Nuclear EOS: uncertainty quantification and applications to neutron stars

Christian Drischler

March 8, 2021 | UK Lockdown Seminar

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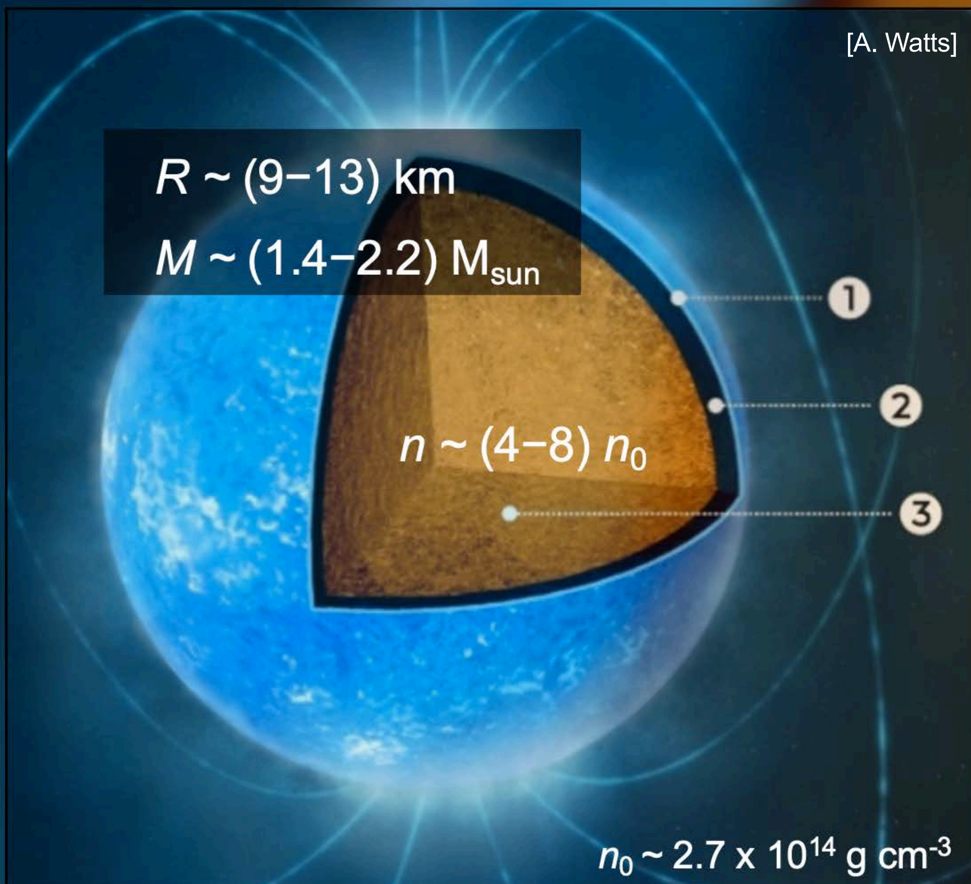

Keywords:

+ Chiral EFT + MBPT
+ infinite nuclear matter
+ Bayesian UQ
+ symmetry energy
+ nuclear saturation
+ N^3LO NN + 3N forces
+ …

Nuclear EOS: uncertainty quantification and applications to neutron stars

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Multimessenger astronomy

ligo.caltech.edu

+ Virgo
+ GEO600
+ KAGRA
+ …

Binary neutron star merger GW170817

$$R_{1.4} \lesssim 13.6\,\mathrm{km}$$

$$M_{\max} \lesssim 2.3\,\mathrm{M}_{\odot}$$

e.g., see:
Margalit, Metzger, APJ **850**, 19
Rezzolla *et. al.*, APJ **852**, L25
De *et al.*, PRL **121**, 091102
Capano *et al.*, NA **4**, 625
Al-Mamun *et al.*, PRL **126**, 061101
…

What is the secondary object in GW190425 and GW190814 ?

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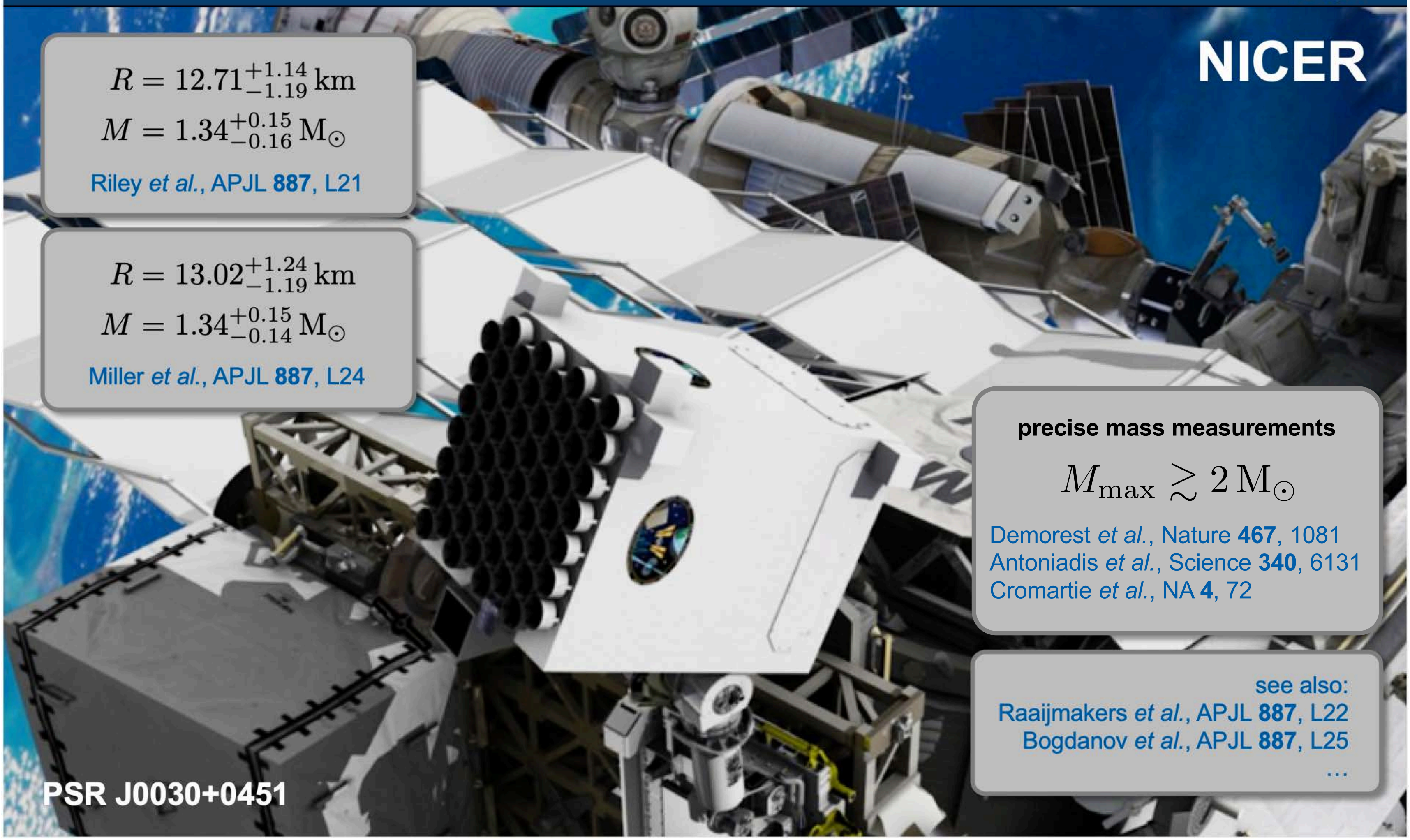
Recent simultaneous *M*–*R* measurement

NASA



$$R = 12.71^{+1.14}_{-1.19}\,\mathrm{km}$$
$$M = 1.34^{+0.15}_{-0.16}\,\mathrm{M}_\odot$$

Riley *et al.*, APJL **887**, L21

$$R = 13.02^{+1.24}_{-1.19}\,\mathrm{km}$$
$$M = 1.34^{+0.15}_{-0.14}\,\mathrm{M}_\odot$$

Miller *et al.*, APJL **887**, L24

precise mass measurements

$$M_{\mathrm{max}} \gtrsim 2\,\mathrm{M}_\odot$$

Demorest *et al.*, Nature **467**, 1081
Antoniadis *et al.*, Science **340**, 6131
Cromartie *et al.*, NA **4**, 72

see also:
Raaijmakers *et al.*, APJL **887**, L22
Bogdanov *et al.*, APJL **887**, L25
…

