Microscopic Equation of State Constraints and Bayesian Uncertainty Quantification

Christian Drischler (drischler@ohio.edu)

NUSYM 2024, XIIth International Symposium on Nuclear Symmetry Energy

September 9, 2024 | Grand Accélérateur National d'Ions Lourds (GANIL)

2025 Glenn T. Seaborg Award for Nuclear Chemistry goes to **ManYee Betty Tsang** (MSU): **Congratulations, Betty!**

Bayesian Model Mixing in SNM

STREAMLINE

SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

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A **Bayesian mixture model** approach to quantifying the *empirical* nuclear **saturation point**

CD, Giuliani, **Bezoui**, Piekarewicz, and Viens, arXiv:2405.02748

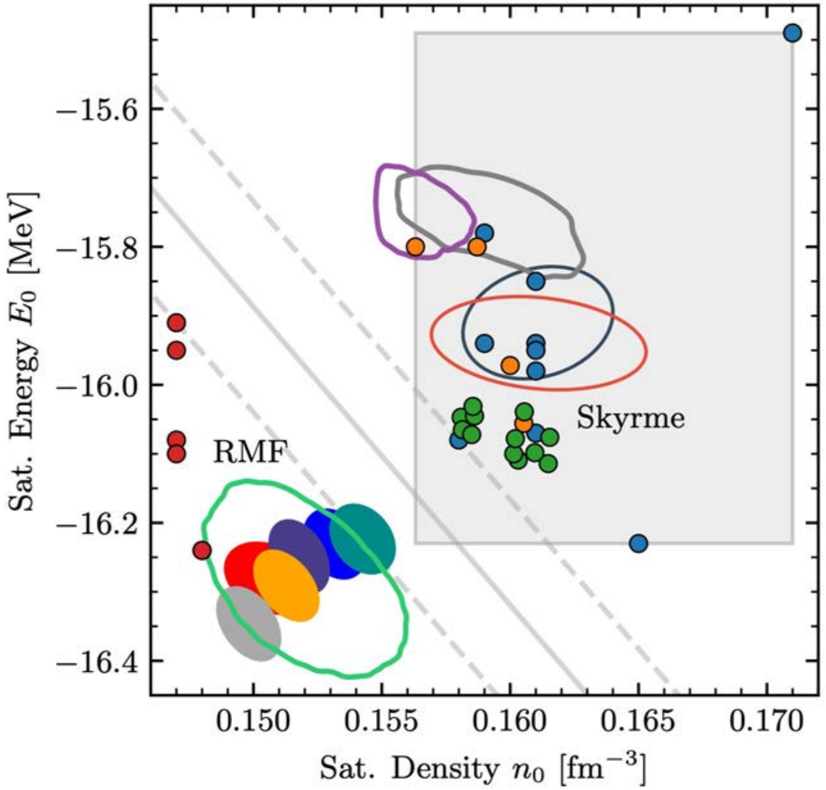
Goal: rigorous benchmarks of saturation properties of chiral NN+3N interactions (using Skyrme & RMF models)

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

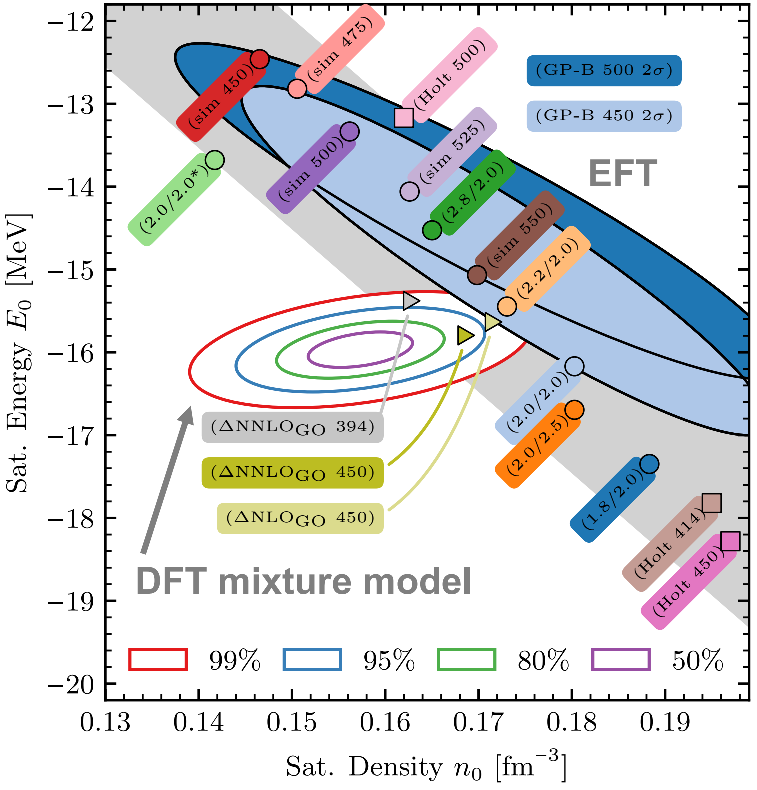
$L = 106 \pm 37\,\mathrm{MeV}$

PREX–II informed

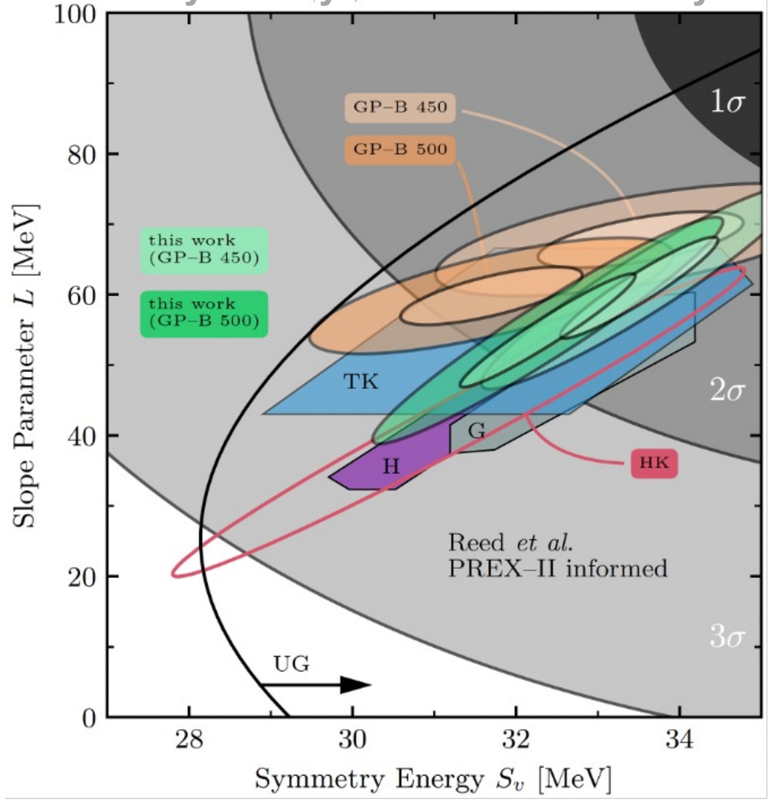
DFT constraints on nuclear saturation



DFT vs EFT: nuclear saturation



symmetry at saturation density



Bayesian Model Mixing in SNM

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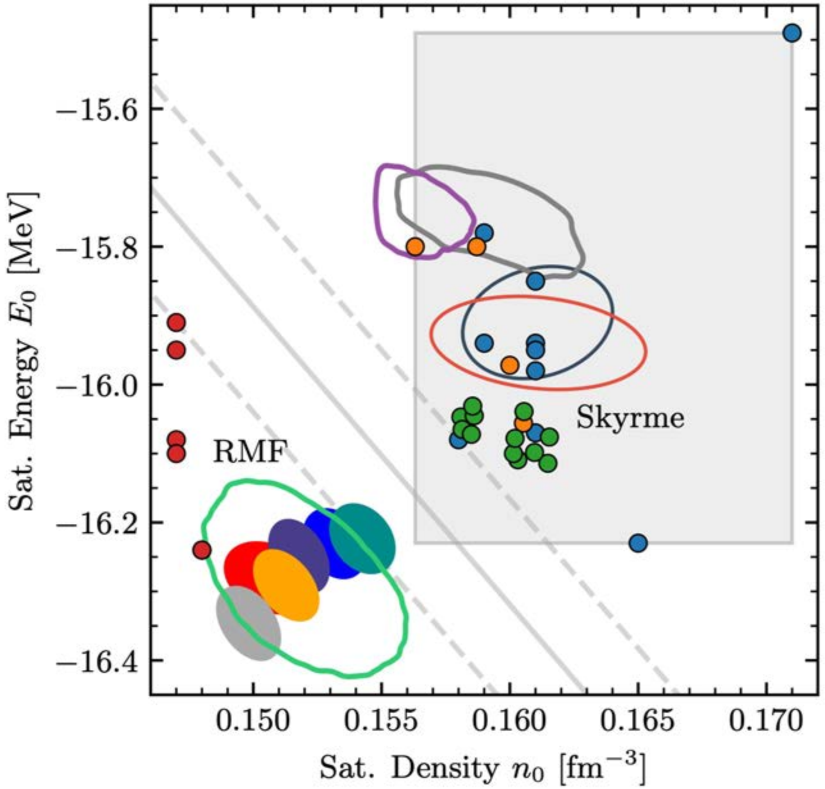

