Quantifying uncertainties in the nuclear-matter equation of state

Berkeley
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Christian Drischler

Online S@INT | Zoom conference | May 28, 2020

nuclear matter

astrophysics
neutron stars,
supernovae, …

EFT

nuclear physics
structure & reactions
of nuclei

correlated EFT uncertainties

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ENERGY

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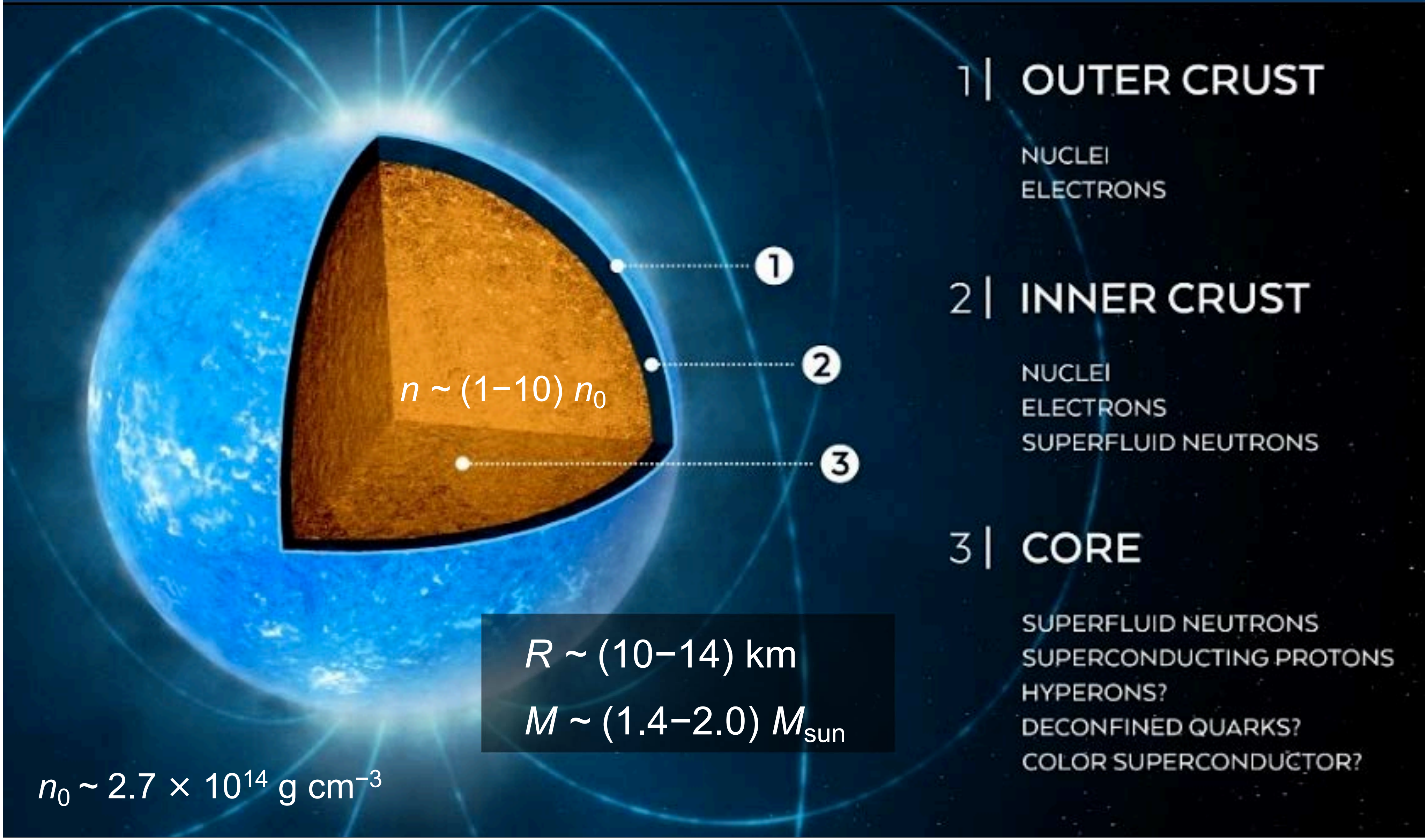
Neutron stars

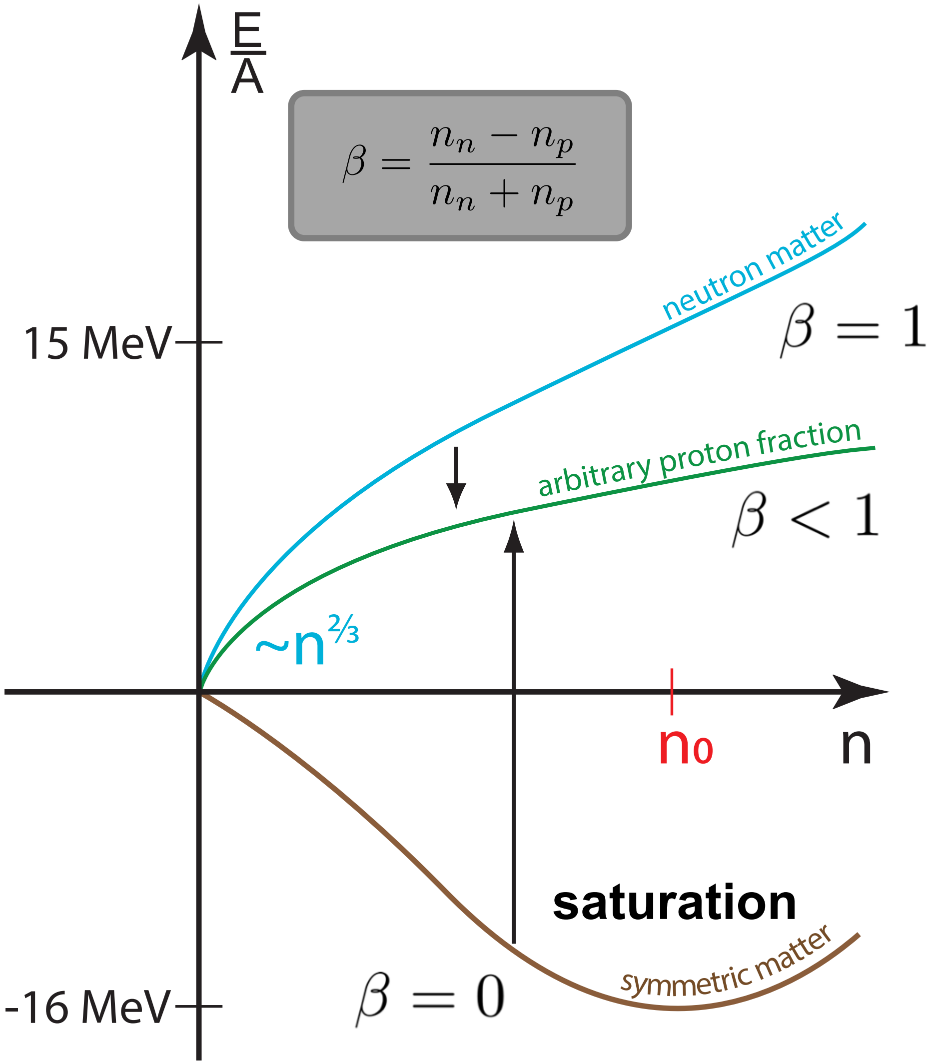
e.g., Watts *et al.*, Rev. Mod. Phys. **88,** 021001



Quantifying uncertainties in the nuclear-matter equation of state

Landscape of nuclear matter

e.g., Hebeler, Holt *et al.*, ARNP **65**, 457



great progress in predicting the **EOS** of infinite matter and the structure of **neutron stars** at densities $\lesssim n_0$

Hebeler, Lattimer *et al.*, APJ **773**, 11
Carbone, Rios *et al.*, PRC **88**, 044302
Hagen, Papenbrock *et al.* PRC **89**, 014319
Coraggio, Holt *et al.*, PRC **89**, 044321
Wellenhofer, Holt *et al.*, PRC **89**, 064009
CD, Carbone *et al.*, PRC **94**, 054307
Ekström, Hagen *et al.*, PRC **97**, 024332
Roggero, Mukherjee *et al.*, PRL **112**, 221103
CD, Hebeler *et al.*, PRL **122**, 042501
Lonardoni, Tews *et al.* PRR **2**, 022033(R)
Piarulli, I. Bombaci *et al.*, PRC **101**, 045801
…

But: existing predictions **only** provided **rough estimates** for the with-density-growing EFT truncation error, without accounting for **correlations**

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Landscape of nuclear matter

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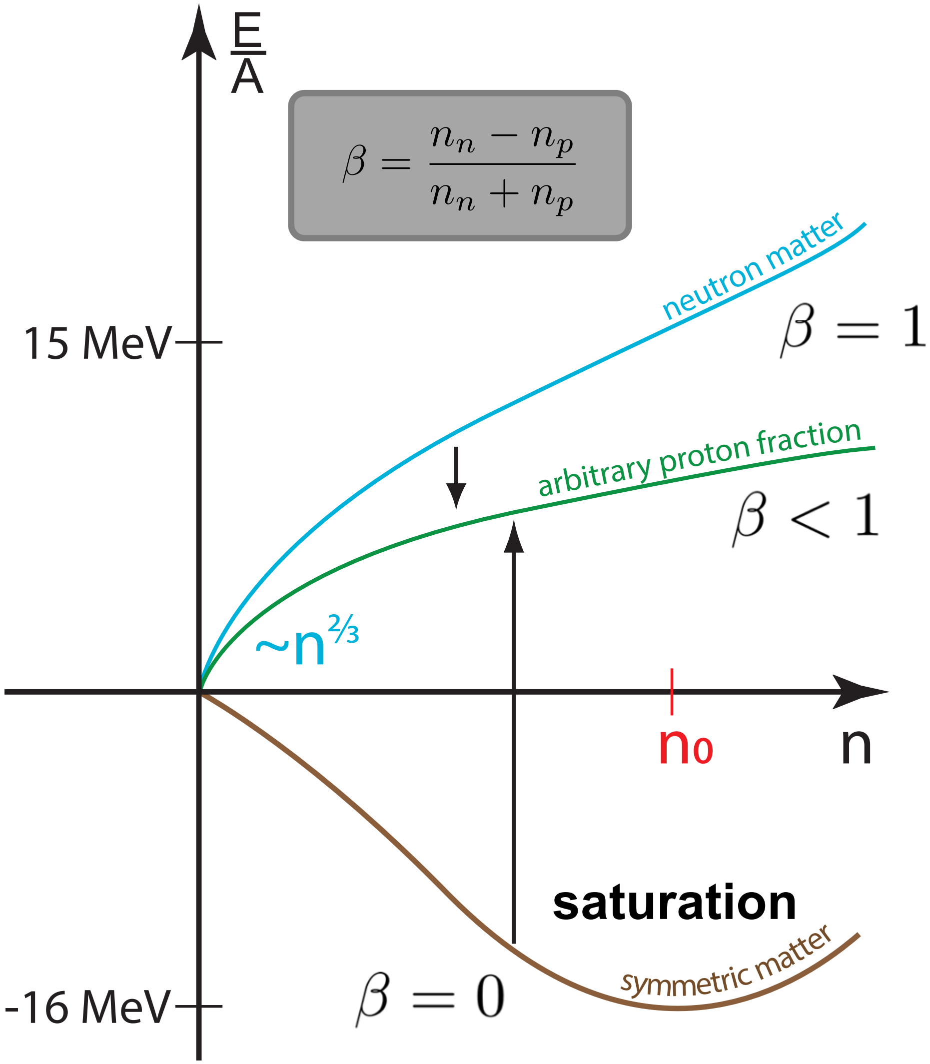

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Hebeler, Lattimer *et al.*, APJ **773**, 11
Carbone, Rios *et al.*, PRC **88**, 044302

needed: *statistically* **meaningful comparisons** between nuclear **theory** and recent **observational constraints**

Lonardoni, Tews *et al.* PRR **2**, 022033(R)
Piarulli, I. Bombaci *et al.*, PRC **101**, 045801
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But: existing predictions **only** provided **rough estimates** for the with-density-growing EFT truncation error, without accounting for **correlations**

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Direct detection of gravitational waves

