Theoretical advances and uncertainty quantification of neutron star properties

Christian Drischler

INT-22-2a: Neutron Rich Matter on Heaven and Earth

July 21, 2022

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BUQEYE Collaboration

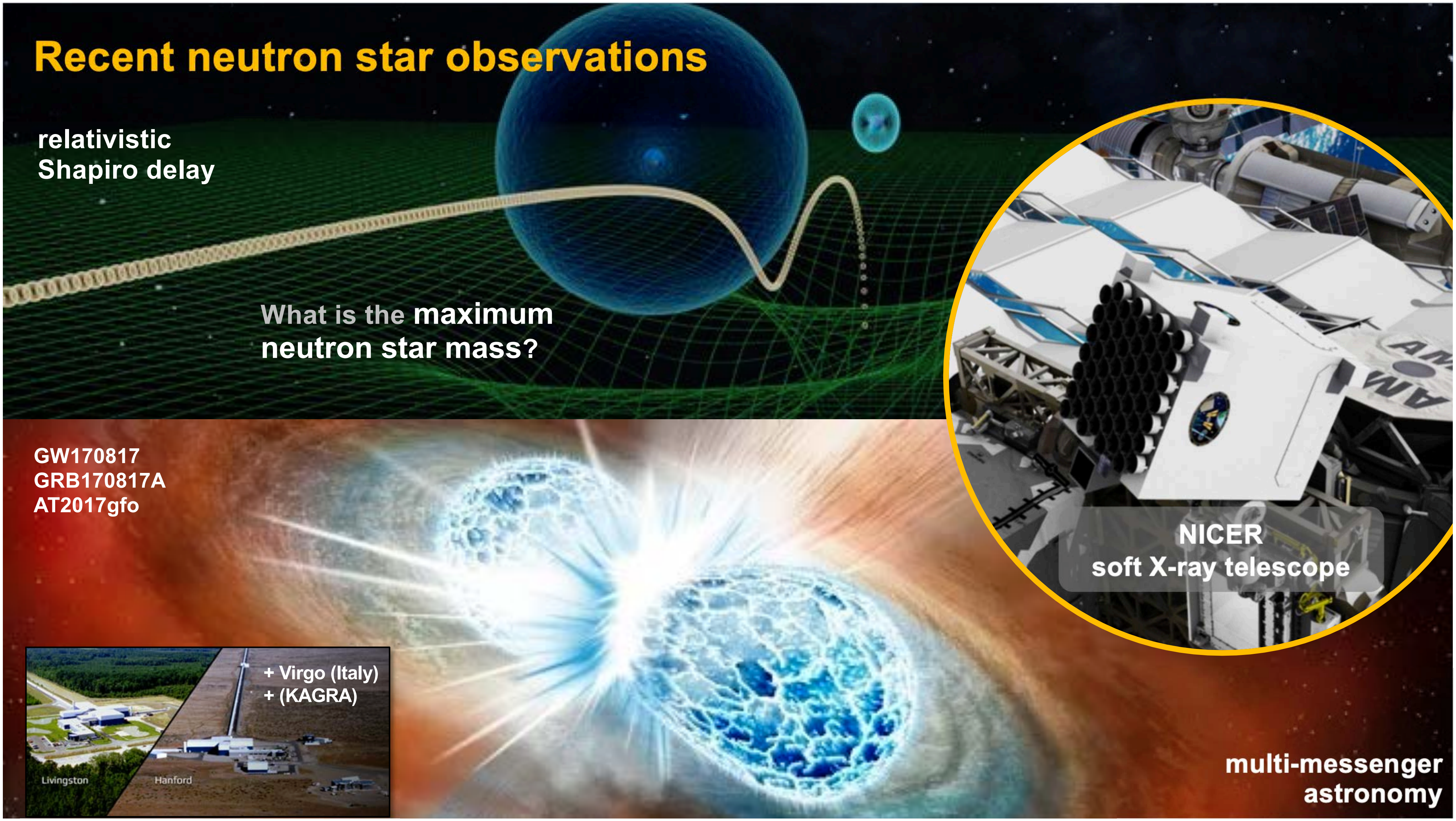
Ribbon-cutting ceremony
May 2, 2022

Facility for Rare Isotope Beams
at Michigan State University

Samuel L. Stanley
President of MSU

Jennifer M. Granholm
Secretary of Energy

Recent neutron star observations



relativistic
Shapiro delay

What is the **maximum neutron star mass?**

GW170817
GRB170817A
AT2017gfo

+ Virgo (Italy)
+ (KAGRA)

NICER
soft X-ray telescope

multi-messenger
astronomy

Nuclear theory in the precision era

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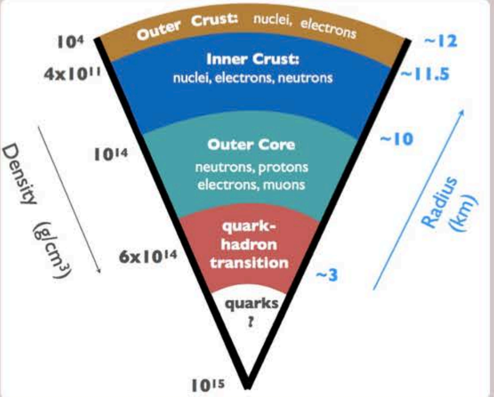
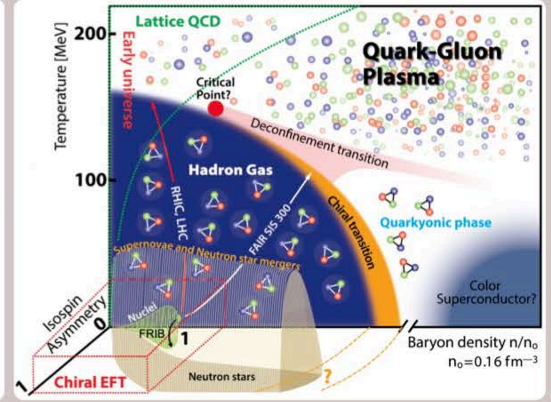
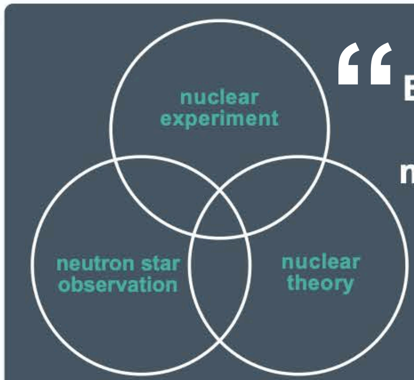
How can neutron star observations help **improve** nuclear **effective field theories** ?

What are the **phases** of neutron star matter below two times normal densities ?

At what density scale does nuclear effective field theory **break down** ?







> “**Enormous progress in theory, experiment, and observation make this new era particularly fruitful for the determination of the equation of state of neutron-rich matter.**”

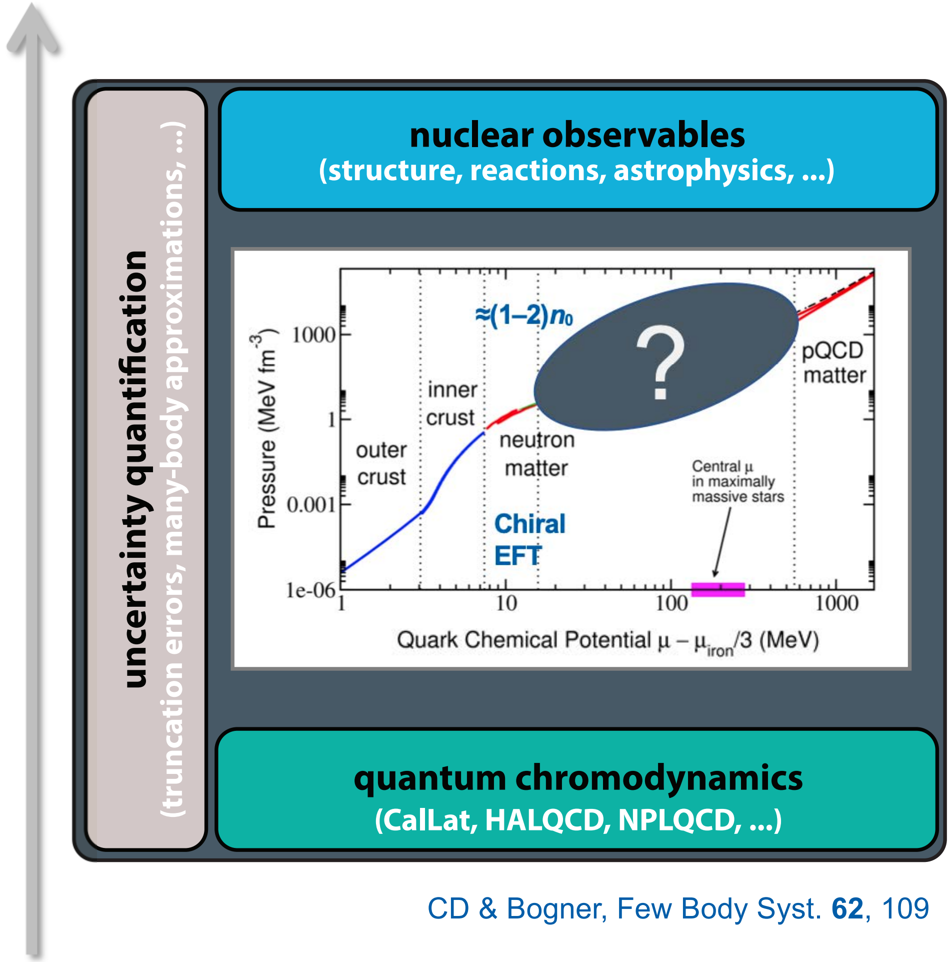
Required: *statistically* meaningful comparisons

Papers presenting the results of theoretical calculations are **expected to include uncertainty estimates**…

- If the authors claim **high accuracy**, or improvements on the accuracy of previous work.
- If the primary motivation for the paper is to make **comparisons with present or future high precision experimental measurements**.
- If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

Phys. Rev. A: Editorial (April 2011)

Ab initio workflow (idealized)



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

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

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

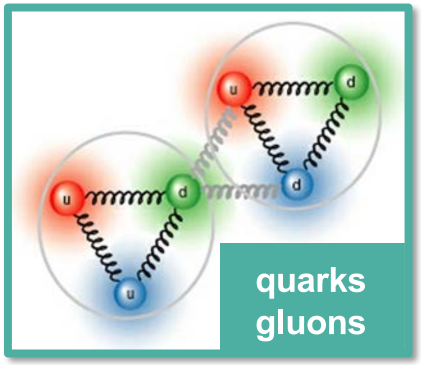
CD & Bogner, Few Body Syst. **62**, 109

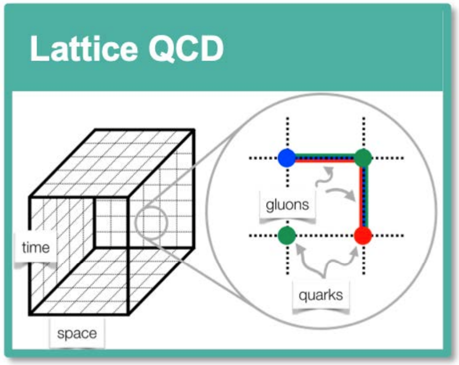
Here: nuclear equation of state (EOS)

energy per particle (and derived quantities)

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

baryon density n
neutron excess δ
temperature T (= 0)





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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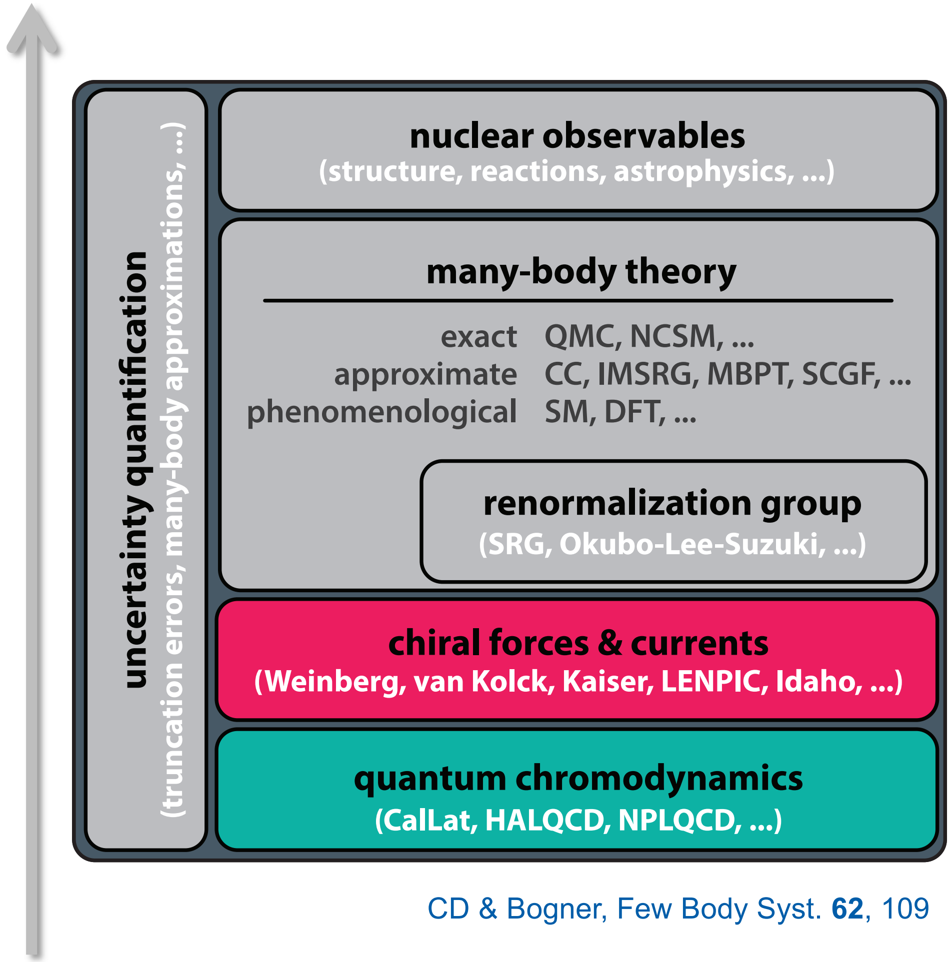

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many-body theory

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

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

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

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baryon density n
neutron excess δ
temperature T (= 0)

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

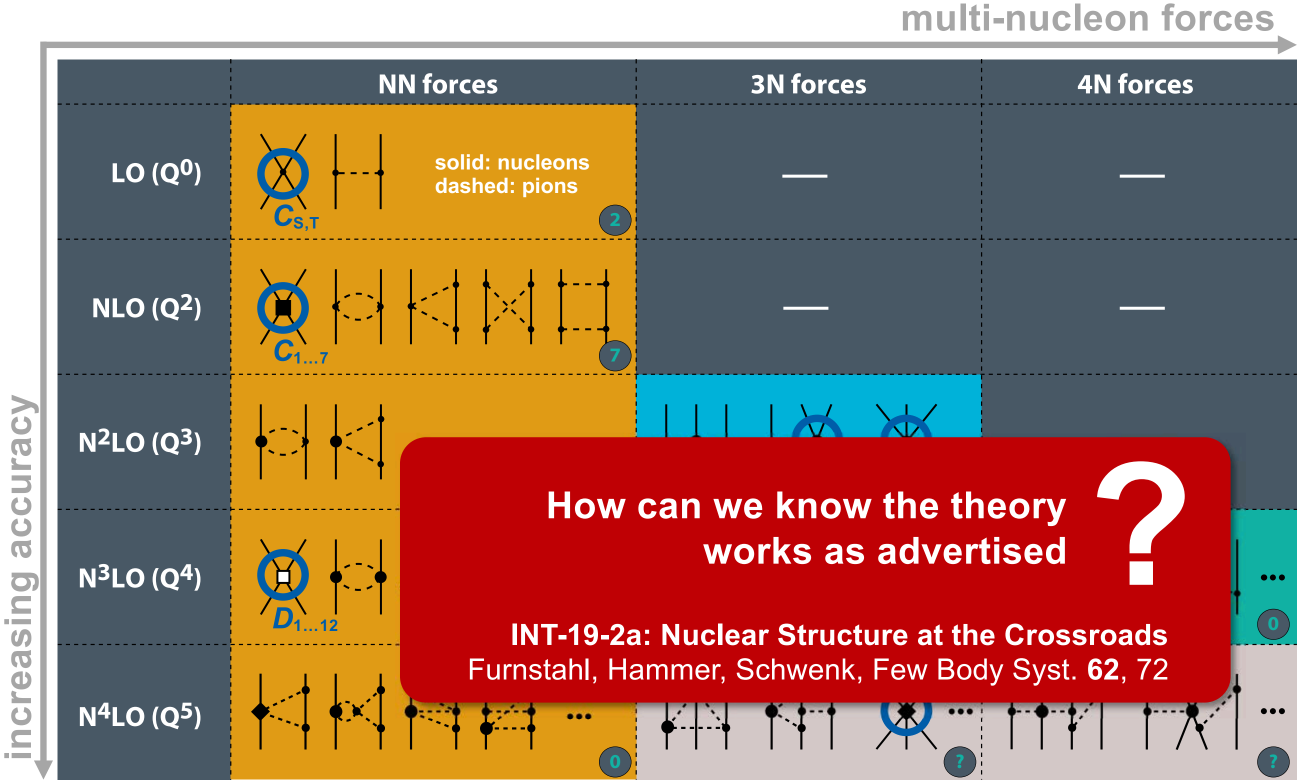
chiral effective field theory
provides microscopic interactions consistent with the symmetries of *low-energy* QCD

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

Modern theory of nuclear forces

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

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



How can we know the theory works as advertised ?