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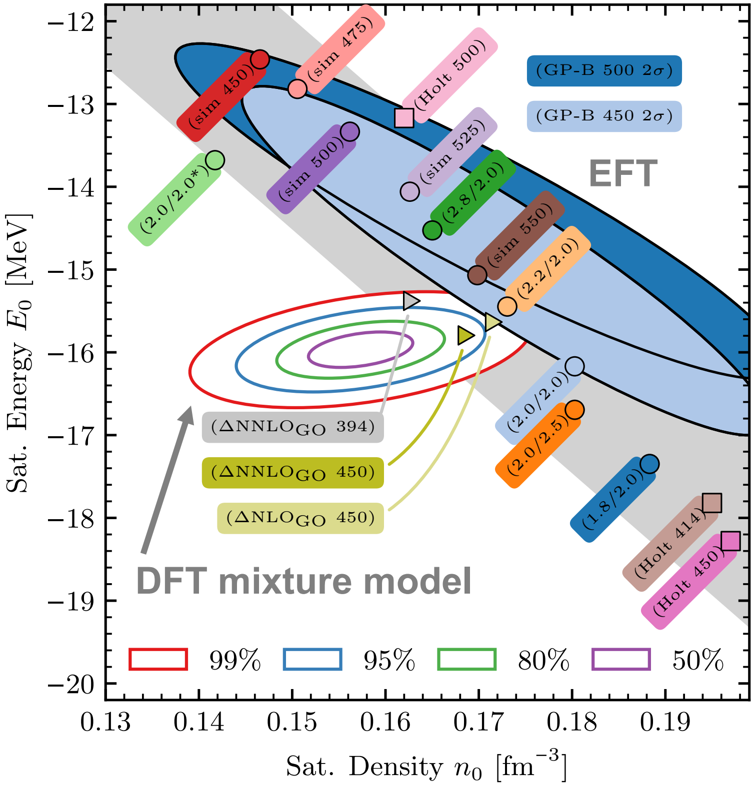
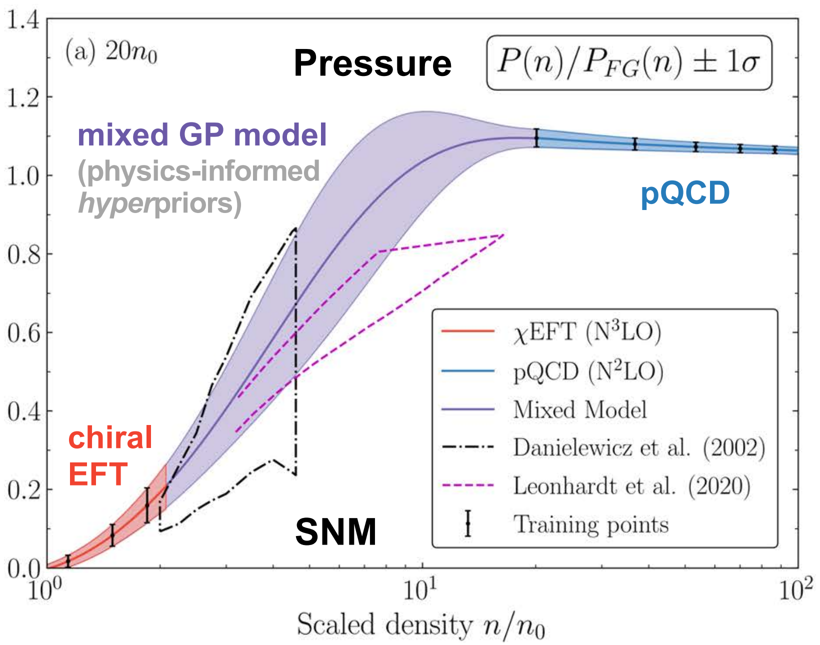


From chiral EFT to perturbative QCD: a **Bayesian model mixing** approach to symmetric matter

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

YouTube Click to watch **Alexandra's FRIB Theory Seminar** (April 14, 2024)



Goal: constructing globally predictive, QCD-based EOSs from individual models

Bridging chiral EFT and pQCD via Bayesian Model Mixing

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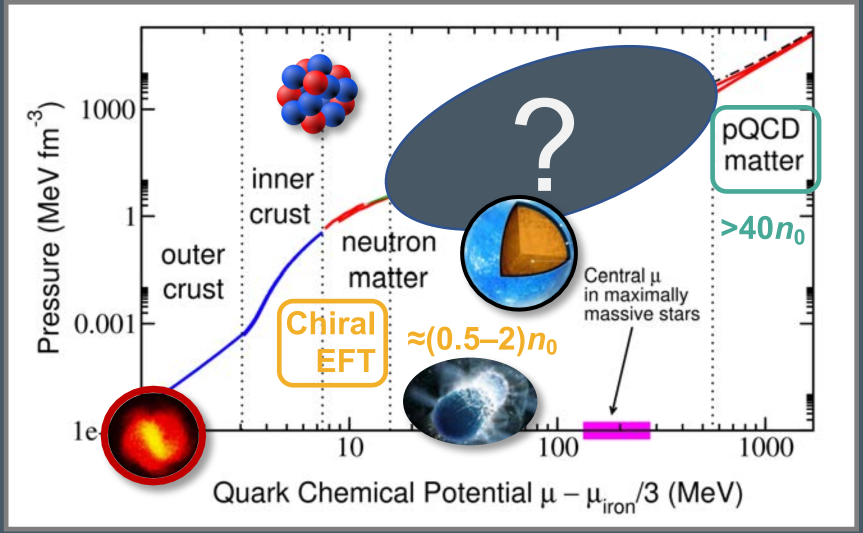
How can we develop *QCD-based* models that are *predictive* across all densities?

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

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

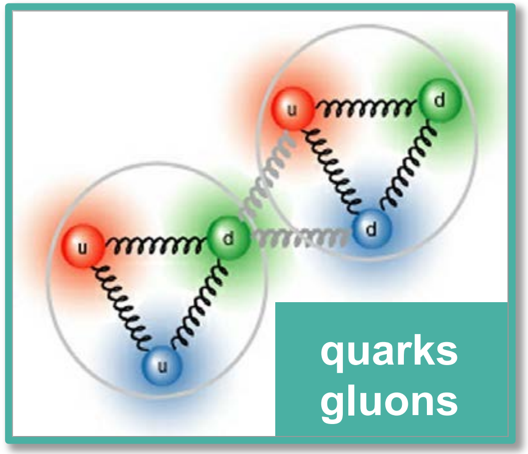


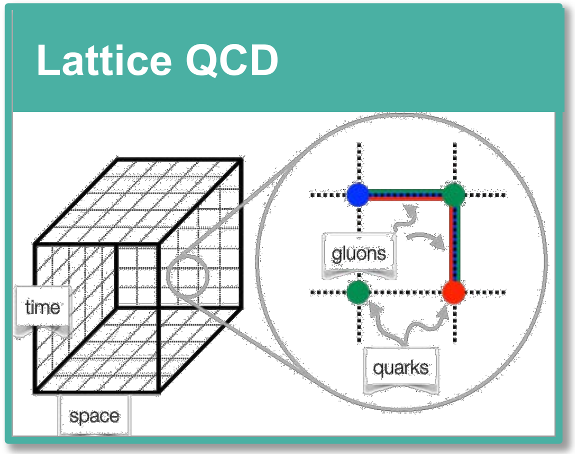
quantum chromodynamics
(CalLat, HALQCD, NPLQCD, ...)

CD & Bogner, Few Body Syst. **62**, 109
e.g., Essick, Tews, Landry, Reddy, Holz, PRC **102**, 055803

Here: nuclear equation of state (EOS)

Pressure, energy per particle, or sound speed





Fujimoto & Reddy, PRD **109**, 014020

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

Low densities: *ab initio* workflow (idealized)

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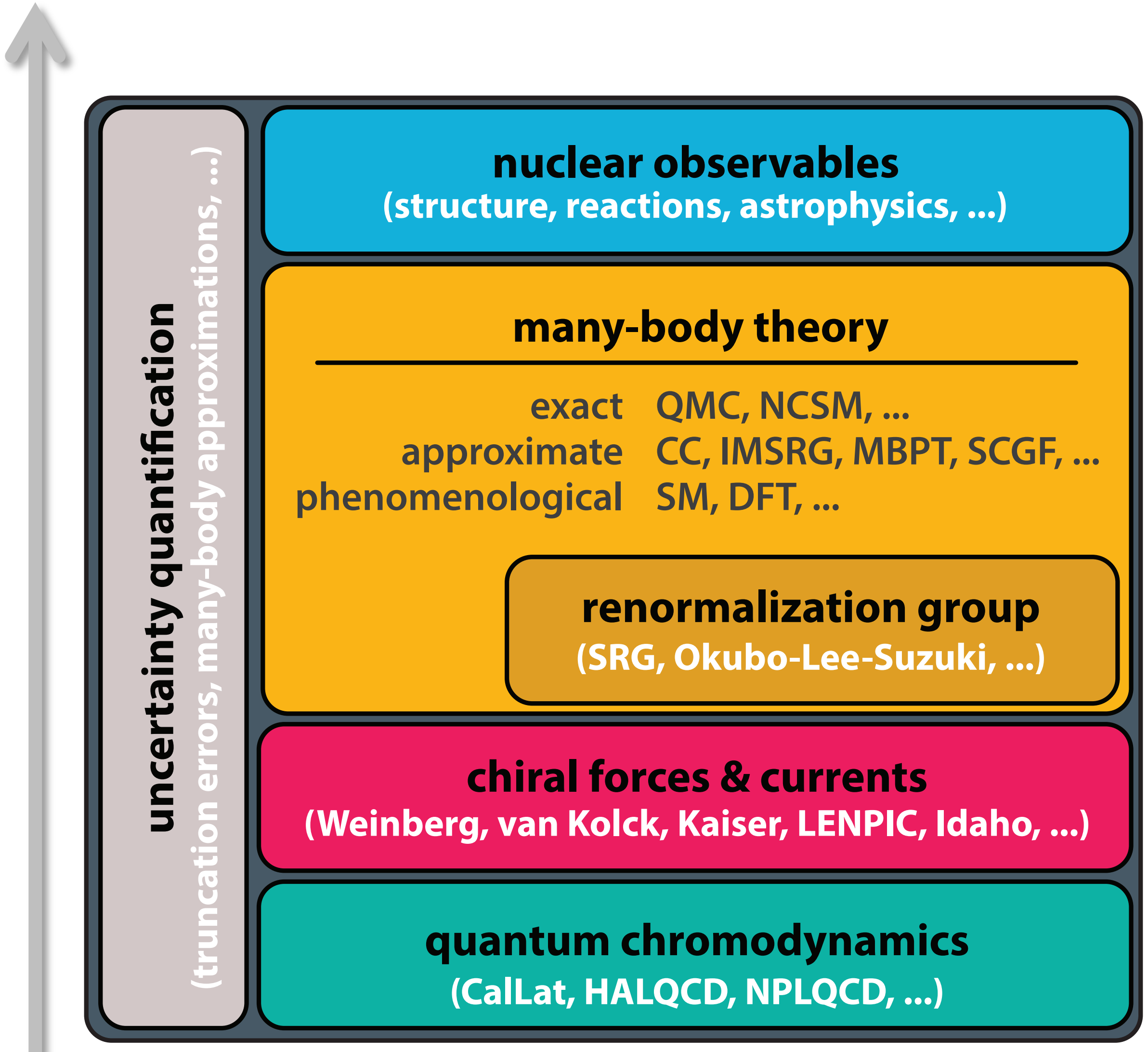

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Here: nuclear equation of state (EOS)

Pressure, **energy per particle**, or sound speed

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

baryon density n

neutron excess δ

temperature T

computational framework

solves the (many-body) Schrödinger equation

requires a nuclear potential as input

chiral effective field theory

provides microscopic interactions consistent with the symmetries of *low-energy* QCD

theory of strong interactions

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

Interesting new ML/MOR applications: *e.g.*, Fore, Kim *et al.*, PRR **5**, 033062