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ligo.caltech.edu

multi-messenger astronomy

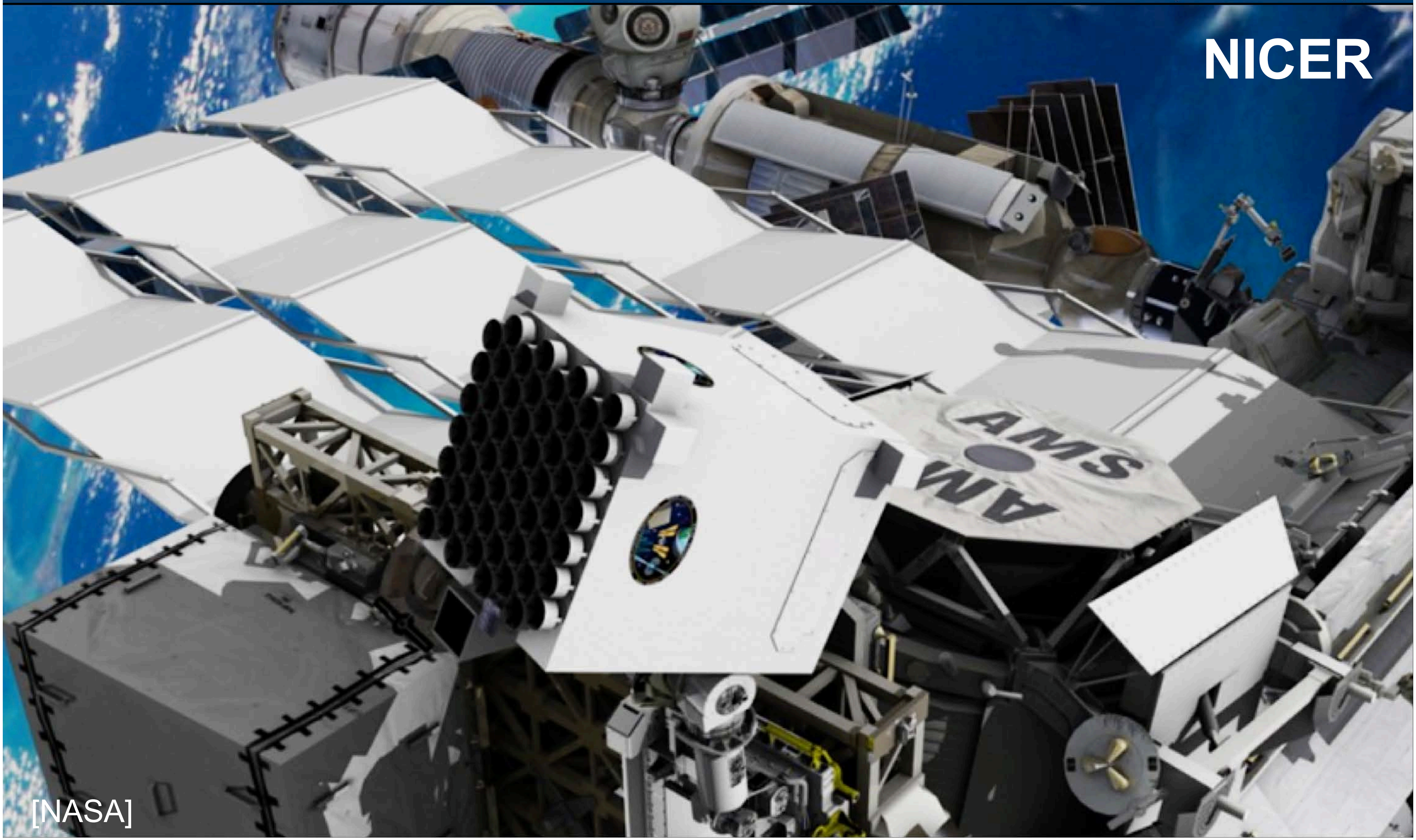
+ Virgo
+ GEO600
+ …

Binary Neutron-Star Merger

Quantifying uncertainties in the nuclear-matter equation of state

(Simultaneous) Mass-radius constraints

see also Greif *et al.*, MNRAS **485**, 4



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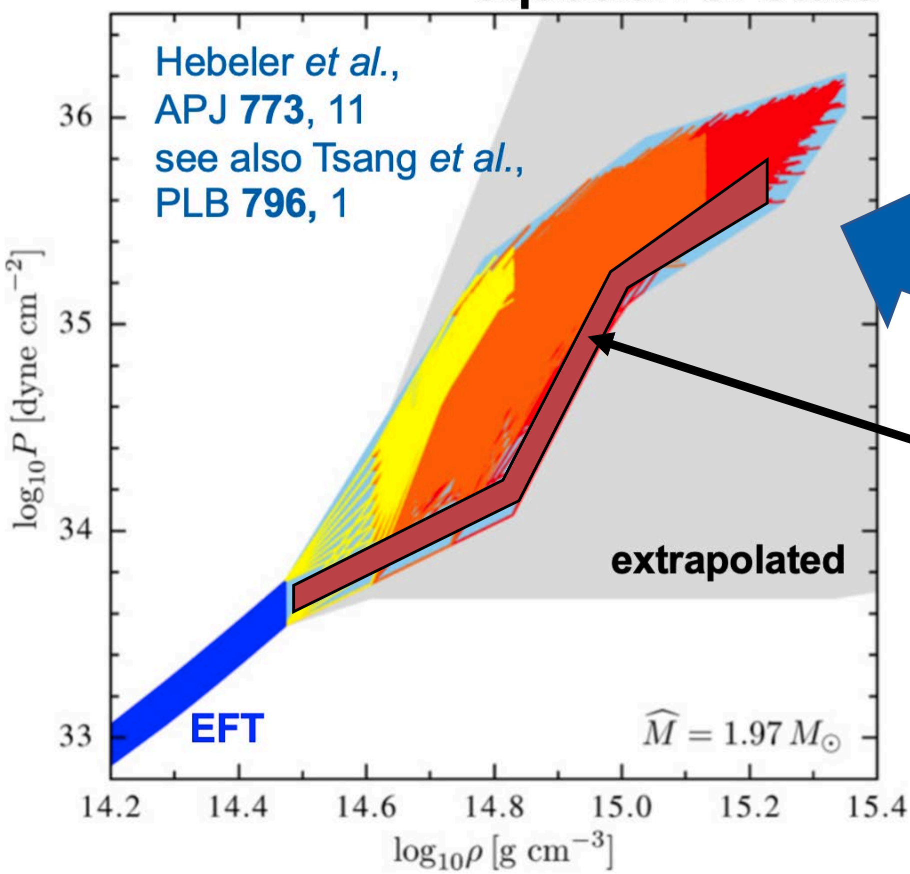
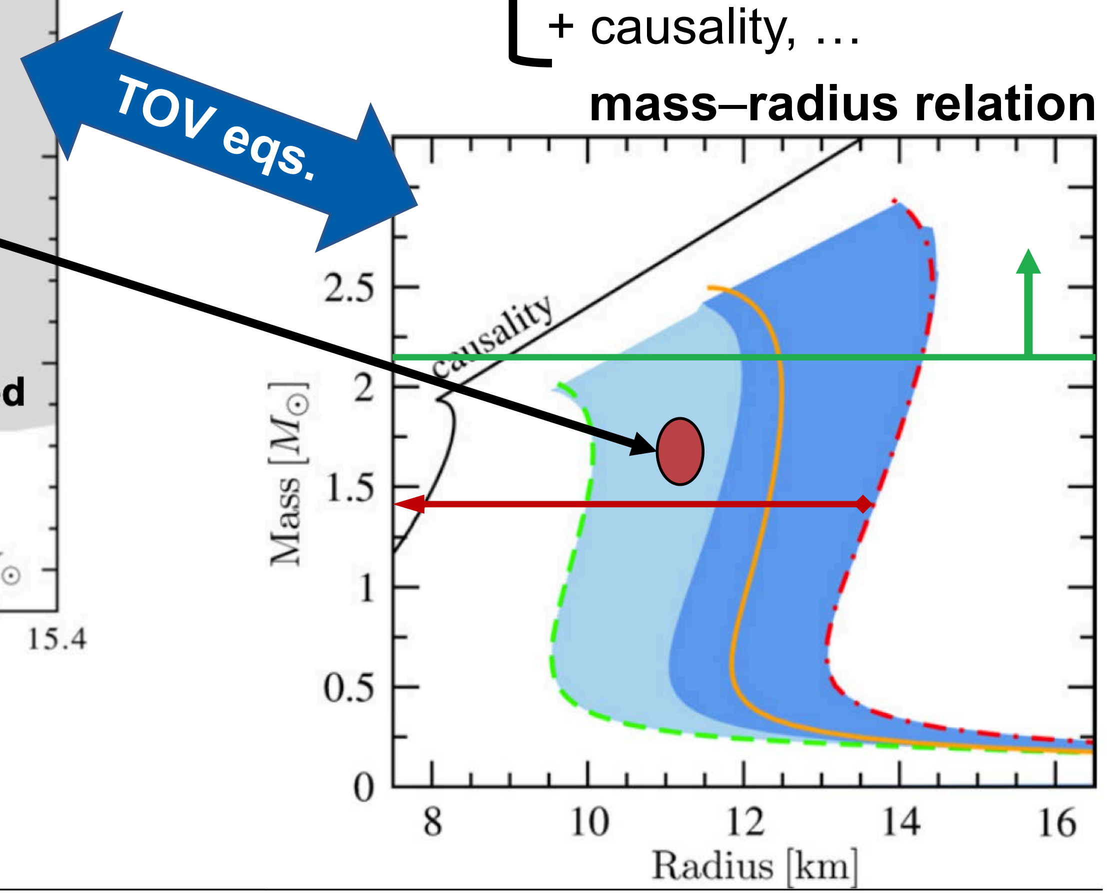
equation of state



constraints from
- + NICER
- + mass measurements
- + GW detections
- + causality, …



Essick, Tews *et al.*, arXiv:2004.07744
Miller, Lamb, Dittmann *et al.*, APJ **887**, L24
Raaijmakers, Riley, Watts *et al.*, APJ **887**, L22
Riley, Watts, Bogdanov *et al.* APJ **887**, L21; …

Quantifying uncertainties in the nuclear-matter equation of state

ISNET: Bringing statisticians and physicists together!

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frib.msu.edu

ISNET 2020

Information and Statistics in Nuclear Experiment and Theory (ISNET 8)

Facility for Rare Isotope Beams
Michigan State University
December 14 to 18, 2020

Local Organizing Committee:

Pawel Danielewicz
Dean Lee
Scott Pratt
Frederi Viens
Morten Hjorth-Jensen
Witek Nazarewicz
Betty Tsang

Bayesian Inference in Subatomic Physics – A Marcus Wallenberg Symposium at Chalmers
September 17-20, 2019, organized by: A. Ekström, C. Forssén, and S. Wesolowski
INT Program INT-16-2a: *Bayesian Methods in Nuclear Physics*

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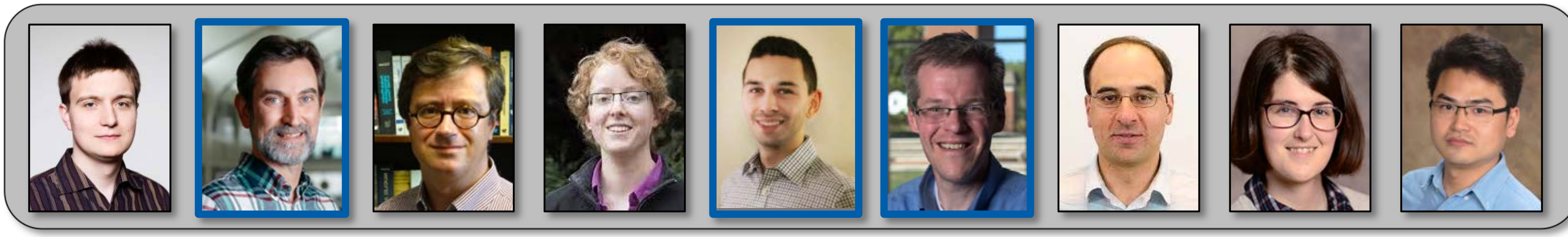
Thanks to my collaborators!

buqeye.github.io

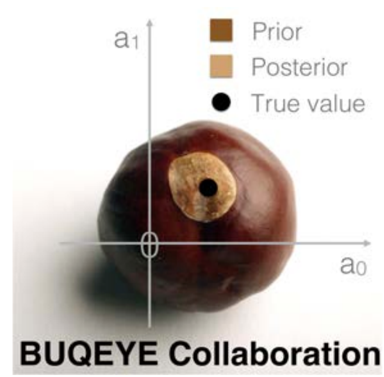


CD, Furnstahl, Melendez, and Phillips

How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties, arXiv:2004.07232.

CD, Melendez, Furnstahl, and Phillips

Effective Field Theory Convergence Pattern of Infinite Nuclear Matter, arXiv:2004.07805.