INT-19-2a: Nuclear Structure at the Crossroads
Furnstahl, Hammer, Schwenk, Few Body Syst. **62**, 72

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

Chiral Effective Field Theory

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

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

fit the unknown couplings $\boldsymbol{\theta}$ to experimental (or lattice) data

- NN: phase shifts & deuteron
- 3N/4N: binding energies, charge radii

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

see also: Low Energy Nuclear Physics International Collaboration (LENPIC)

Bayesian statistics is ideal for quantifying and propagating theoretical uncertainties

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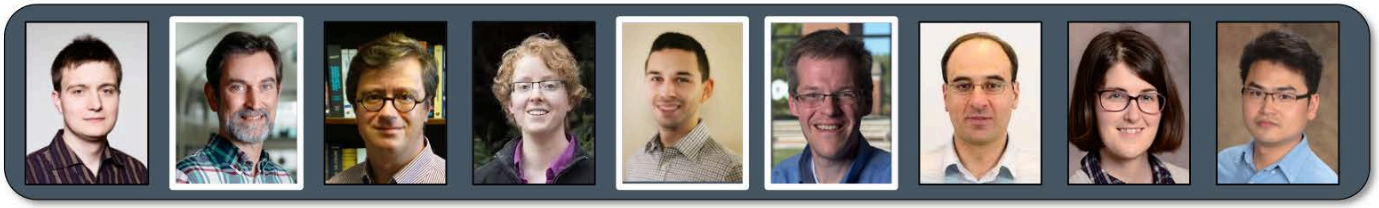
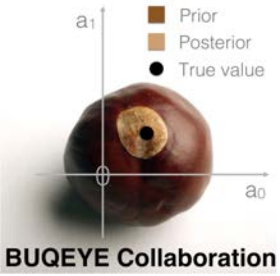




Bayesian
Uncertainty
Quantification:
Errors for
Your
EFT

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

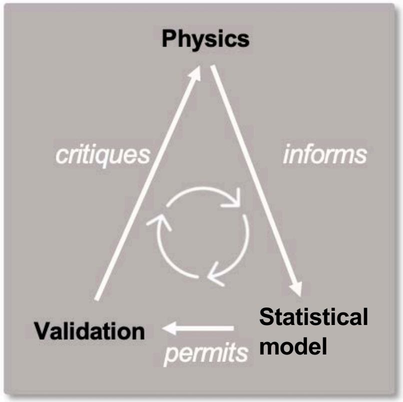
Select papers for UQ in EFT-based calculations:

How well do we know the neutron-matter EOS at the densities inside neutron stars? A Bayesian approach with correlated uncertainties, CD, Furnstahl, Melendez, Phillips, PRL **125**, 202702.

Rigorous constraints on 3N forces […] calculations of few-body observables, Wesolowski, Svensson, Ekström *et al.*, PRC **104**, 064001.

Fast & accurate emulation of two-body scattering observables without wave functions, Melendez, CD, Garcia, Furnstahl, Zhang, PLB **821**, 136608.

Designing Optimal Experiments: An Application to Proton Compton Scattering, Melendez, Furnstahl, Grießhammer, McGovern, Phillips, Pratola, EPJ **57**, 81.



BUQEYE aims to use (Bayesian) statistical tools to **answer fundamental problems** in the **construction and application of** EFTs in nuclear physics. The tools include:

- **parameter estimation**
- **model checking & selection**
- **fast & accurate emulators**
- **experimental design**

BAND
Bayesian Analysis of Nuclear Dynamics

An NSF Cyberinfrastructure Framework designed to facilitate:

- **Bayesian Model Mixing** to quantify model uncertainty;
- **full UQ** for experimentally inaccessible environments such as neutron stars;
- Bayesian **experimental design** to assess the impact of proposed experiments.

BAND Manifesto,
Phillips, Furnstahl, Heinz *et al.*,
JGP: NP **48** 072001

Spotlight: rigorous constraints on chiral forces

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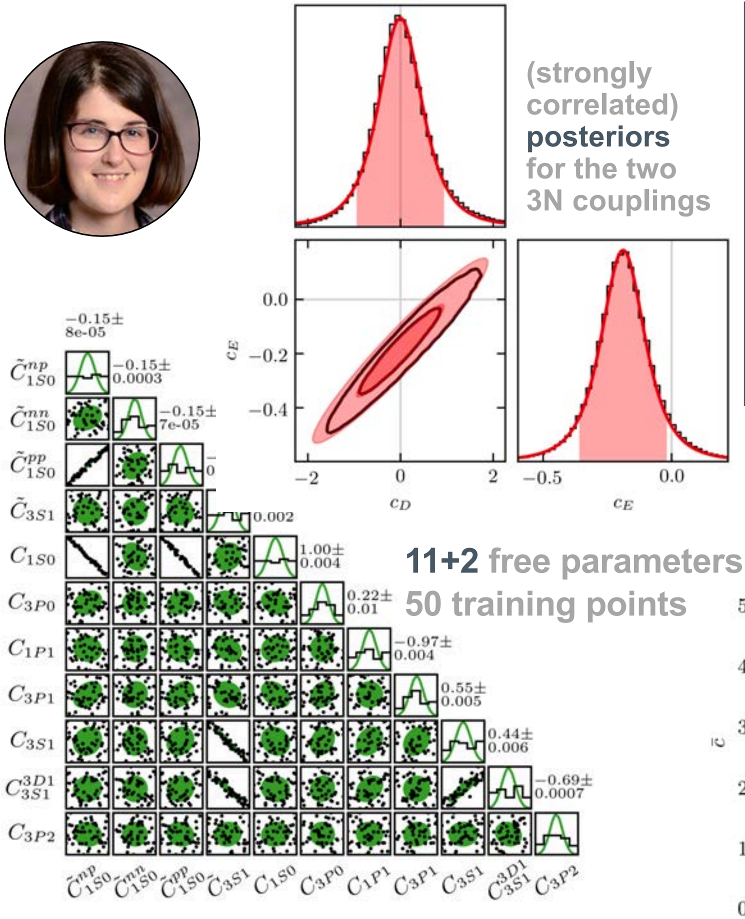


(strongly correlated) **posteriors** for the two 3N couplings

11+2 free parameters

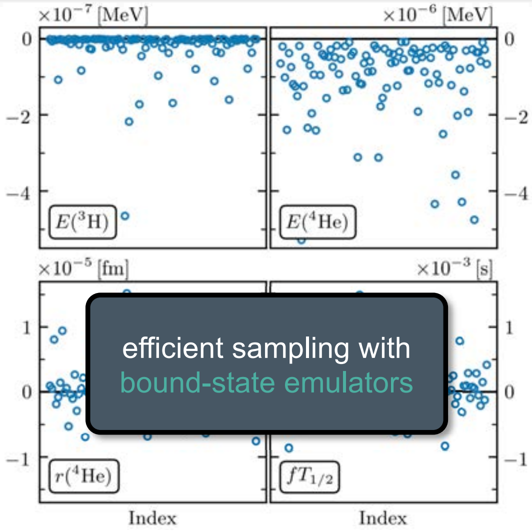
50 training points

Wesolowski, Svensson *et al.*, PRC **104**, 064001

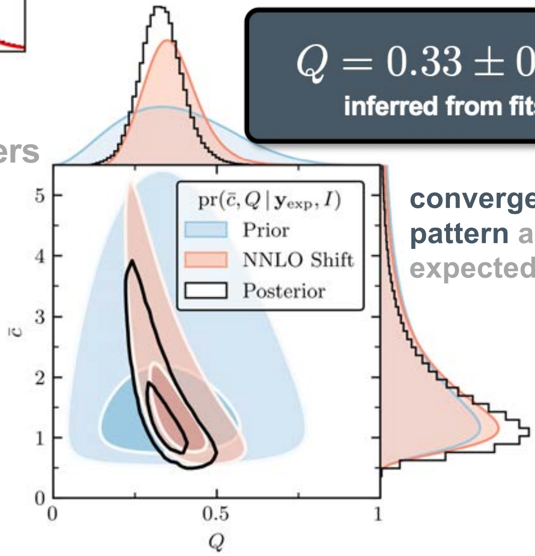
First chiral potentials (up to N^{2}LO) with uncertainties fully quantified

- ✓ EFT truncation errors
- ✓ data errors (LEC fits)
- ✓ method uncertainties

Applications to *A* = *6* nuclei:
Djärv, Ekström *et al.*, PRC **105**, 014005



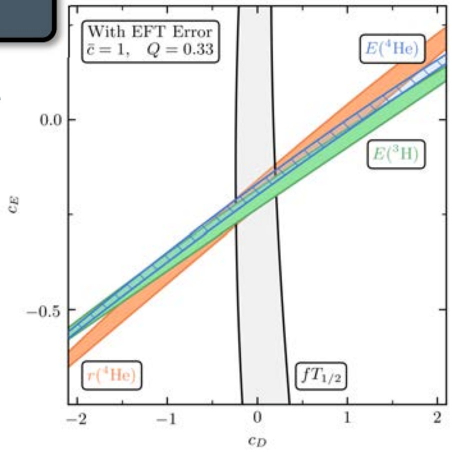
efficient sampling with bound-state emulators



$$Q = 0.33 \pm 0.06$$

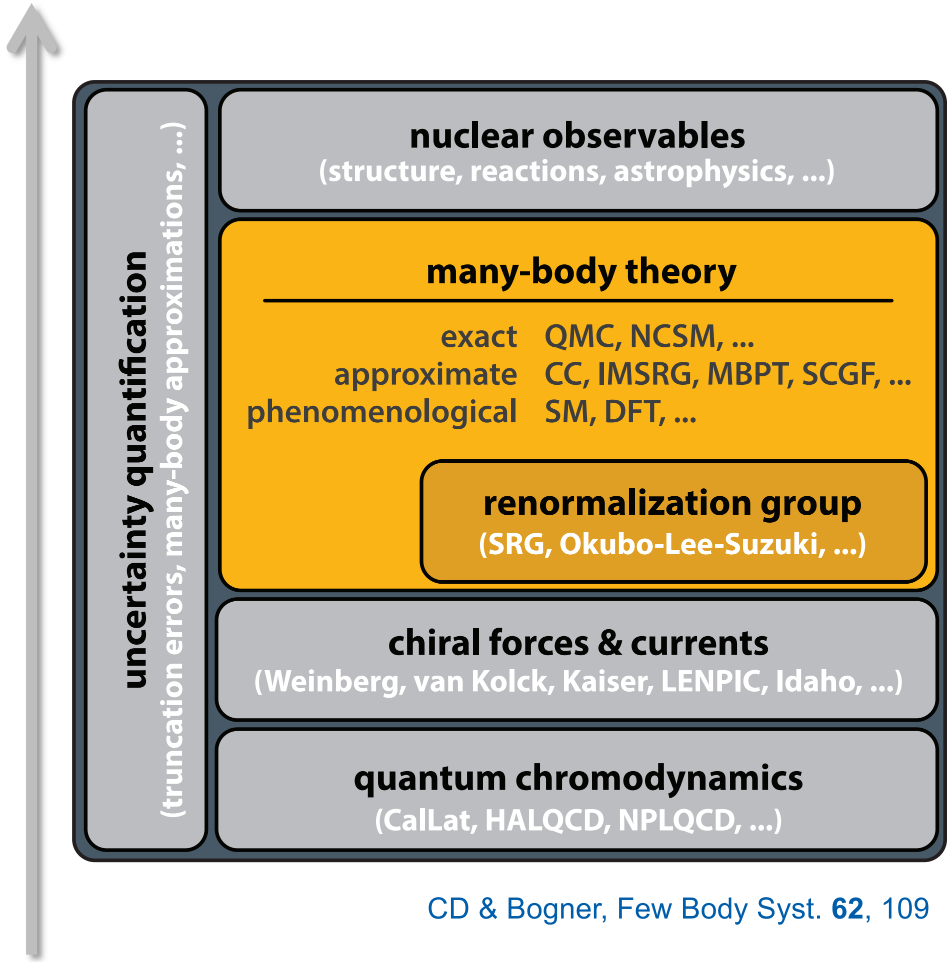
inferred from fits

convergence pattern as expected



Simultaneous fits can be problematic without EFT truncation errors

Ab initio workflow (idealized)



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

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(structure, reactions, astrophysics, ...)