Modern theory of nuclear forces

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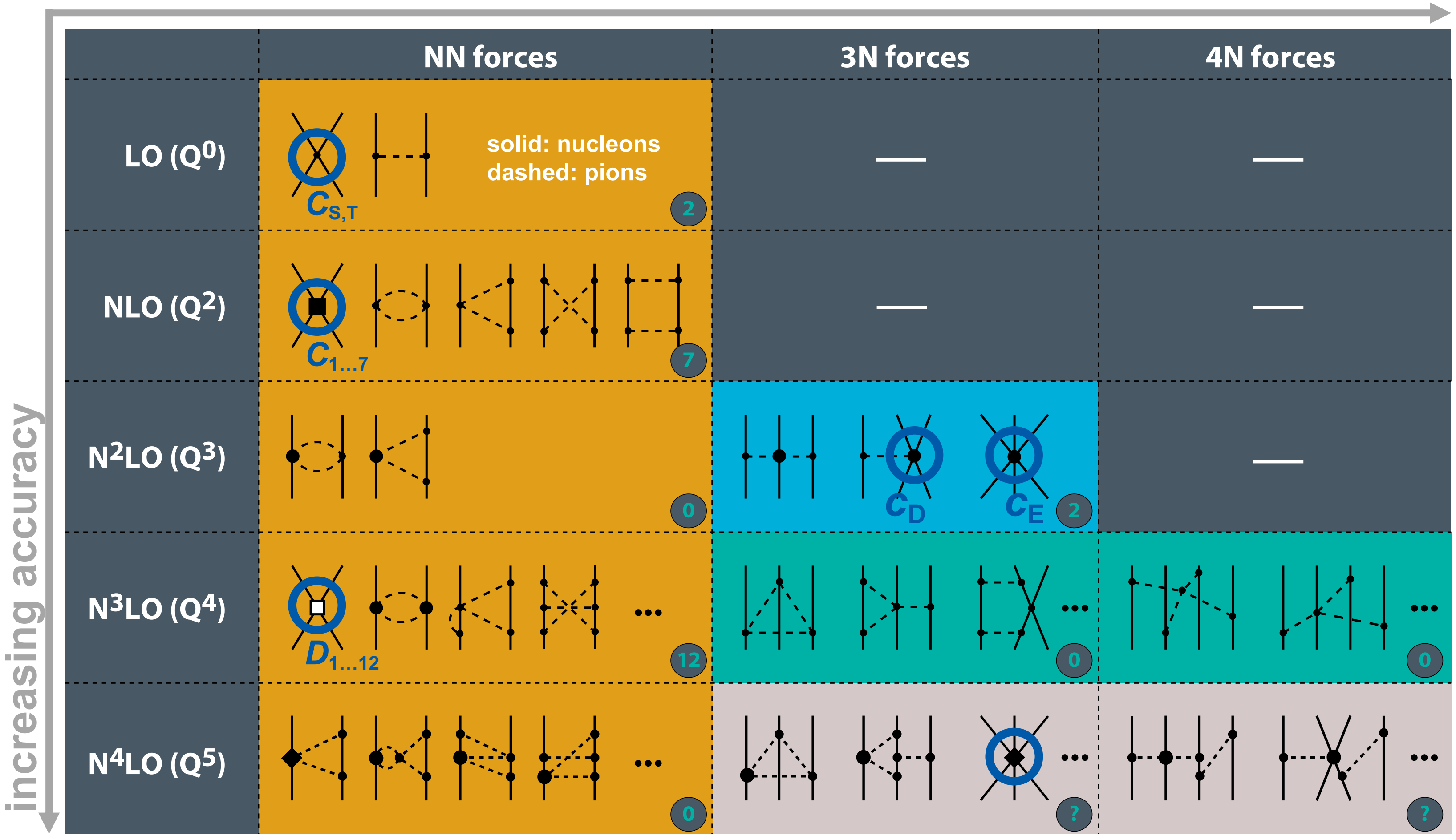
Hierarchy of chiral nuclear forces up to N⁴LO

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

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



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

Chiral *effective* field theory

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

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

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

fit the unknown couplings to experimental (or lattice) data

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

First rigorous uncertainty quantification

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

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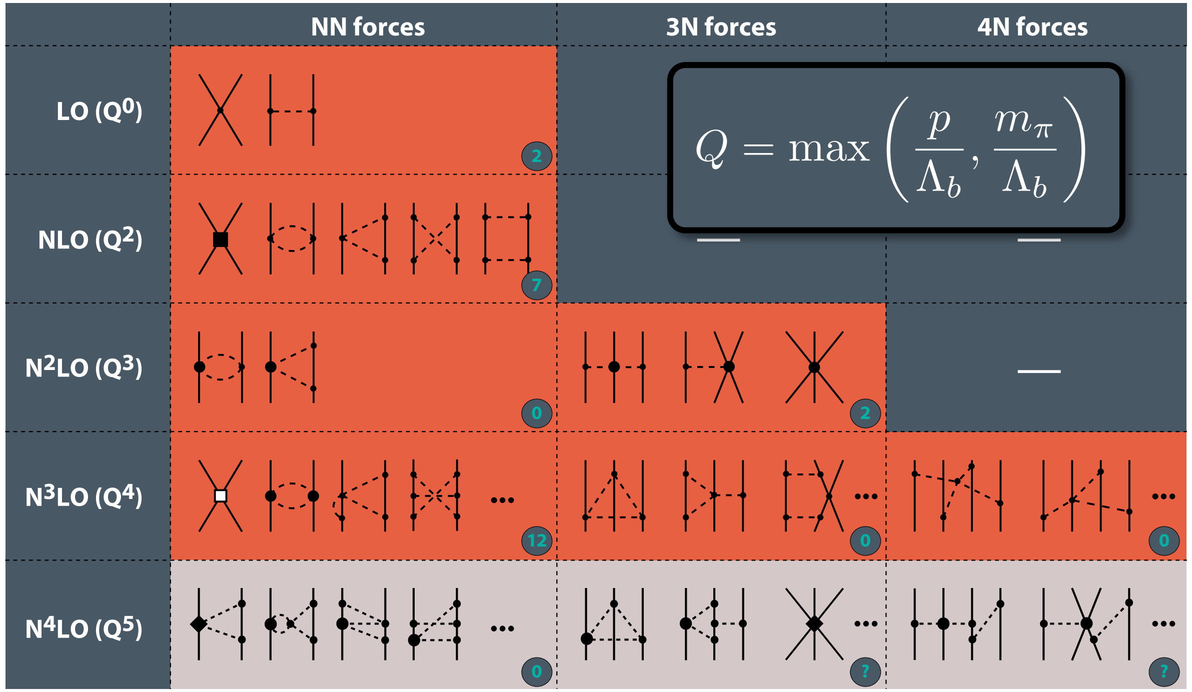
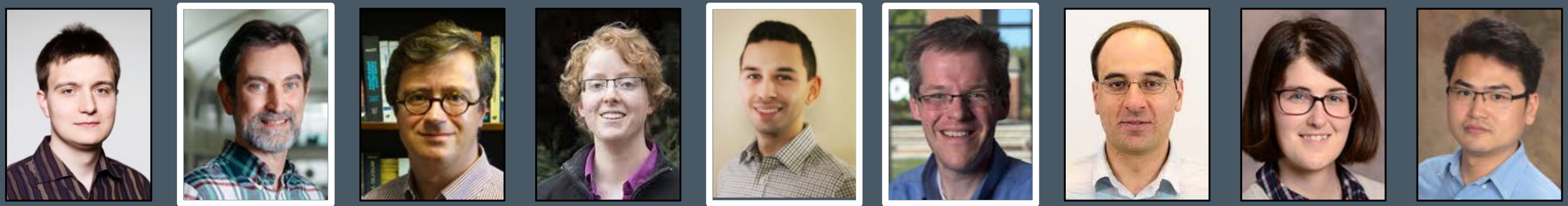
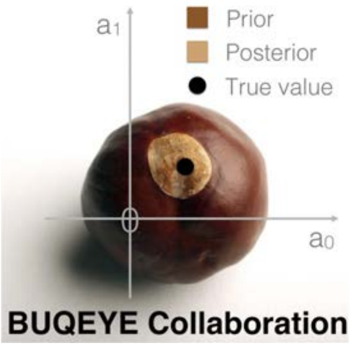


$$Q = \max\left(\frac{p}{\Lambda_b}, \frac{m_\pi}{\Lambda_b}\right)$$

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



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



Bayesian Uncertainty Quantification: Errors for Your EFT

First rigorous uncertainty quantification

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

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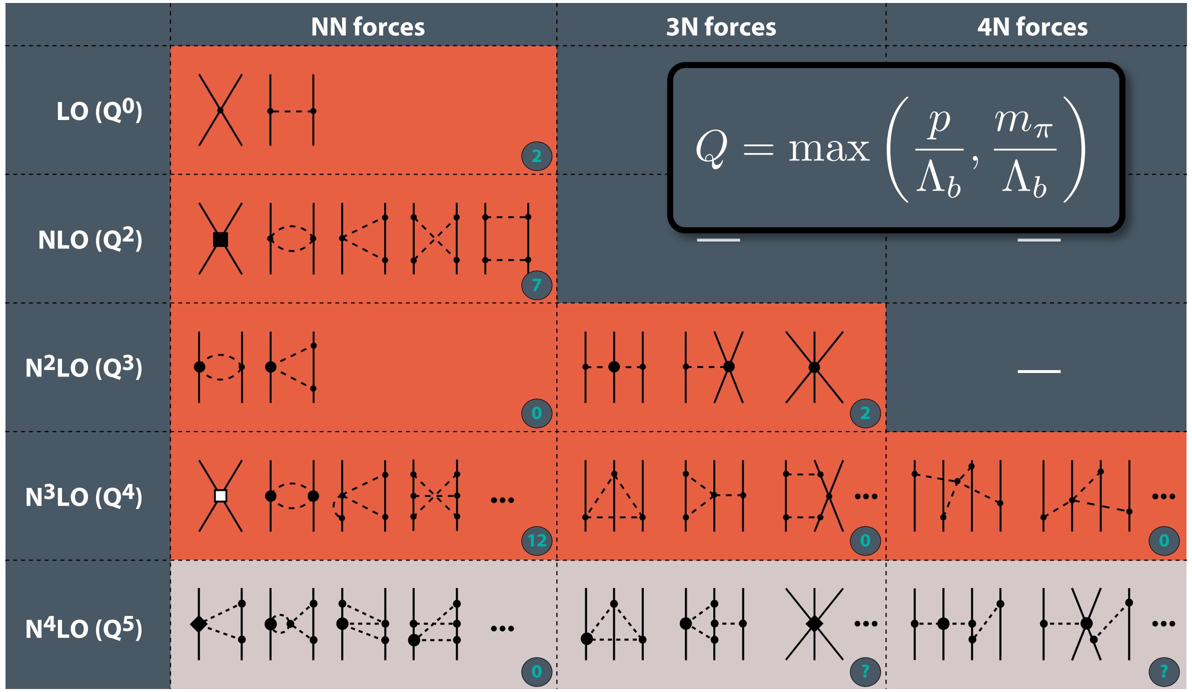