Bayesian
Uncertainty
Quantification:
Errors for
Your
EFT

UQ framework available at https://buqeye.github.io

Quantifying uncertainties in the nuclear-matter equation of state

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CD, Haxton, McElvain, Mereghetti *et al.*, arXiv:1910.07961

nuclear-matter equation of state
statistically rigorous UQ for chiral EFT

many-body perturbation theory
controlled and computational efficient method
many-body uncertainty estimates

chiral effective field theory
systematic expansion of nuclear forces
order-by-order nuclear potentials

CalLat NPLQCD ...

observables

many-body framework

effective field theory

quantum chromodynamics

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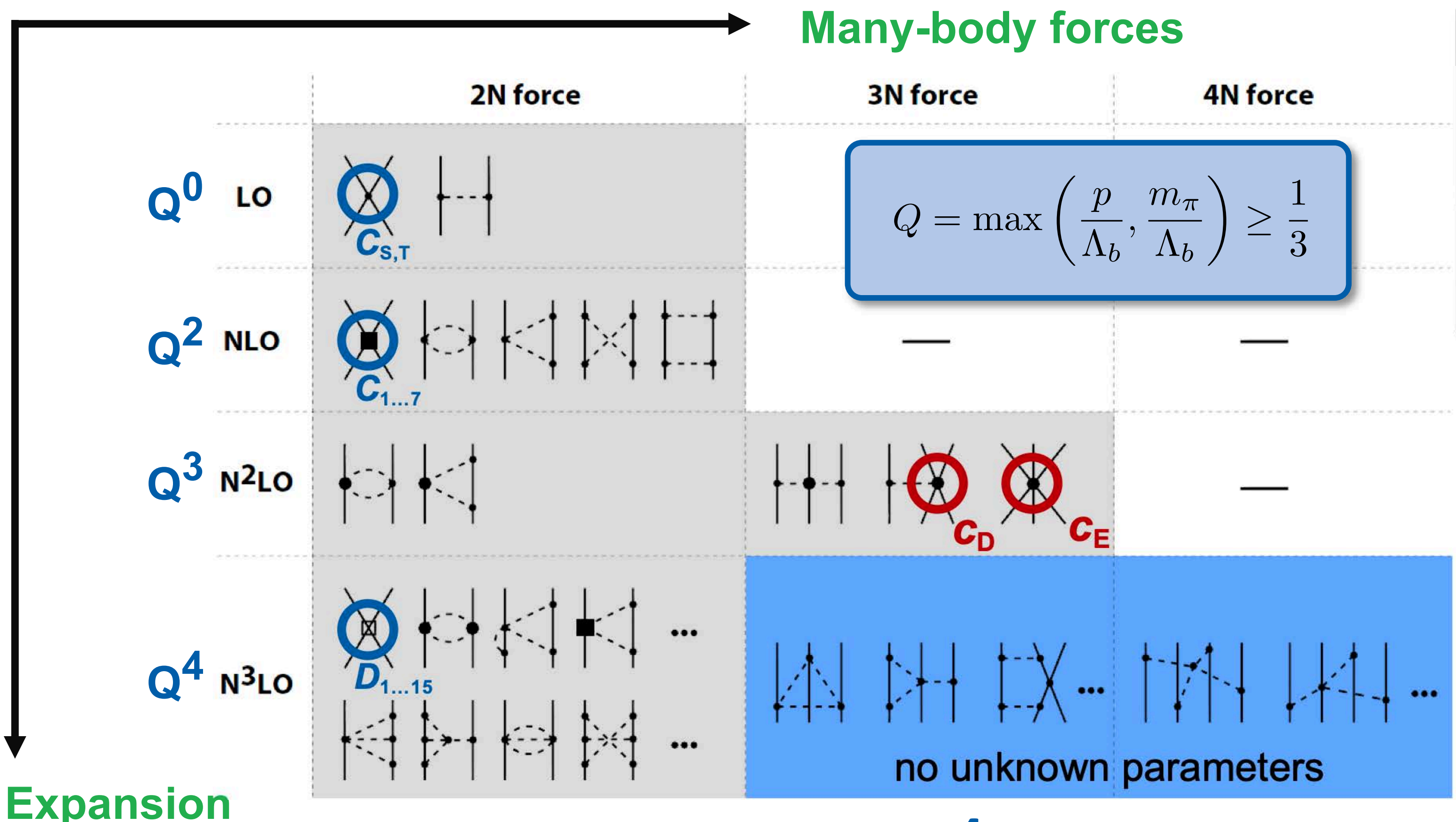
Hierarchy of nuclear forces in chiral EFT

e.g., Machleidt, Entem, Phys. Rep. **503**, 1



S. Weinberg

… and ongoing work at N^{4}LO and even N^{5}LO…

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

Quantifying uncertainties in the nuclear-matter equation of state

Including correlations in UQ is important!

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CD, Melendez *et al.*, arXiv:2004.07805

$$\delta y_{i\geqslant 2}(x) = \max_{2\leqslant j\leqslant i}\left(Q^{i+1}(x)|y_0(x)|,\, Q^{i+1-j}(x)\,|\Delta y_j(x)|\right)$$

$$\delta y_0(x) = Q^2(x)\,|y_0(x)|$$

Epelbaum, Krebs, Meißner, EPJ A 51, 53

x : generic sampling point
$y_n(x)$: n-th order prediction

The "standard EFT" uncertainty does *not* account for correlations:

Type-x:

Correlations between $y(x)$ and $y(x')$; *e.g.*, $y = E/A(n^{(')})$;

quantified and **propagated** using the ML truncation-error model proposed by BUQEYE

Melendez, Furnstahl *et al.*, PRC **100**, 044001
Melendez's GSUM, github.com/buqeye/gsum

Type-y:

Correlations between discrete observables $y_i(x)$ and $y_j(x')$; *e.g.*, an observable i and its derivative j

extension of the truncation error model: now **quantified** and **propagated** using **multi-output Gaussian Processes** (GPs)

github.com/buqeye/nuclear-matter-convergence

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BUQEYE's EFT truncation-error model

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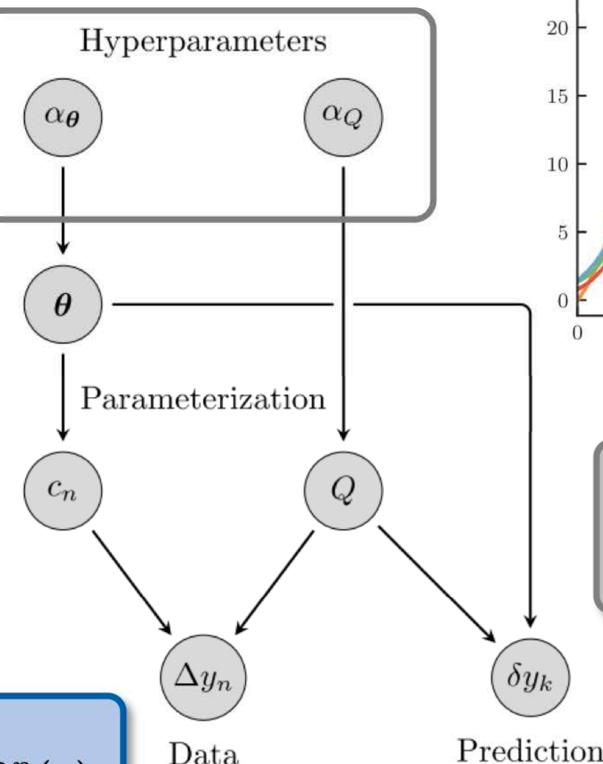
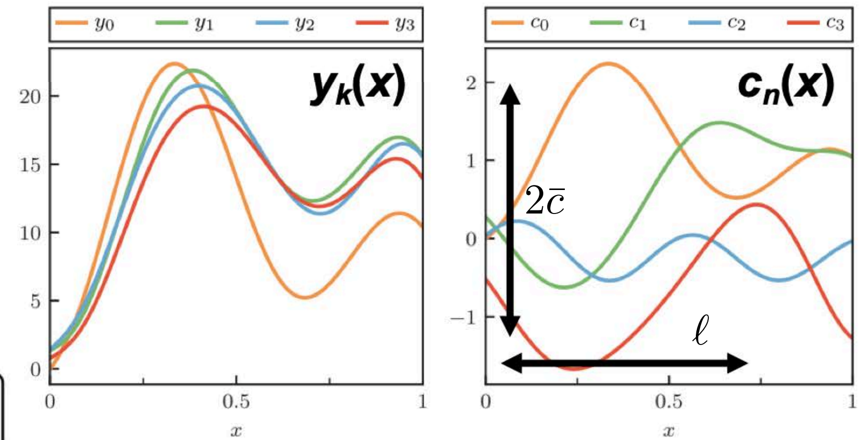
Melendez, Furnstahl *et al.*, PRC **100**, 044001

prior information

learn ϑ and Q from data





$$c_n(x) = \frac{\Delta y_n(x)}{y_{\mathrm{ref}}(x) Q^n(x)}$$

$$c_n(x) \,|\, \bar{c}^2, \ell \overset{\mathrm{iid}}{\sim} \mathcal{GP}[0, \bar{c}^2 r(x, x'; \ell)]$$

model all $c_n(x)$ as independent draws from a single GP

$$y_k(x) = y_{\mathrm{ref}}(x) \sum_{n=0}^{k} c_n(x) Q^n(x)$$

calculate observable $y_k(x)$ order by order

evaluate geometric series

$$\delta y_k(x) = y_{\mathrm{ref}}(x) \sum_{n=k+1}^{\infty} c_n(x) Q^n(x)$$

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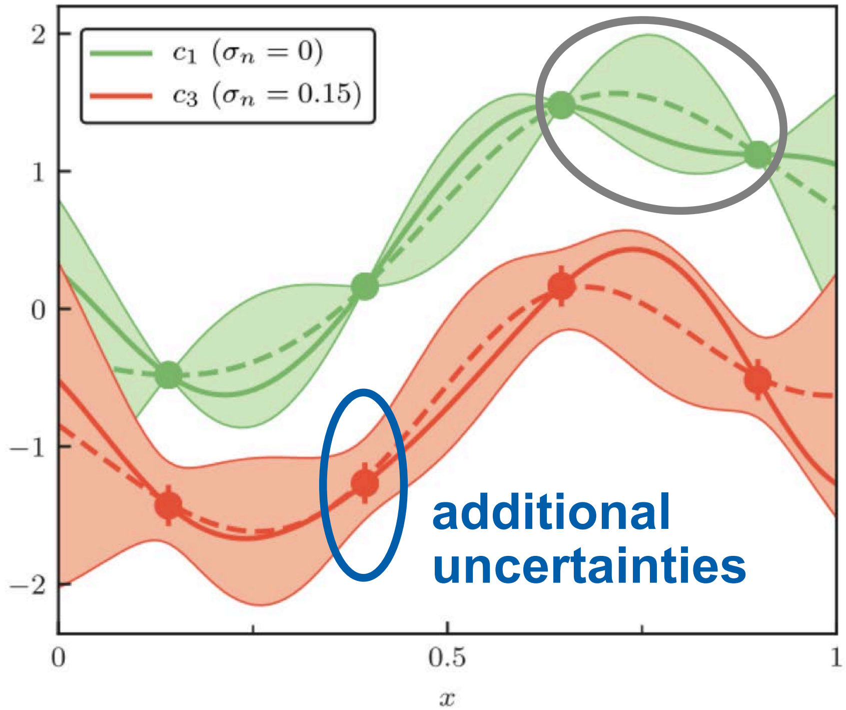
Using GPs for interpolation

CD, Melendez *et al.*, arXiv:2004.07805

interpolation uncertainties



additional (many-body) **uncertainties** can be **easily included**

GPs are **closed** under **differentiation**

straightforward to compute derivatives with correlations accounted for

e.g., **pressure** and **speed of sound**

» **in contrast to other methods**

Gaussian Process interpolates the EOS while quantifying uncertainties, including **to-all-orders EFT truncation errors**

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

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Quantifying uncertainties in the nuclear-matter equation of state

Efficient Monte Carlo framework

CD, Hebeler, Schwenk, PRL **122**, 042501

efficient evaluation of **MBPT diagrams**
with **NN**, **3N**, and **4N forces** (single-particle basis)

- **implementing diagrams** has become **straightforward** (incl. particle-hole terms)
- multi-dimensional momentum integrals: (improved) Lepage's VEGAS algorithm
- **controlled computation** of arbitrary interaction and many-body diagrams

EOS up to high orders

automatic code generation

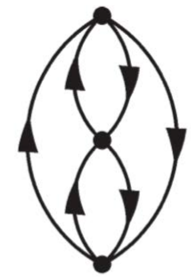
analytic form of the diagrams

Quantifying uncertainties in the nuclear-matter equation of state

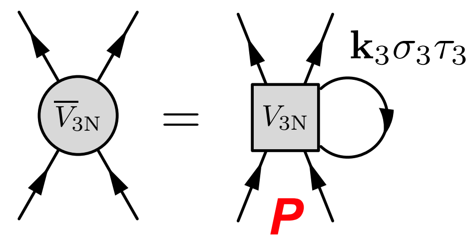
Significant challenges are past!

