From Low to High Densities: an Application of Bayesian Model Mixing to the Dense Matter EOS

Christian Drischler (drischler@ohio.edu)

INT-24-89W: EOS Measurements with Next-Generation GW Detectors

August 26, 2024 | Institute for Nuclear Theory (INT)

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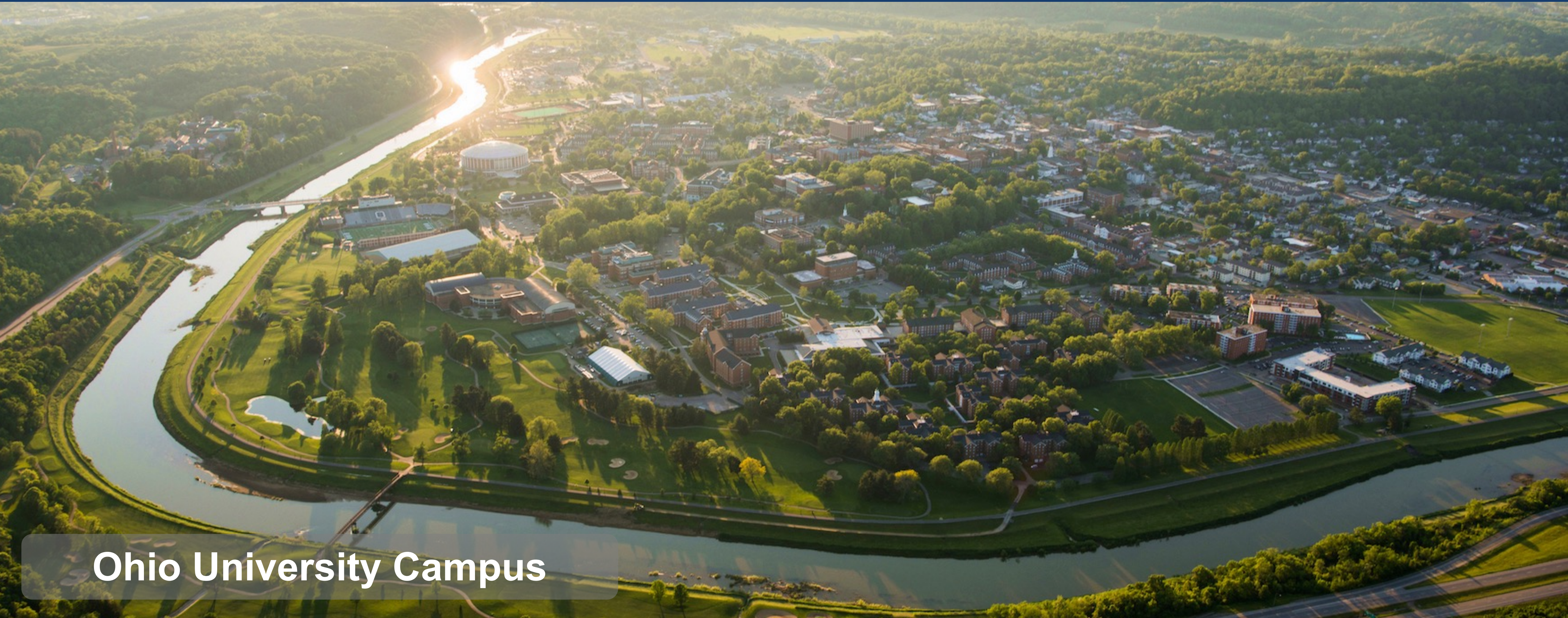
BUQEYE Collaboration