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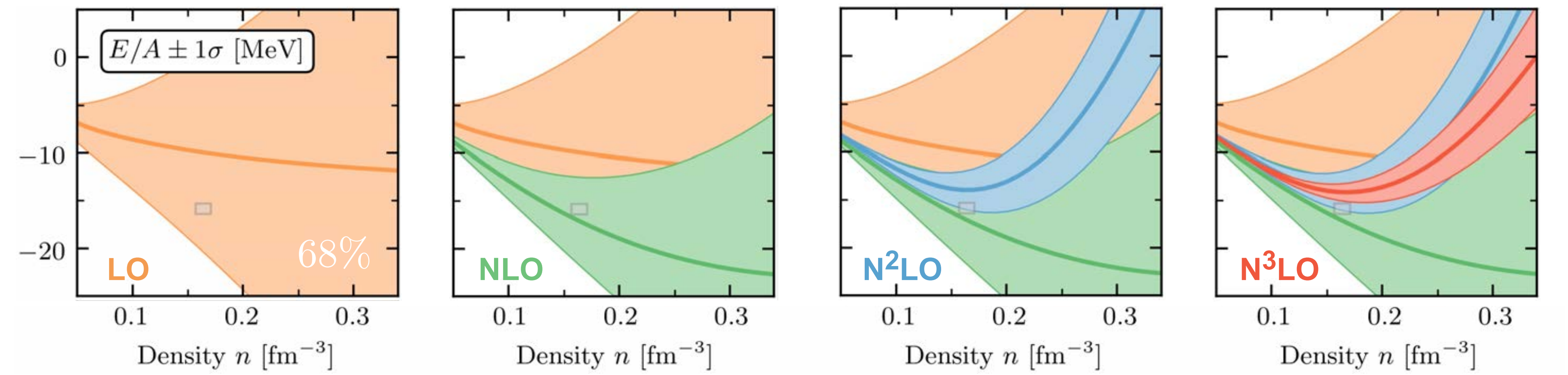
An example: symmetric matter

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

Uncertainty bands depict 68% credibility regions

$$y = y_k + \delta y_k$$



Correlated EFT truncation error model (revisited)

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your EFT

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

Increasing accuracy

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

EFT prediction at k^{th} order

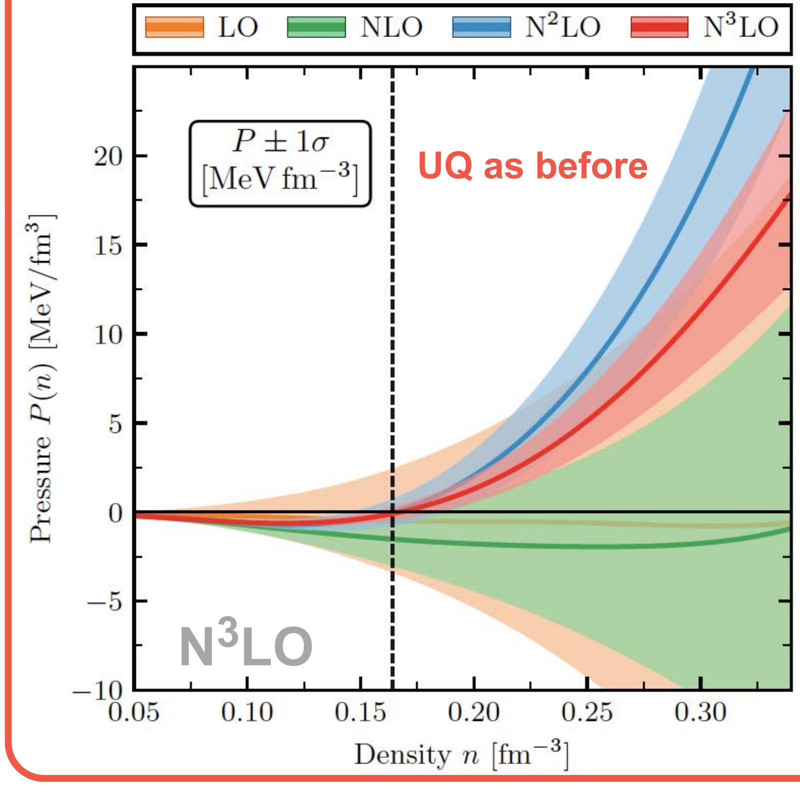
want full prediction: $y = y_k + \delta y_k$

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

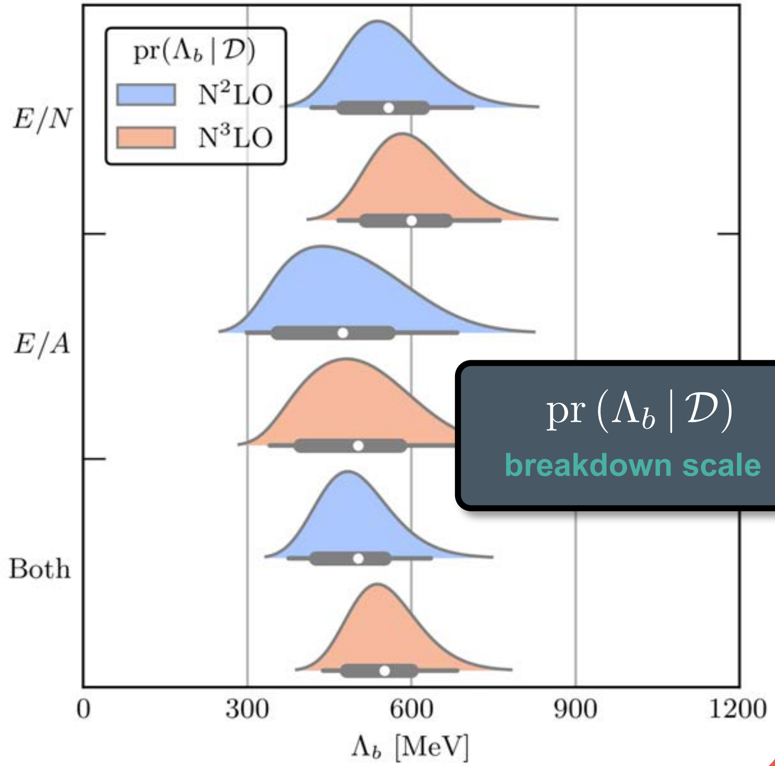
$$\delta y_k = y_{\text{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

to-all-orders truncation error

Chiral EFT



Bayesian inference of the in-medium breakdown scale



$\text{pr}\,(\Lambda_b \,|\, \mathcal{D})$

breakdown scale

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

$$y_{\text{ref}}(k_F) = 16 \text{ MeV} \left(\frac{k_F}{k_{F,0}}\right)^2$$

GPs are closed under differentiation:

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

At what *density* does chiral EFT break down, and why?

CD, Furnstahl *et al.*, PRL **125**, 202702 | CD, Melendez *et al.*, PRC **102**, 054315

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need to infer theo

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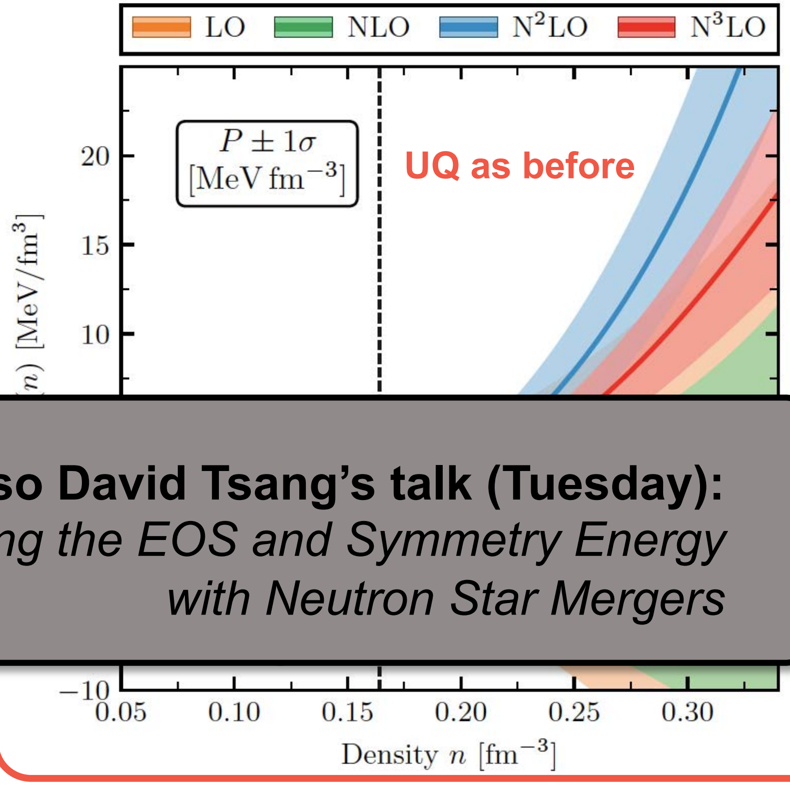
See also Duncan Neill's talk (Thursday):
Resonant shattering flares as asteroseismic tests of chiral effective field theory

Chiral EFT



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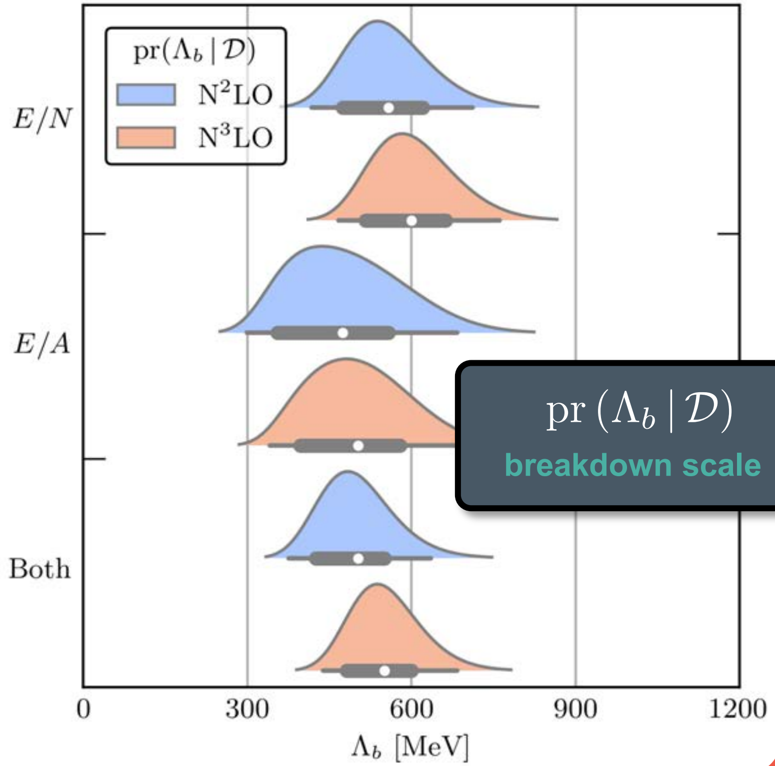

$$\mathrm{pr}\left(\Lambda_b \,|\, \mathcal{D}\right)$$

breakdown scale

See also David Tsang's talk (Tuesday):
Constraining the EOS and Symmetry Energy with Neutron Star Mergers