CD, Hebeler, Schwenk, PRL **122**, 042501

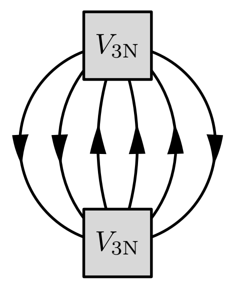
Higher orders: particle-hole contributions
Coraggio *et al.*, PRC **89**, 044321; Holt, Kaiser, PRC **95**, 034326



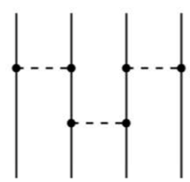
No approximations for 3N normal ordering
CD *et al.*, PRC **93**, 054314; Holt *et al.*, PRC **81**, 024002



Include residual 3N diagram(s)
Hagen *et al.*, PRC **89**, 014319; Kaiser, EPJ A **48**, 58



Higher many-body forces
Hebeler *et al.*, PRC **91**, 044001



development of a novel Monte Carlo framework

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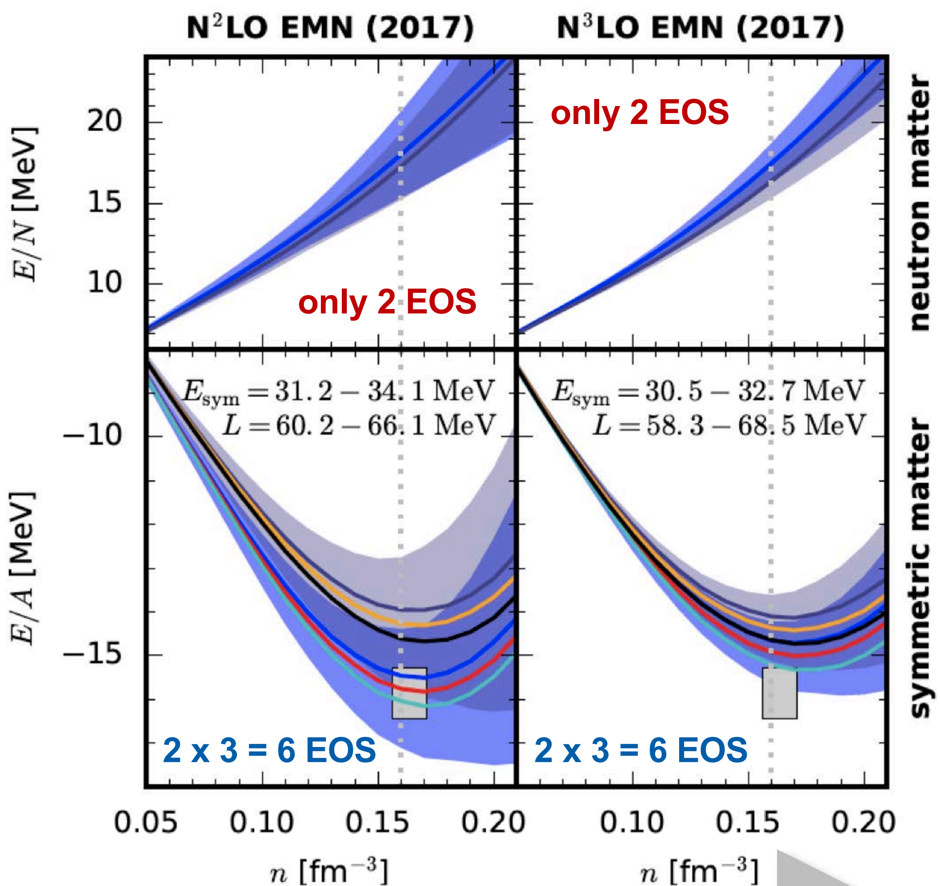
Many-body input of our UQ

CD, Hebeler, Schwenk, PRL **122**, 042501



extended up to $2n_0$

use the Monte Carlo framework to evaluate the EOS up to N^{3}LO

bare N^{2}LO / N^{3}LO EMN potentials

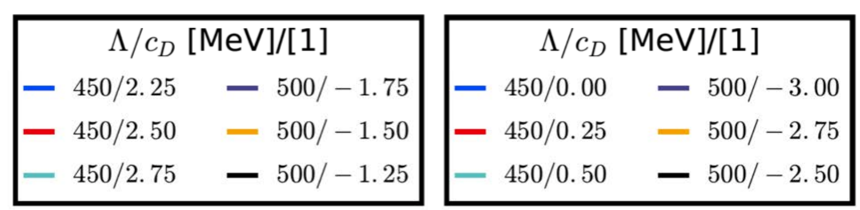
Entem, Machleidt, Nosyk, PRC **96**, 024004

Hoppe, CD, Furnstahl *et al.*, PRC **96**, 054002

fit 3N interactions to the triton and nuclear **saturation point**

identified (c_D,c_E) which **saturate** close to the empiral **saturation point**

3 Hamiltonians available for each cutoff and chiral order; **in total: 12**



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Quantifying uncertainties in the nuclear-matter equation of state

Extracting the observable coefficients

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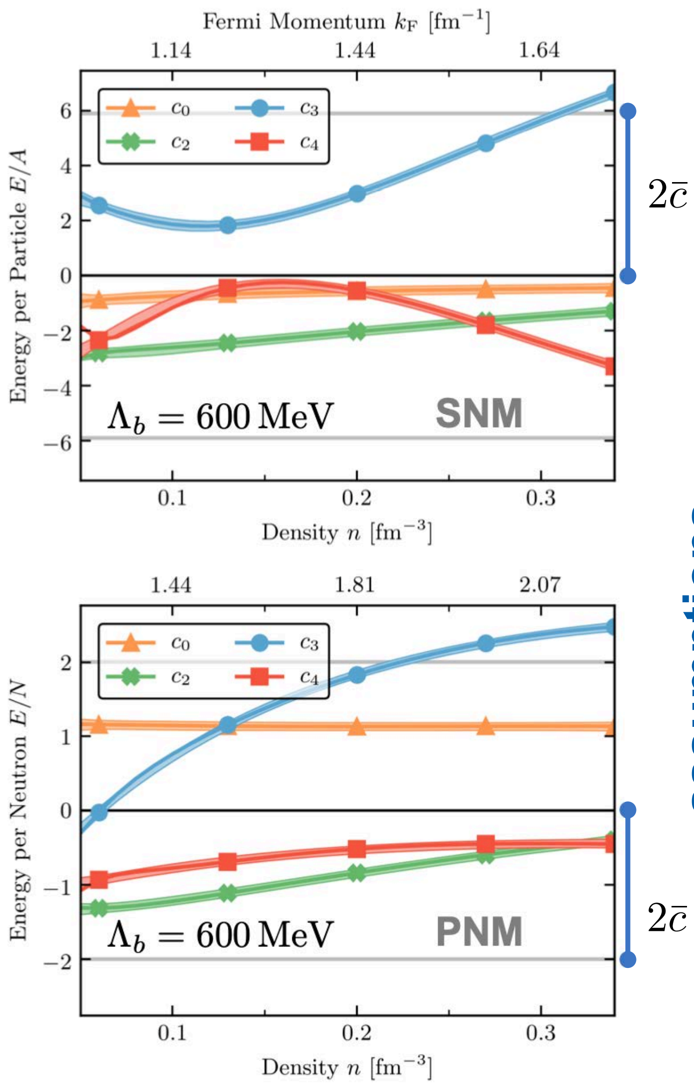
CD, Melendez *et al.*, arXiv:2004.07805



$$c_n(x) = \frac{\Delta y_n(x)}{y_\mathrm{ref}(x) Q^n(x)}$$

We need to choose:

assumptions

feedback

x : γk_F or $n = g\dfrac{k_\mathrm{F}^3}{6\pi^2}$ $\quad \gamma > 0$

stationary kernel: same curviness across entire range

y

$y_\mathrm{ref}(x)$: $y_\mathrm{ref}(k_\mathrm{F}) = 16\,\mathrm{MeV} \times \left(\dfrac{\gamma k_\mathrm{F}}{k_{\mathrm{F},0}}\right)^2$

naturalness: overall scale for $c_n(x)$

$Q(x)$: $Q(k_\mathrm{F}) = \dfrac{p}{\Lambda_b}$ $\quad p = \gamma k_\mathrm{F}$

What is the *soft scale* of nuclear matter?

Trust, but verify
model-checking diagnostics $\quad \gamma = 1$

Quantifying uncertainties in the nuclear-matter equation of state

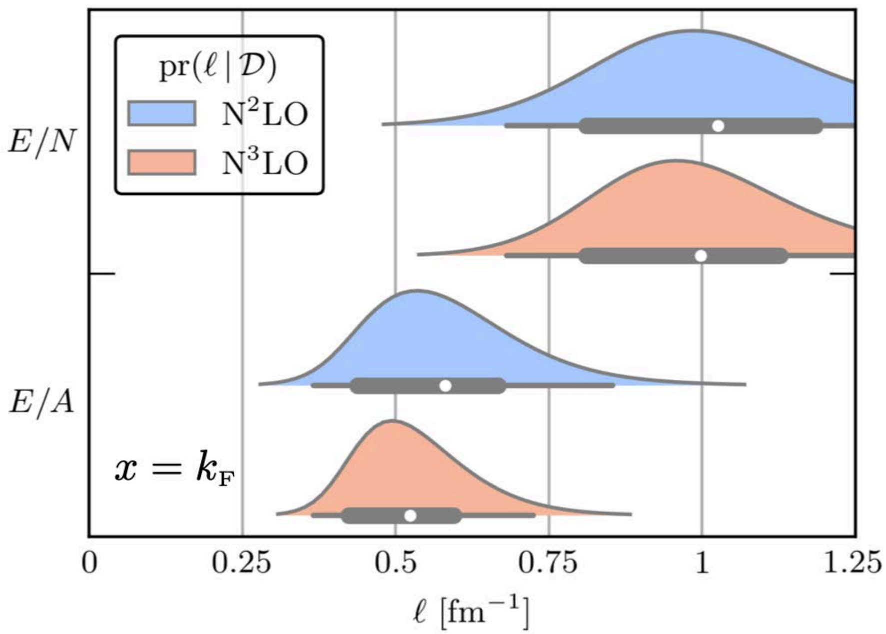
Bayesian inference from the data

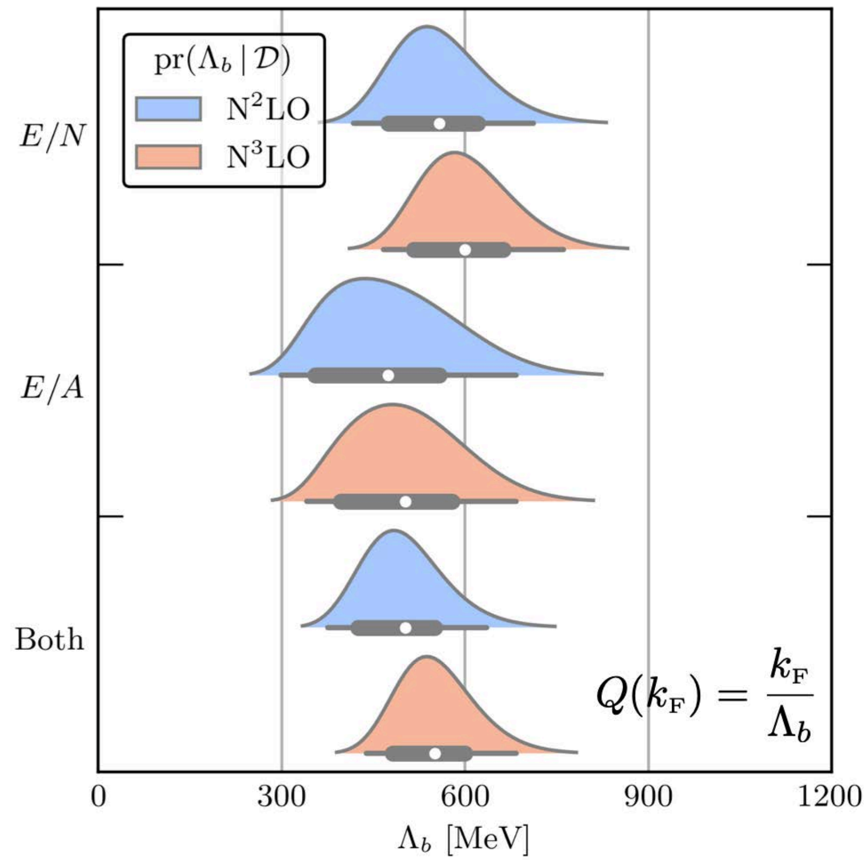
How correlated is nuclear matter ?

$\mathrm{pr}\,(\ell \,|\, \mathcal{D})$
correlation length

Where does the EFT break down ?

