^5)

$$y_k = y_{\rm ref} \sum_{n=0}^{k} c_n Q^n$$

EFT prediction at $k^{\rm th}$ order

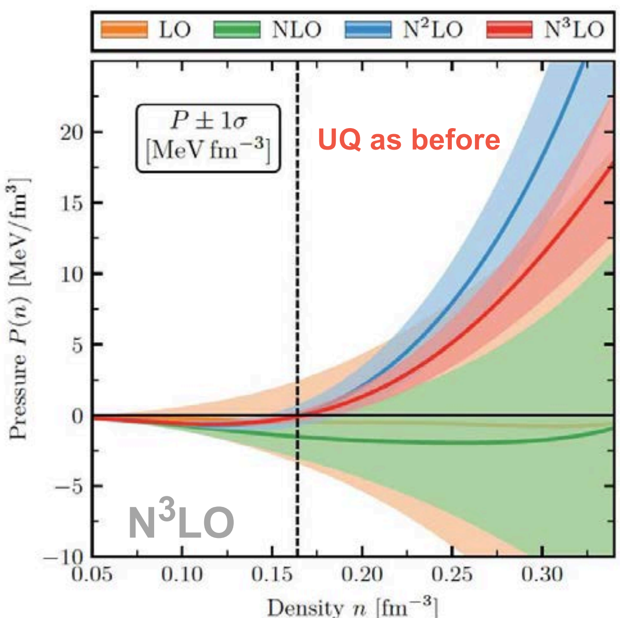
want full prediction: $y = y_k + \delta y_k$

need to infer theory uncertainty from the *computed* EFT orders

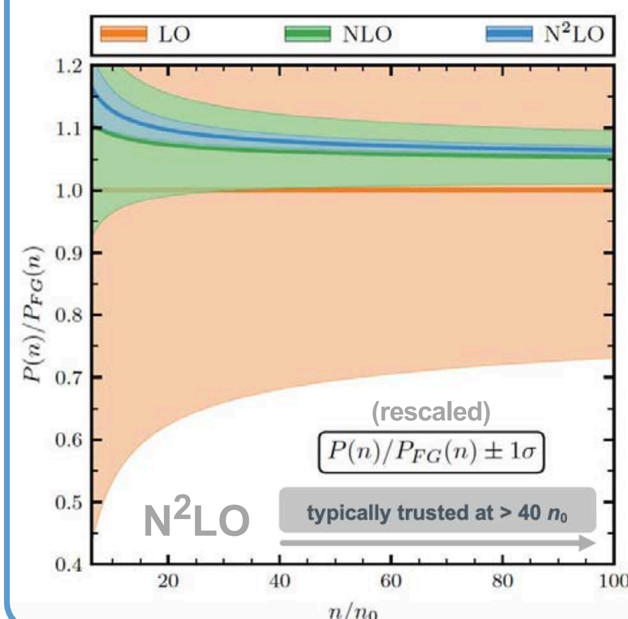
$$\delta y_k = y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

to-all-orders truncation error

Chiral EFT



pQCD



Truncation error estimation:

$$Q = \frac{N_f}{\pi} \alpha_s\left(\bar{\Lambda}(\mu_{\rm FG})\right)$$

$$y_{\rm ref} = P_{\rm FG}(n)$$ (two-loop level)

Kohn-Luttinger-Ward inversion:

$$P(\mu) \to P(n)$$

(consistent up to the desired order in pQCD)

pQCD prediction:

$$P(\mu)$$

workflow

cf. Bayesian analysis using the MiHO framework: Gorda *et al.*, PRL **131**, 181902; JHEP **06**, 002

Mixing of random variables (pointwise)

Semposki, Furnstahl, and Phillips, PRC **106**, 044002

Bayesian Model (*pointwise* in density)

$$Y_i = F + \delta Y_i \qquad i \in [1, M]$$

e.g.,
1: Chiral EFT
2: pQCD

random variable corresponding to the predictions of model *i*

truth, with **prior** $F \sim \mathcal{N}[0, \sigma_f^2]$

BUQEYE **truncation error** $\delta Y_i \sim \mathcal{N}[0, \sigma_i^2]$

(all σ_i's are known and uncorrelated)

$$\vec{y} = \{y_i\}_{i=1}^{M} \qquad K_y = \mathrm{diag}(\sigma_i^2)$$

set of **model predictions** at each point and associated **inter-model covariance matrix**

$$\mathrm{pr}(f \,|\, \vec{y}, K_y) \propto \mathrm{pr}(\vec{y} \,|\, f, K_y)\, \mathrm{pr}(f)$$