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

Here: nuclear equation of state (EOS)
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neutron excess δ
temperature T (= 0)

Here: many-body perturbation theory (MBPT)

computationally efficient method (HPC-friendly)
allows to estimate many-body uncertainties

Widely applicable:

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

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

Many-body perturbation theory (MBPT) in a nutshell

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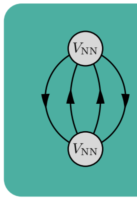
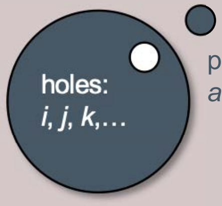
$$\frac{E^{(0)}}{V} = +\frac{1}{2}\sum_{ij} \langle ij \,|\, \overline{V}_{\rm NN} \,|\, ij \rangle$$

Hartree-Fock



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

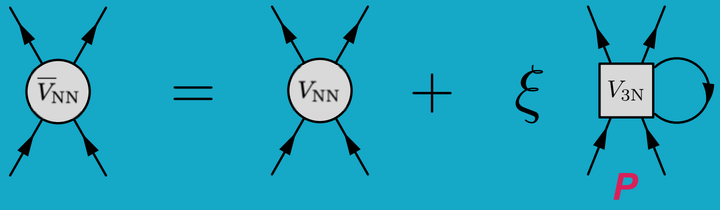
second order



holes: *i, j, k,…*

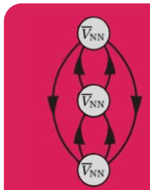
particles: *a, b, c,…*

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



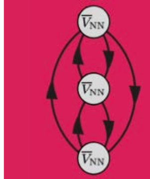
effective potential **genuine NN forces** **normal-ordered 3N forces**

typically requires approximations | involved at N^{3}LO+



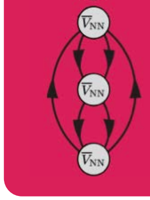
$$\frac{E^{(3)}_{hh}}{V} = +\frac{1}{8}\sum_{\substack{ab\\ijkl}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab\rangle \langle kl \,|\, \overline{V}_{\rm NN} \,|\, ij\rangle \langle ab \,|\, \overline{V}_{\rm NN} \,|\, kl\rangle}{D_{ijab}D_{klab}}$$

involved partial-wave decomposition



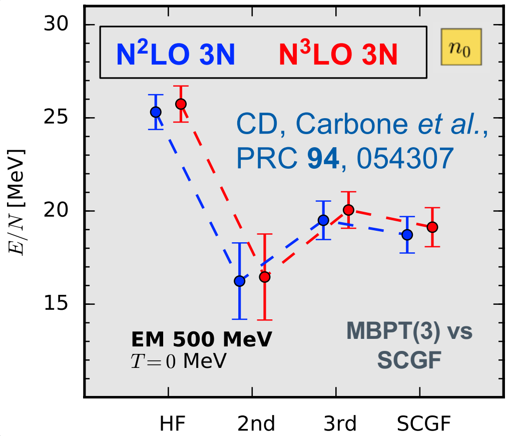
$$\frac{E^{(3)}_{ph}}{V} = +\sum_{\substack{abc\\ijk}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab\rangle \langle ak \,|\, \overline{V}_{\rm NN} \,|\, ic\rangle \langle bc \,|\, \overline{V}_{\rm NN} \,|\, jk\rangle}{D_{ijab}D_{jkbc}}$$

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

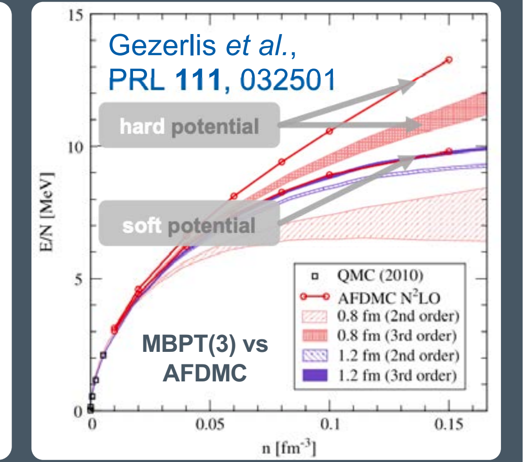


$$\frac{E^{(3)}_{pp}}{V} = +\frac{1}{8}\sum_{\substack{abcd\\ij}} \frac{\langle ij \,|\, \overline{V}_{\rm NN} \,|\, ab\rangle \langle ab \,|\, \overline{V}_{\rm NN} \,|\, cd\rangle \langle cd \,|\, \overline{V}_{\rm NN} \,|\, ij\rangle}{D_{ijab}D_{ijcd}}$$

third order



CD, Carbone *et al.*, PRC **94**, 054307

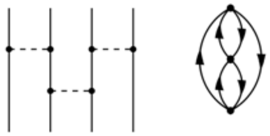


Gezerlis *et al.*, PRL **111**, 032501

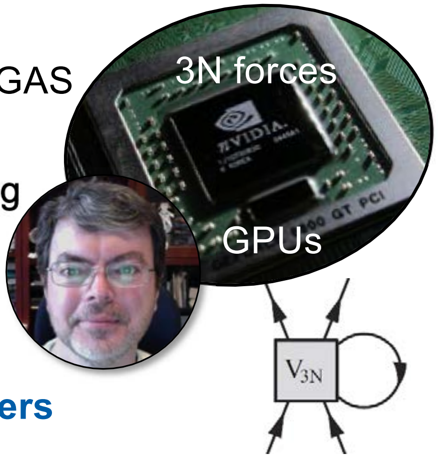
nonperturbative benchmarks in neutron matter

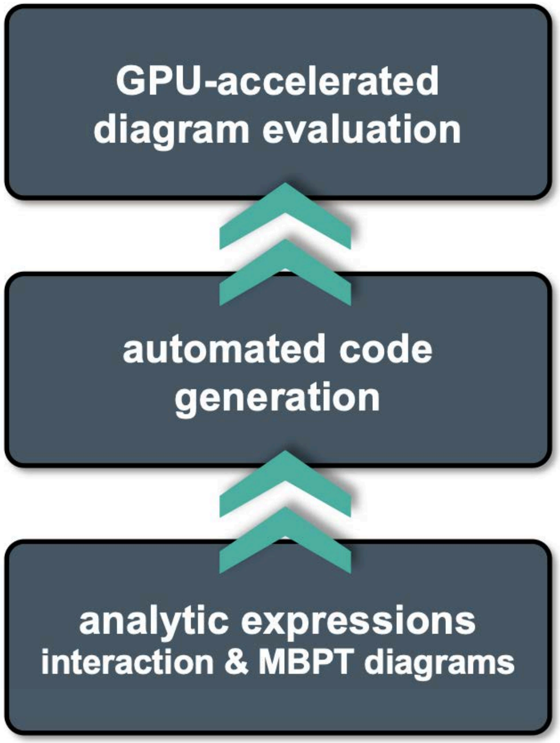
Monte Carlo framework for MBPT (second generation)

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



- **implementation of arbitrary diagrams** has become **straightforward** (numerically exact)
- multi-dimensional momentum integrals: improved VEGAS with CUDA, OpenMP, and MPI support
- hybrid, GPU-accelerated approach for normal ordering
- propagation of importance sampling distributions (*e.g.*, for mapping the EOS efficiently in density)
- **fast EOS calculations at low MBPT orders; controlled MBPT calculations at higher MBPT orders**





GPU-accelerated diagram evaluation

automated code generation

analytic expressions interaction & MBPT diagrams

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

For applications to the dilute Fermi Gas:
Wellenhofer, CD, Schwenk,
PRC **104**, 014003 & PLB **802**, 135247

High-order MBPT

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.

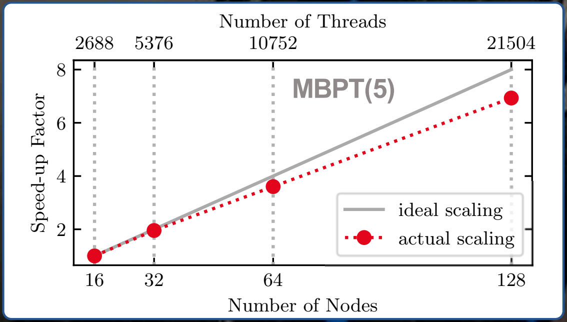
with automated diagram generation

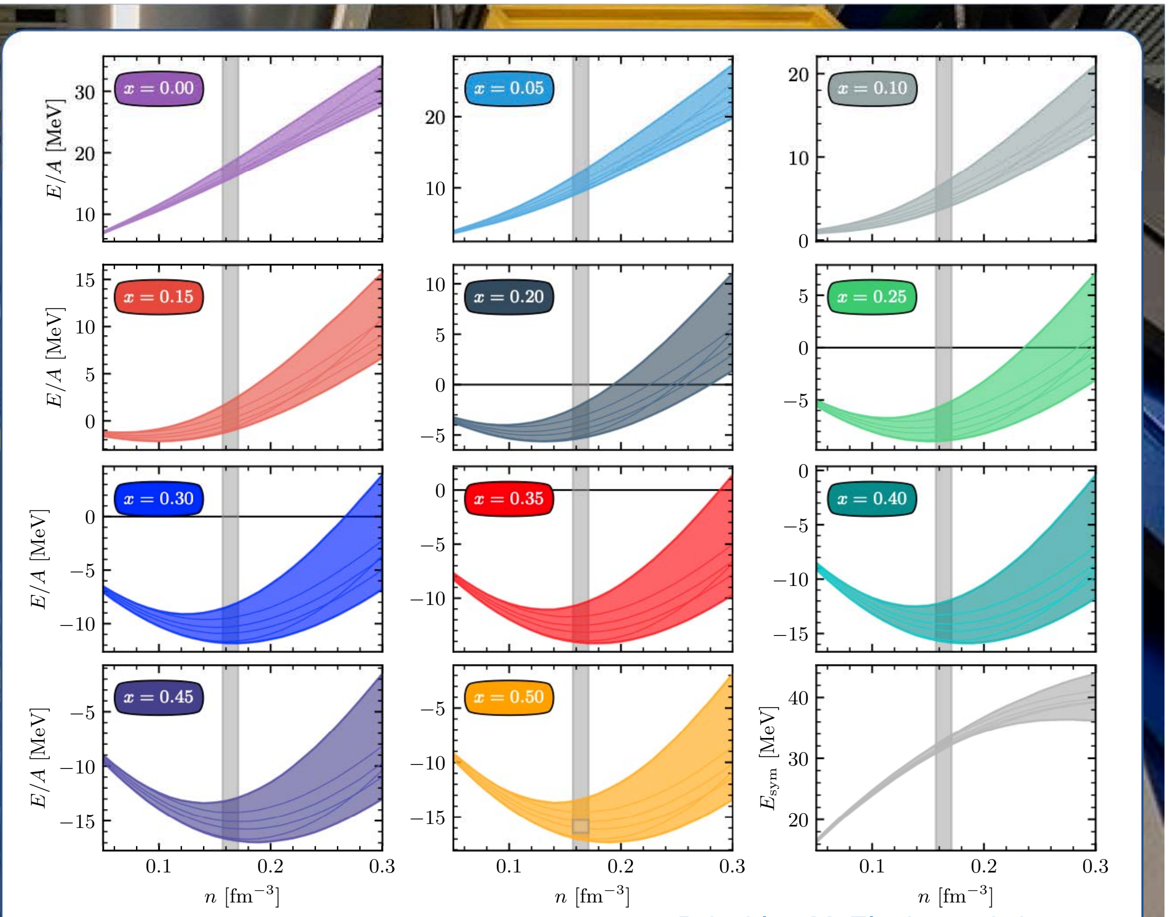
Stevenson, Int. J. Mod. Phys. C **14**, 1135
Arthuis *et al.*, Comput. Phys. **240**, 202

»

fully automated approach to MBPT for nuclear matter

MBPT: an HPC application





Drischler, McElvain *et al.*, in prep.

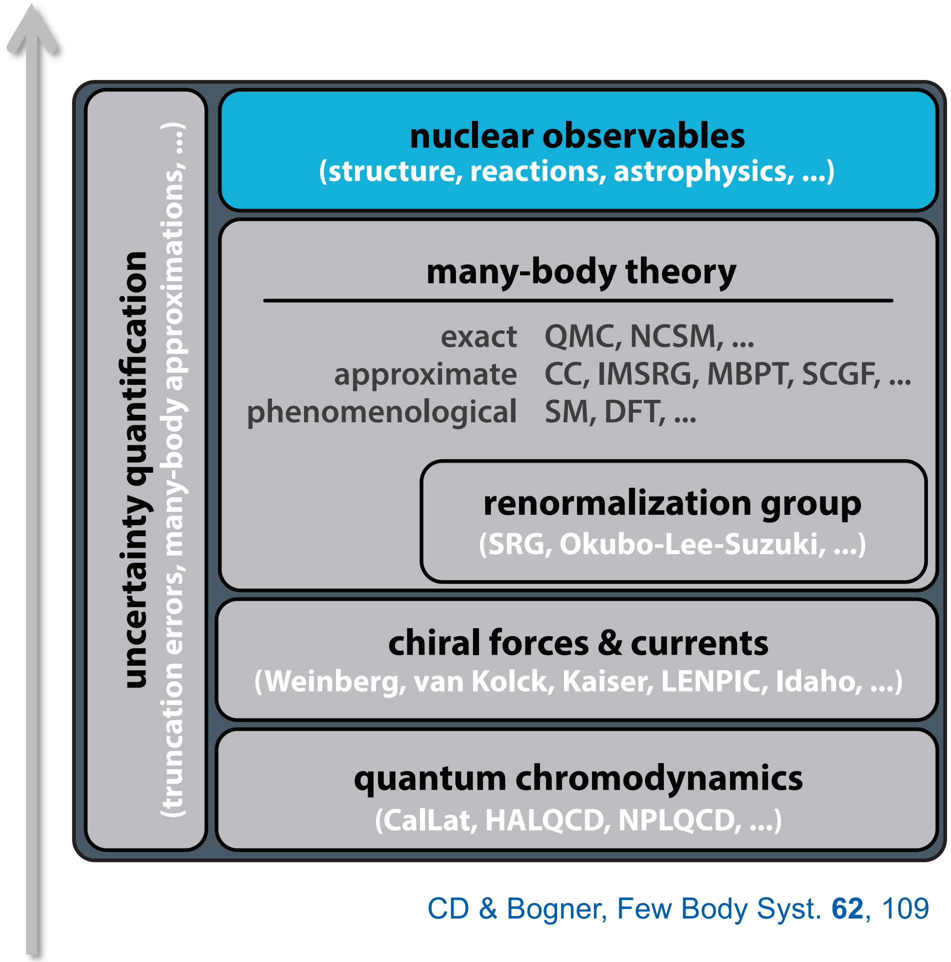
#2 (U.S.)

Summit @ Oak Ridge Leadership Computing Facility

202 752 CPU Cores
27 648 Nvidia GPUs

122.3 peta flops

Ab initio workflow (idealized)



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

nuclear EOS with quantified uncertainties
energy per particle (and derived quantities)

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baryon density n
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Uncertainty quantification

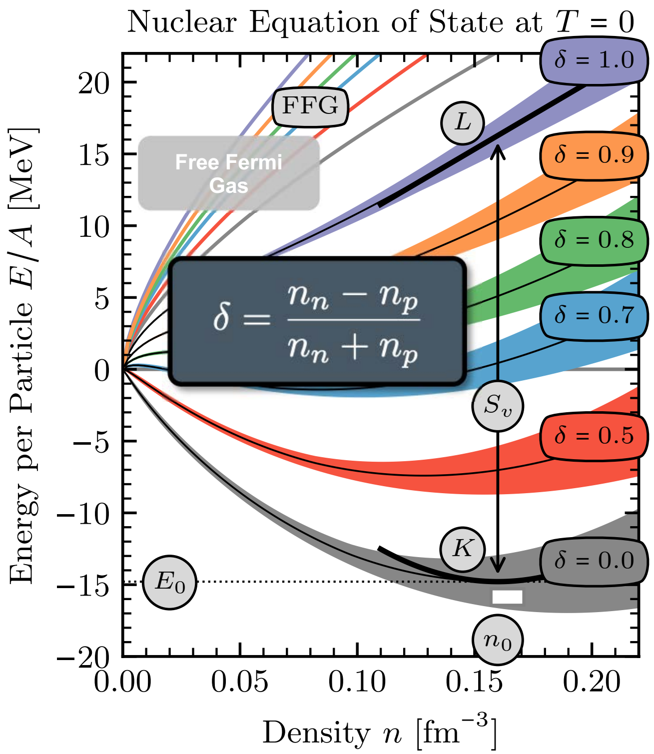
robust estimates of theoretical uncertainties using Bayesian machine learning via Gaussian Processes

uncertainties in EFT-based calculations due to:

- **truncating the EFT expansion**
- **applying many-body (and other) approximations**
- **fitting LECs to experimental data**

First chiral potentials with uncertainties
fully quantified and their application:
Wesolowski, Svensson *et al.*, PRC **104**, 064001
Djärv, Ekstöm *et al.*, PRC **105**, 014005

Microscopic EOS calculations

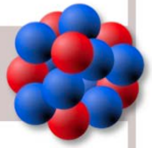


Great progress in **microscopic EOS calculations** at densities $\lesssim 2n_0$ and predictions for the neutron star structure

low-density EOS parameters

- symmetry energy S_v
- slope parameter L
- saturation point (n_0, E_0)
- incompressibility K

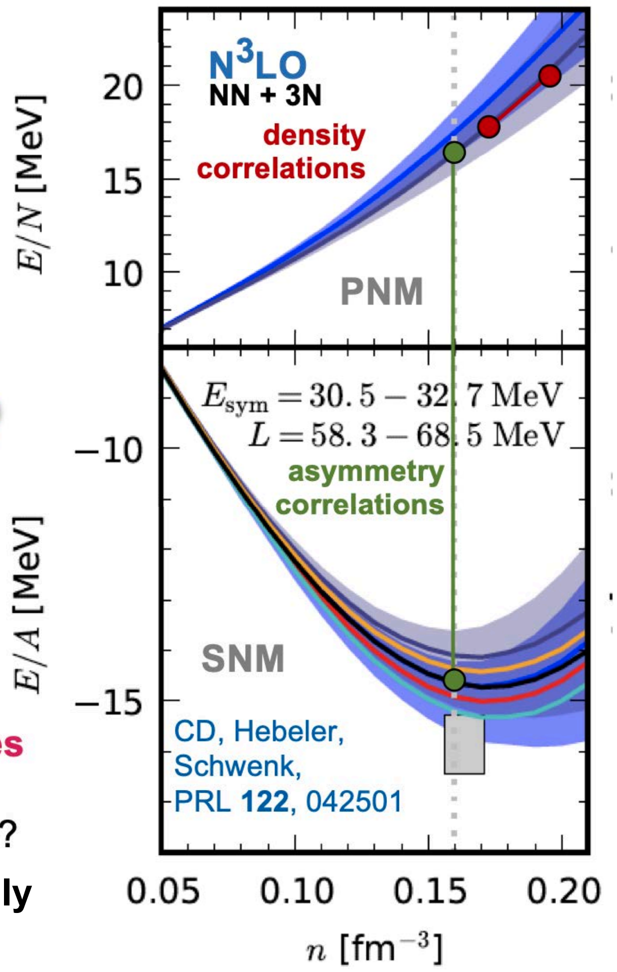
connection to experiment



- binding energies
- neutron skin thicknesses
- giant resonances
- heavy-ion collisions

But: the existing **uncertainty estimates** had only *limited* statistical meaning; *clean* propagation to derived quantities?