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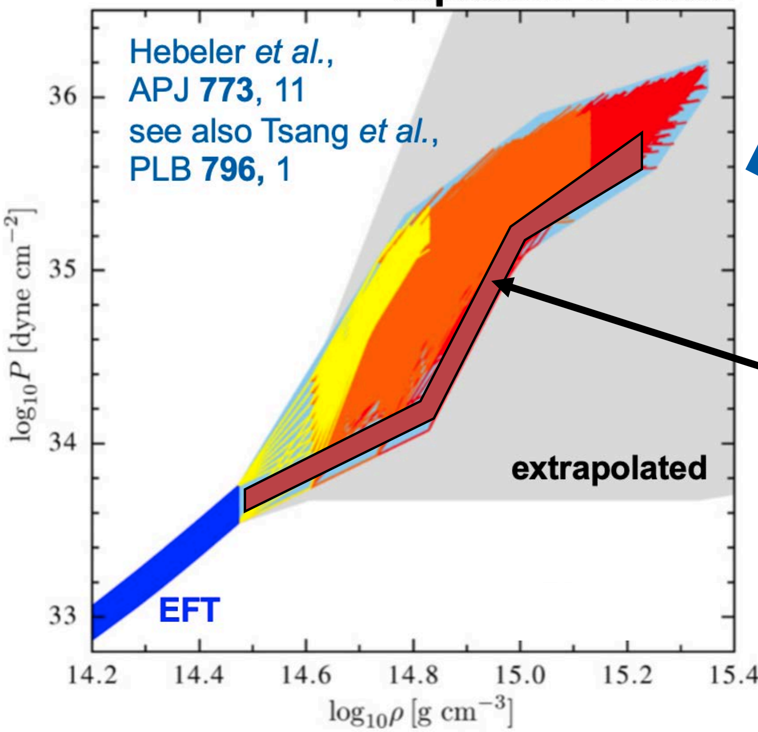
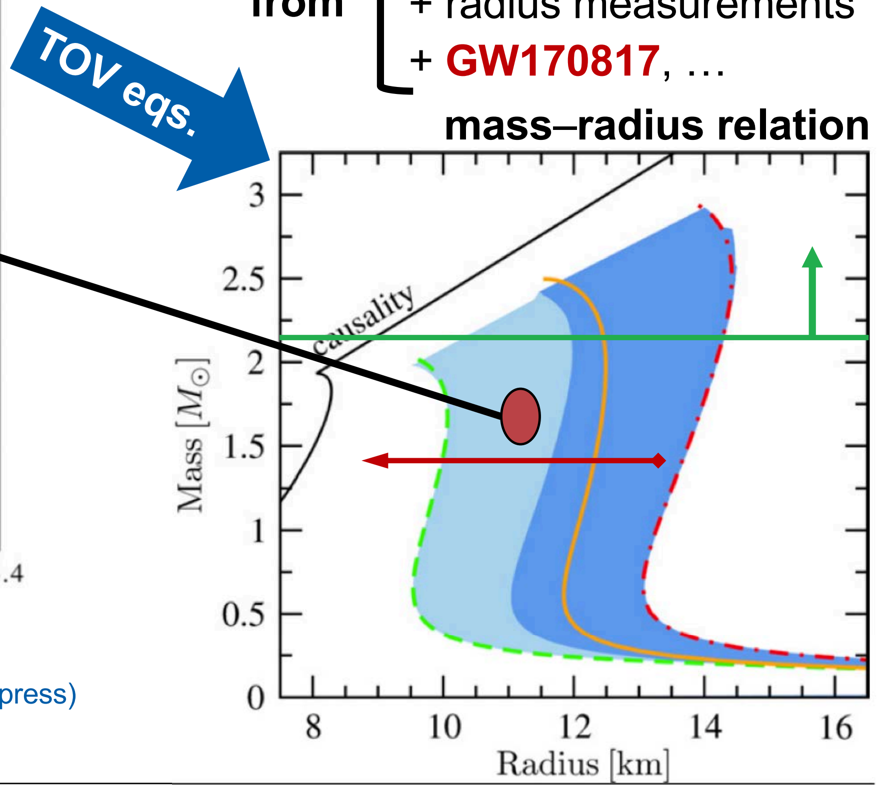
Direct correspondence: *M–R* relation and EOS

equation of state



constraints from
- + causality
- + mass measurements
- + radius measurements
- + GW170817, …

mass–radius relation



recent reviews:
CD, Holt, and Wellenhofer, arXiv:2101.01709 (ARNPS in press)
Hebeler, Holt *et al.*, ARNPS **65**, 457

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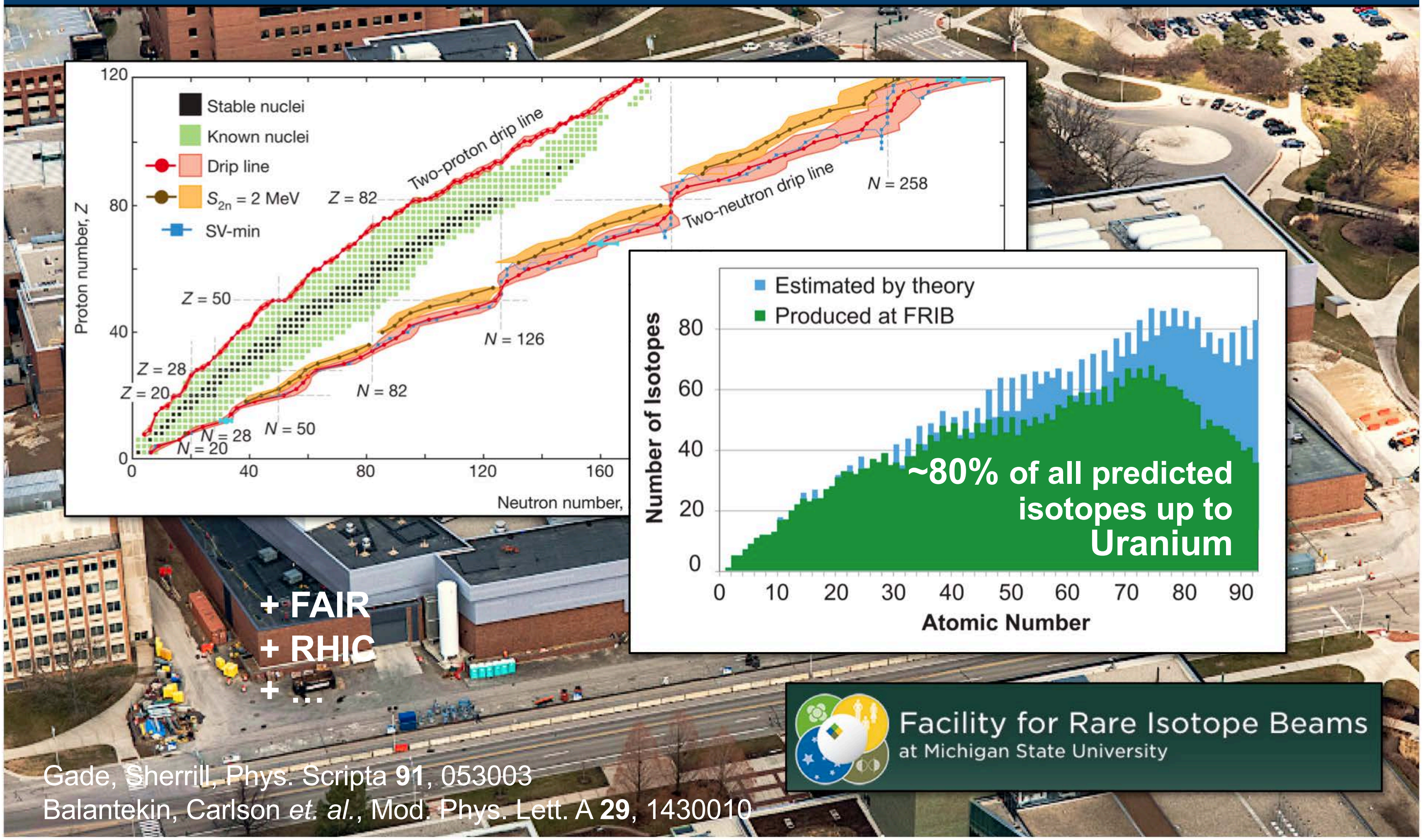
Beam facilities