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Correlated EFT truncation errors (for pQCD)

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

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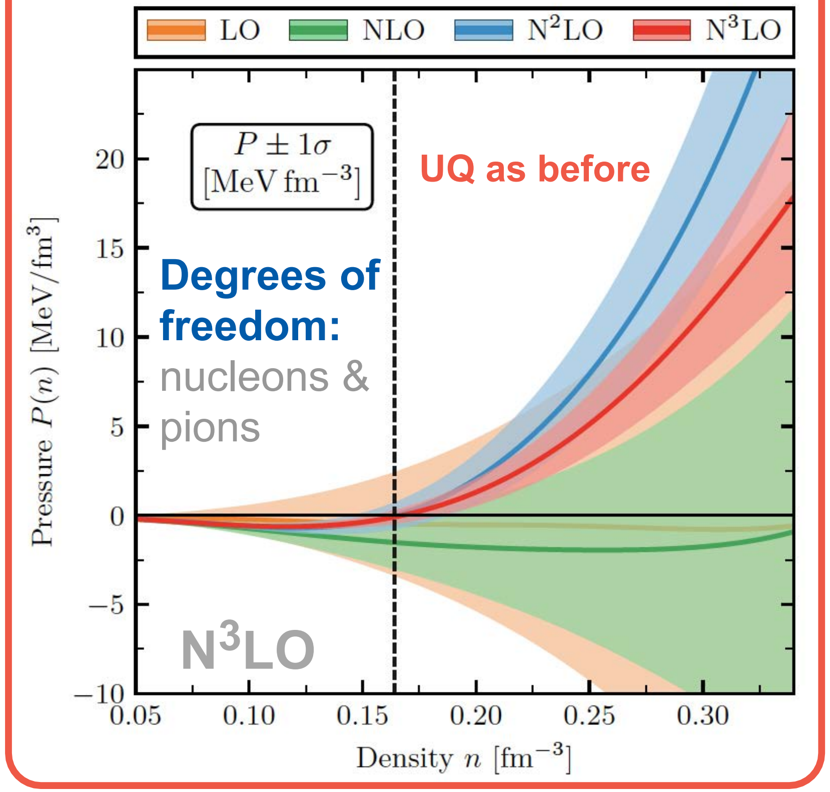

pQCD

Perturbative expansion in the strong coupling constant (at the two-loop level)

$$\alpha_s(\bar\Lambda) = \frac{4\pi}{\beta_0 L}\left[1 - \frac{2\beta_1}{\beta_0^2}\frac{\ln L}{L}\right]$$

$$L = \ln(\bar\Lambda^2/\Lambda^2_{\overline{MS}}), \quad \bar\Lambda = 2X\mu,$$

$$\frac{P(\mu)}{P_{FG}(\mu)} \simeq 1 + a_{1,1}\left(\frac{\alpha_s(\bar\Lambda)}{\pi}\right) + N_f\left(\frac{\alpha_s(\bar\Lambda)}{\pi}\right)^2\left[a_{2,1}\ln\left(\frac{N_f\alpha_s(\bar\Lambda)}{\pi}\right) + a_{2,2}\ln\frac{\bar\Lambda}{2\mu} + a_{2,3}\right] + \mathcal{O}(\alpha_s^3),$$

$$a_{1,1} = -2$$
$$a_{2,1} = -1$$
$$a_{2,2} = -4.8333$$
$$a_{2,3} = -8.0021$$

Degrees of freedom: massless **quarks** (*up* & *down*, with equal chemical potential μ) and **gluons**

cf. Bayesian analysis using the MiHO framework: Gorda *et al.*, PRL **131**, 181902; JHEP **06**, 002 (see also more recent work)

Correlated EFT truncation errors (for pQCD)

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to-all-orders truncation error

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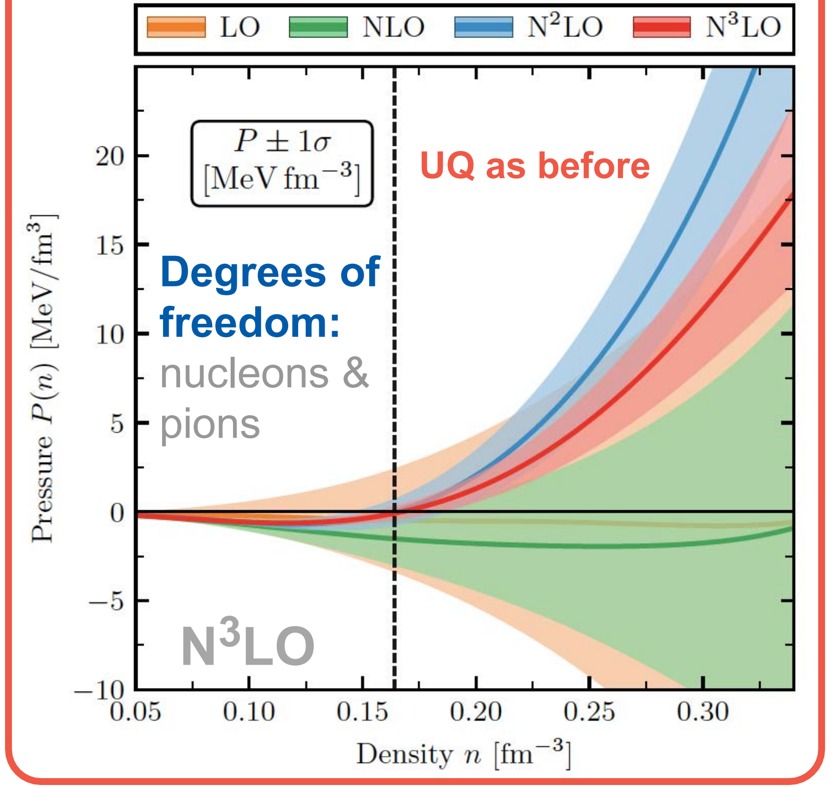
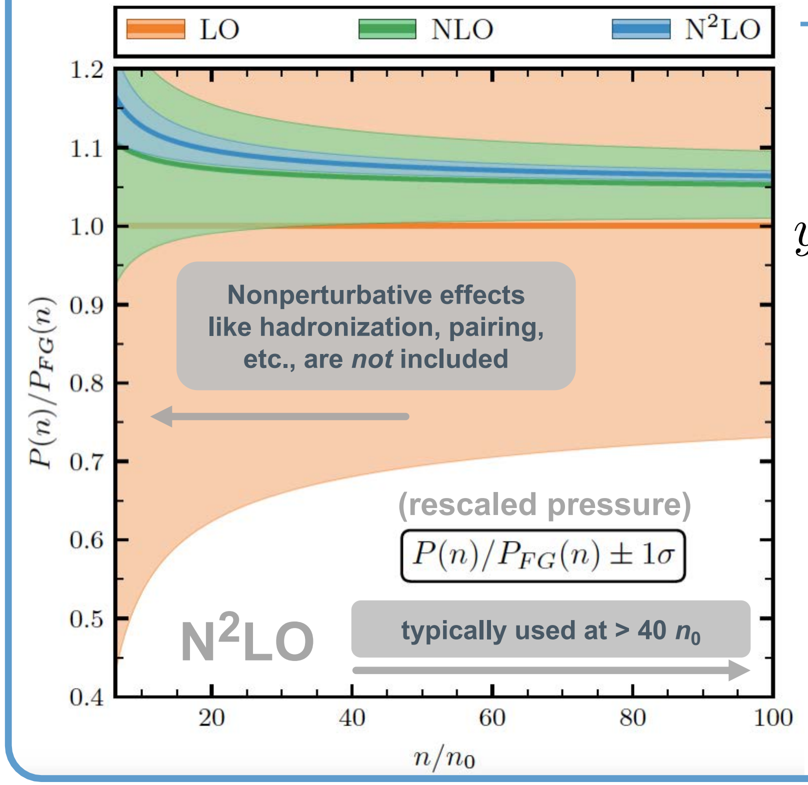


pQCD



Truncation error estimation:

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

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

Kohn-Luttinger-Ward inversion:

$$P(\mu) \rightarrow P(n)$$

(consistent up to the desired order in pQCD)

pQCD prediction:

$$P(\mu)$$

workflow

cf. Bayesian analysis using the MiHO framework: Gorda *et al.*, PRL **131**, 181902; JHEP **06**, 002 (see also more recent work)

Curvevise mixing of random variables

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

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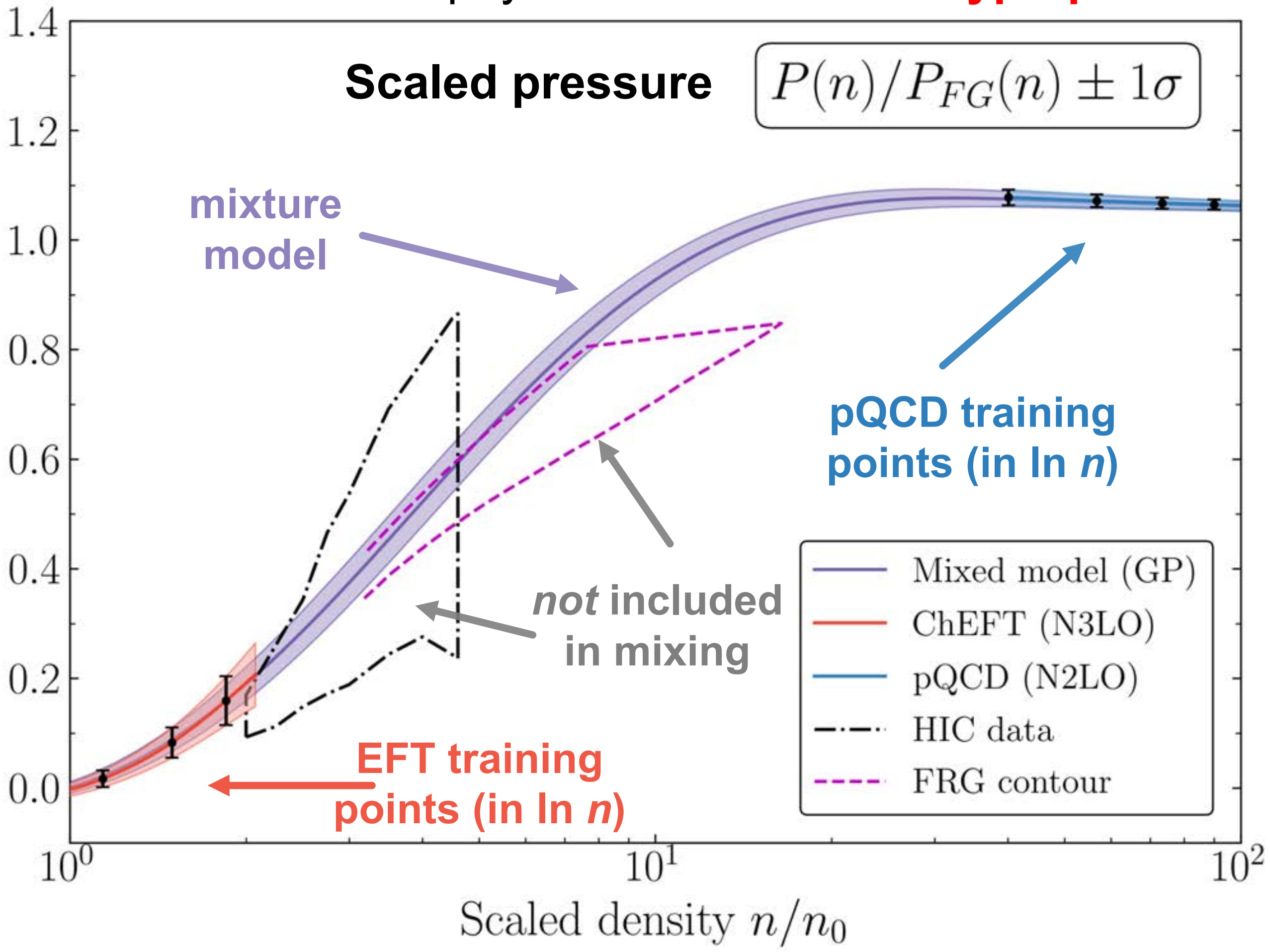
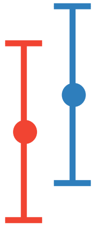
One can include physics constraints via **hyperpriors**