EFT truncation errors increase rapidly with increasing density



Rigorous UQ for nuclear matter

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

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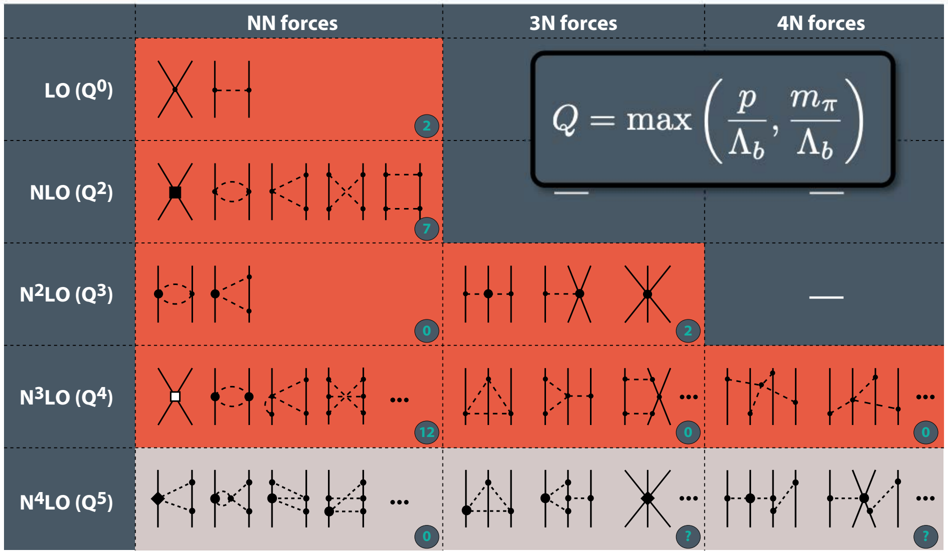

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

$\{y_0, y_2, y_3, \ldots, y_k\}$	**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**
$\mathcal{GP}\left[0, \bar{c}^2\, r(x, x'; l)\right]$	**treat all c_n as independent draws from a single Gaussian Process**
$\delta y_k = y_{\rm ref}\sum_{n=k+1}^{\infty} c_n Q^n$	**learn hyperparameters of that GP & compute to-all-orders truncation error**

Recent applications of BUQEYE's GP model for correlated EFT truncation errors:

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

***Ab initio* predictions link the neutron skin of ^{208}Pb to nuclear forces**
Hu, Jiang, Miyagi *et al.*, arXiv:2112.01125

***Ab initio* nucleon-nucleus elastic scattering with chiral EFT uncertainties**
Baker, McClung, Elster *et al.*, arXiv:2112.02442

Rigorous UQ for nuclear matter

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

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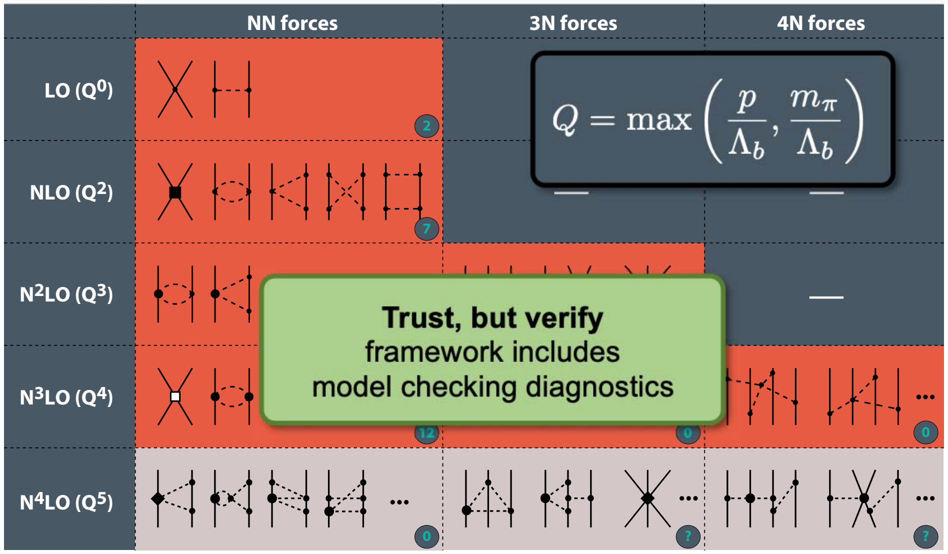

$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

Trust, but verify
framework includes
model checking diagnostics

$$\{y_0, y_2, y_3, \ldots, y_k\}$$

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make a *falsifiable* model assumption for the convergence pattern

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

treat all c_n as independent draws from a single Gaussian Process

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

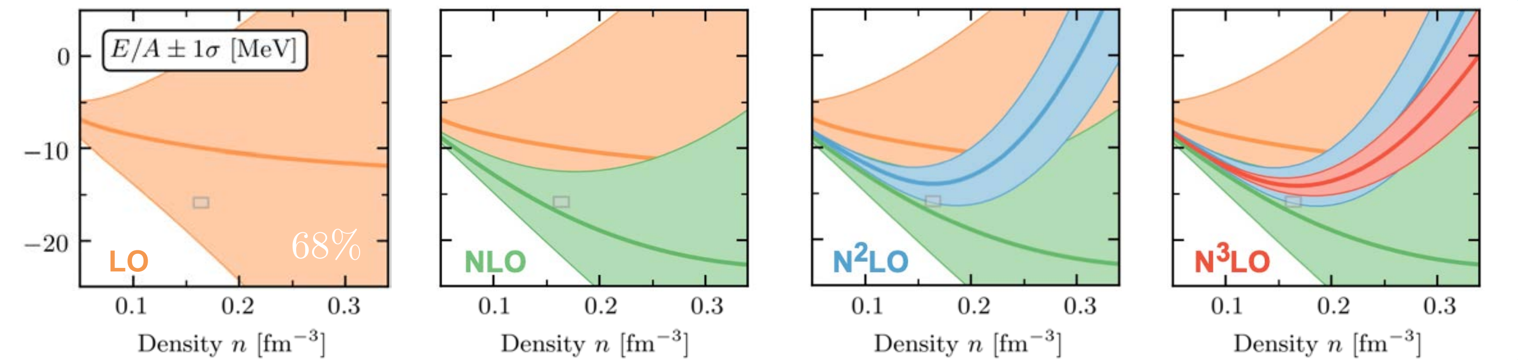
learn hyperparameters of that GP & compute to-all-orders truncation error

An example: symmetric matter

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

Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$



Rigorous UQ for nuclear matter

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

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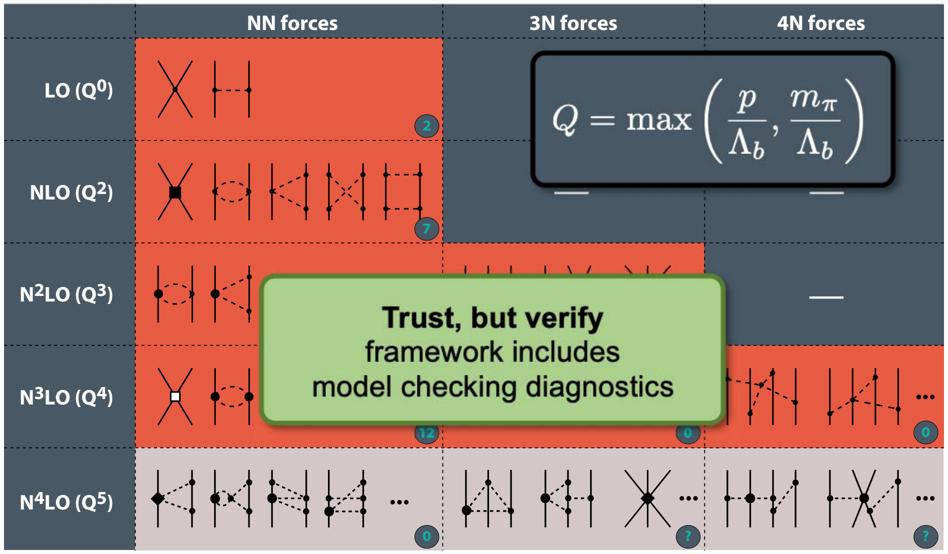


$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

Trust, but verify
framework includes
model checking diagnostics

$$\{y_0, y_2, y_3, \ldots, y_k\}$$

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

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

treat all c_n as independent draws from a single Gaussian Process

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

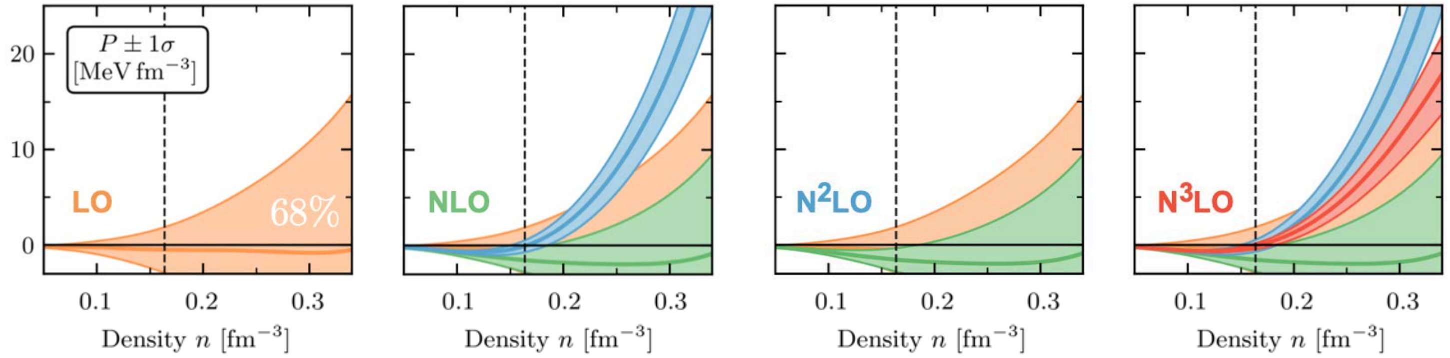
learn hyperparameters of that GP & compute to-all-orders truncation error

An example: symmetric matter

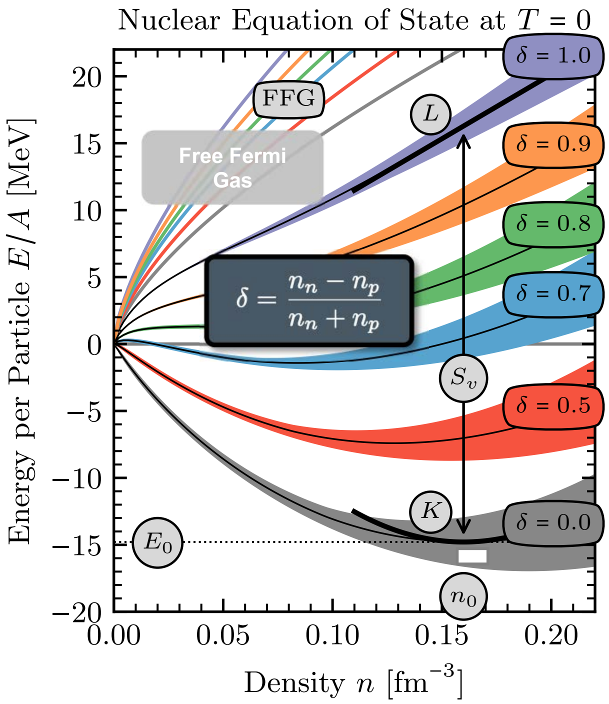
$$y = P \equiv n^2 \frac{\mathrm{d}}{\mathrm{d}n}\frac{E}{A}, \quad k = 4$$

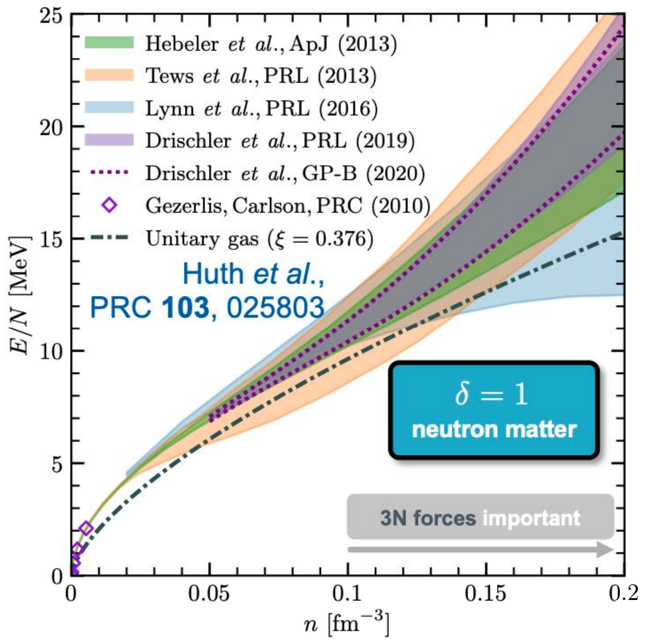
Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$