Erler *et al.*, Nature **486**, 509–512



+ FAIR
+ RHIC
+ …

Facility for Rare Isotope Beams
at Michigan State University

Gade, Sherrill, Phys. Scripta **91**, 053003
Balantekin, Carlson *et. al.*, Mod. Phys. Lett. A **29**, 1430010

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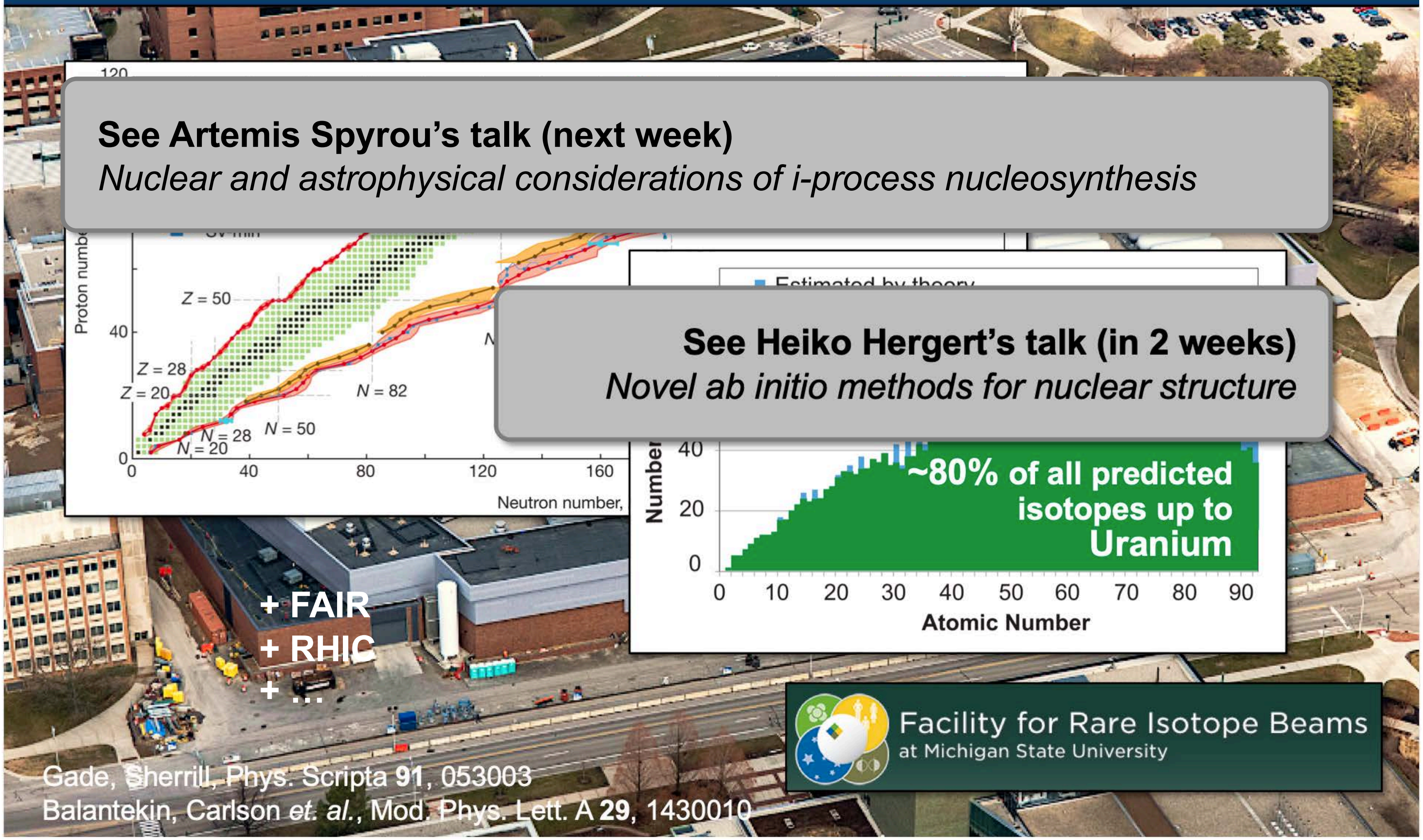

See Artemis Spyrou's talk (next week)
Nuclear and astrophysical considerations of i-process nucleosynthesis

See Heiko Hergert's talk (in 2 weeks)
Novel ab initio methods for nuclear structure

+ FAIR
+ RHIC
+ …

Gade, Sherrill, Phys. Scripta **91**, 053003
Balantekin, Carlson *et. al.*, Mod. Phys. Lett. A **29**, 1430010

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CD, Haxton, McElvain *et al.*, arXiv:1910.07961 (PPNP in press)

equation of state
neutron-star matter | nuclear saturation

many-body perturbation theory
computational efficient
many-body uncertainty estimates

chiral effective field theory
systematic expansion of nuclear forces
truncation error estimates

NPLQCD …

observables

many-body framework

effective field theory

quantum chromodynamics

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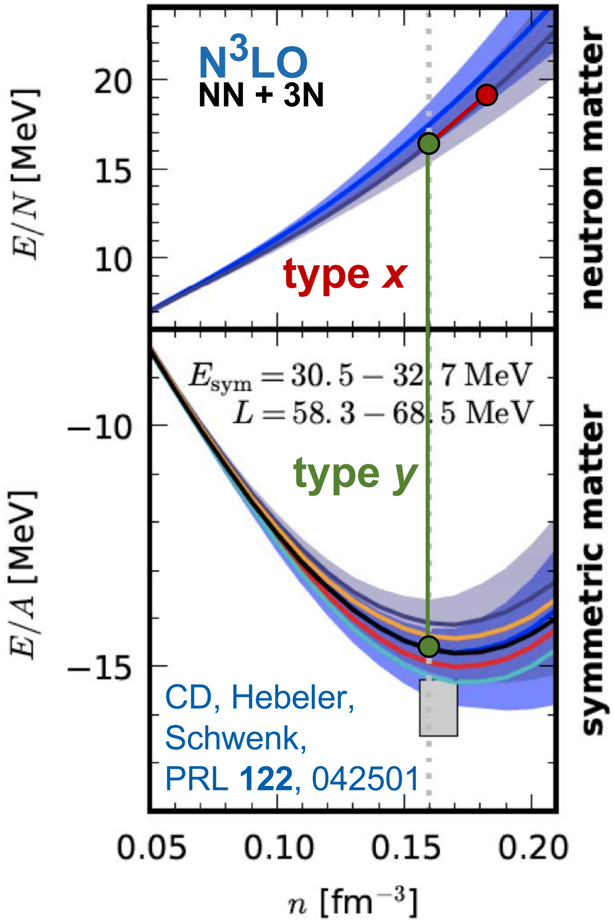
Nuclear matter calculations

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

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

Lonardoni, Tews *et al.*, PRR **2**, 022033(R)
Piarulli, Bombaci *et al.*, PRC **101**, 045801
…

But: existing predictions **only** provided **rough estimates** for the with-density-growing **EFT truncation error**, and did *not* account for **correlations**

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New framework for UQ of the infinite-matter EOS

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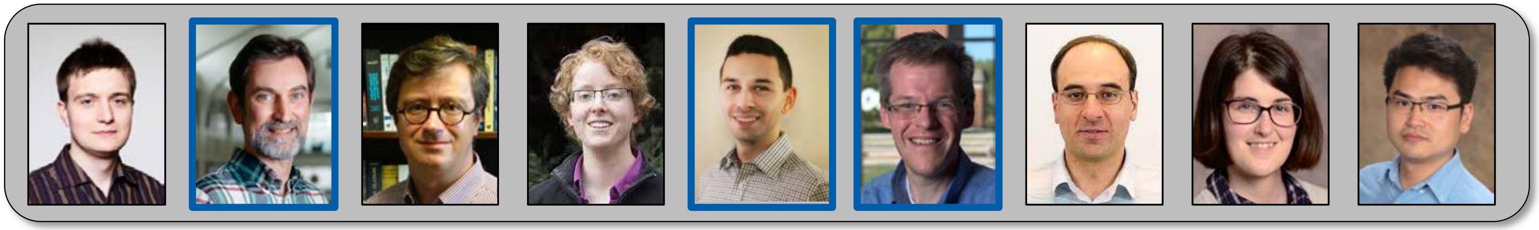
buqeye.github.io