Here, only 2 models: 1: Chiral EFT 2: pQCD



random variable (at a given density) corresponding to the predictions of model *i*

$$i \in [1, M]$$

(assumes common mean)

$$Y^{(i)} = F + \delta Y^{(i)}$$

QCD, with **prior**

$$\sim \mathrm{GP}[0, \kappa_f(x, x')]$$

kernel choice: here, RBF (hyperparameters estimated from data)

BUQEYE **truncation error**

$$\sim \mathrm{GP}[0, \kappa_y^{(i)}(x, x')]$$

full, block-diagonal covariance matrix

We found for the BMM:

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

$$\vec{\mu} \equiv \Sigma B_t^T K_y^{-1} \vec{y}, \qquad \Sigma \equiv (K_f^{-1} + B_t^T K_y^{-1} B_t)^{-1}$$

Assumptions (*not* necessarily satisfied, validation needed):

- *F* is smooth, precluding *discontinuous* phase transitions
- stationarity: persistence in size & length scale of EOS's variability

Sensitivity on physics-informed priors

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

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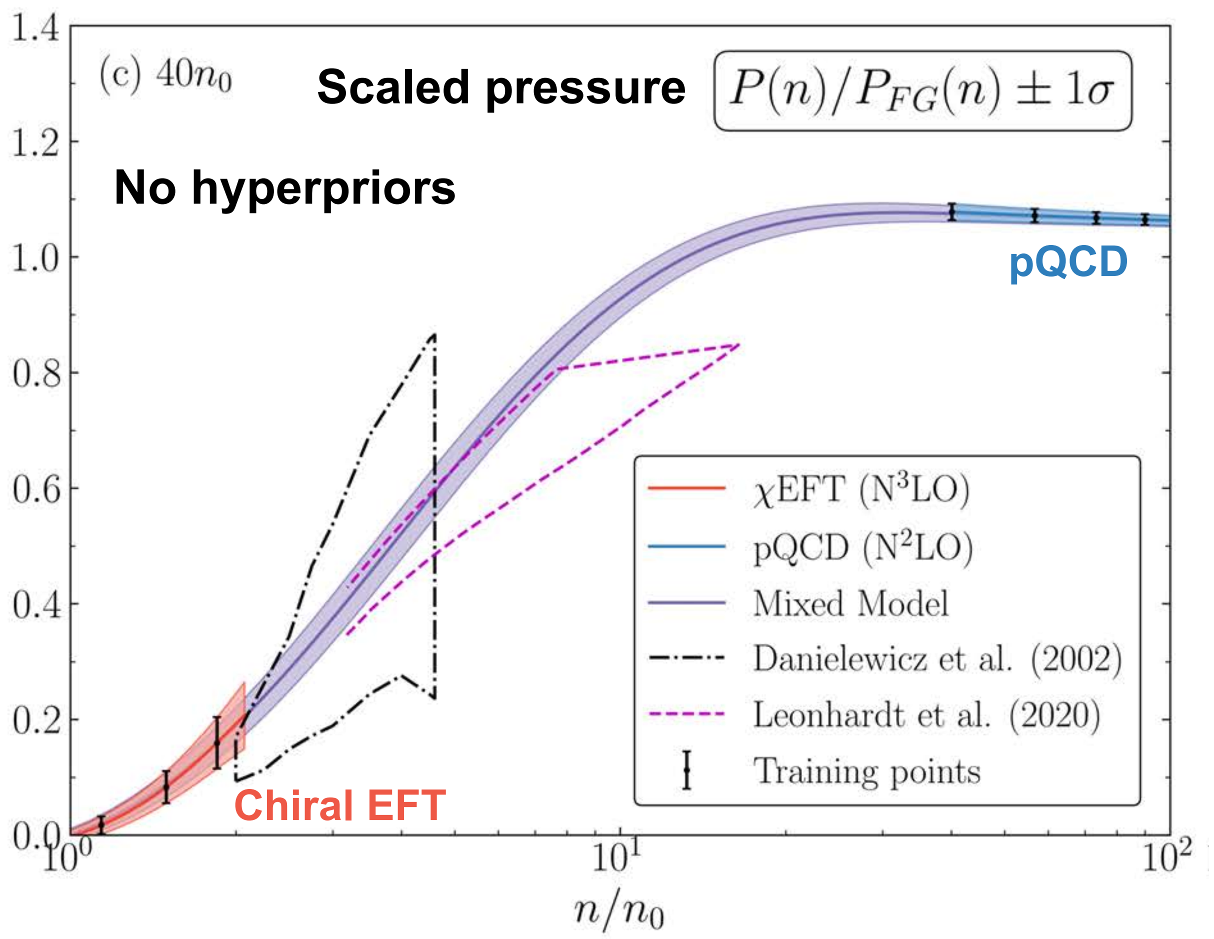

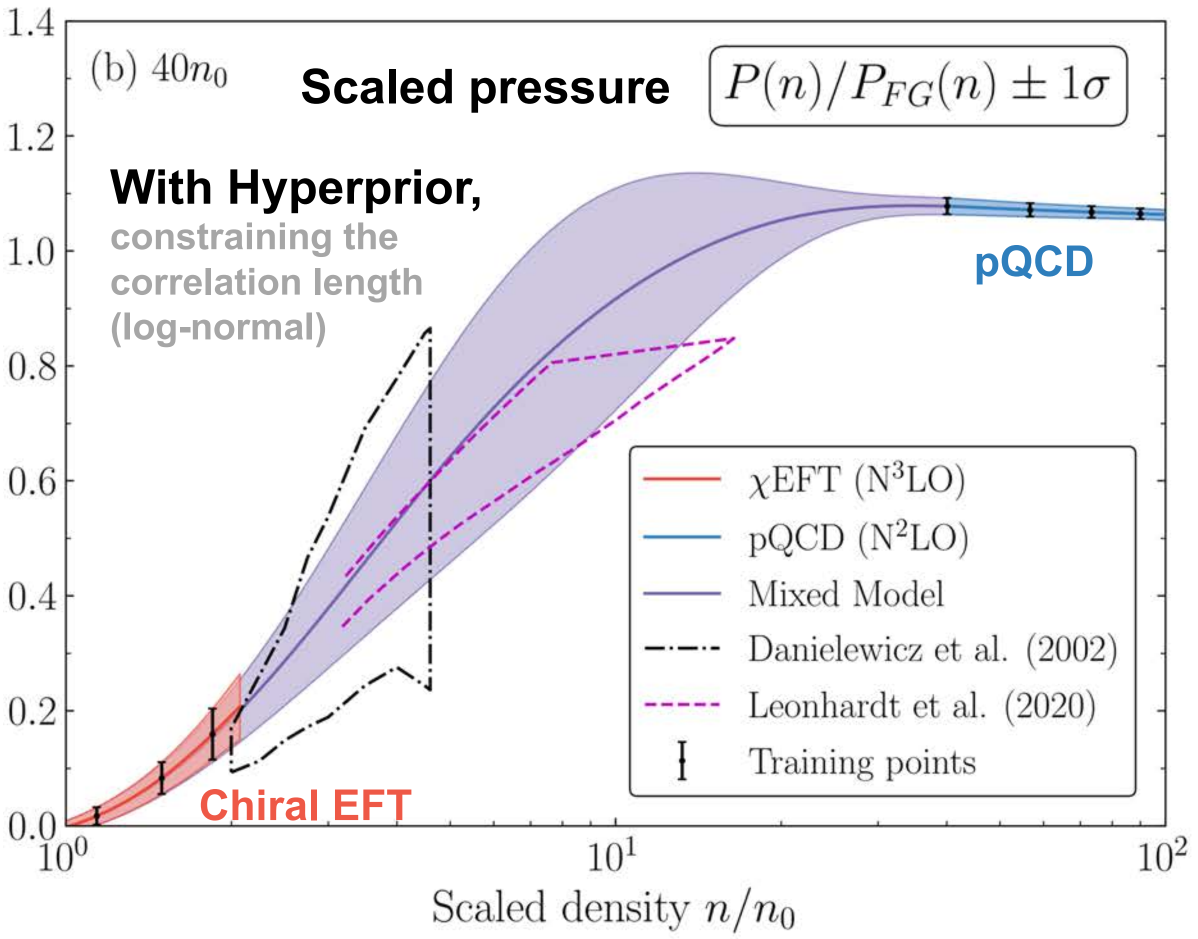

Inferred **long correlation lengths** render uncertainty on the mixed EOS very small due, even smaller than each model

Unrealistic, large impact of pQCD on chiral EFT region

We placed a *hyperprior* on the correlation length to **enforce small covariances between EFT & pQCD**

Smaller length scales result in larger uncertainty bands

Training points in pQCD region

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

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The pQCD uncertainties do *not* account for nonperturbative effects (such as hadronization and pairing)