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





to be compared with

$$k_\mathrm{F}^\mathrm{max} = \begin{cases} 2.2\,\mathrm{fm}^{-1} & \text{PNM} \\ 1.7\,\mathrm{fm}^{-1} & \text{SNM} \end{cases}$$

Quantifying uncertainties in the nuclear-matter equation of state

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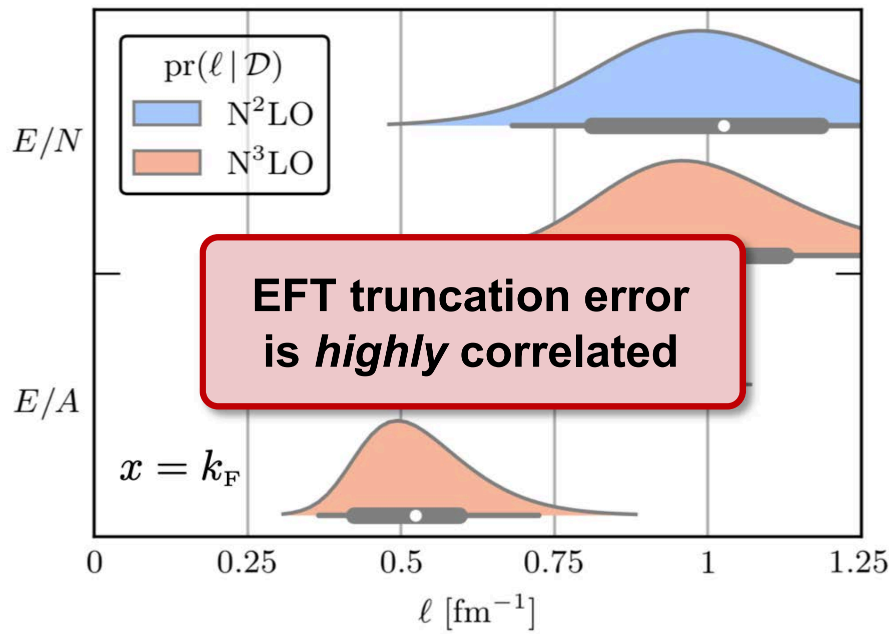
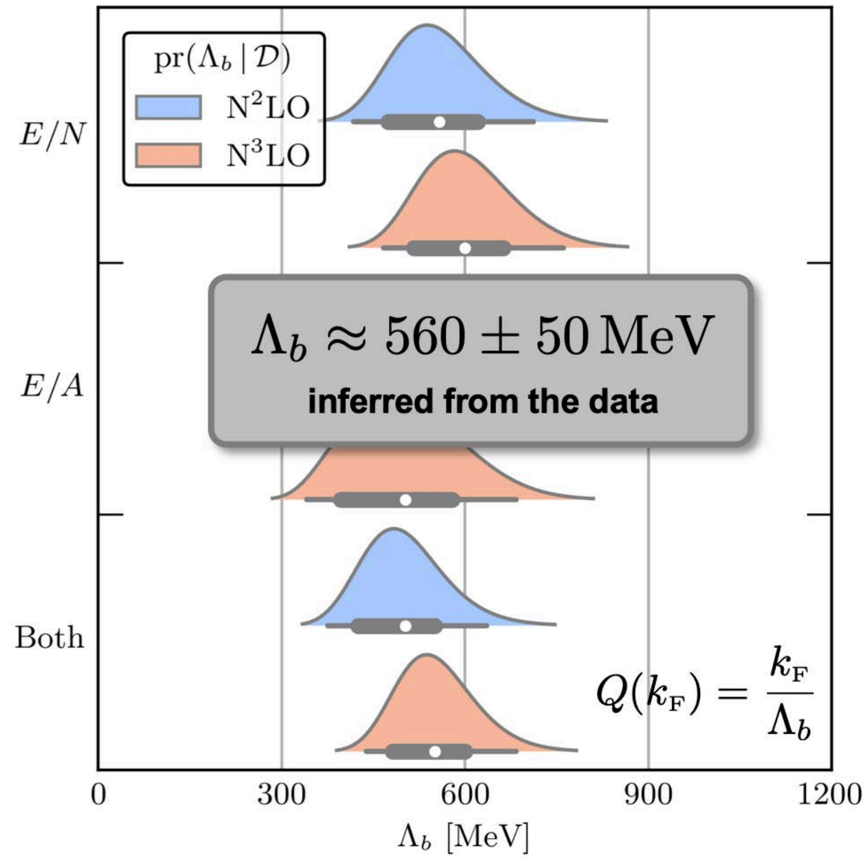


EFT truncation error is *highly* correlated



$\Lambda_b \approx 560 \pm 50\,\mathrm{MeV}$
inferred from the data

to be compared with

$$k_\mathrm{F}^\mathrm{max} = \begin{cases} 2.2\,\mathrm{fm}^{-1} & \mathrm{PNM} \\ 1.7\,\mathrm{fm}^{-1} & \mathrm{SNM} \end{cases}$$

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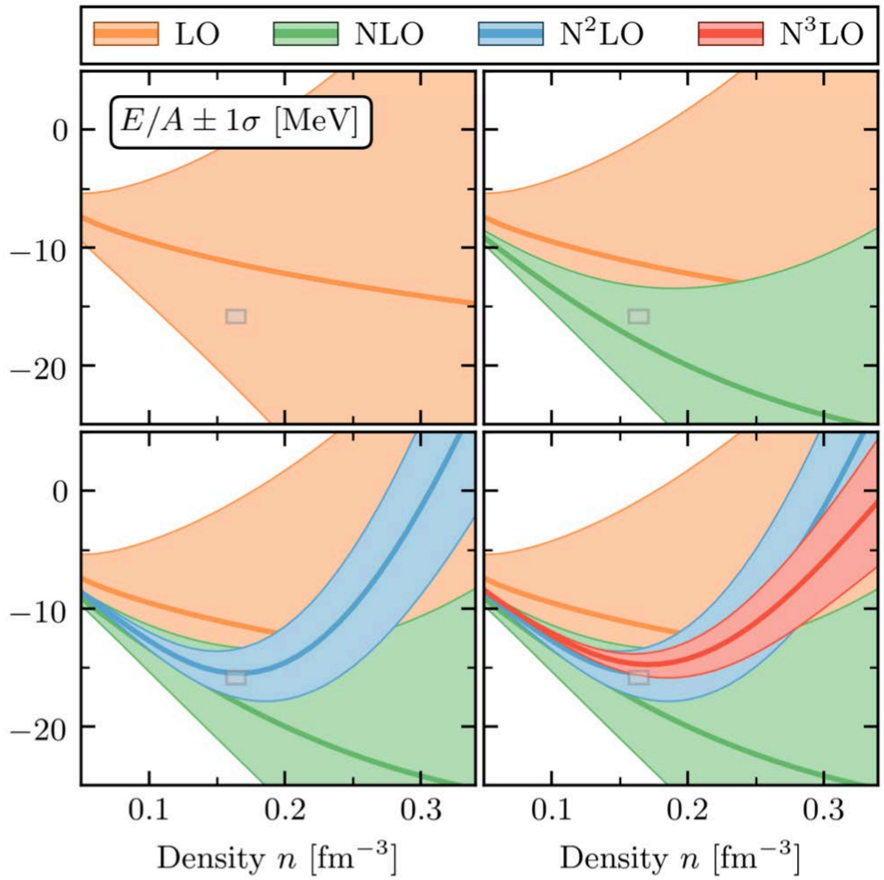
SNM and the saturation point

CD, Melendez *et al.*, arXiv:2004.07805

Λ = 450 MeV



$$\mathrm{pr}\left(\frac{E}{A}(n_0), n_0 \,|\, \mathcal{D}\right)$$

see also CD, Hebeler, Schwenk, PRL **122**, 042501

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SNM and the saturation point

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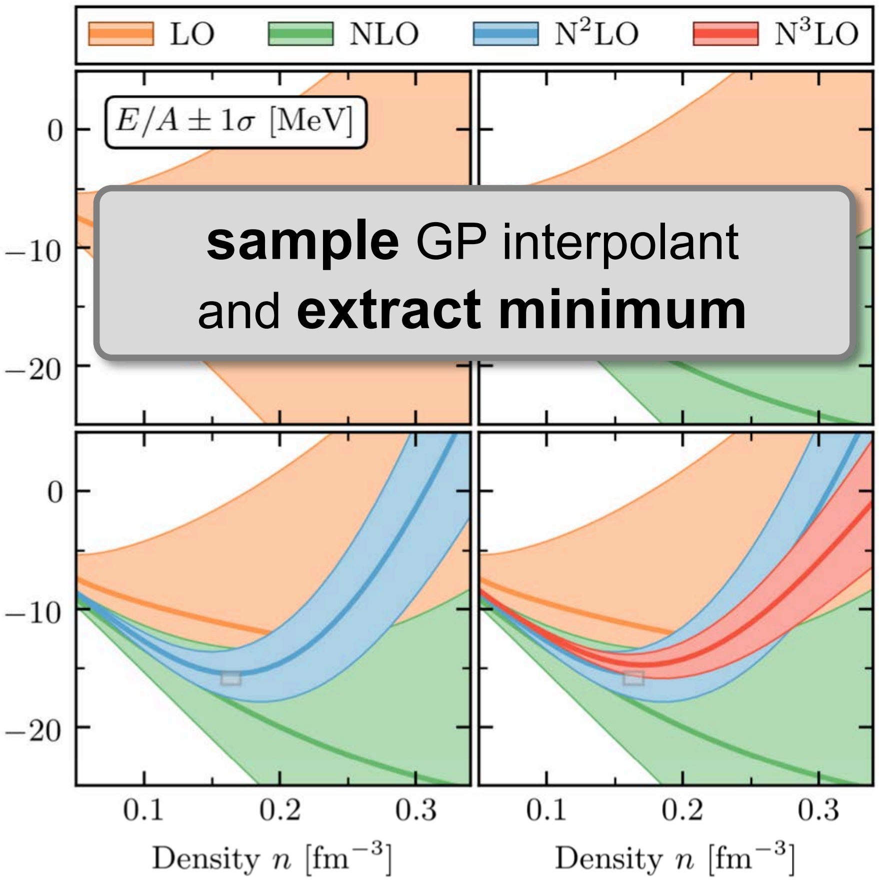
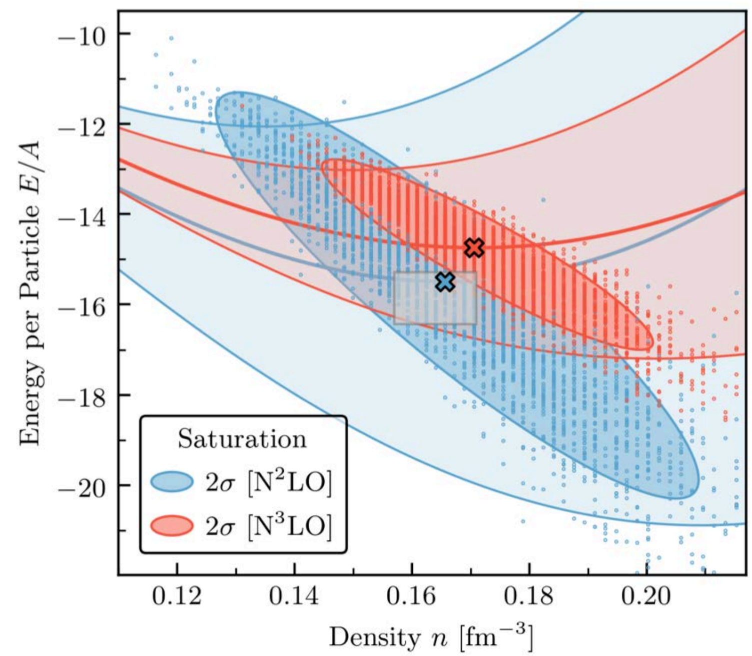


sample GP interpolant and **extract minimum**



two-dimensional Gaussian

$$\begin{bmatrix} n_0 \\ \frac{E}{A}(n_0) \end{bmatrix} \approx \begin{bmatrix} 0.173 \\ -14.9 \end{bmatrix} \qquad \Sigma \approx \begin{bmatrix} 0.014^2 & -0.014 \\ -0.014 & 1.1^2 \end{bmatrix}$$

see also CD, Hebeler, Schwenk, PRL **122**, 042501

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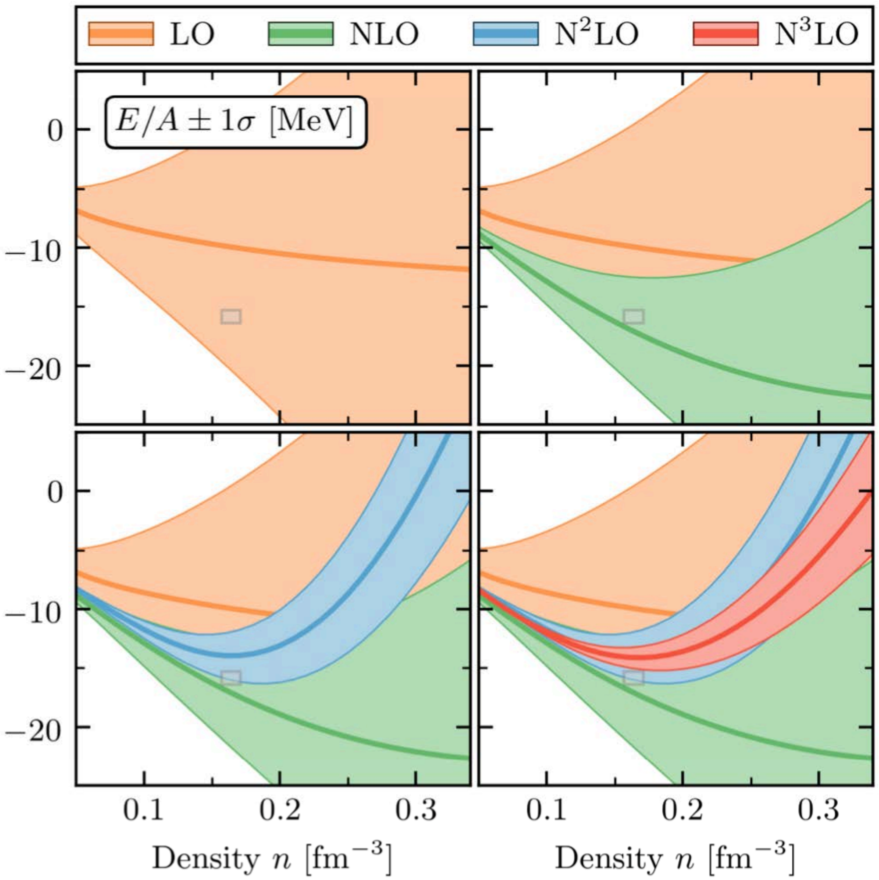
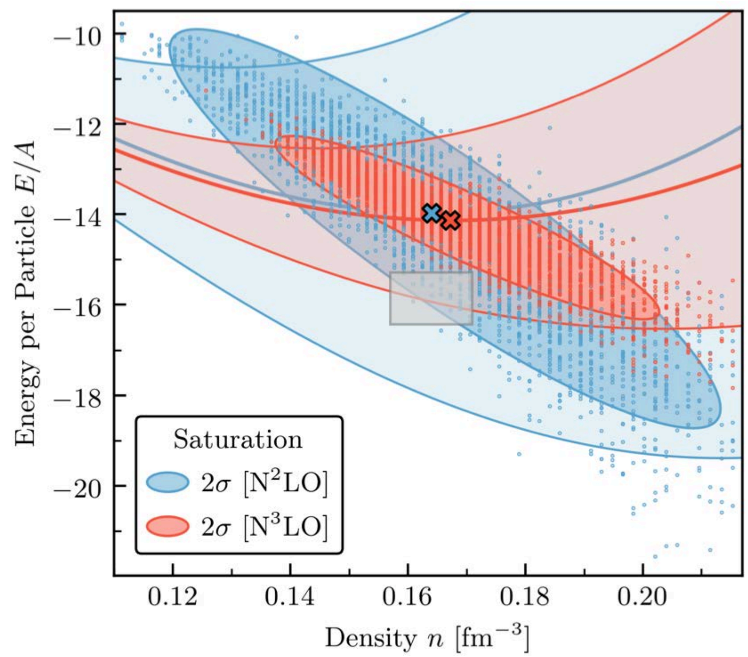