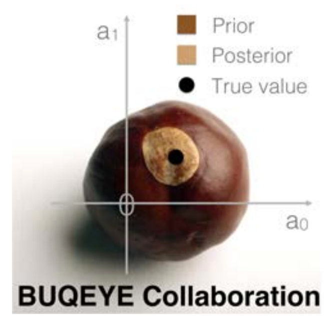


CD, Furnstahl, Melendez, and Phillips

How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties, PRL **125**, 202702

CD, Melendez, Furnstahl, and Phillips

Effective Field Theory Convergence Pattern of Infinite Nuclear Matter, PRC **102**, 054315



Bayesian
Uncertainty
Quantification:
Errors for
Your
EFT

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

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New framework for UQ of the infinite-matter EOS

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buqeye.github.io

CD, Furnstahl, Melendez, and Phillips

How w … n
equat … inty
stars? … cation:
uncer … or

CD, M

Effect
Infinit

…allows us to…

…efficiently **quantify** *and* **propagate** theoretical **uncertainties** of the EOS (such as EFT truncation errors) to derived quantities

» *statistically* **robust uncertainty estimates** for key quantities of **neutron stars**

ble at
https://buqeye.github.io

Nuclear EOS: uncertainty quantification and applications to neutron stars

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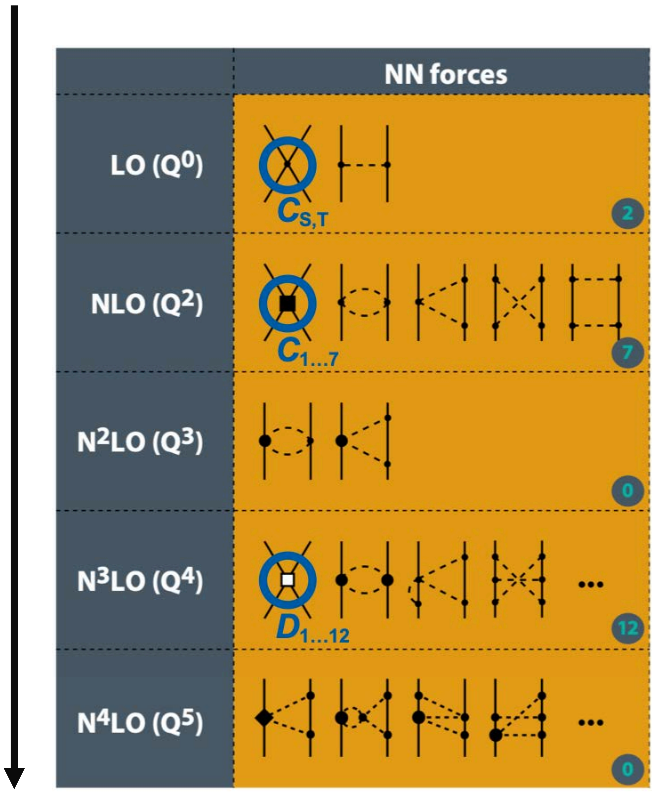
Hierarchy of nuclear forces in chiral EFT

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



modern approach to nuclear forces:

- QCD is nonperturbative at the low-energy scales of nuclear physics
- use relevant instead of the fundamental degrees of freedom: *e.g.*, **nucleons** and **pions**
- **pion exchanges** and short-range **contact interactions** ($\propto$ LECs)
- **systematic expansion** enables improvable **uncertainty estimates**

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

Expansion

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

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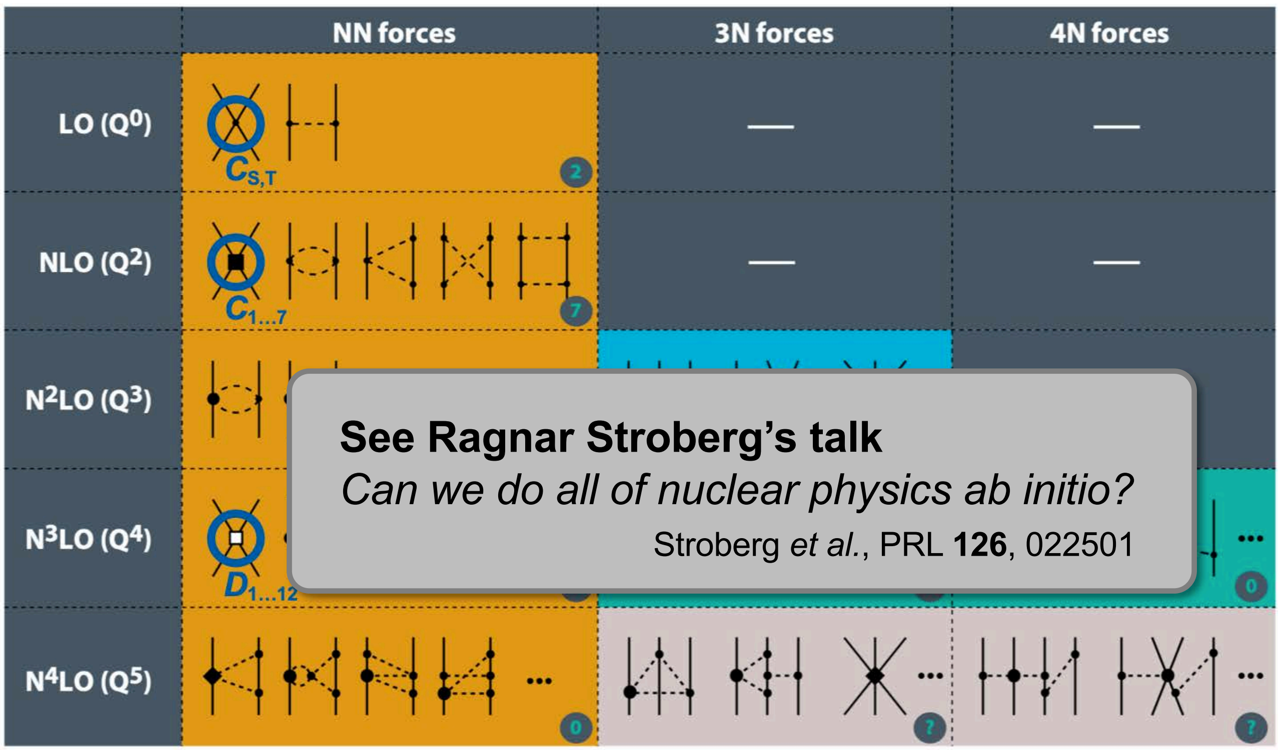
e.g., Machleidt, Entem, Phys. Rep. **503**, 1

Many-body forces



See Ragnar Stroberg's talk

Can we do all of nuclear physics ab initio?

Stroberg *et al.*, PRL **126**, 022501

no unknown parameters

S. Weinberg

Expansion

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

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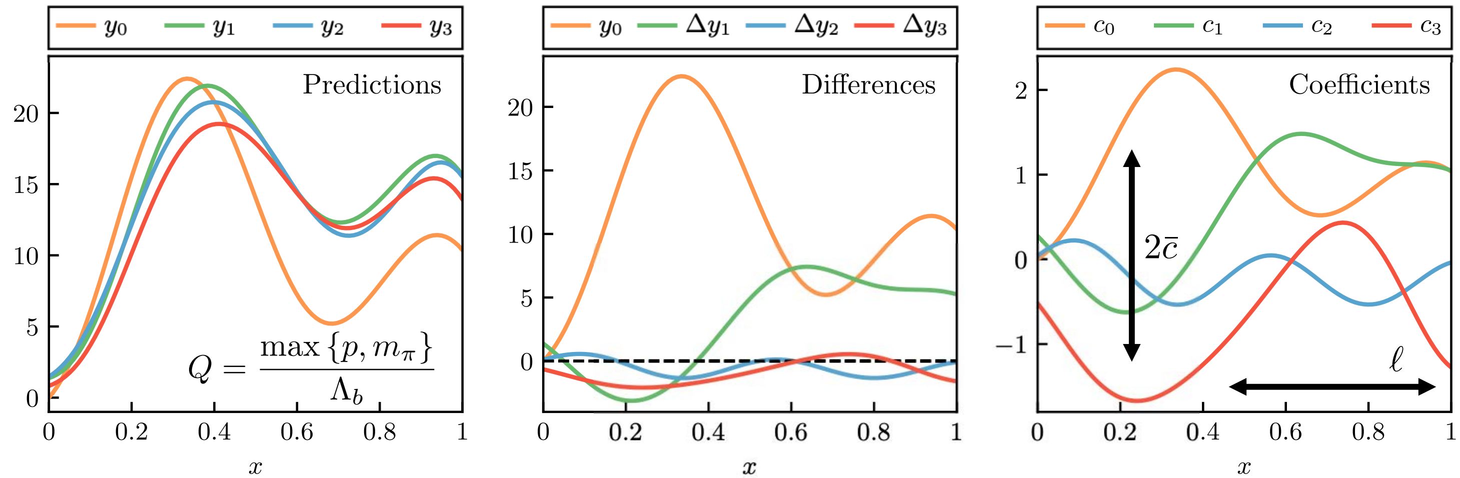
In a nutshell: EFT truncation-error model