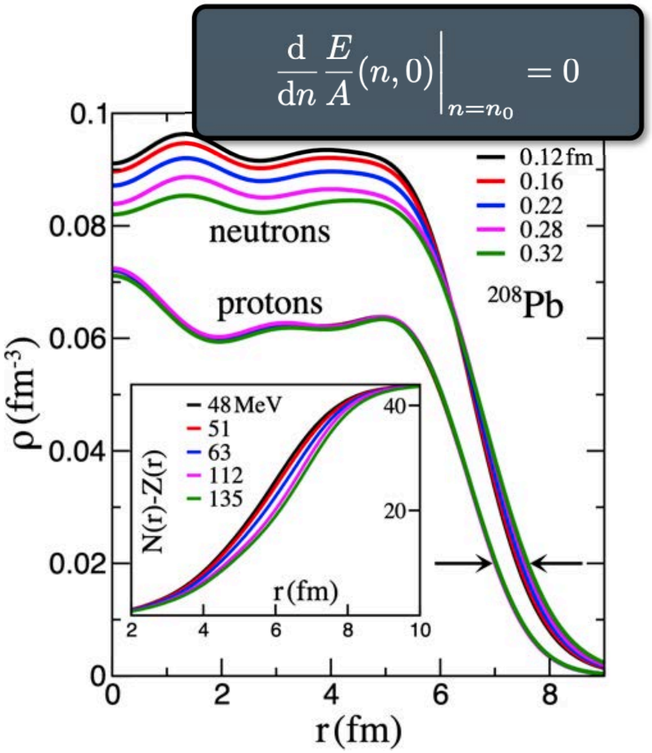


Neutron matter | saturation in symmetric matter





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



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

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

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

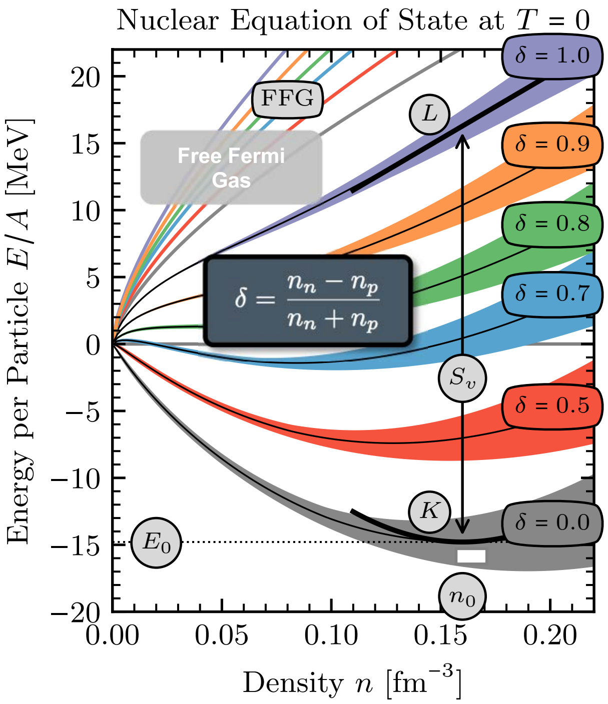
saturation point: **fine-tuned cancellation** between the kinetic and interaction contributions (ideal testbed for chiral EFT)

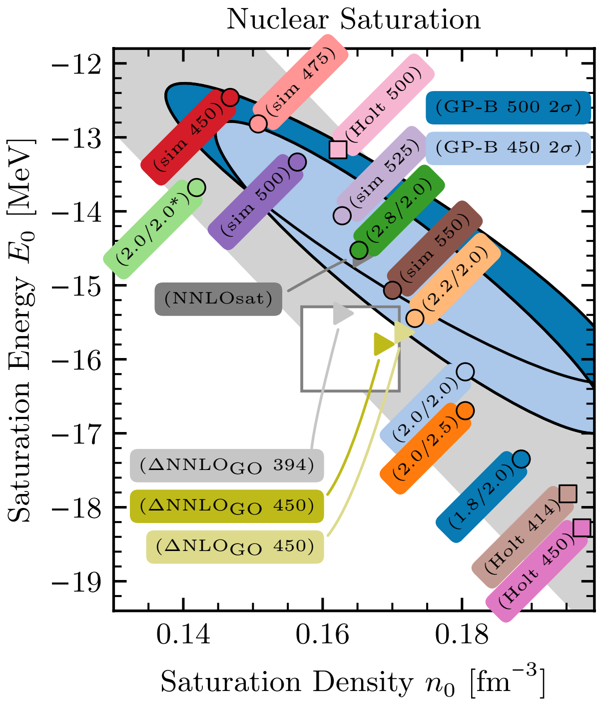
Coester band overlaps with the empirical box (but limited meaning without errors)

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

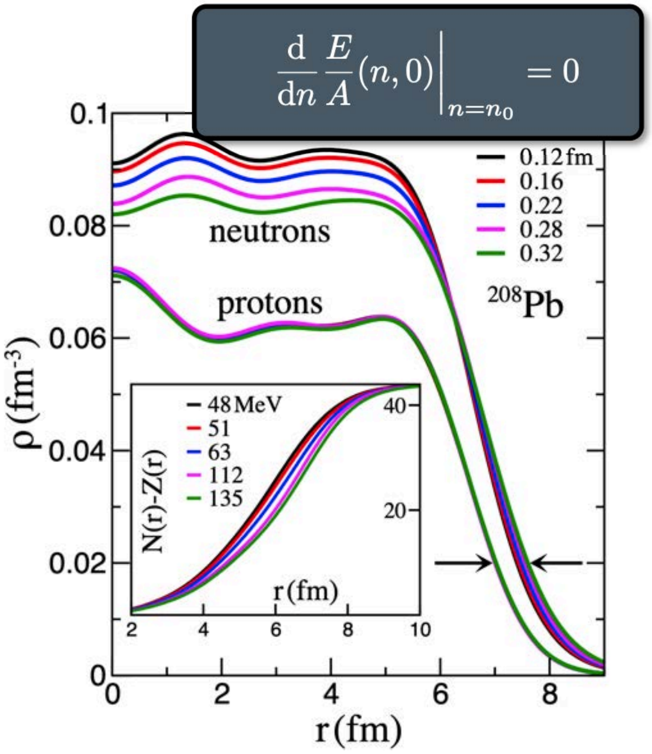
needed: improved predictions with novel NN+3N interactions and robust uncertainty quantification

Neutron matter | saturation in symmetric matter


Nuclear Equation of State at $T = 0$


Nuclear Saturation

CD, Holt, and Wellenhofer, Annu. Rev. Nucl. Part. Sci. **71**, 403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Piekarewicz & Fattoyev, Phys. Today **72**, 7

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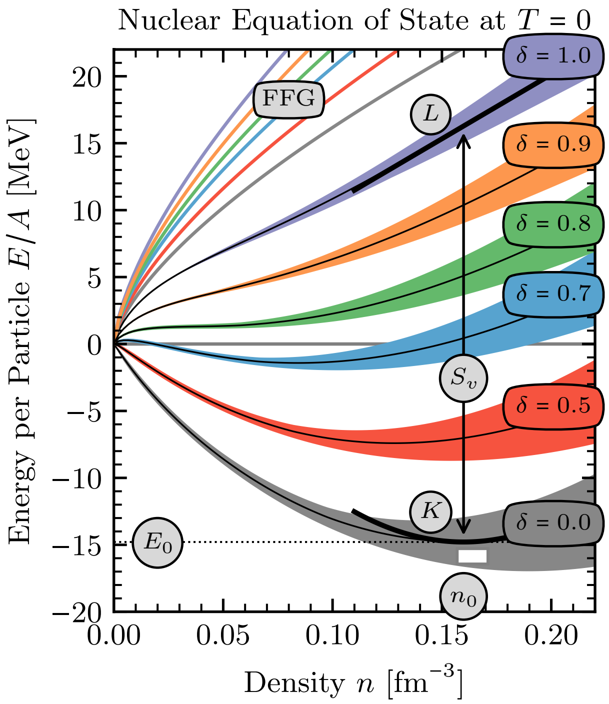
Annotations: (λ / Λ_{3N}) in fm^{-1} or (Λ) in MeV

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

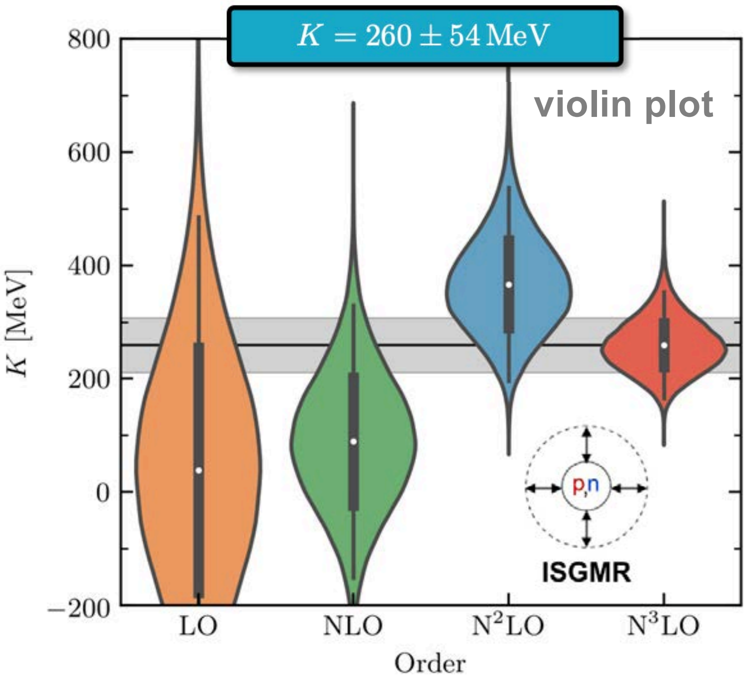
Incompressibility (in symmetric matter)



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

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

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

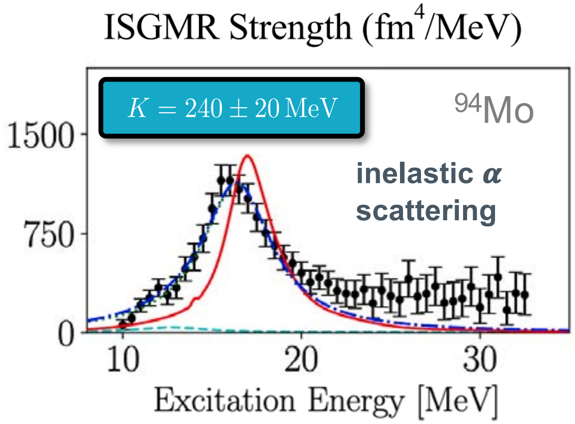


CD, Melendez *et al.*, PRC **102**, 054315

order-by-order convergence pattern

uncertainties due to the predicted saturation density included via marginalization

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



Howard, Garg *et al.*, PLB **807** 135608
Roca-Maza & Paar, PPNP **101**, 96

Approved FRIB experiment:
“The ISGMR in ^{132}Sn: Implications on the Nuclear Incompressibility”
Randhawa *et al.* (experiment: 21056)

Why correlations are important: symmetry energy

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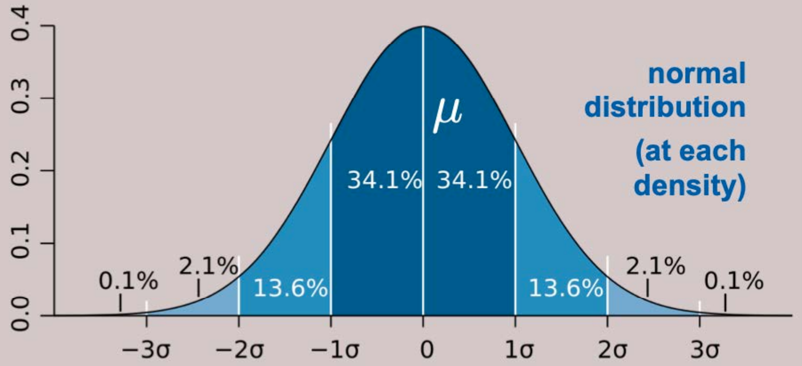
Reminder: Statistics 101



normal distribution

(at each density)

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

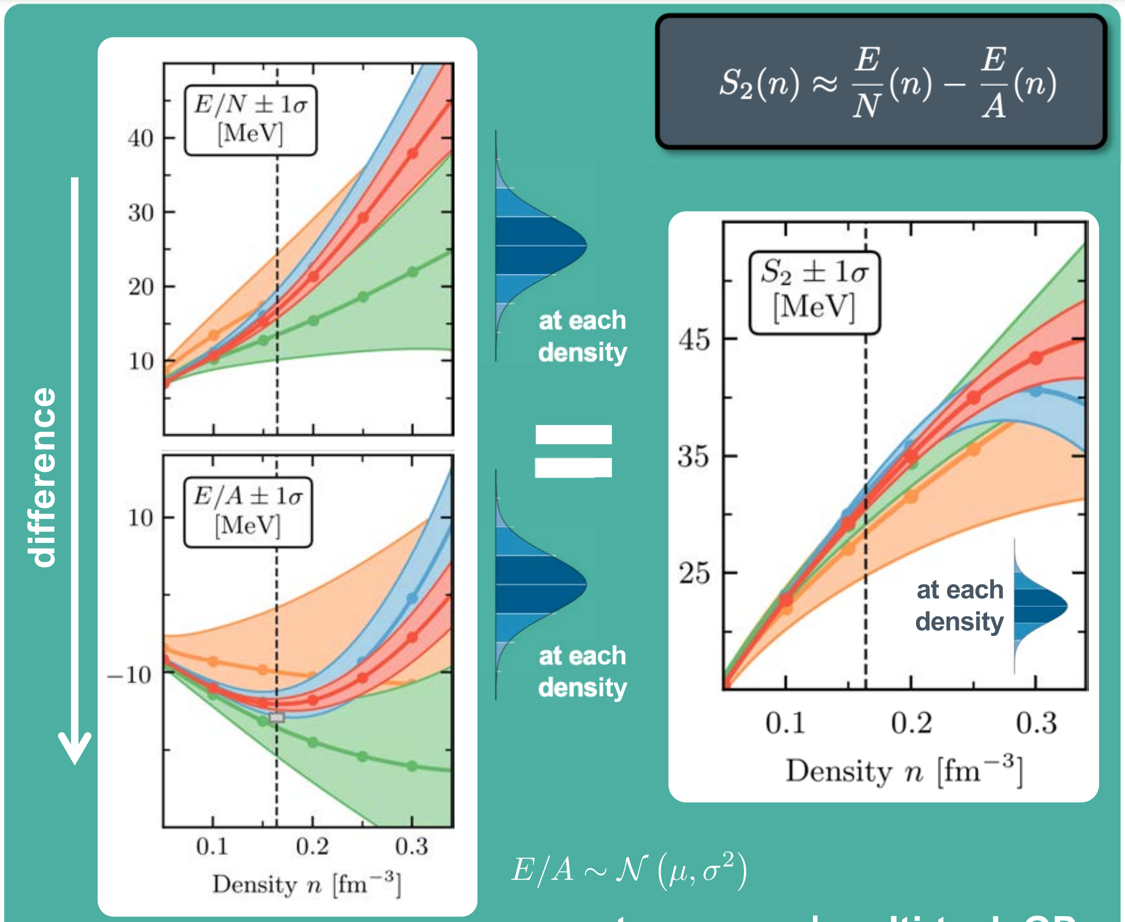
$$\mu_{S_2} = \mu_{\text{PNM}} - \mu_{\text{SNM}}$$

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

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

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

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



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

symmetry energy | multi-task GPs

Nuclear symmetry energy

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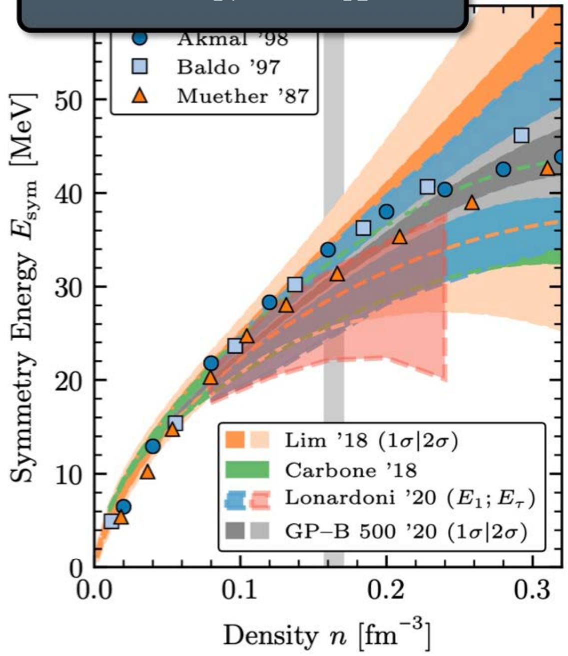
$$S_2(n) \approx \frac{E}{N}(n) - \frac{E}{A}(n)$$