$$\mathrm{pr}\left(\frac{E}{A}(n_0), n_0 \,|\, \mathcal{D}\right)$$



two-dimensional Gaussian

$$\begin{bmatrix} n_0 \\ \frac{E}{A}(n_0) \end{bmatrix} \approx \begin{bmatrix} 0.170 \\ -14.3 \end{bmatrix} \qquad \Sigma \approx \begin{bmatrix} 0.016^2 & -0.015 \\ -0.015 & 1.0^2 \end{bmatrix}$$

see also CD, Hebeler, Schwenk, PRL **122**, 042501

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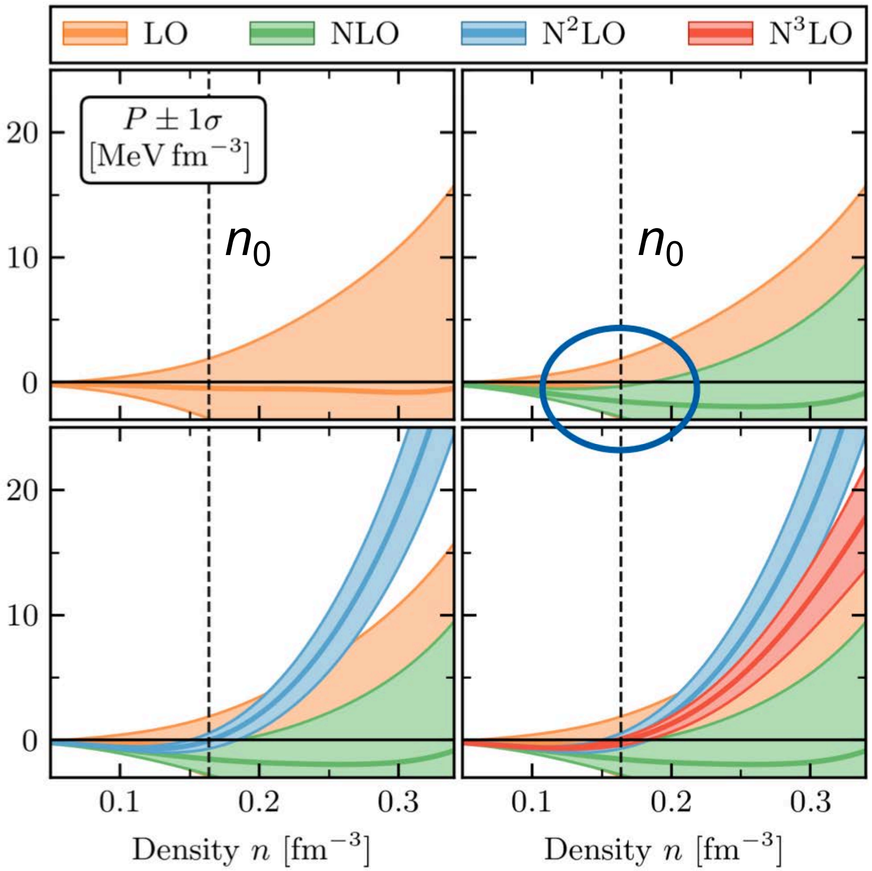
Pressure of SNM

CD, Melendez *et al.*, arXiv:2004.07805

Λ = 500 MeV



$$P(n) = n^2 \frac{\mathrm{d}}{\mathrm{d}n}\frac{E}{A}(n)$$

!

LO / NLO: nuclear saturation at ~n_0 could be achieved within the large uncertainties

possible zero-crossing over a wide range of densities suggests that the nuclear **saturation point is *fine tuned***

N^2LO / N^3LO: consistently within the bands of the previous orders, $n \lesssim n_0$, but diverge beyond

be careful: bands are difficult to gauge due to the *long* correlation length (small effective sample size)

» **model-checking diagnostics**

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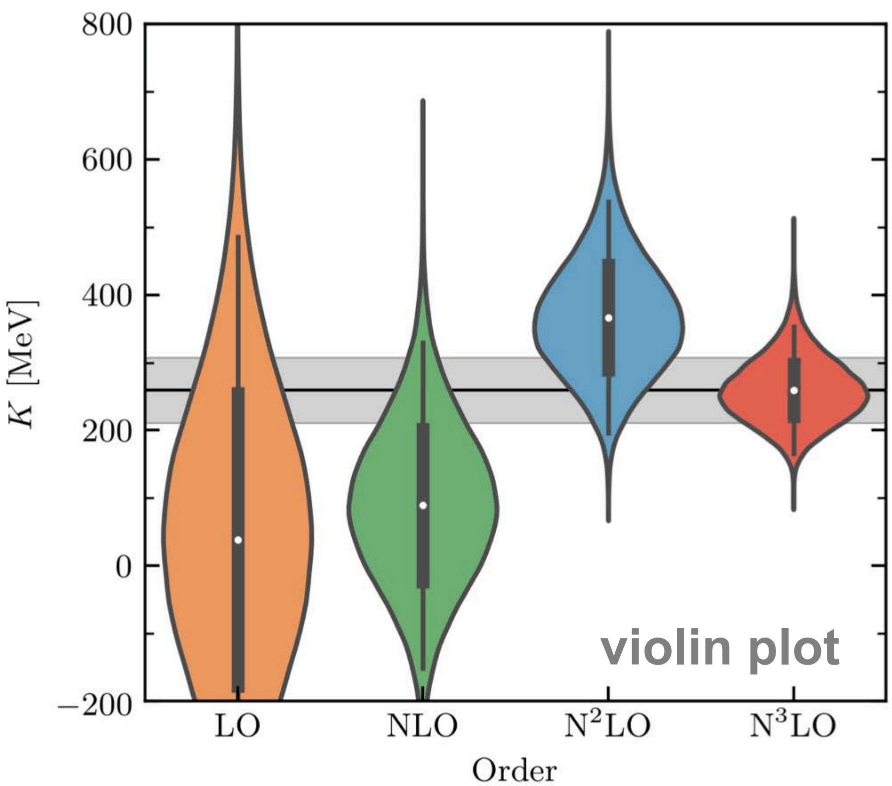
Incompressibility of SNM

CD, Melendez *et al.*, arXiv:2004.07805

$$K = 9n_0^2 \frac{\mathrm{d}^2}{\mathrm{d}n^2}\frac{E}{A}(n)\Big|_{n=n_0}$$

Λ = 500 MeV



! bands are consistent across orders

$$\mathrm{pr}(K \mid \mathcal{D}) = \int \mathrm{pr}(K \mid \mathcal{D}, n_0)\, \mathrm{pr}(n_0 \mid \mathcal{D})\, \mathrm{d}n_0$$

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

LO / NLO: the empirical saturation point is typically *not* well reproduced…

… leading to **wide-spread distributions** whose 1σ regions reach $K < 0$, even though saturation requires $K > 0$

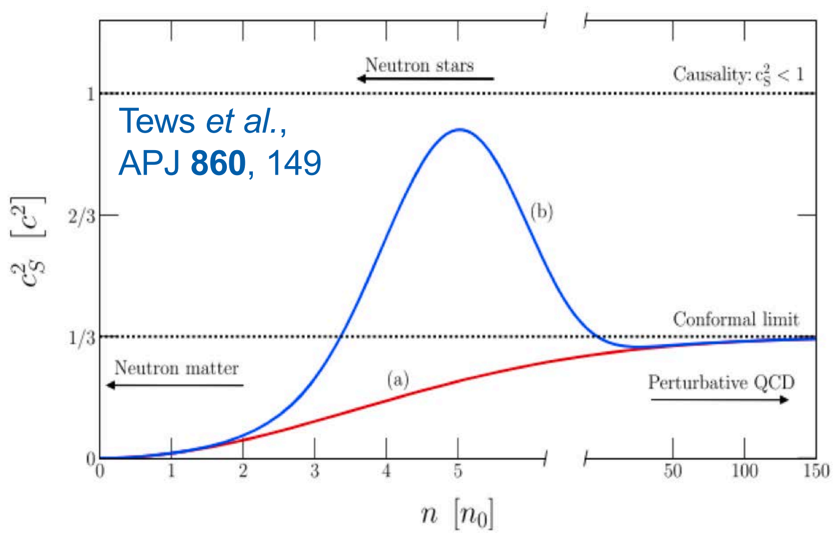
$$K = 260 \pm 54\,\mathrm{MeV} \quad (\Lambda = 500\,\mathrm{MeV})$$
$$K = 292 \pm 54\,\mathrm{MeV} \quad (\Lambda = 450\,\mathrm{MeV})$$

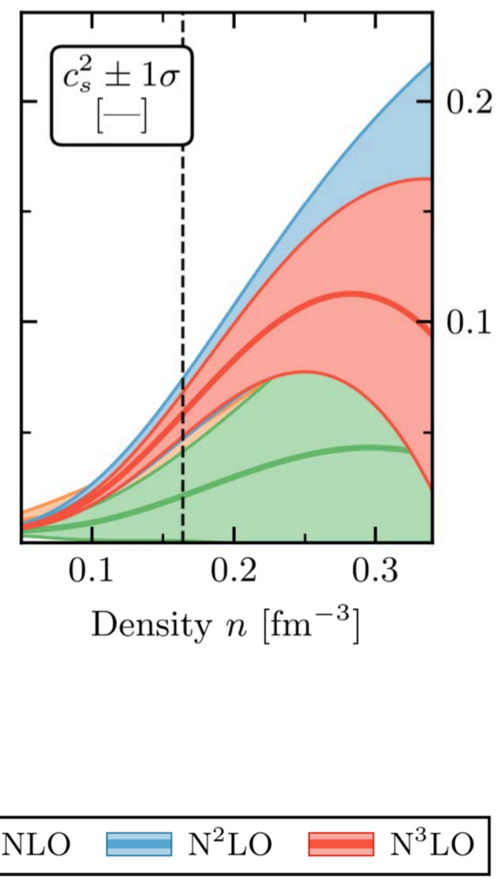
Quantifying uncertainties in the nuclear-matter equation of state