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

predict observable y_k order by order in EFT

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

treat all c_n as independent draws from a Gaussian Process



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

infer EFT truncation error

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

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

geometric sum

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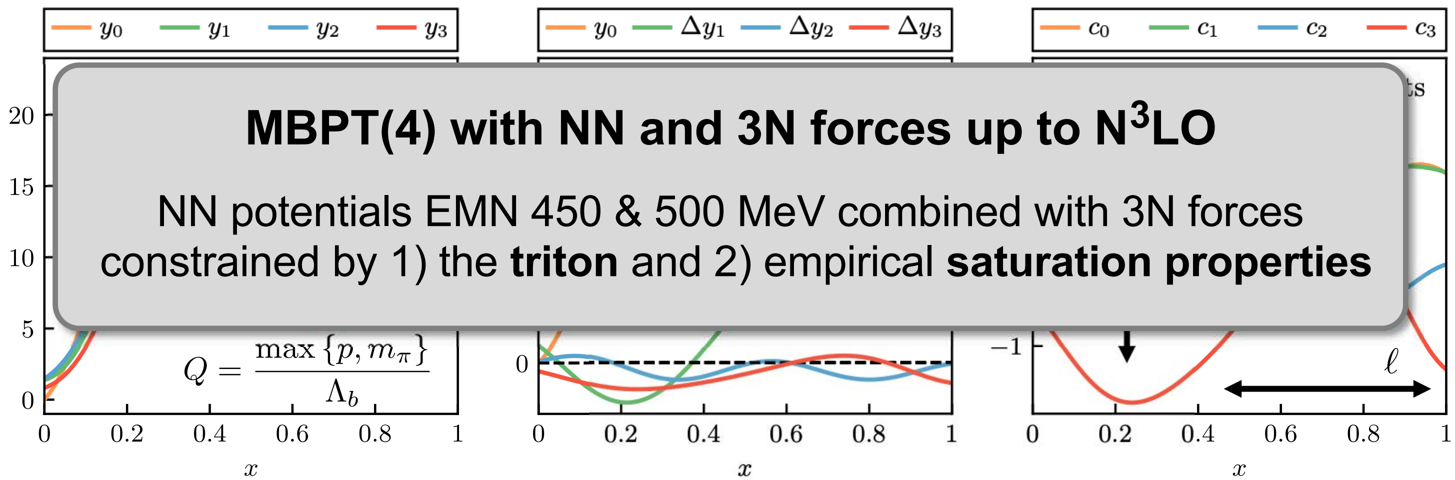

MBPT(4) with NN and 3N forces up to N^{3}LO

NN potentials EMN 450 & 500 MeV combined with 3N forces constrained by 1) the **triton** and 2) empirical **saturation properties**

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

infer EFT truncation error

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

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

geometric sum

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Efficient Monte Carlo framework

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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) VEGAS algorithm
- acceleration: openMP, MPI, and CUDA
- **controlled computation** of arbitrary interaction and many-body diagrams

EOS up to high orders

↑

automatic code generation

↑

analytic form of the diagrams

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Significant challenges are past!

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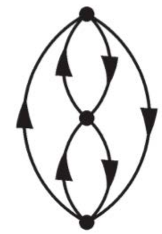
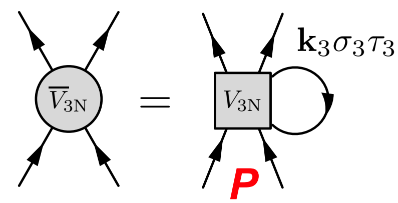
CD, Hebeler, Schwenk, PRL **122**, 042501

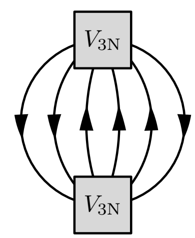
- **Higher orders: particle-hole contributions**
  Coraggio *et al.*, PRC **89**, 044321; Holt, Kaiser, PRC **95**, 034326, ...



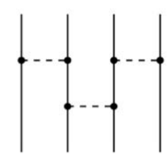
- **No approximations for 3N normal ordering**
  CD *et al.*, PRC **93**, 054314; Holt *et al.*, PRC **81**, 024002, …



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



- **Higher many-body forces**
  Epelbaum, PLB **639**, 256, ...



application of a novel Monte Carlo framework

Number of diagrams in MBPT

Stevenson, Int. J. Mod. Phys. C **14**, 1135

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.

ADG: 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

Important physics questions

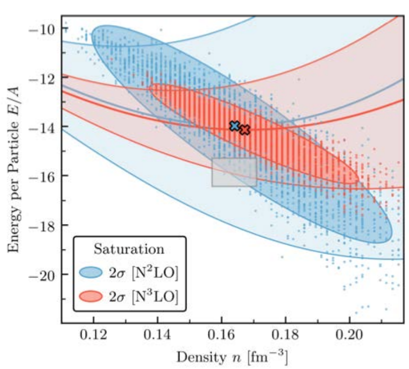
CD, Melendez *et al.*, PRC **102**, 054315

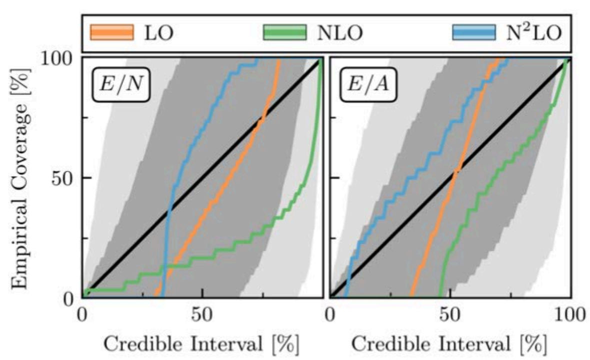
Does chiral EFT perform as advertised in medium? If so, where does it break down? If not, how to identify a more efficient EFT?

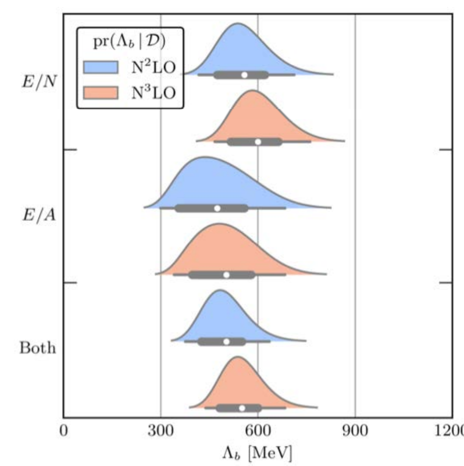
How well can chiral EFT reproduce the *empirical* properties at the 1σ level? Can we trust the uncertainty estimates?

How predictive is chiral EFT at ~$2n_0$? And what are the astrophysical implications?