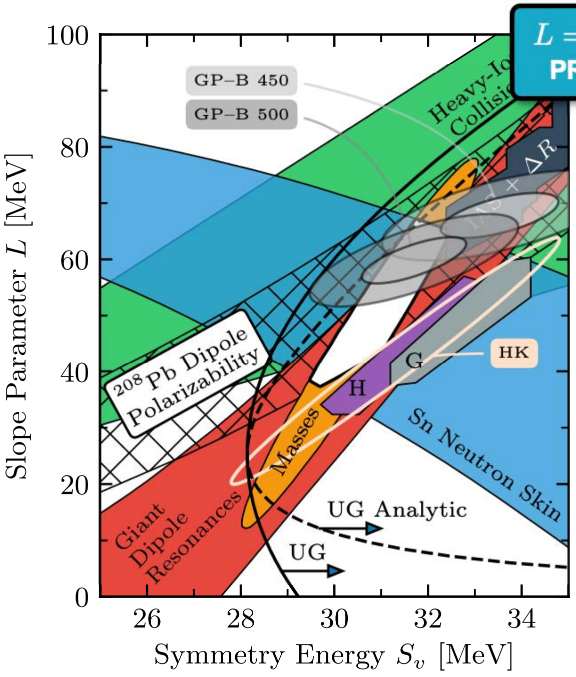
CD, Holt *et al.*, ARNPS **71**, 403

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

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

excellent agreement with experiment

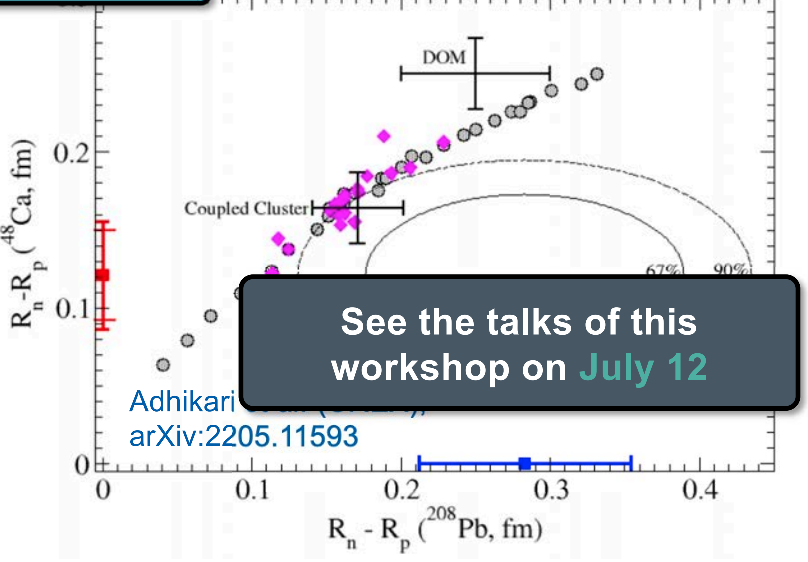
$L = 106 \pm 37$ MeV
PREX–II informed



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

marginalization over predicted saturation density

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



Adhikari
arXiv:2205.11593

See the talks of this workshop on July 12

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

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

3N forces beyond normal ordering?

Drischler, McElvain *et al.*, in prep.

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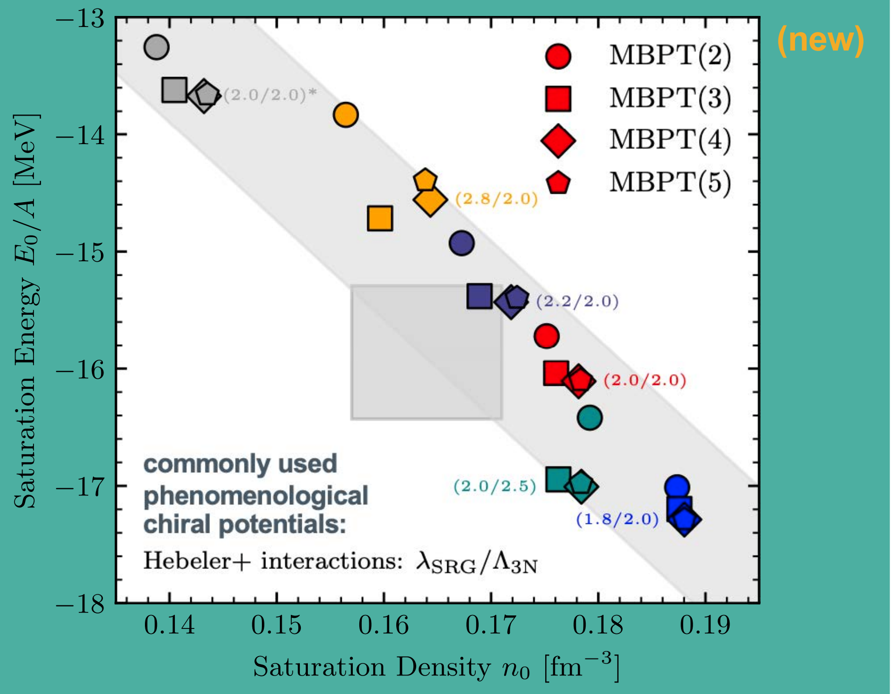
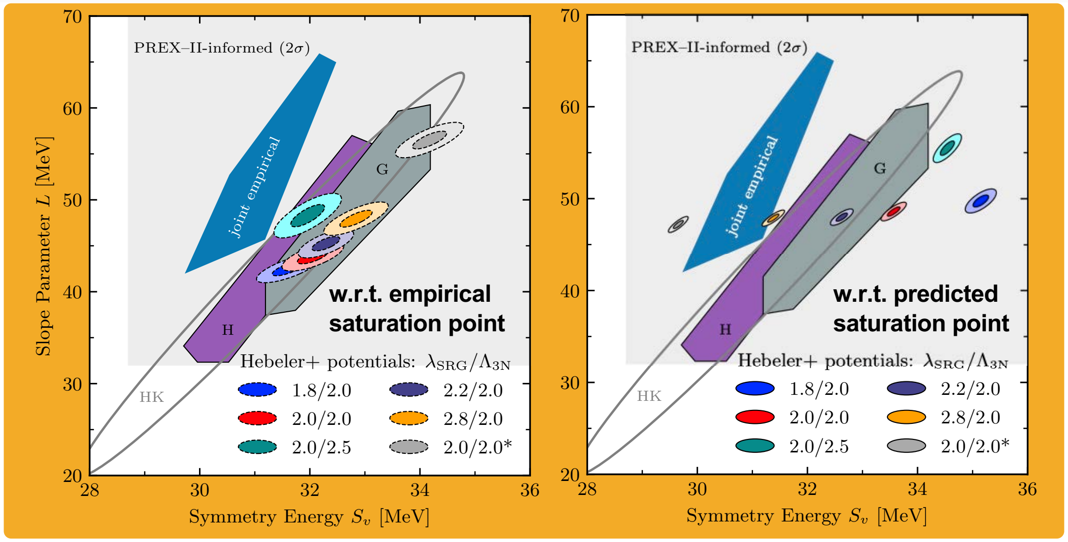
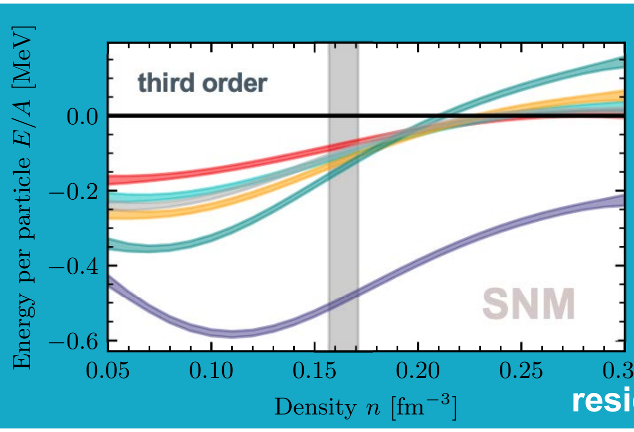
MBPT(*n*)	2	3	4	5
NN+3N norm. ord.	✓	✓	(✓, 3N)	✓
residual 3N	✓ (1)	✓ (14)	✗	✗

(new)



nuclear saturation | symmetric nuclear matter





14 new diagrams

first studied in closed-shell nuclei: from ^{4}He to ^{48}Ca

Hu, Li, Xu,
arXiv:1810.08804

residual 3N contributions

Exploring the limits of chiral EFT

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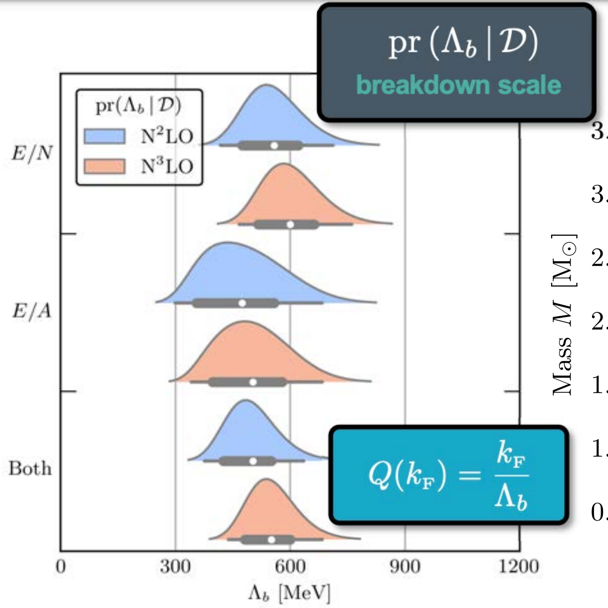
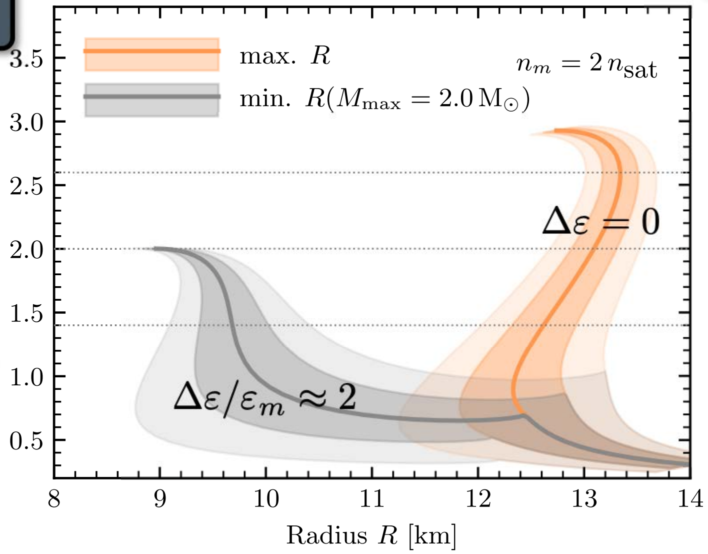


CD, Melendez *et al.*, PRC **102**, 054315

Bayesian inference of the in-medium breakdown scale

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

χEFT at N^{3}LO + causal EOS



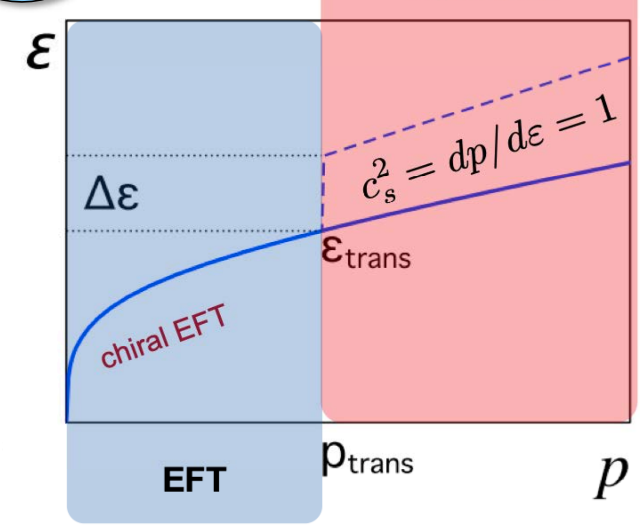
CD, Han, Lattimer *et al.*, PRC **103**, 045808
CD, Han, and Reddy, PRC **105**, 035808

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

could already be challenged by NICER

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

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



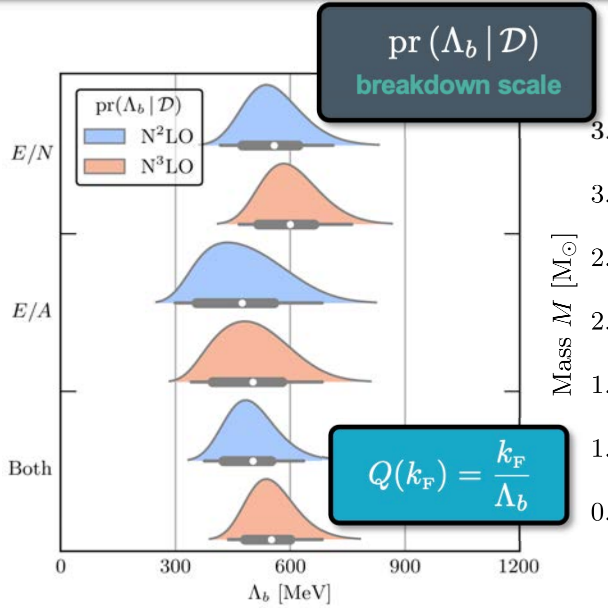
Han & Prakash, APJ **899**, 2
Alford *et al.*, JPG: NPP **46**, 114001

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 $R_{\min}$

Exploring the limits of chiral EFT



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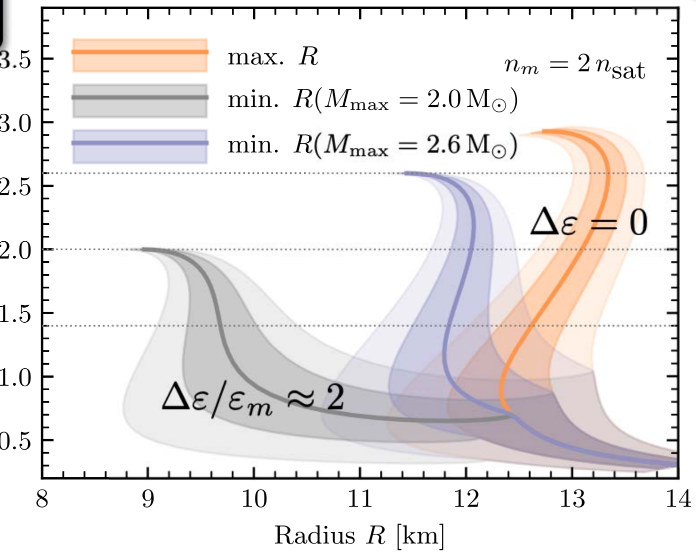