Posterior

$$F \,|\, \vec{y}, K_y, K_f \sim \mathcal{N}[\mu, \Sigma]$$

Mixed Model

$$\left.\begin{aligned} \mu &\equiv \Sigma\, \vec{1}^\intercal K_y^{-1} \vec{y} \\ \Sigma &\equiv (\sigma_f^{-2} + \vec{1}^\intercal K_y^{-1} \vec{1})^{-1} \end{aligned}\right\}$$

estimation of a **common mean** from measurements of ***different* precision**

precision weighting $\longrightarrow$ $\sigma_f^{-2} \to 0$

$$\mu = \Sigma \sum_{i=1}^{M} \frac{1}{\sigma_i^2} y_i \qquad \Sigma^{-1} \equiv \sum_{i=1}^{M} \frac{1}{\sigma_i^2}$$

Pointwise Bayesian Model Mixing

Semposki, CD, Furnstahl, Melendez and Phillips, in prep.

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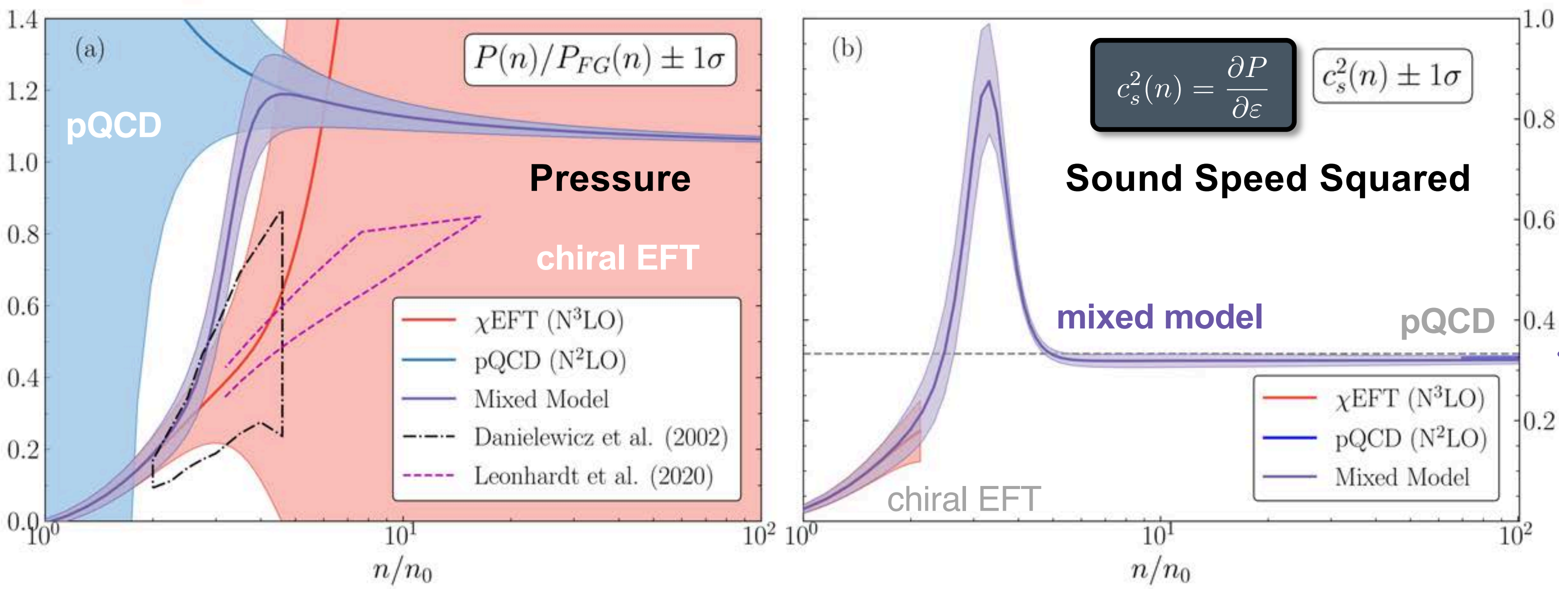
Bayesian Model Mixing combines the two predictive models in different density regions into one **overall predictive composite model!**