CD, Han, Lattimer, Prakash, Reddy, Zhao, arXiv:2009.06441







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Bayesian inference

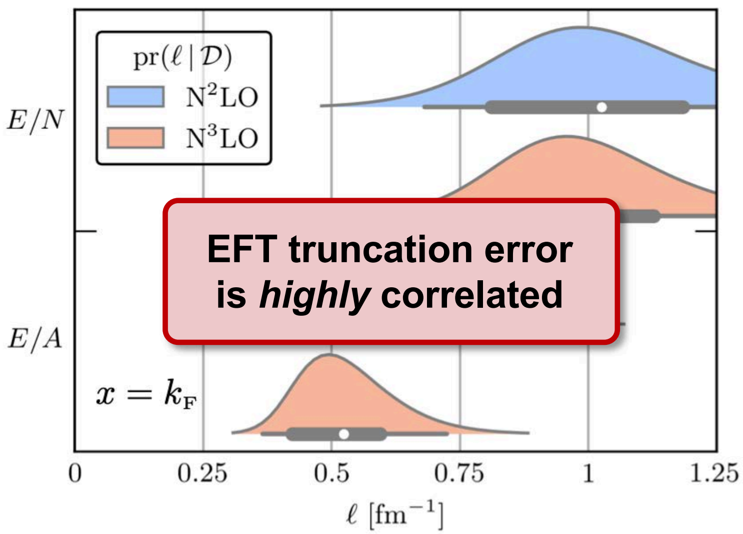
CD, Melendez *et al.*, PRC **102**, 054315

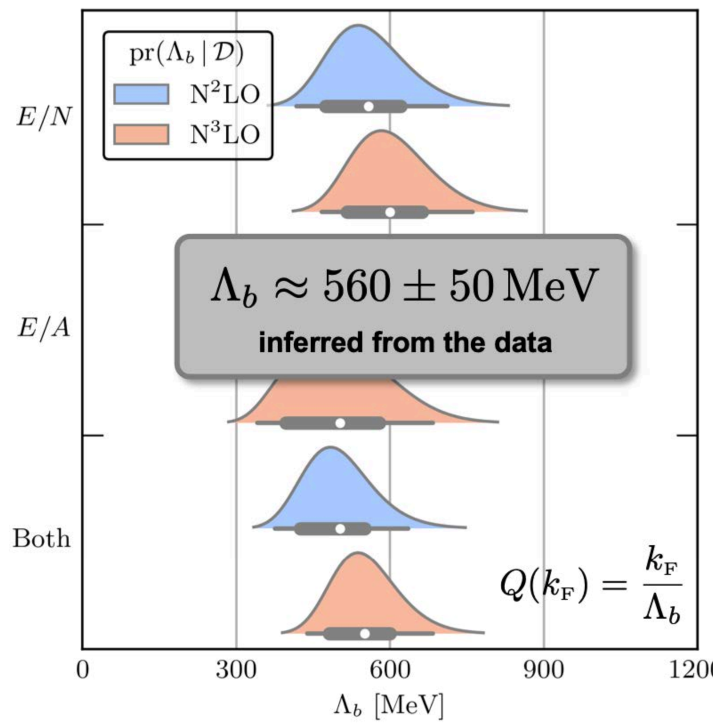
How correlated is nuclear matter **?**

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

Where does the EFT break down **?**

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





to be compared with

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

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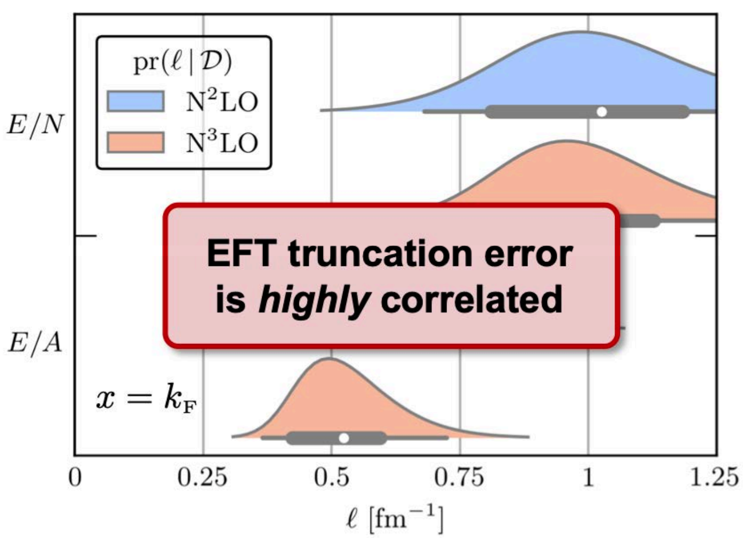
Propagating type-*x* uncertainties

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

How correlated is nuclear matter ?

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

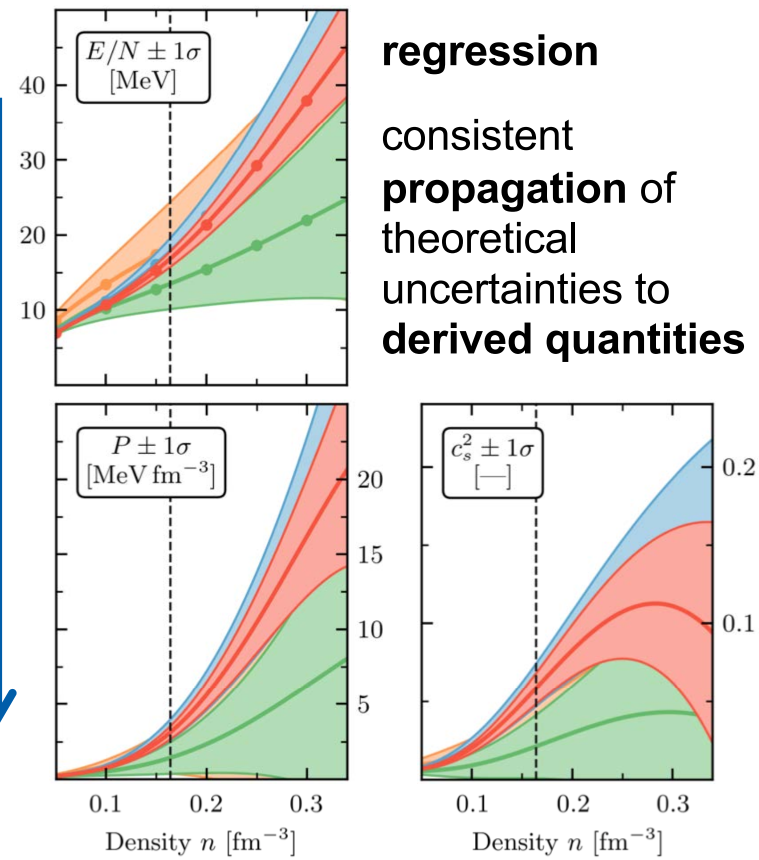


EFT truncation error is *highly* correlated

to be compared with

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

derivative(s)



regression

consistent **propagation** of theoretical uncertainties to **derived quantities**

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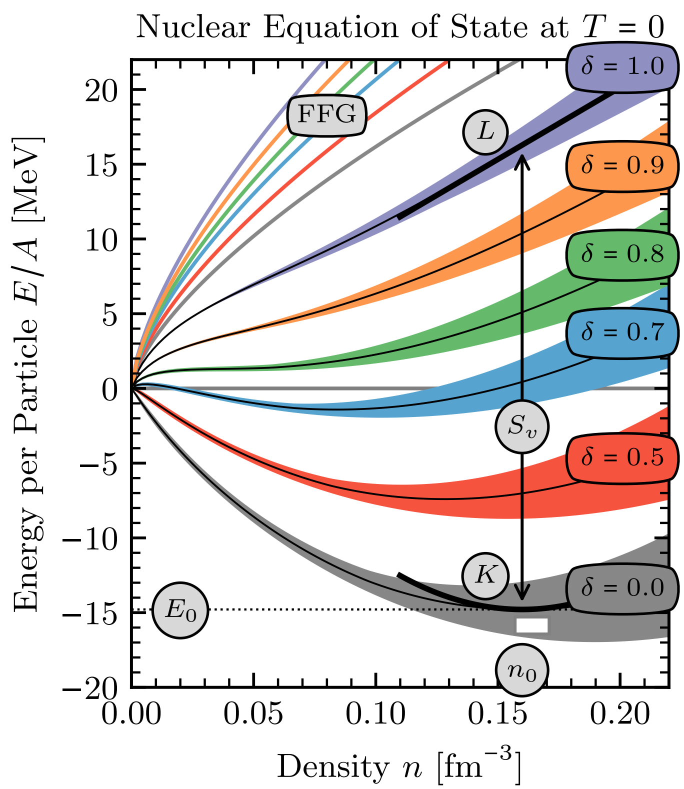
Parameters of the low-density EOS