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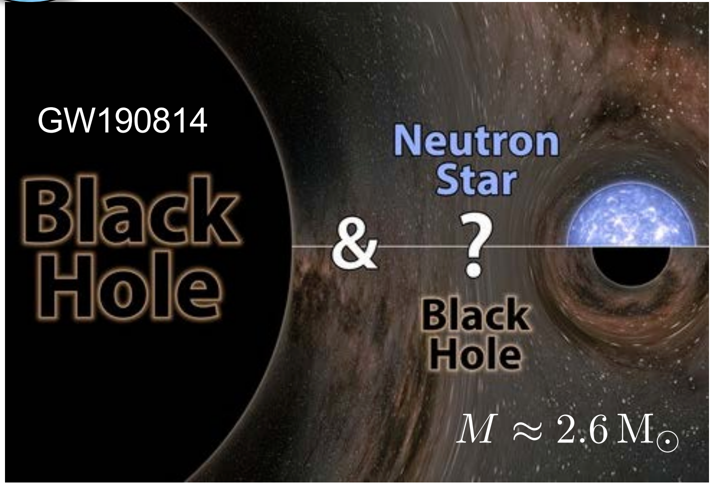

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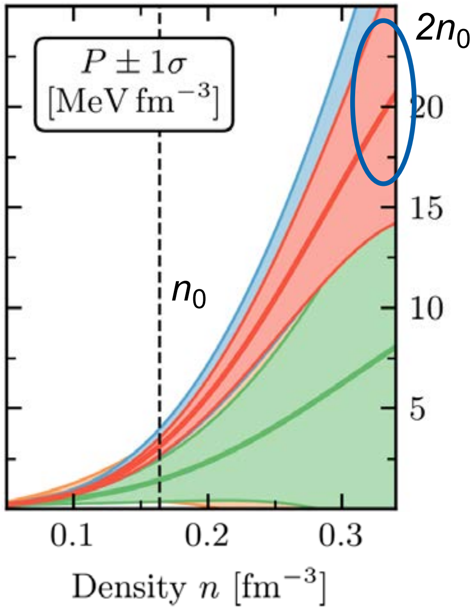
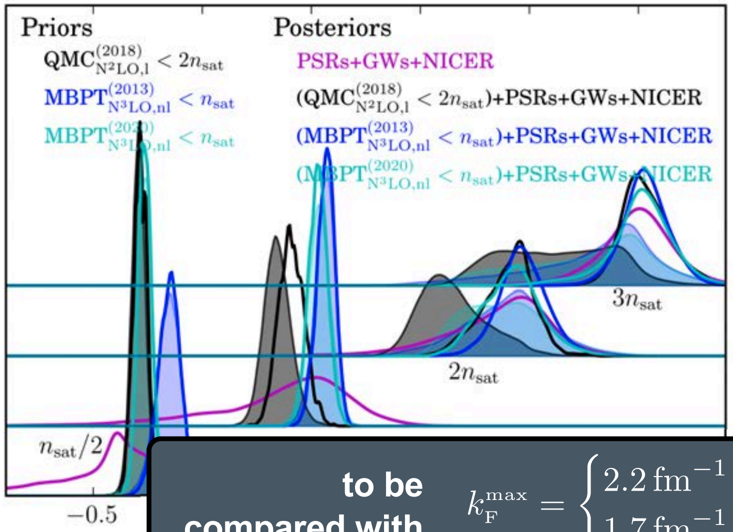
Direct astrophysical tests at supranuclear densities



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

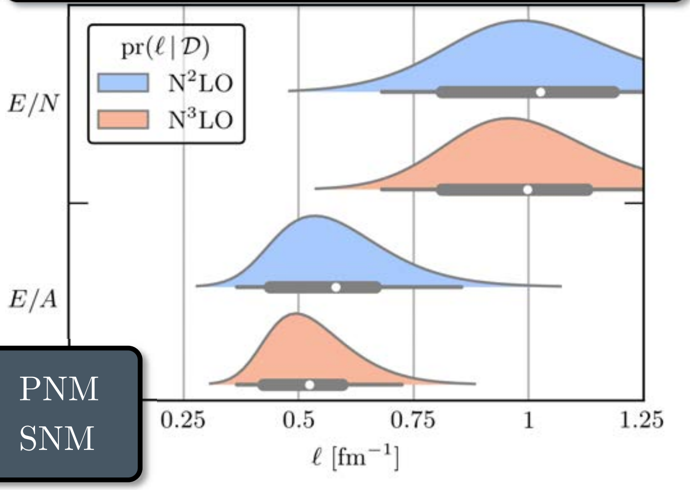
🟧 LO 🟩 NLO 🟦 N²LO 🟥 N³LO



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

see also: Essick *et al.*, PRC **102**, 055803

How correlated is nuclear matter? $\mathrm{pr}\,(\ell\,|\,\mathcal{D})$ correlation length



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

EFT truncation error is *highly* correlated

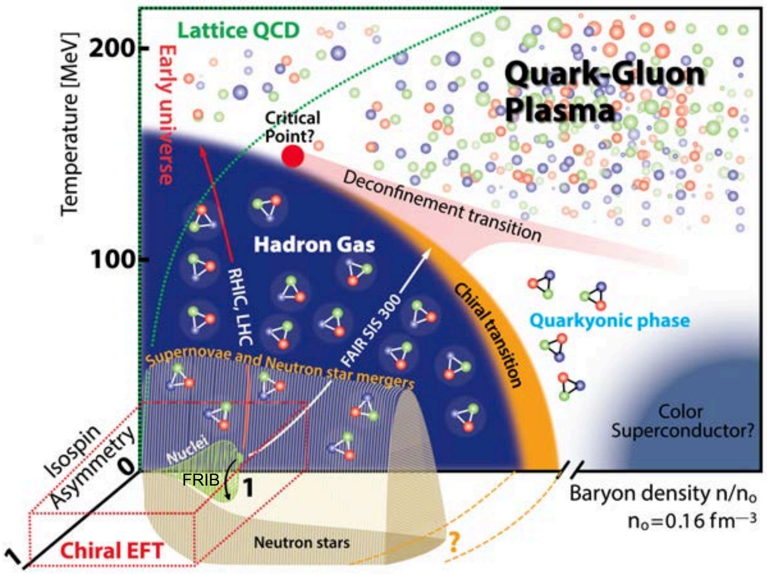
$$P(n = 0.32\,\mathrm{fm}^{-3}) \approx \begin{cases} 20 \pm 6\,\mathrm{MeV\,fm}^{-3} & \mathrm{MBPT:\ nonlocal} \\ 15 \pm 5\,\mathrm{MeV\,fm}^{-3} & \mathrm{QMC:\ local}\ V_{E,\mathbb{1}} \end{cases}$$

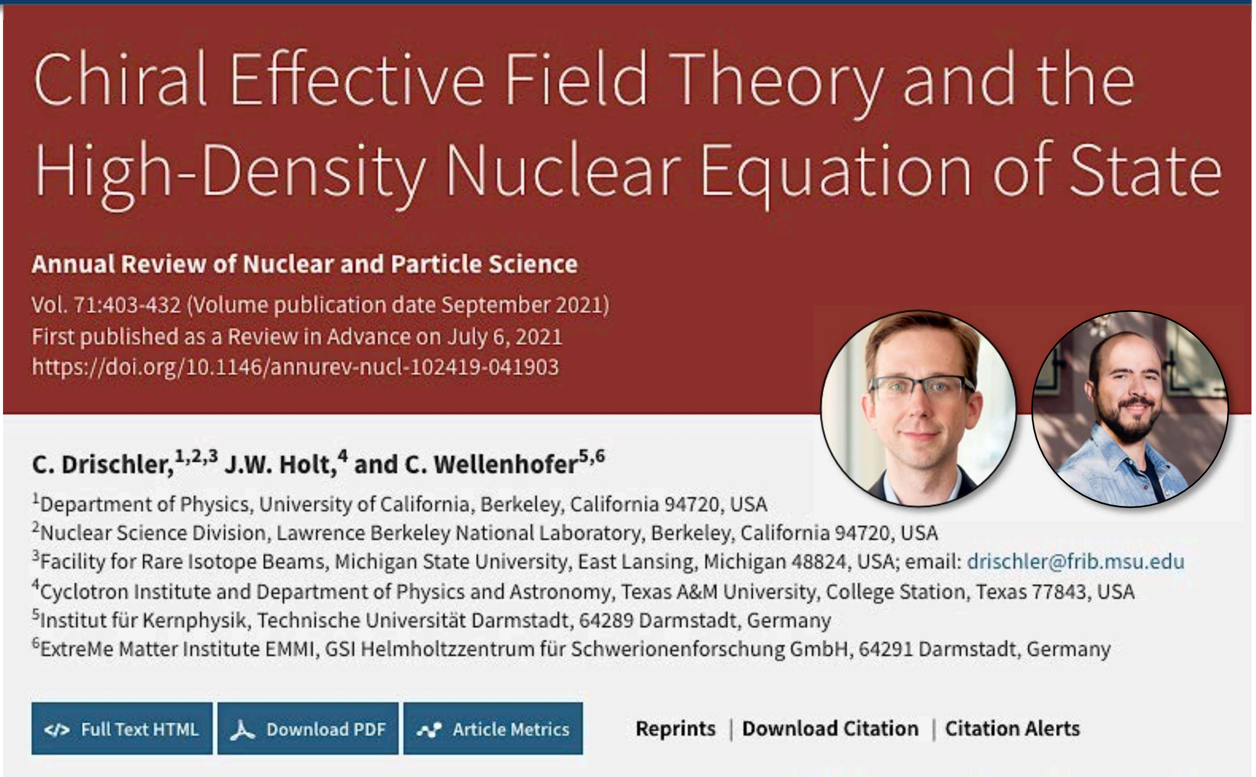
Neutron star observations could be used for:

Model checking & selection of chiral interactions

Constraints on coupling constants in nuclear forces

More details? Recent review article





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

Annual Review of Nuclear and Particle Science
Vol. 71:403-432 (Volume publication date September 2021)
First published as a Review in Advance on July 6, 2021
https://doi.org/10.1146/annurev-nucl-102419-041903

C. Drischler,[1,2,3] J.W. Holt,[4] and C. Wellenhofer[5,6]
[1]Department of Physics, University of California, Berkeley, California 94720, USA
[2]Nuclear Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
[3]Facility for Rare Isotope Beams, Michigan State University, East Lansing, Michigan 48824, USA; email: drischler@frib.msu.edu
[4]Cyclotron Institute and Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843, USA
[5]Institut für Kernphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany
[6]ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

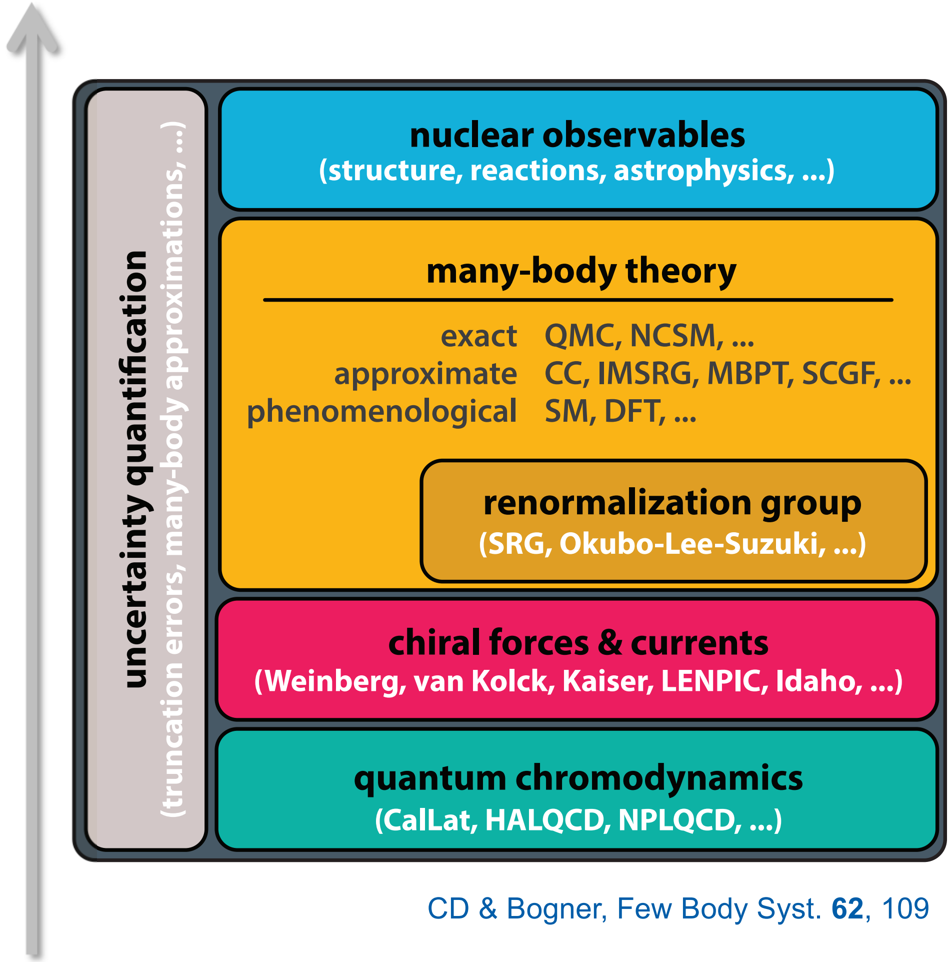
Keywords:

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

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

Open Access

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* (=0)

Emulators for nuclear physics

computationally *inexpensive* algorithms capable of approximating exact model calculations with *high accuracy*

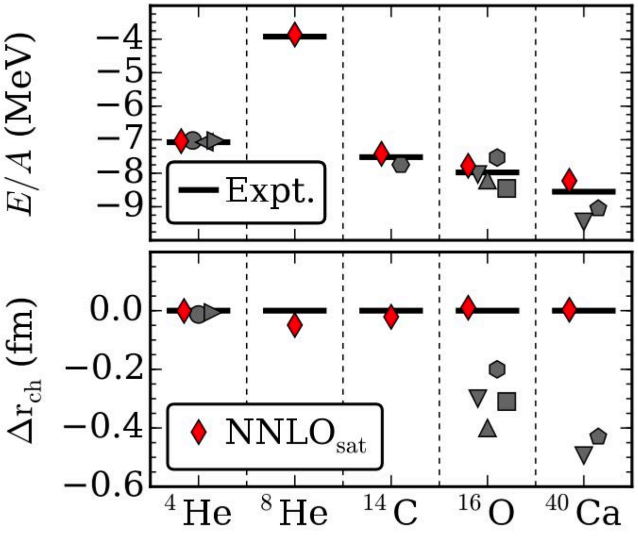
surrogate models

See also applications in GW astronomy, such as:

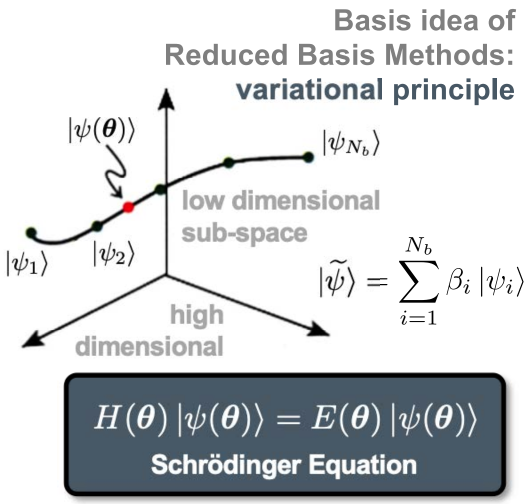
Fast Prediction and Evaluation of Gravitational Waveforms Using Surrogate Models
Field, Galley, Hesthaven, Kaye, Tiglio, PRX **4**, 031006

Frequency-domain reduced order models for gravitational waves from aligned-spin compact binaries
Pürrer, Class. Quantum Grav. **31**, 195010

Game changers in nuclear physics: emulators



Ekström *et al.*, PRC **91**, 051301(R)