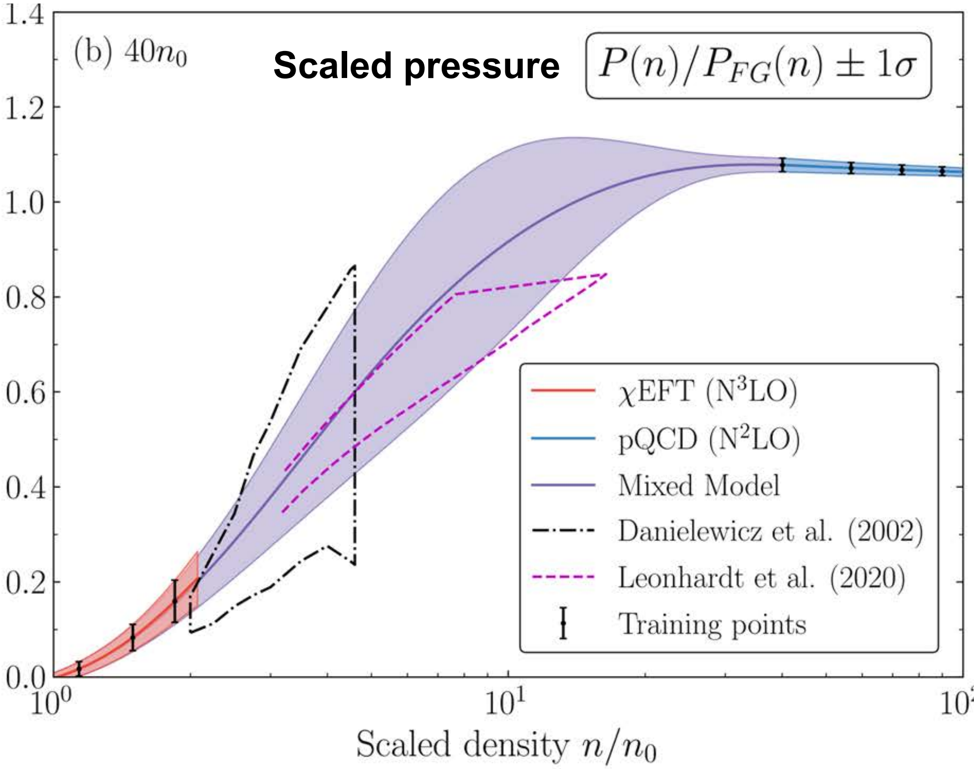
These effects become more important as the density is lowered

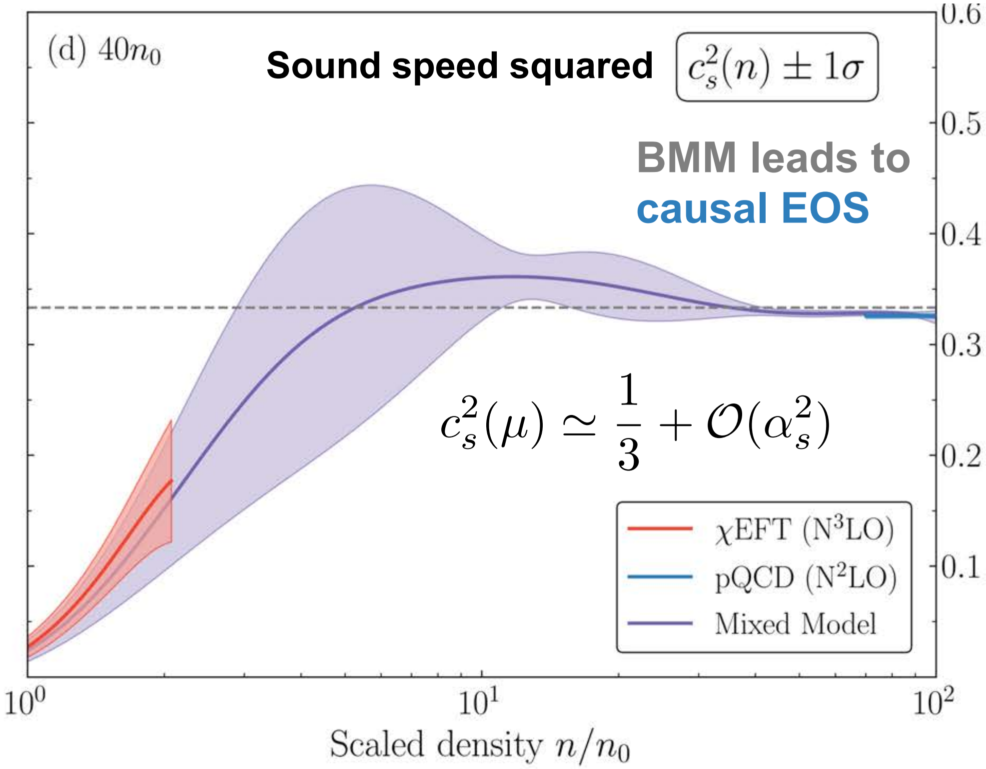
Open-Source Software: **Taweret** (BAND framework)

Bayesian Analysis of Nuclear Dynamics

What is the lowest density for including pQCD constraints?

$$n \geqslant 40 n_0$$





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

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

pQCD:
two massless quark flavors

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

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

Training points in pQCD region

Semposki, CD, Furnstahl,
Melendez, and Phillips,
arXiv:2404.06323

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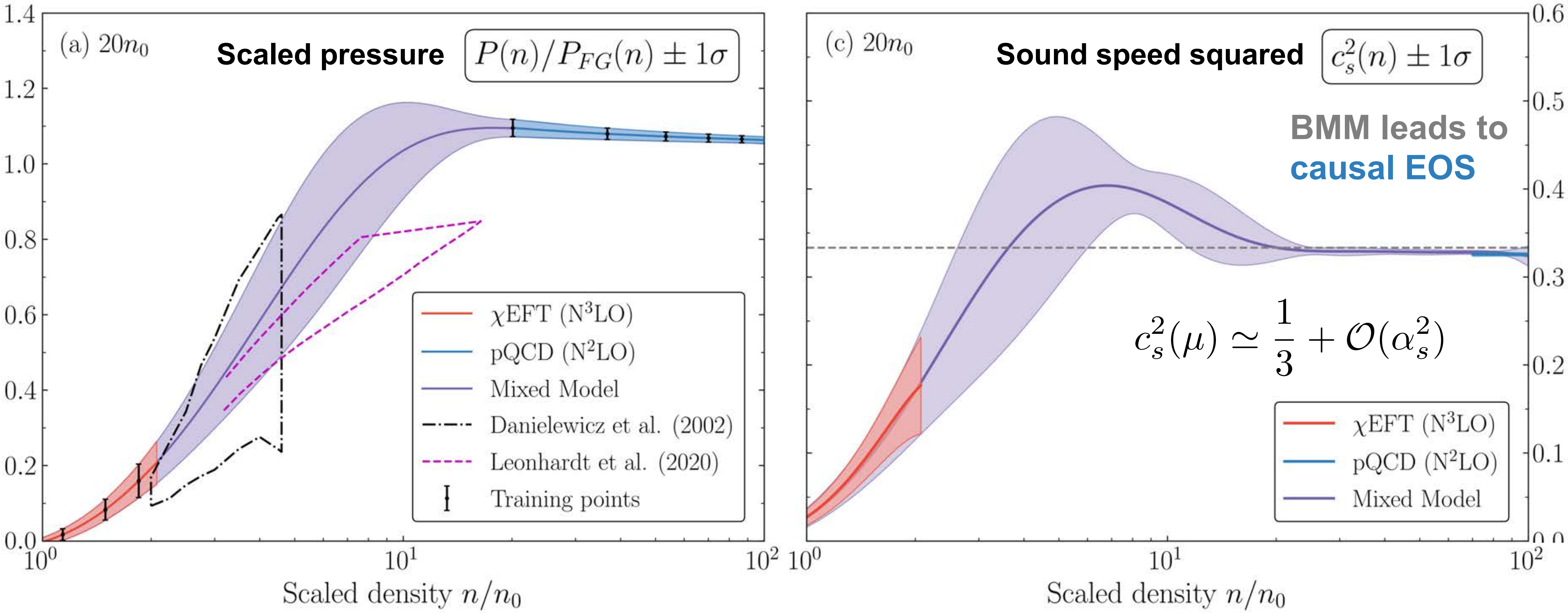
BAND Bayesian Analysis of Nuclear Dynamics

What is the lowest density for including pQCD constraints?

$$n \geqslant 20 n_0$$



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Take-away points

Semposki, CD, Furnstahl, Melendez, and Phillips, arXiv:2404.06323

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1. **Chiral EFT enables microscopic calculations of nuclei and infinite matter at n $\lesssim 2n_0$ (and finite temperature) with quantified uncertainties**

2. **BMM combines multiple predictive models in different regions into one overall predictive composite model. Not limited to the EOS, MBPT, or EFT!**

3. **Promising method for constructing globally predictive, QCD-based EOSs with rigorous UQ to study the structure & evolution of neutron stars**

   Uncertainties in the mixed region depend significantly on *physics-informed* priors. Guidance needed.

4. **Requires extension to neutron star matter (and finite temperatures) and inclusion of recent neutron star observations & nuclear experiments**

Many thanks to: **R. Furnstahl** **J. Melendez** **D. R. Phillips** **A. Semposki**

BUQEYE Collaboration

More details? Recent review article

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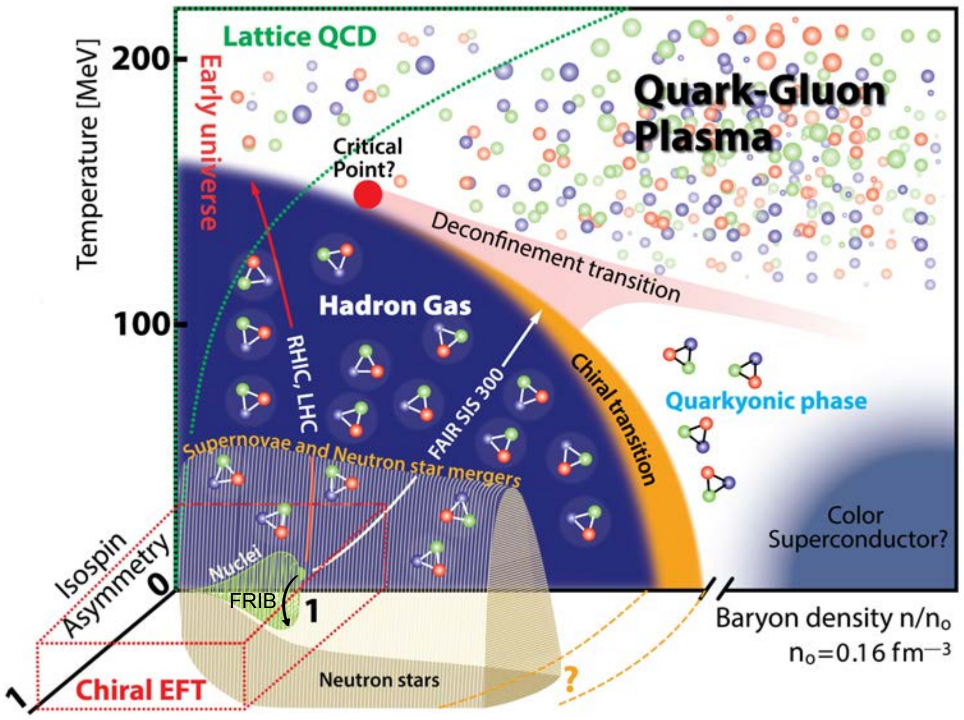