Open-Source Software: **Taweret** (BAND framework)

BAND Bayesian Analysis of Nuclear Dynamics



The **mixed model** approaches the **conformal limit** from below, as expected

$$c_s^2 = \frac{1}{3}$$

pQCD: two massless quark flavors

The FRG & HIC constraints are only shown as references as they do *not* provide a C.L.

A non-constant mean function is *needed* to **extend chiral EFT in** densities (series in the density)

The **two limits are well-reproduced,** but the HIC and fRG constraints do *not* favor the observed **rapid stiffening of the EOS**

Correlated Bayesian Model Mixing

Semposki, CD, Furnstahl, Melendez and Phillips, in prep.

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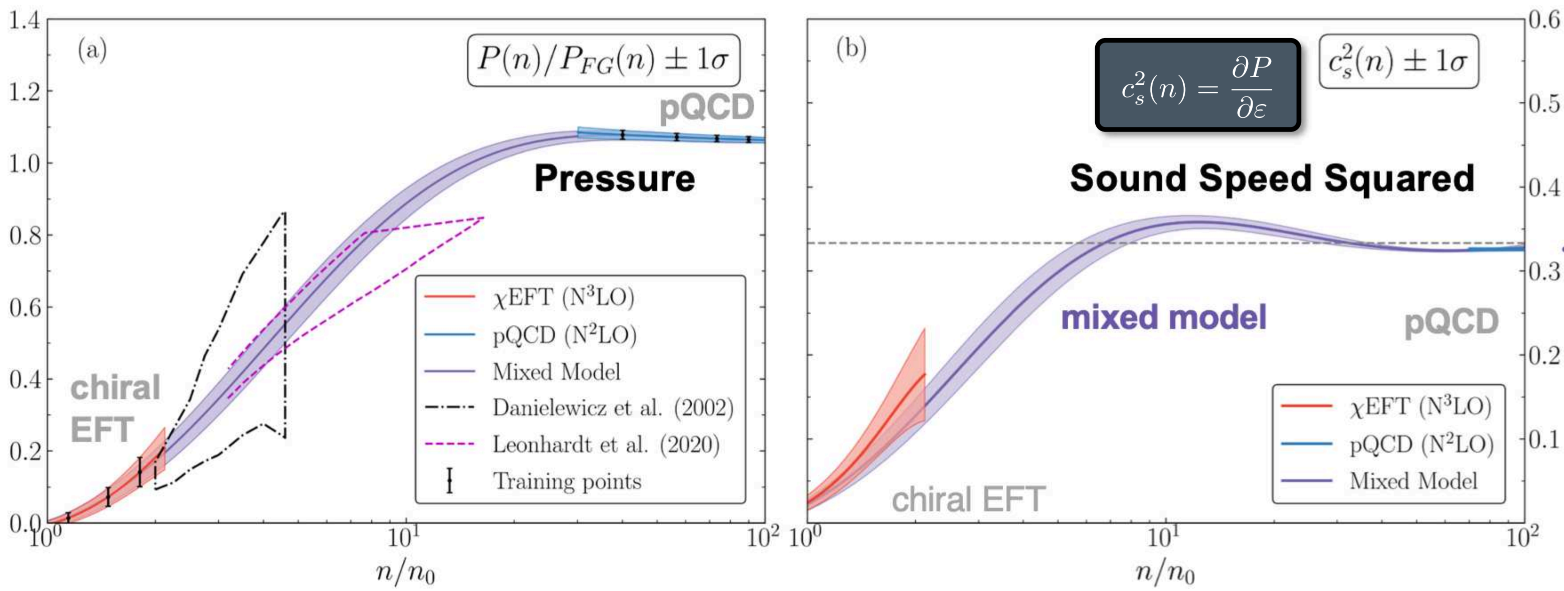
Promising method for **constructing globally predictive, QCD-based EOSs** with full UQ **to study the structure and evolution of neutron stars**

Much-needed **microscopic input for simulations** of supernovae and mergers

Open-source software soon available via:

BAND
Bayesian Analysis of Nuclear Dynamics



The **mixed model** approaches the

$$c_s^2 = \frac{1}{3}$$

conformal limit from below, as expected

pQCD:
two massless quark flavors

The FRG & HIC constraints are only shown as references as they do *not* provide a C.L.