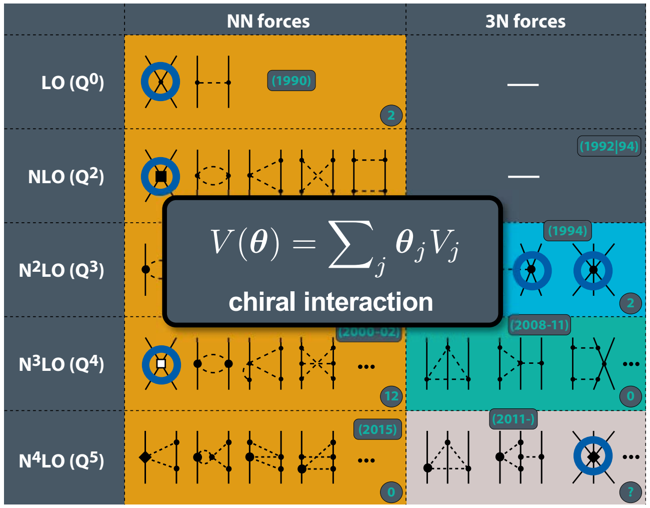

Basis idea of Reduced Basis Methods: **variational principle**

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

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

Schrödinger Equation

Frame *et al.*, PRL **121**, 032501
Melendez, CD *et al.*, arXiv:2203.05528



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

chiral interaction

CD, Holt, and Wellenhofer, ARNPS **71**, 403

Open questions in chiral EFT: power counting, regulator artifacts, and differing predictions for medium-mass nuclei

statistical analyses of scattering data could provide valuable insights

Here: Reduced Basis Methods (Eigenvector Continuation)

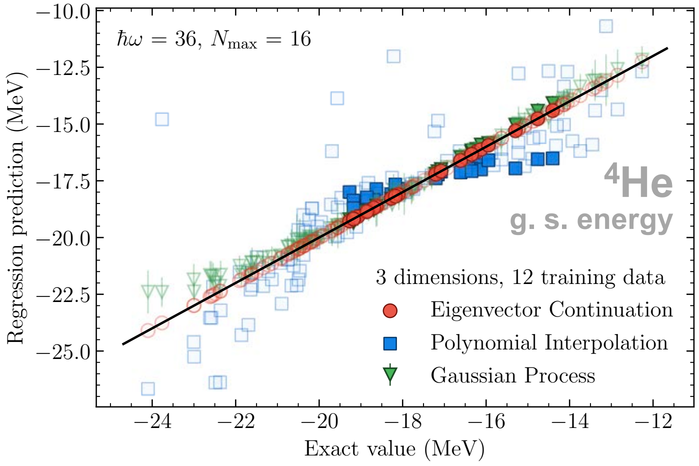
Construct **reduced-order models** by removing superfluous information in HiFi models

Emulators enable applications thought to be prohibitively slow (MC sampling)

Example: **Bayesian parameter estimation**

Emulators for bound-state calculations

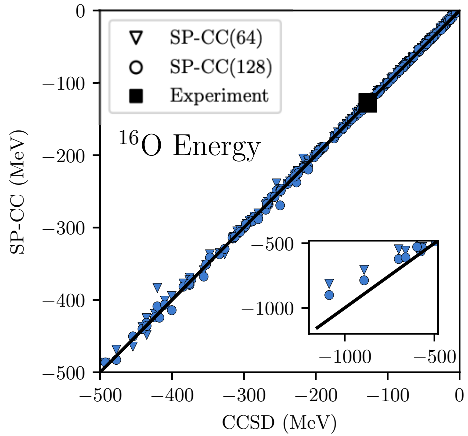
efficient subspace projection

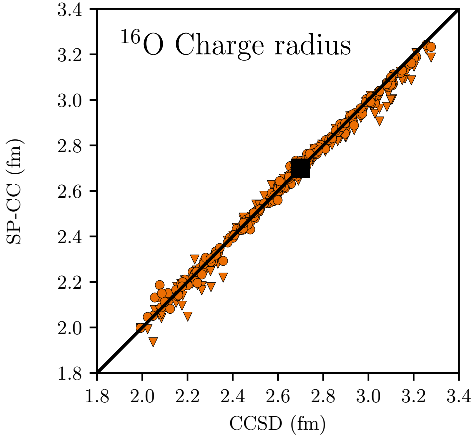


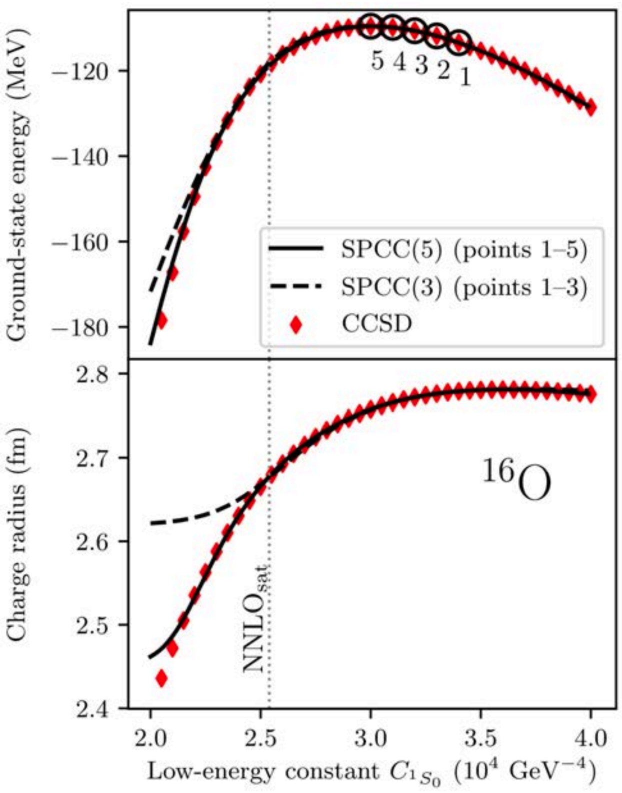
König, Ekström *et al.*, PLB **810**, 135814

Fast & accurate emulation via subspace projection methods (RBM)

RBM-driven emulators have **accurately approximated g. s. properties** binding energies and charge radii







Ekström & Hagen, PRL **123**, 252501

Millions of sampling points computed in one hour on a standard laptop.
An equivalent set of exact CC computations would require 20 years.

Emulators: mining scattering & reaction data, and more

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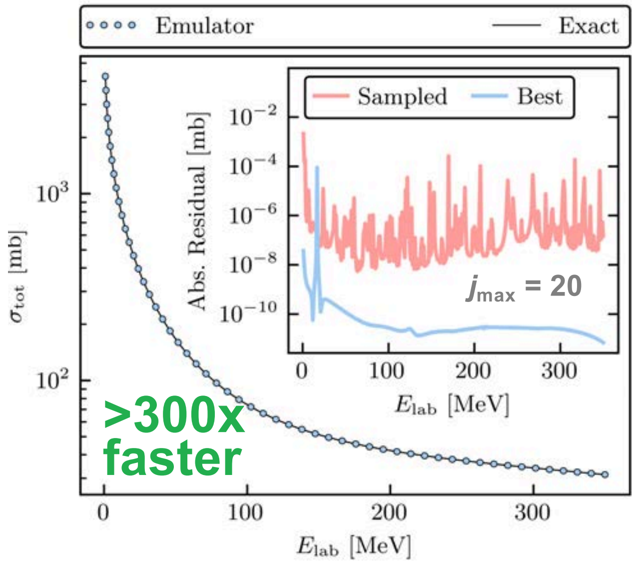
N^{4}LO+ SMS chiral NN potential
(26 free parameters (LECs) varied)

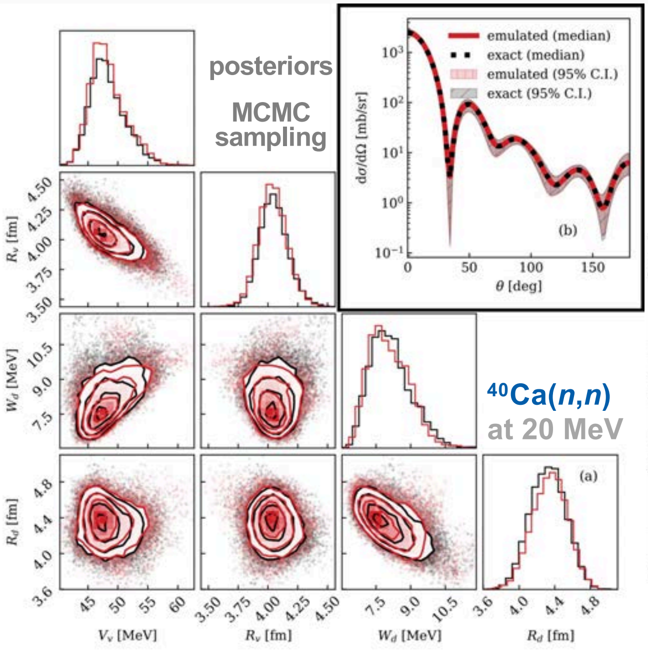


>300x faster

Melendez, CD *et al.*, PLB **821**, 136608

Proof of principle: emulation of two-body scattering observables with and without wavefunctions (KVP vs NVP)

26 free parameters (LECs) varied (N^{4}LO+ SMS chiral NN potential)



posteriors

MCMC sampling

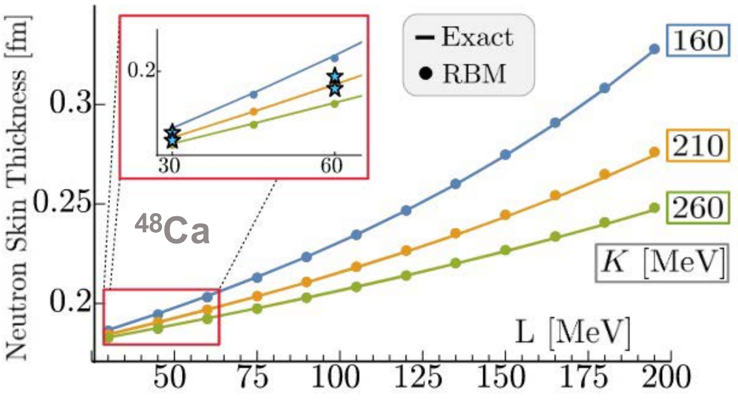
^{40}Ca(n,n) at 20 MeV

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

both interpolation and extrapolation in the parameter space $\boldsymbol{\theta}$ with negligible errors

efficient Bayesian parameter estimation for improving next-generation chiral interactions and optical models

BAND
Bayesian Analysis of Nuclear Dynamics



^{48}Ca

Bonilla, Giuliani, Godbey, Lee, arXiv:2203.05284
Anderson, O'Donnell, Piekarewicz, arXiv:2206.14889
see also: J. Melendez on GitHub

towards **calibrating modern EDFs** using Bayesian optimization and RBM emulators

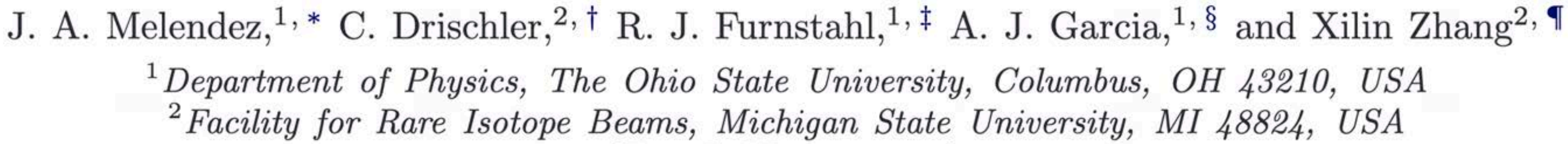
Proof of principle: emulated the entire single-particle spectrum of a variety of nuclei

Model reduction for nuclear emulators

Emulator classification

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

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



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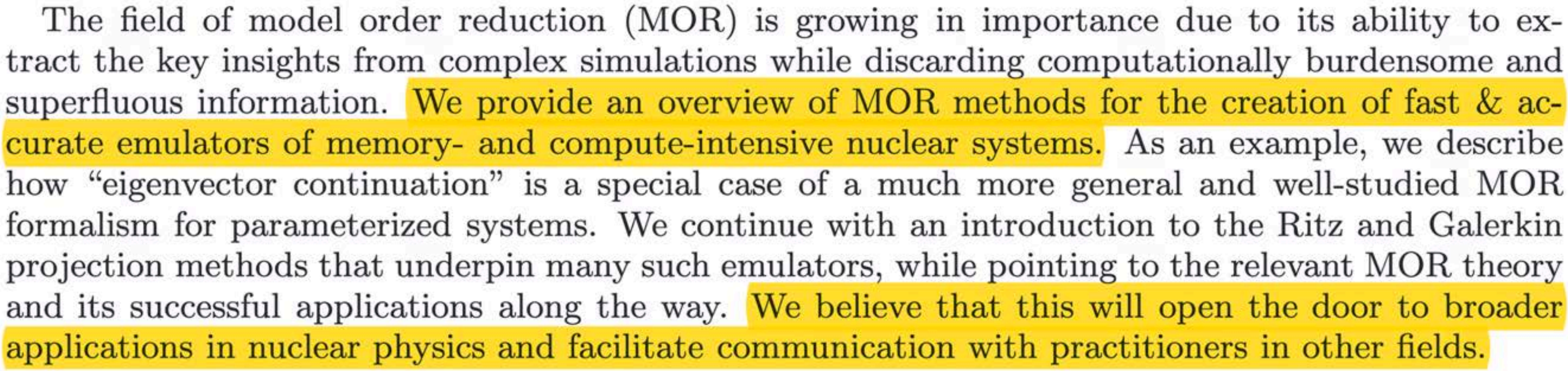
Many pointers to the MOR literature: arXiv:2203.05528 (accepted Guide in J. Phys. G Nucl. Part.)

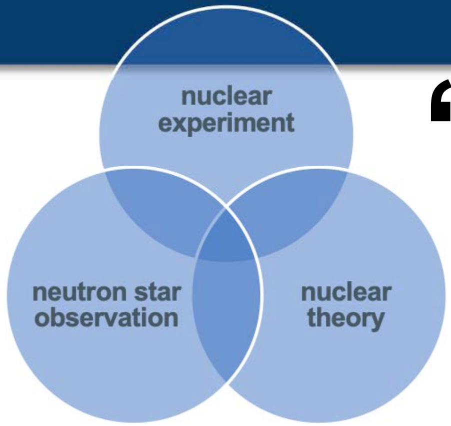


The field of model order reduction (MOR) is growing in importance due to its ability to extract the key insights from complex simulations while discarding computationally burdensome and superfluous information. We provide an overview of MOR methods for the creation of fast & accurate emulators of memory-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

see also: CD & Zhang, Chap. 8, pp. 29–36, in arXiv:2202.01105 (collective pieces edited by Tews, Davoudi, Ekström, Holt)

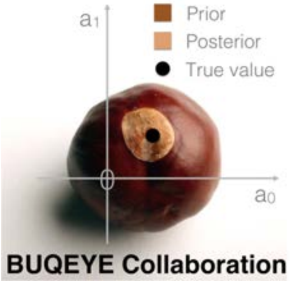
Take-away points

multi-messenger
nuclear precision
FRIB
} era



> “Enormous progress in theory, experiment, and observation make this new era particularly fruitful for the determination of the equation of state of neutron-rich matter.”

1. **Upcoming observational (and experimental) campaigns will provide stringent constraints on the properties of neutron stars**
2. **Chiral EFT enables microscopic predictions of nuclear matter (and nuclei) with quantified uncertainties to interpret these empirical constraints**
3. **Bayesian methods are powerful tools for quantifying & propagating correlated uncertainties in EFT-based calculations (*model checking* is important)**
4. **Emulators have been game changers in nuclear physics; and much can be learned from the well-established MOR field in applied mathematics.**



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