CD, Holt, and Wellenhofer, arXiv:2101.01709



FFG: free Fermi gas; ***δ*** = (n_n – n_p)/n: isospin asymmetry

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

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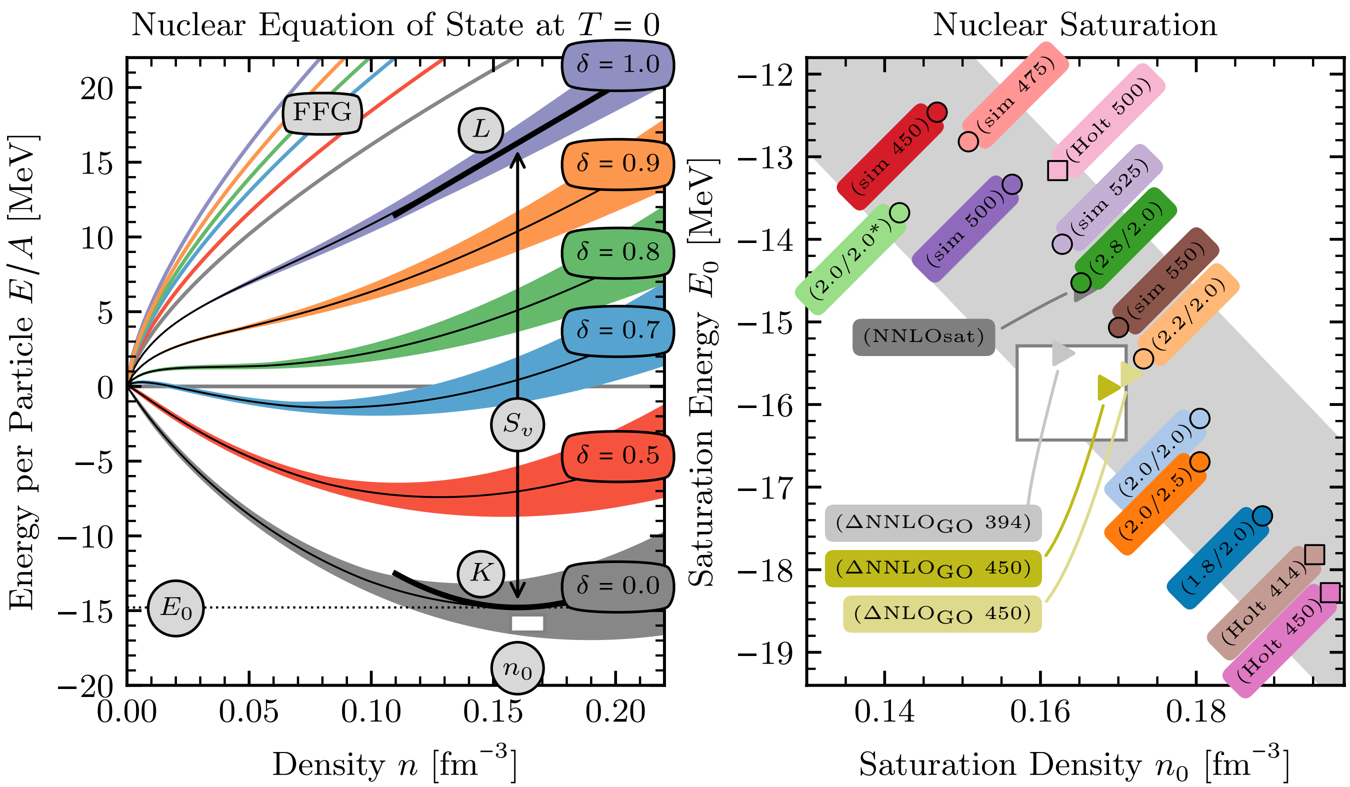

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Annotations: (λ / Λ_{3N}) in fm^{-1} or (Λ) in MeV

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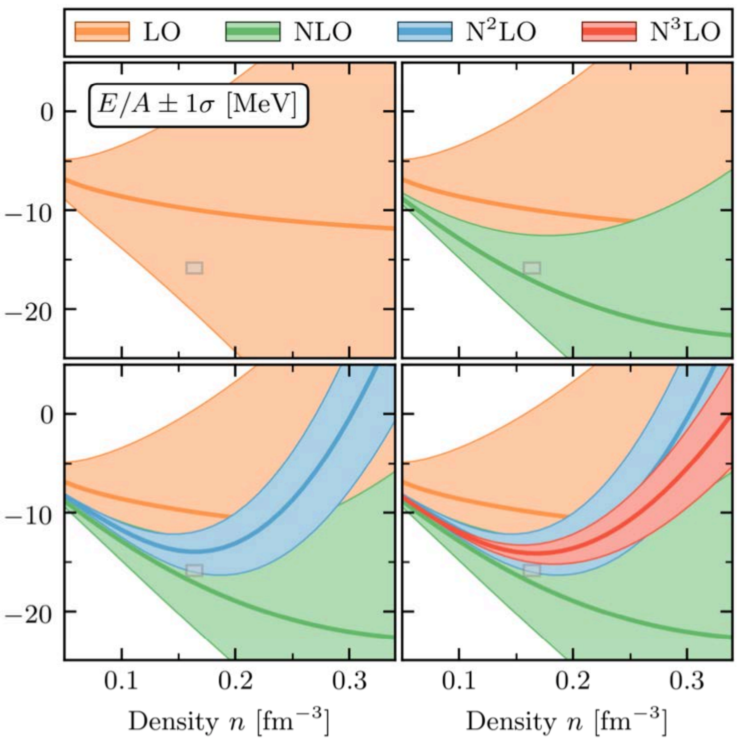
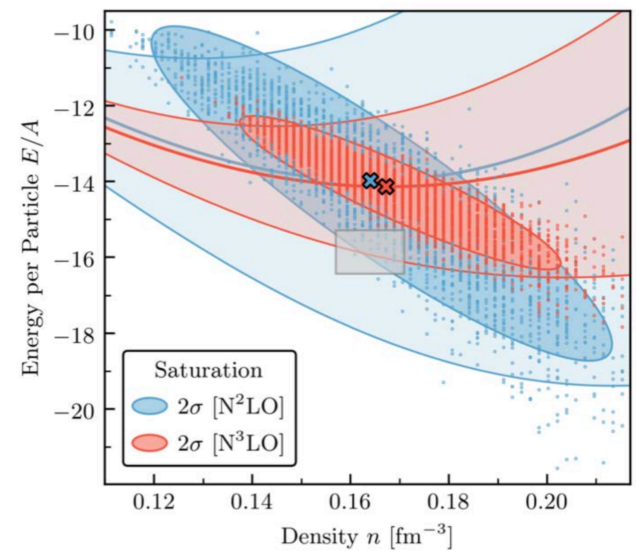
SNM and the saturation point

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

Λ = 500 MeV



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



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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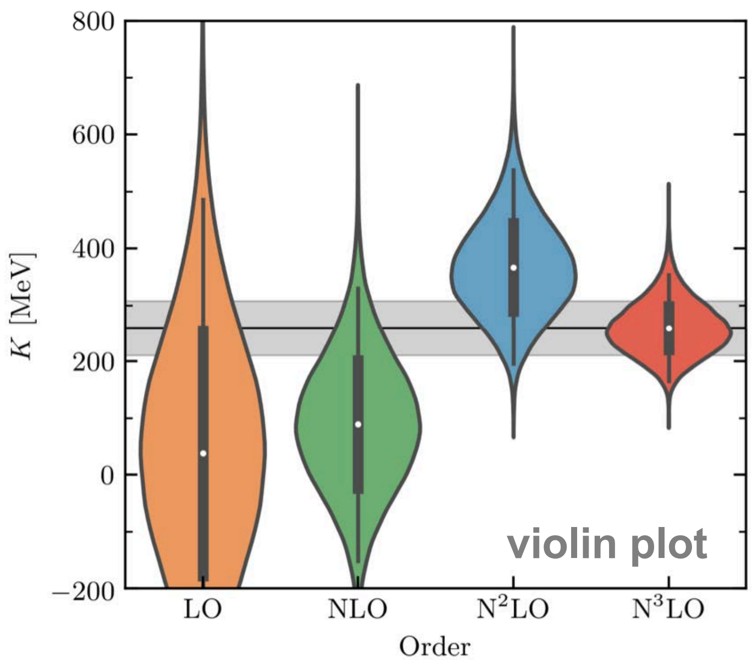
Incompressibility of SNM