New GP-based mixing uses the two models' covariance structure *and* GP prior on the truth

Requires **only a few GP training points** in the regions **where the to-be-mixed theories are predictive** (cf. error bars)

Take-away points

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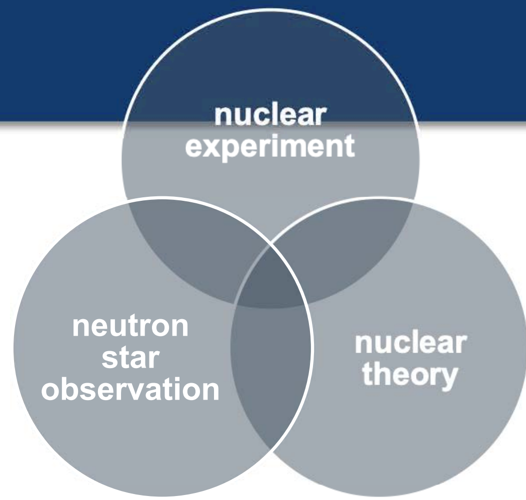
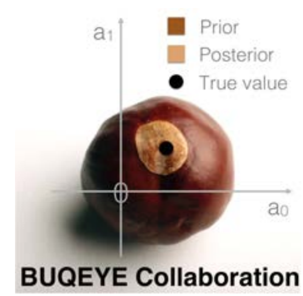
nuclear precision
multi-messenger
exascale
FRIB

} era



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

1. Upcoming observational and experimental campaigns will provide **stringent constraints** on the properties of neutron stars.
2. Chiral EFT enables **microscopic calculations** of nuclei and infinite matter at $n \lesssim 2n_0$ **with quantified uncertainties** to interpret these empirical constraints.
3. **Automated MBPT**: efficient EOS calculations across a wide range of densities, isospin asymmetries, and temperatures, as well as nuclear interactions.
4. Bayesian methods: powerful tools for quantifying & propagating **correlated uncertainties** in EFT calculations (facilitated by fast & accurate emulators).



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More details? Recent review article

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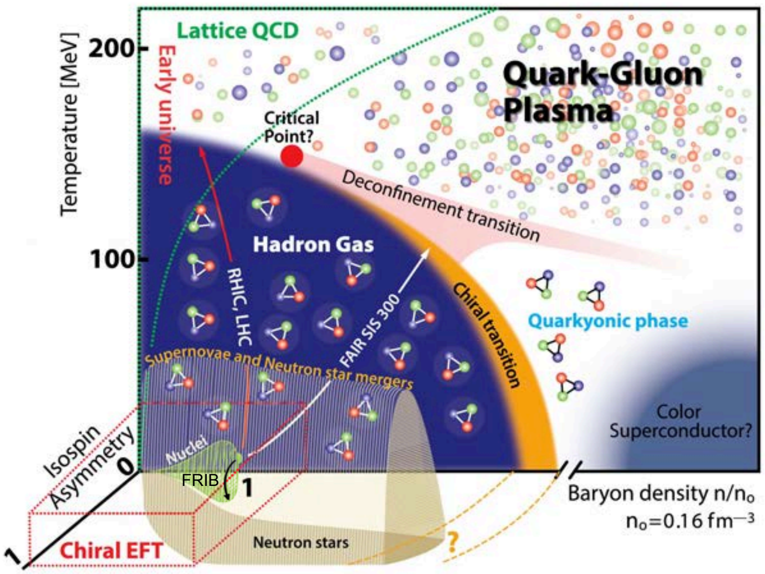

Keywords:

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

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