Bayesian Model Mixing in SNM

STREAMLINE SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

BAND Bayesian Analysis of Nuclear Dynamics

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

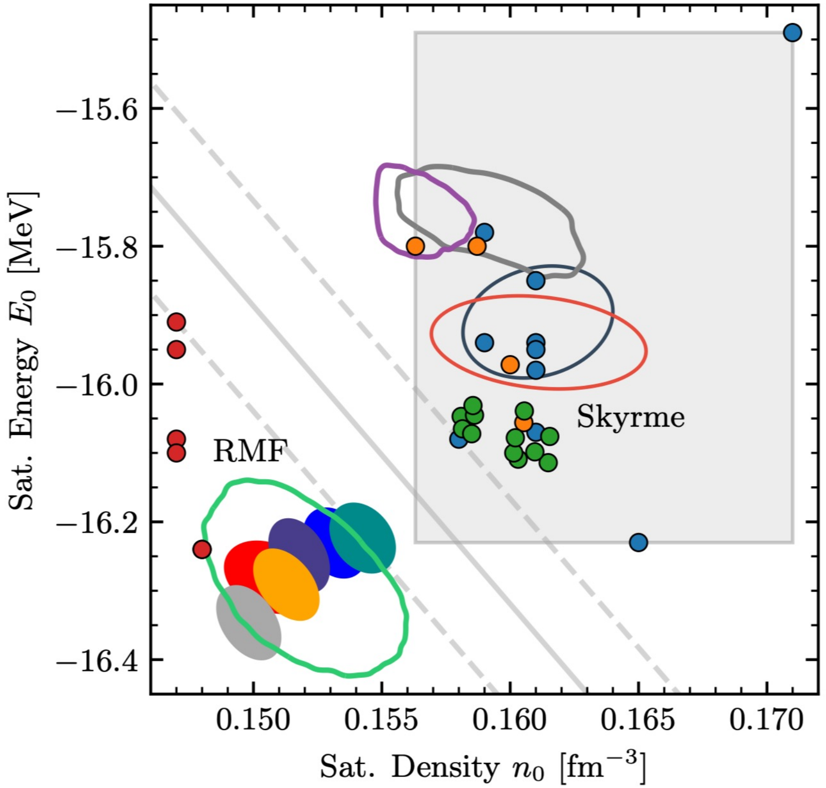
CD, Giuliani, **Bezoui**, Piekarewicz, and Viens, arXiv:2405.02748

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

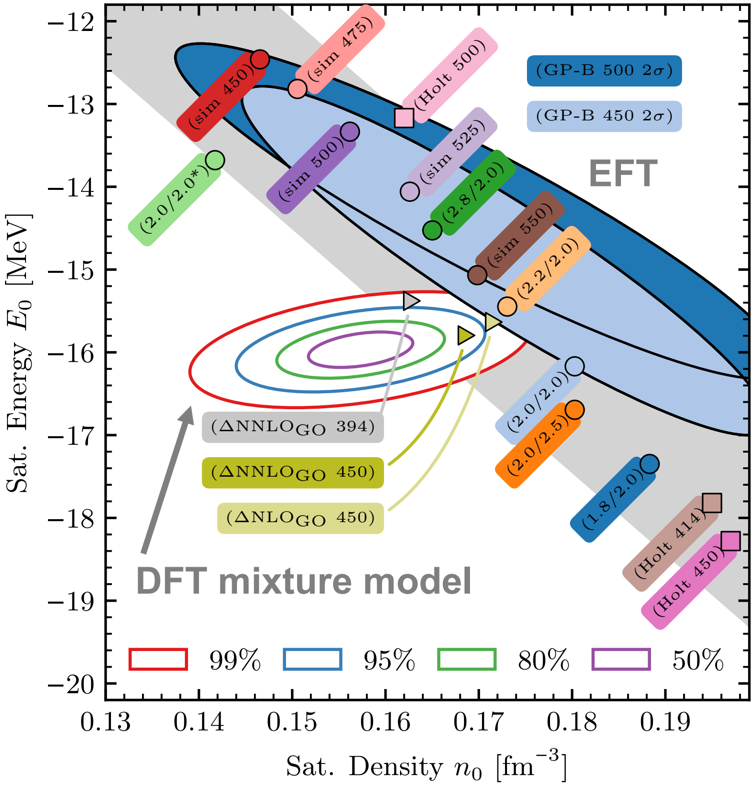
From chiral EFT to perturbative QCD: a **Bayesian model mixing** approach to symmetric matter