Chiral Effective Field Theory and the High-Density Nuclear Equation of State

Annual Review of Nuclear and Particle Science

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

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Keywords:

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

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James Lattimer, Annu. Rev. Nucl. Part. Sci. **71**, 433

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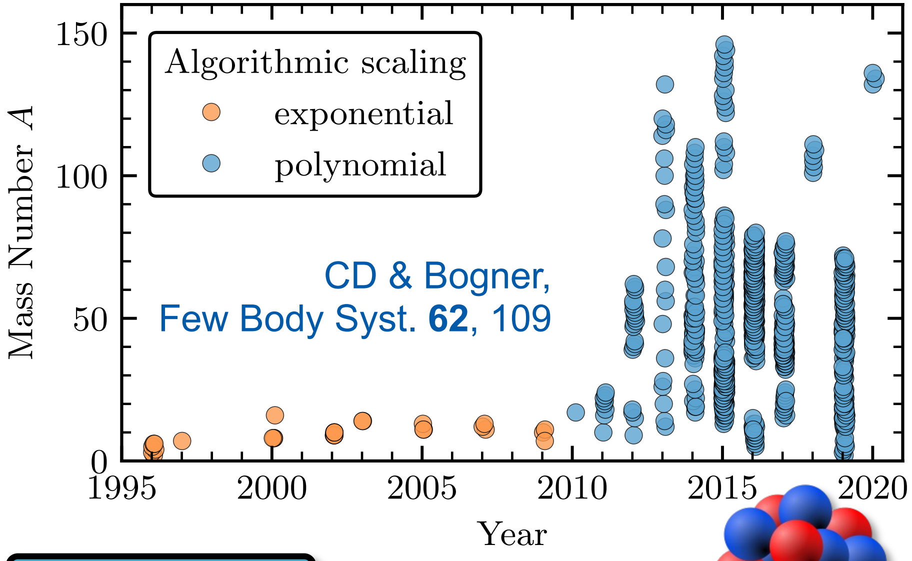
Major process: χEFT, many-body theory, and UQ!



CD & Bogner,
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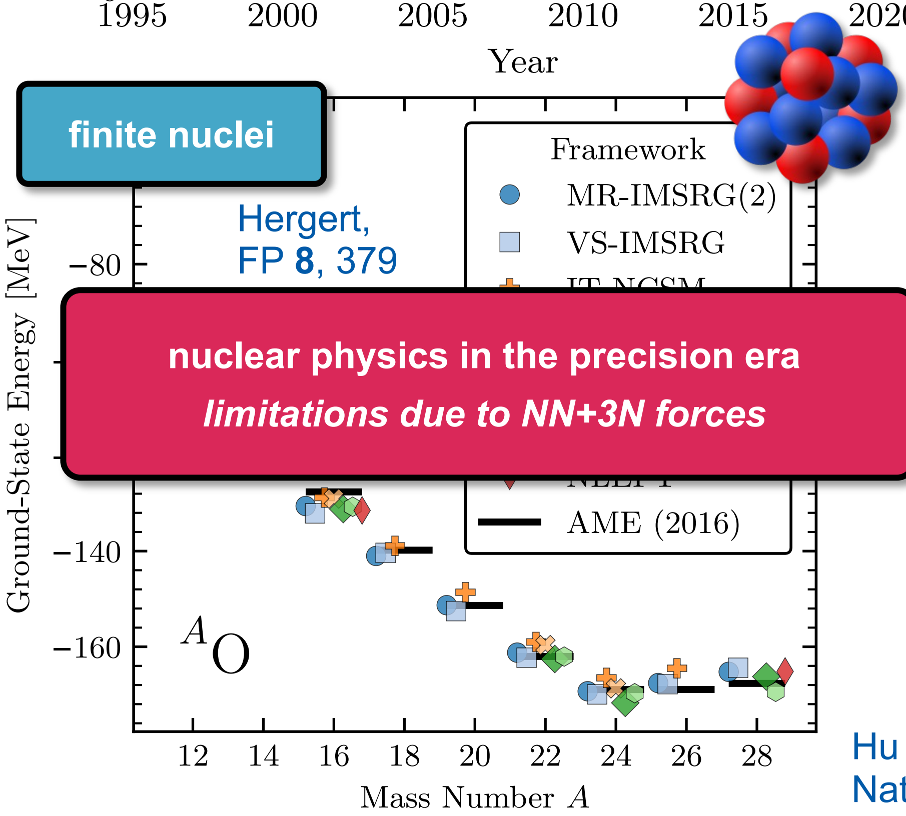
finite nuclei



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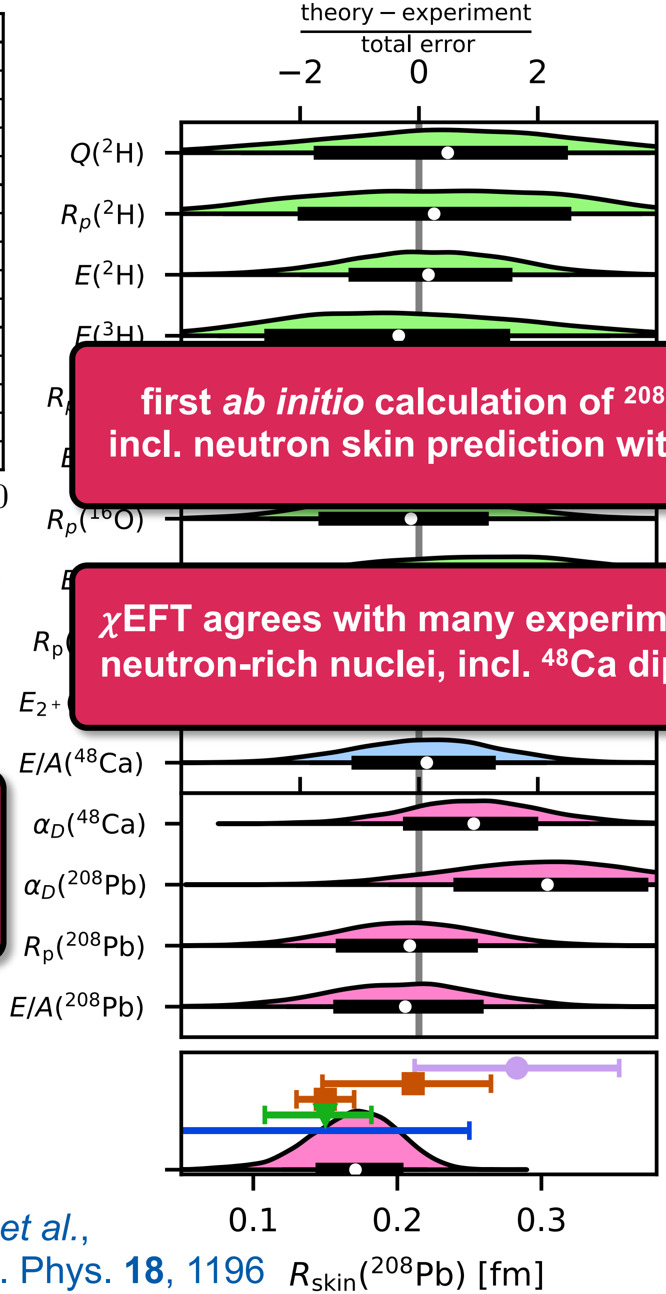
nuclear physics in the precision era

limitations due to NN+3N forces



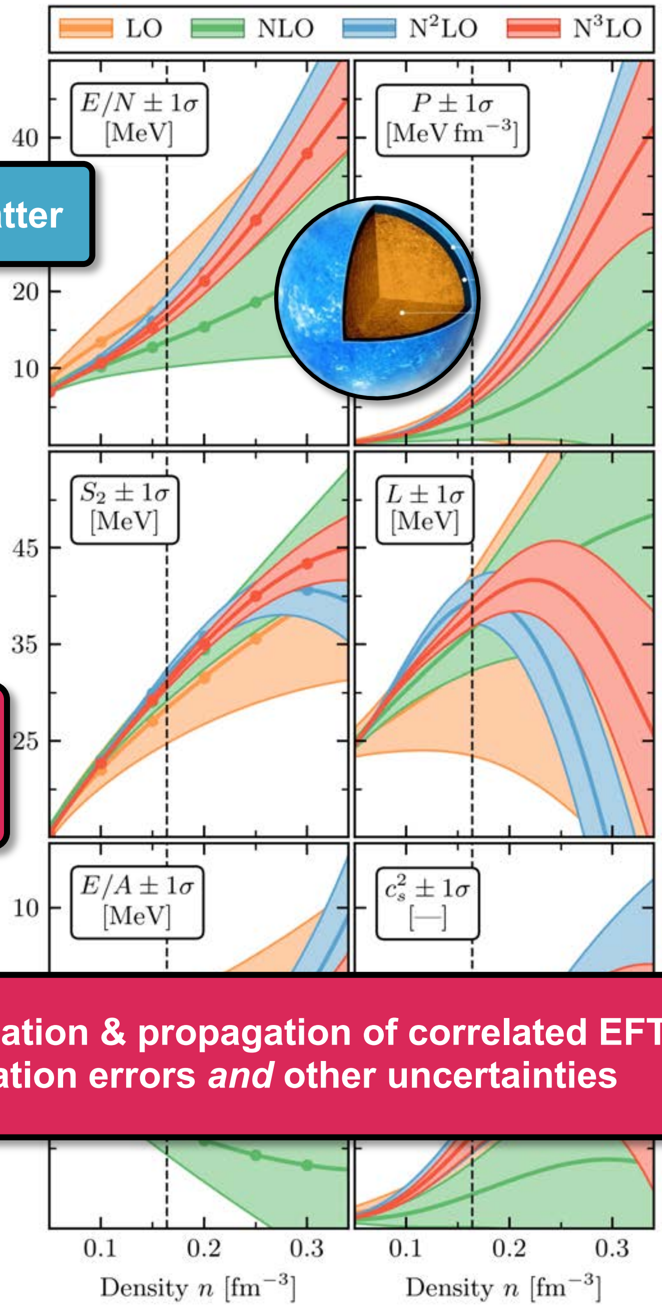
first *ab initio* calculation of ^{208}Pb,
incl. neutron skin prediction with UQ

χEFT agrees with many experiments probing neutron-rich nuclei, incl. ^{48}Ca dipole pol.

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

electroweak
hadronic
electromagnetic
gravitational waves

infinite matter



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

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