Speed of sound and pressure in PNM

CD, Furnstahl *et al.*, arXiv:2004.07805

$$c_s^2(n) = \frac{\partial P(n)}{\partial \varepsilon(n)}$$





Quantifying uncertainties in the nuclear-matter equation of state

Speed of sound and pressure in PNM

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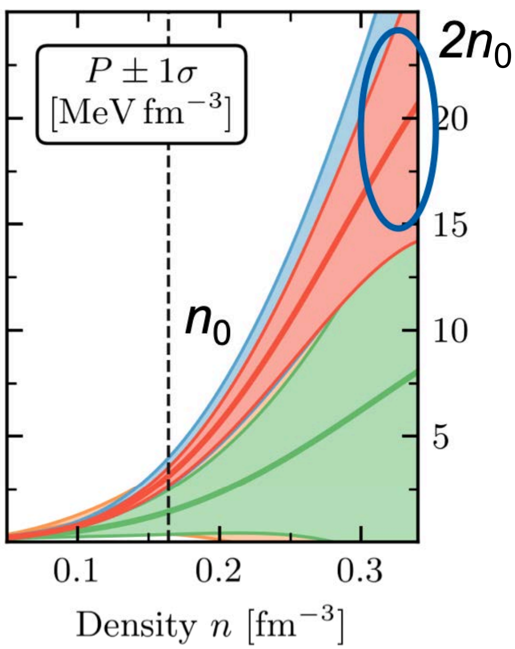
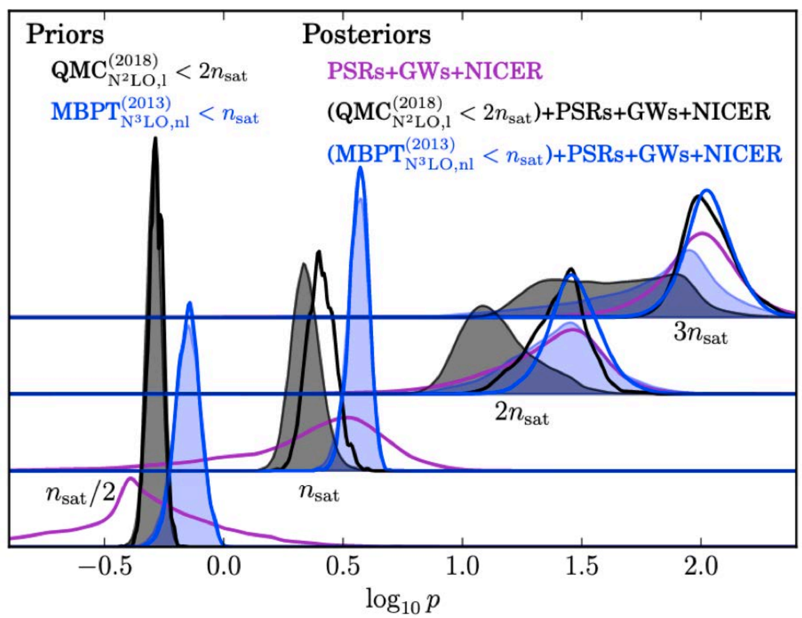
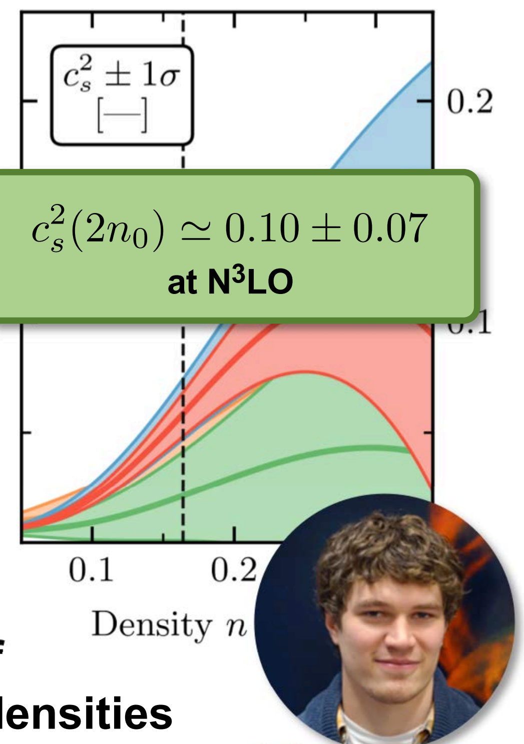
CD, Furnstahl *et al.*, arXiv:2004.07805

$$P(n = 0.32\,\mathrm{fm}^{-3}) \approx \begin{cases} 20 \pm 6\,\mathrm{MeV\,fm}^{-3} & \text{MBPT: nonlocal} \\ 15 \pm 5\,\mathrm{MeV\,fm}^{-3} & \text{QMC: local } V_{E,\mathbb{1}} \end{cases}$$

$$c_s^2(n) = \frac{\partial P(n)}{\partial \varepsilon(n)}$$







$$c_s^2(2n_0) \simeq 0.10 \pm 0.07$$

at N^{3}LO

$$P(n) = n^2 \frac{\mathrm{d}}{\mathrm{d}n} \frac{E}{N}(n)$$

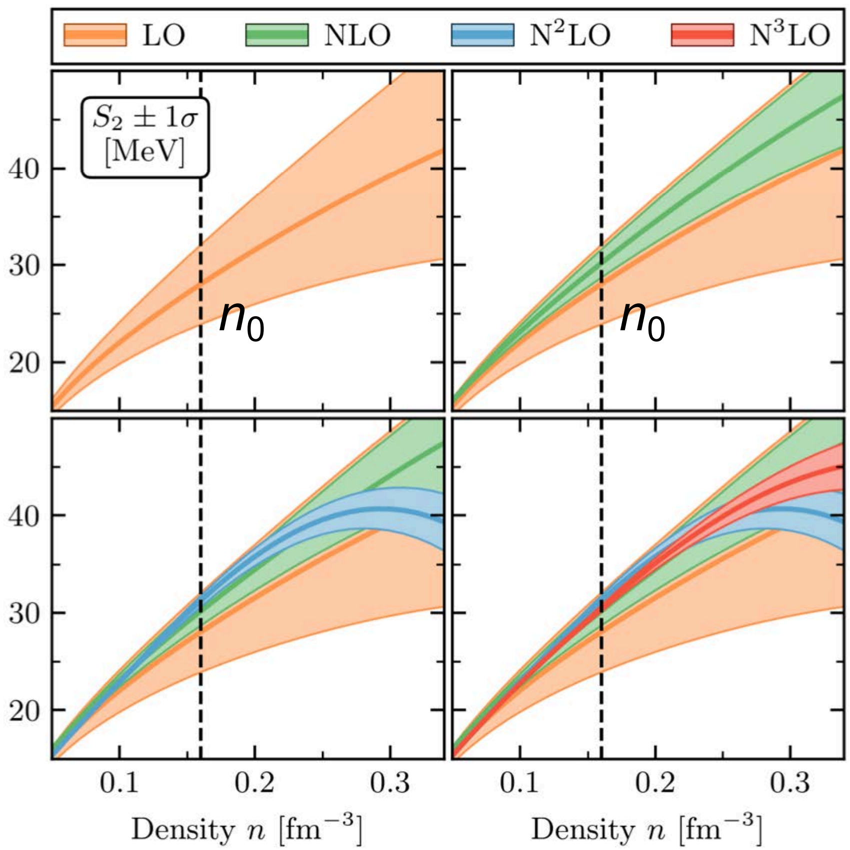
Direct astrophysical tests of chiral EFT at supranuclear densities

Essick, Tews, Landry, Reddy, Holz, arXiv:2004.07744

Quantifying uncertainties in the nuclear-matter equation of state

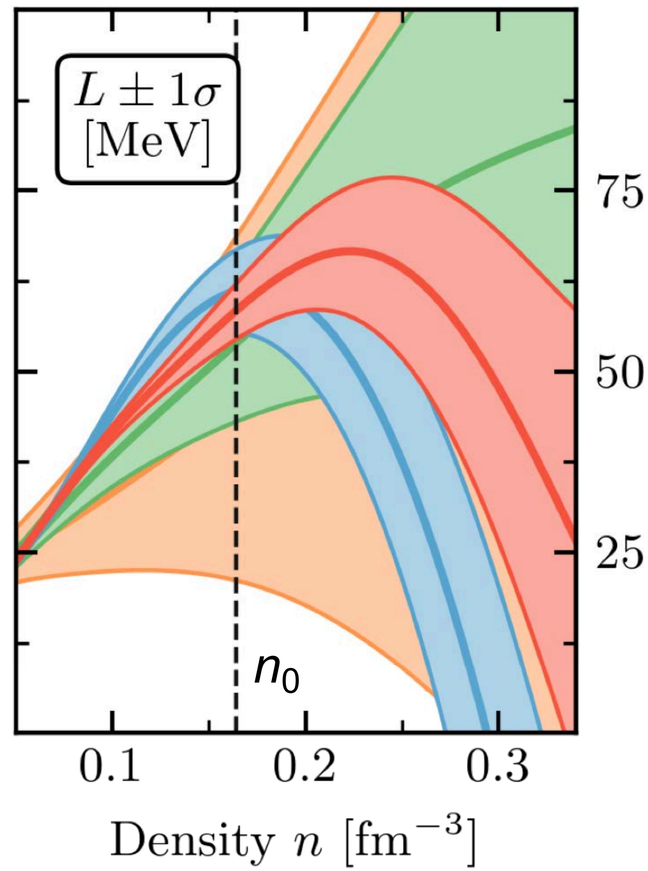
Nuclear symmetry energy

CD, Furnstahl *et al.*, arXiv:2004.07805



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

$$L(n) \equiv 3n \frac{\mathrm{d}}{\mathrm{d}n} S_2(n)$$



Quantifying uncertainties in the nuclear-matter equation of state

Nuclear symmetry energy

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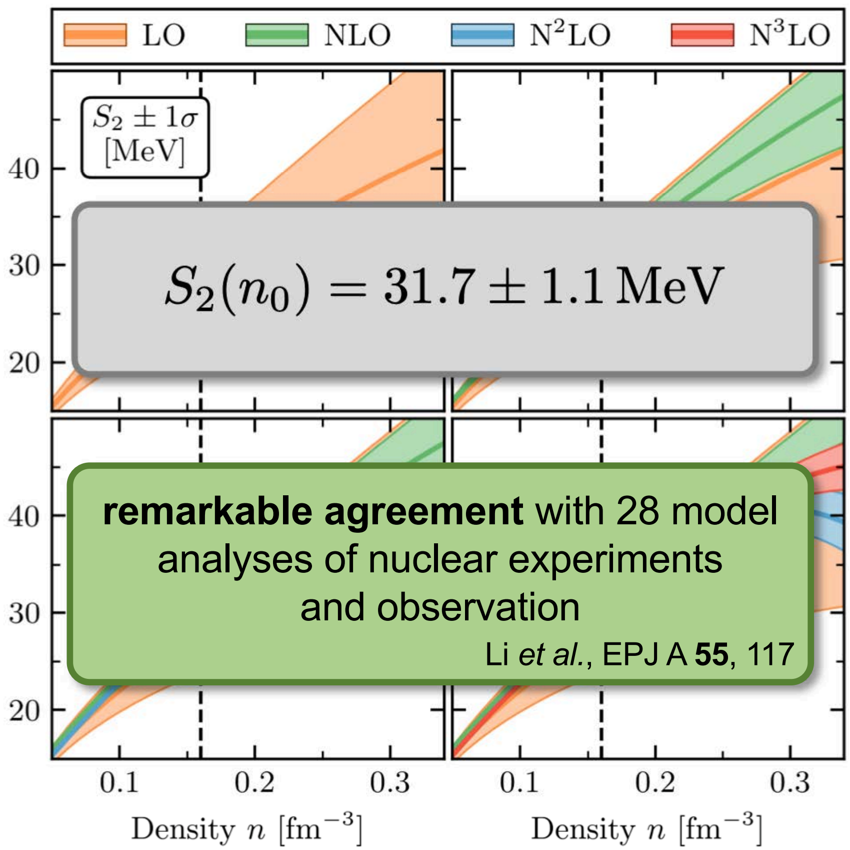
CD, Furnstahl *et al.*, arXiv:2004.07805



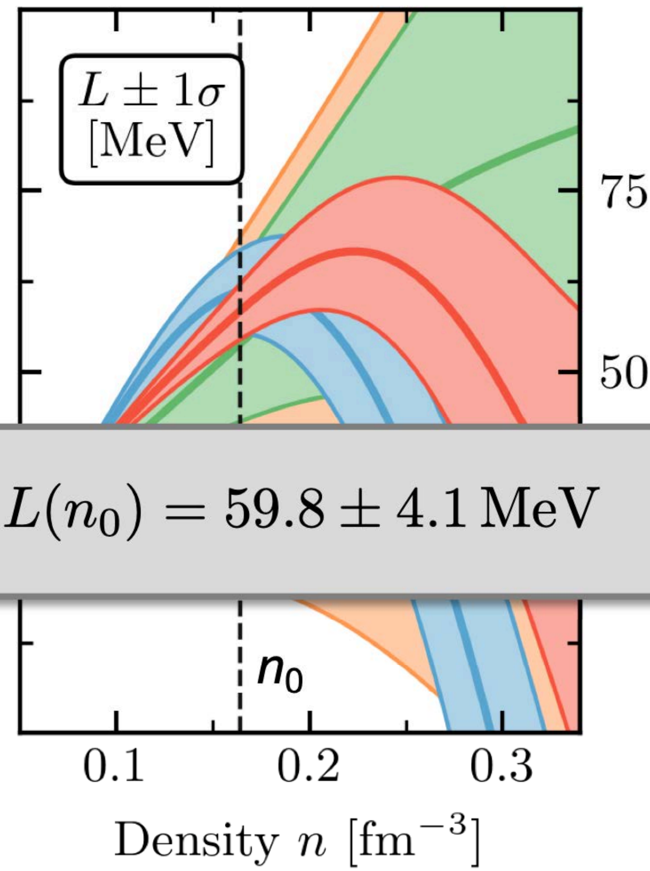
$$S_2(n_0) = 31.7 \pm 1.1\,\mathrm{MeV}$$

remarkable agreement with 28 model analyses of nuclear experiments and observation