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

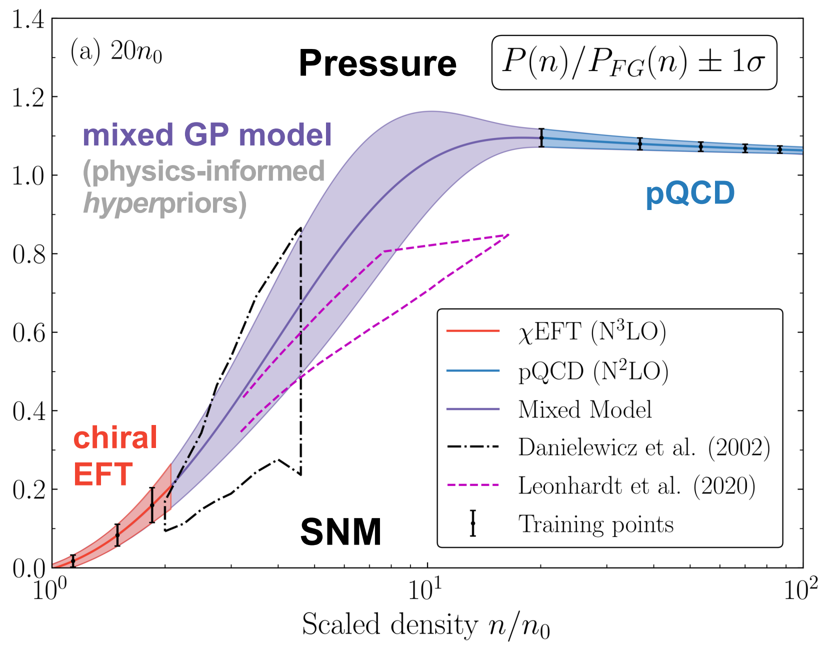
DFT constraints on nuclear saturation



DFT vs EFT: nuclear saturation



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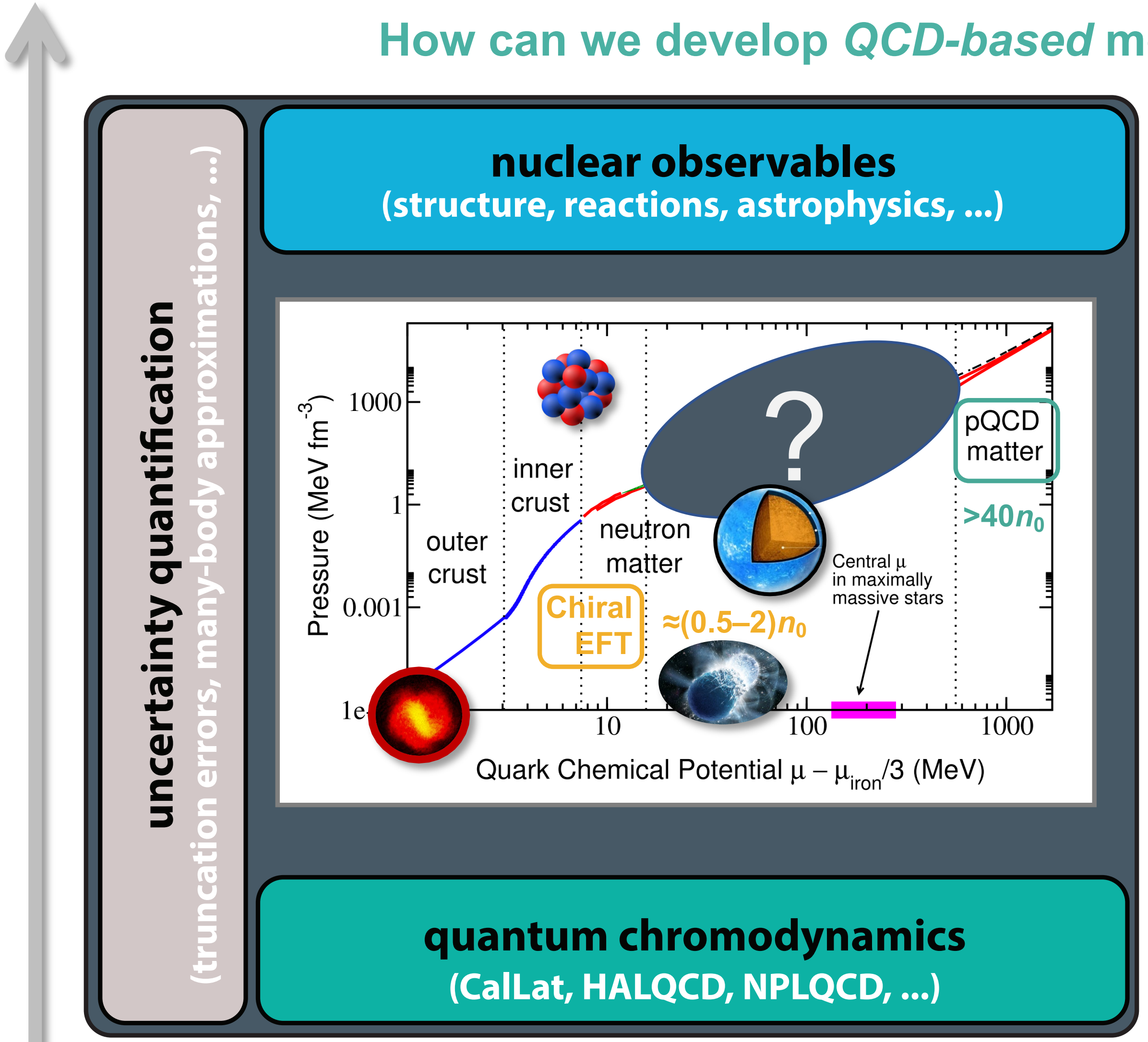