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

Λ = 500 MeV



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

! 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 $K > 0$

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

for connections to experiment, see, *e.g.*, Roca-Maza and Paar, PPNP **101,** 96

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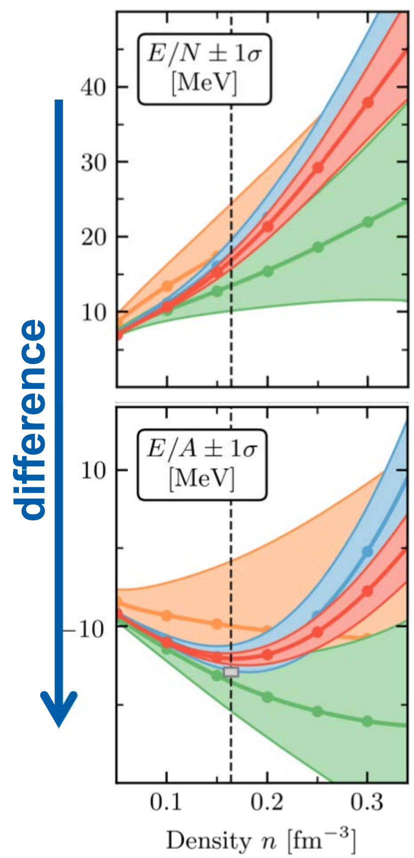
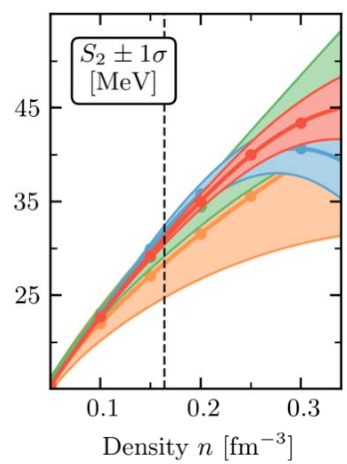
Type-*y*: nuclear symmetry energy

CD, Furnstahl *et al.*, PRL **125**, 202702



$$E_{\mathrm{PNM}} \sim \mathcal{N}\left(\mu, \sigma^2\right)$$
$$E_{\mathrm{SNM}} \sim \mathcal{N}\left(\mu, \sigma^2\right)$$

at a given density



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

Reminder: Statistics 101

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

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

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

Can result in smaller uncertainties than one might *naively* expect.

See, *e.g.*, Wen & Holt, arXiv:2012.02163; Somasundaram, CD, Tews *et al.*, arXiv:2009.04737 for $S_{2k>2}(n)$

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

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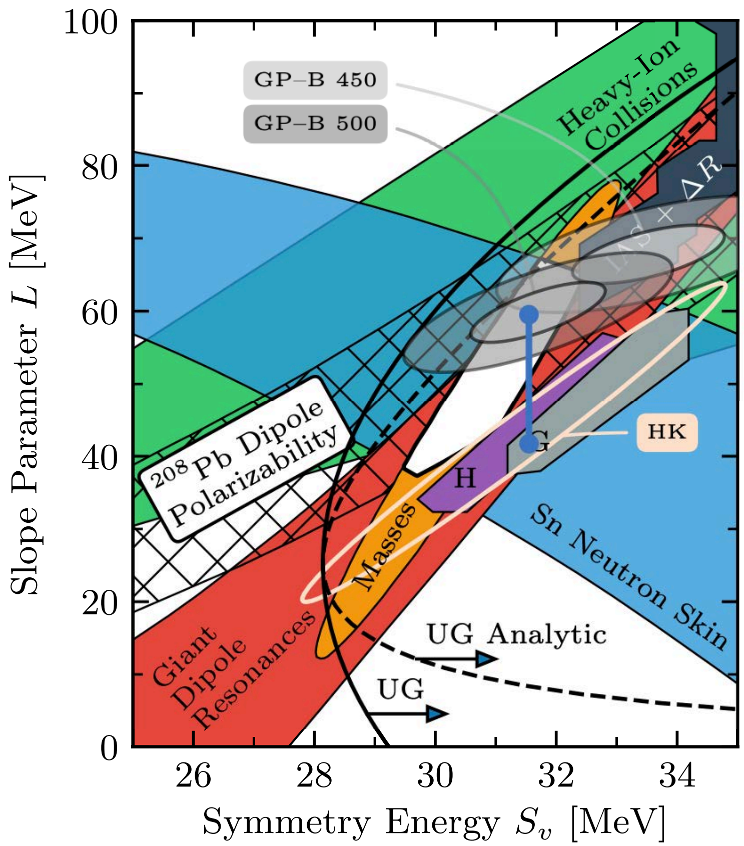
CD, Furnstahl *et al.*, PRL **125**, 202702



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

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 $S_2(n_0)$

GP–B (500): two-dimensional Gaussian

$$\begin{bmatrix}\mu_{S_v}\\ \mu_L\end{bmatrix} = \begin{bmatrix}31.7\\ 59.8\end{bmatrix} \qquad \Sigma = \begin{bmatrix}1.11^2 & 3.27\\ 3.27 & 4.12^2\end{bmatrix}$$

Nuclear EOS: uncertainty quantification and applications to neutron stars

Constraints derived from PREX–II

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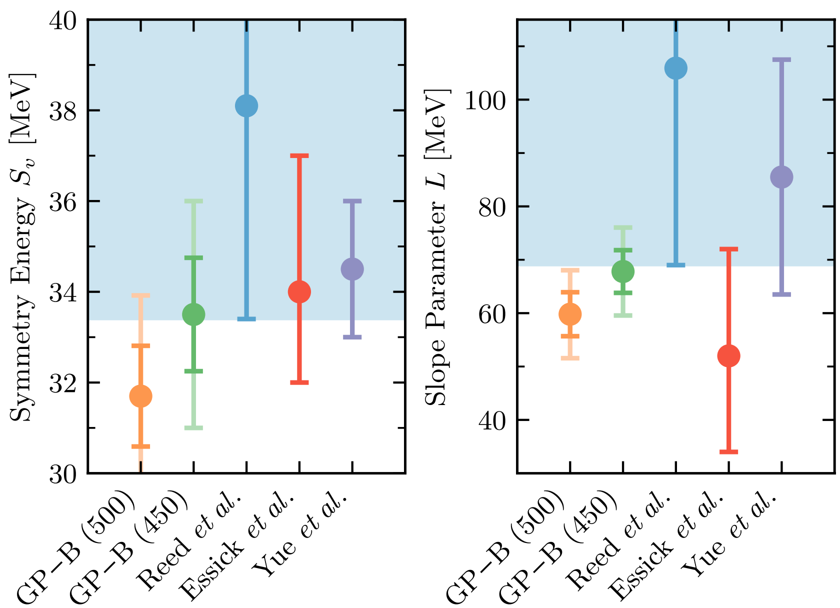
see also Yue *et al.*, arXiv:2102.05267



Parity violating elastic e scattering

$$R_{\rm skin}\left({}^{208}\mathrm{Pb}\right) = 0.283 \pm 0.071\,\mathrm{fm}$$

PREX collaboration, arXiv:2102.10767

Exploiting strong correlations (EDFs)

$$S_v = 38.1 \pm 4.7\,\mathrm{MeV}$$
$$L = 105.9 \pm 36.9\,\mathrm{MeV}$$

Reed *et al.*, arXiv:2101.03193

Astron. data + chiral EFT only (incl. GP-B)

$$R\left({}^{208}\mathrm{Pb}\right) = 0.18^{+0.04}_{-0.04}\,\mathrm{fm}$$
$$S_v = 34^{+3}_{-2}\,\mathrm{MeV} \quad L = 52^{+20}_{-18}\,\mathrm{MeV}$$

Essick *et al.*, arXiv:2102.10074

$$\begin{bmatrix}\mu_{S_v}\\ \mu_L\end{bmatrix} = \begin{bmatrix}31.7\\ 59.8\end{bmatrix} \qquad \Sigma = \begin{bmatrix}1.11^2 & 3.27\\ 3.27 & 4.12^2\end{bmatrix}$$

PREX–II:

- **uncertainties are still large**
- **extracted $R_{\rm skin}$ (and L) consistent with joint posterior (1σ level) but overall allows for stiffer EOS at ~n_0**

Nuclear EOS: uncertainty quantification and applications to neutron stars

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Summary and outlook

buqeye.github.io

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

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

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

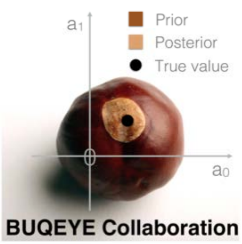
- excellent agreement of predicted S_v–L correlation with experiment
- PNM and SNM show a regular EFT convergence pattern with increasing order
- extracted Λ_b is consistent with NN scattering ● N^2LO coefficient may be an outlier

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

- Hüther *et al.*, PLB **808**, 135651; 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



thanks to my collaborators:

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