Li *et al.*, EPJ A **55**, 117

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

$$L(n) \equiv 3n \frac{\mathrm{d}}{\mathrm{d}n} S_2(n)$$



$$L(n_0) = 59.8 \pm 4.1\,\mathrm{MeV}$$

Quantifying uncertainties in the nuclear-matter equation of state

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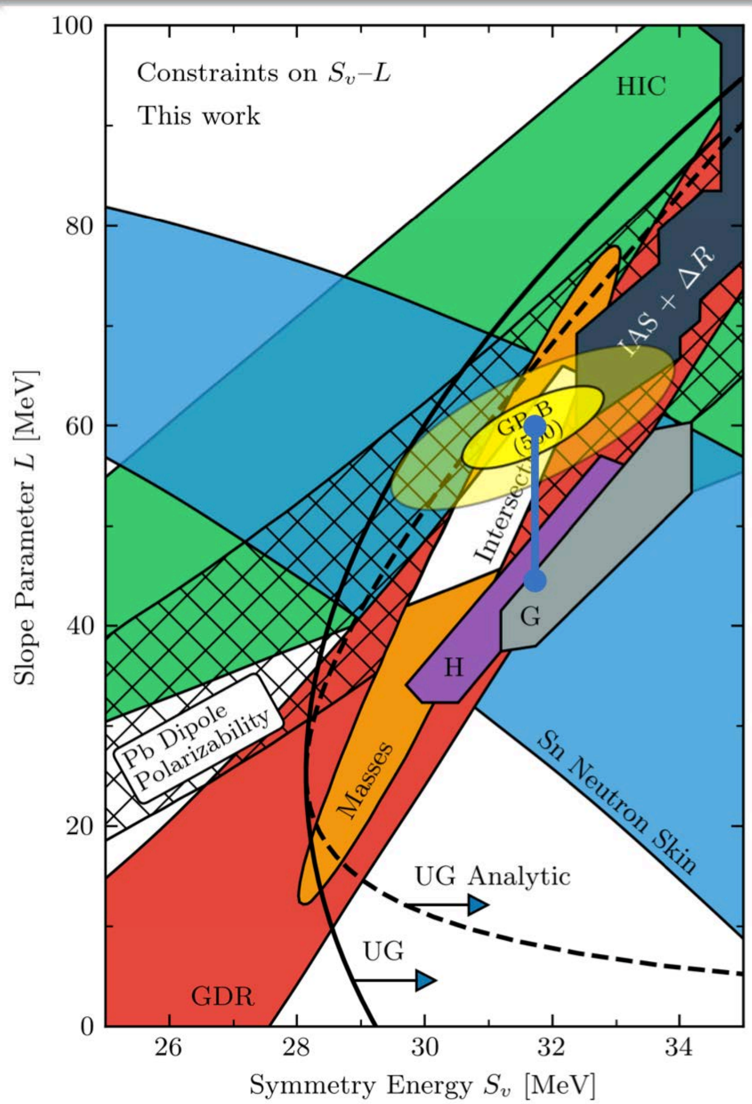
S_v–L correlation (as compiled by Lattimer *et al.*)

CD, Furnstahl *et al.*, arXiv:2004.07805



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

! Excellent agreement with experiment

Lattimer and Lim, APJ **771**, 51

$$\mathrm{pr}(S_v, L \,|\, \mathcal{D}) = \int \mathrm{d}n_0\, \mathrm{pr}(S_2, L \,|\, n_0, \mathcal{D})\, \mathrm{pr}(n_0 \,|\, \mathcal{D})$$

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

2σ ellipse (light yellow) is completely within the *conjectured* unitary gas limit

predicted range in ***S_v* agrees** with other **theoretical constraints**; but ~15 MeV stronger density-dependence of $S_2(n_0)$

two-dimensional Gaussian

$$\begin{bmatrix}\mu_{S_v}\\ \mu_L\end{bmatrix} = \begin{bmatrix}31.7\\ 59.8\end{bmatrix} \qquad \Sigma = \begin{bmatrix}1.24 & 3.27\\ 3.27 & 16.95\end{bmatrix}$$

Quantifying uncertainties in the nuclear-matter equation of state

Results for nuclei with these potentials

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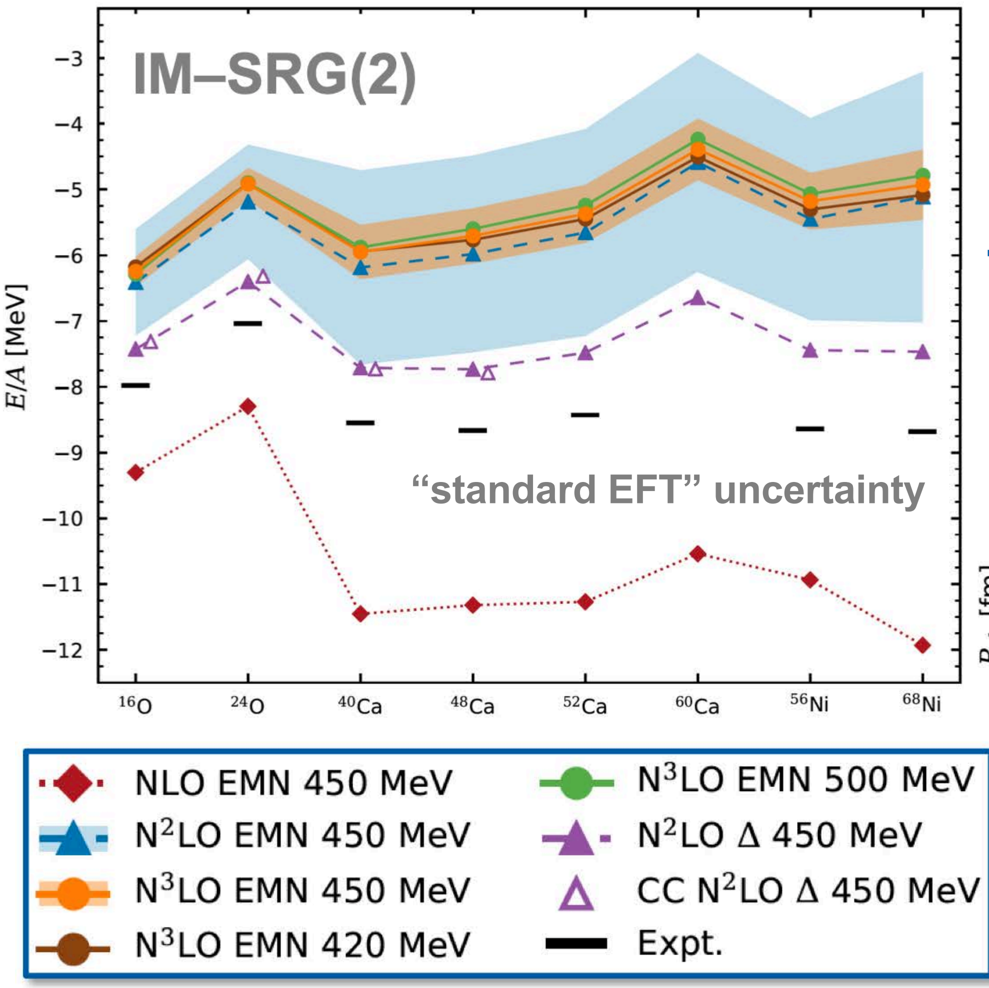
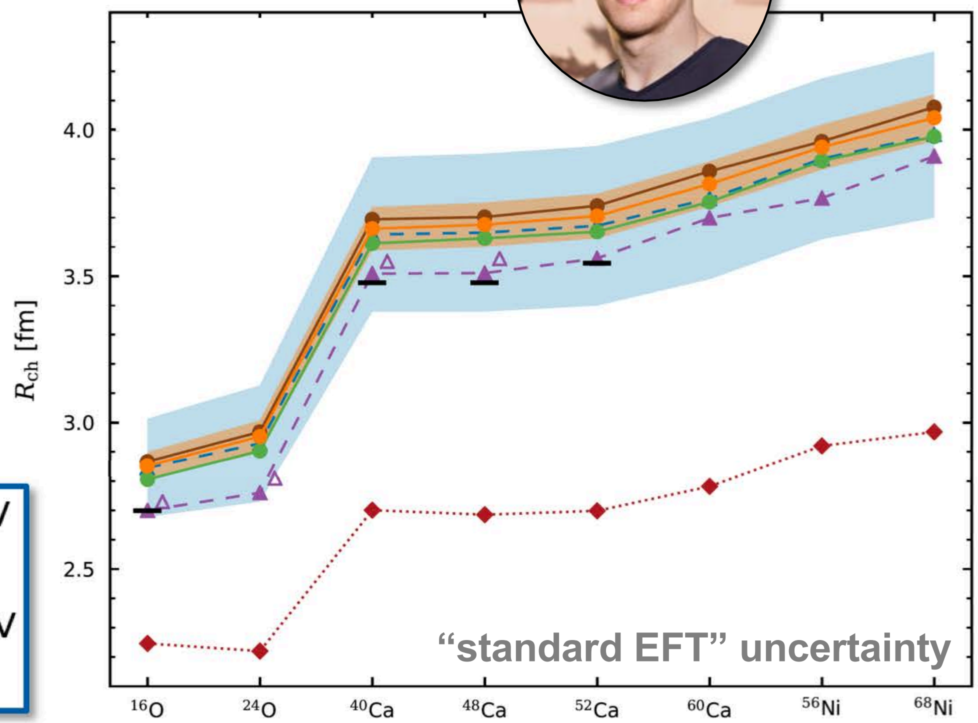
Hoppe, CD *et al.*, PRC **100**, 024318

binding energies



realistic **saturation properties** may **not suffice** for medium-mass nuclei **!**

charge radii



Quantifying uncertainties in the nuclear-matter equation of state

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Summary and outlook

1 set a new standard for UQ in infinite-matter calculations

- correlations within *and* between observables are crucial for reliable UQ
- need for *statistically* meaningful comparisons between theory and observation
- efficiently quantify and propagate EOS uncertainties to derived quantities

2 *statistically rigorous* analysis of the EOS up to N^3LO

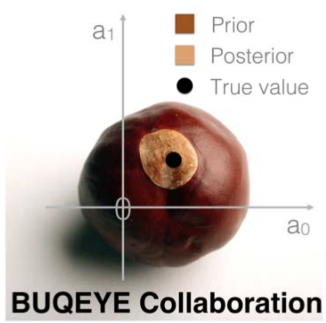
- excellent agreement of predicted S_v–L correlation with experiment
- PNM and SNM show a regular EFT convergence pattern with increasing order
- extracted Λ_b is consistent with NN scattering ● N^2LO coefficient may be an outlier

3 improved NN+3N potentials up to N^3LO are needed

- Hüther *et al.*, arXiv:1911.04955; Hoppe *et al.*, PRC **100**, 024318; …

4 full Bayesian UQ: MCMC for LECs & hyperparameters

- consistently include uncertainties in the LECs of chiral interactions
- compute nuclear saturation properties using Bayesian optimization



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K. McElvain D. Phillips A. Schwenk **C. Wellenhofer**

Quantifying uncertainties in the nuclear-matter equation of state

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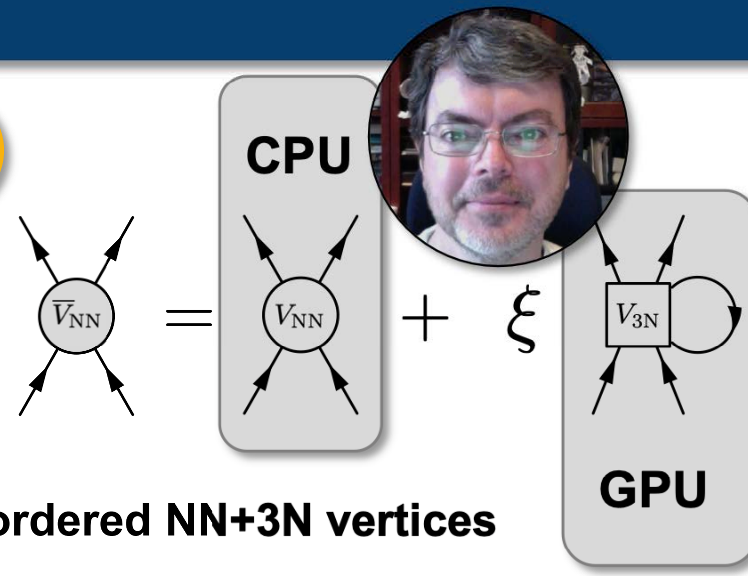
Next-generation MBPT calculations

MBPT(*n*)*	2	3	4	5
NN only	✓(1)	✓(3)	✓(24)	✓(375)
norm. ord. 3N	✓	✓	✓	✓
residual 3N	✓(1)	✓(14)	–	–

1

✓ past
✓ 2020



scalable multi-CPU/-GPU application

normal-ordered NN+3N vertices

complete third order

MC framework 2.0

SQL-based data repository

asymmetric-matter EOS

openMP, MPI, and CUDA

MPI-JM

self error detecting

significantly improved accuracy

2

Automated generation and evaluation of many-body diagrams I. Bogoliubov many-body perturbation theory

Pierre Arthuis, Thomas Duguet, Alexander Tichai, Raphaël-David Lasseri, Jean-Paul Ebran

Comput. Phys. **240**, 202

highly optimized: > 100x faster

3N partial-wave calculations

...