How can we develop *QCD-based* models that are *predictive* across all densities?

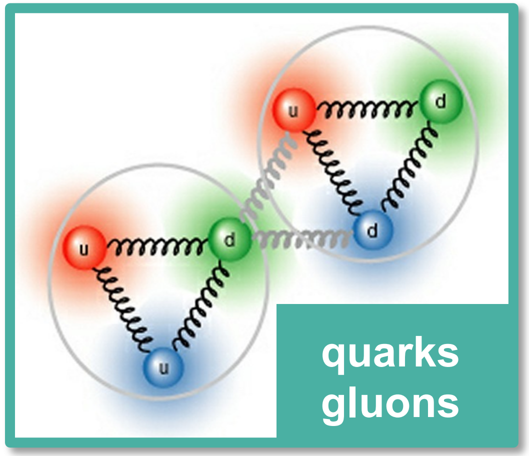


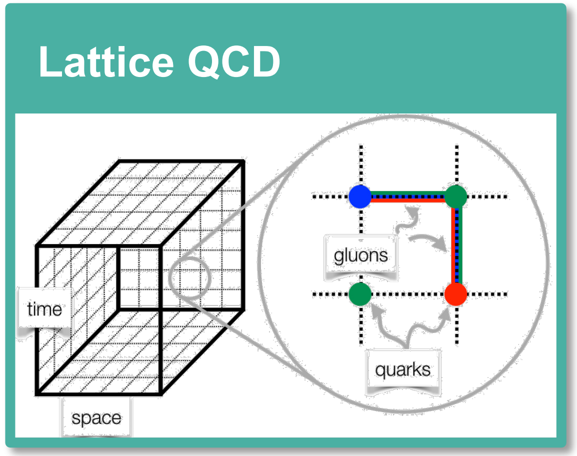
CD & Bogner, Few Body Syst. **62**, 109

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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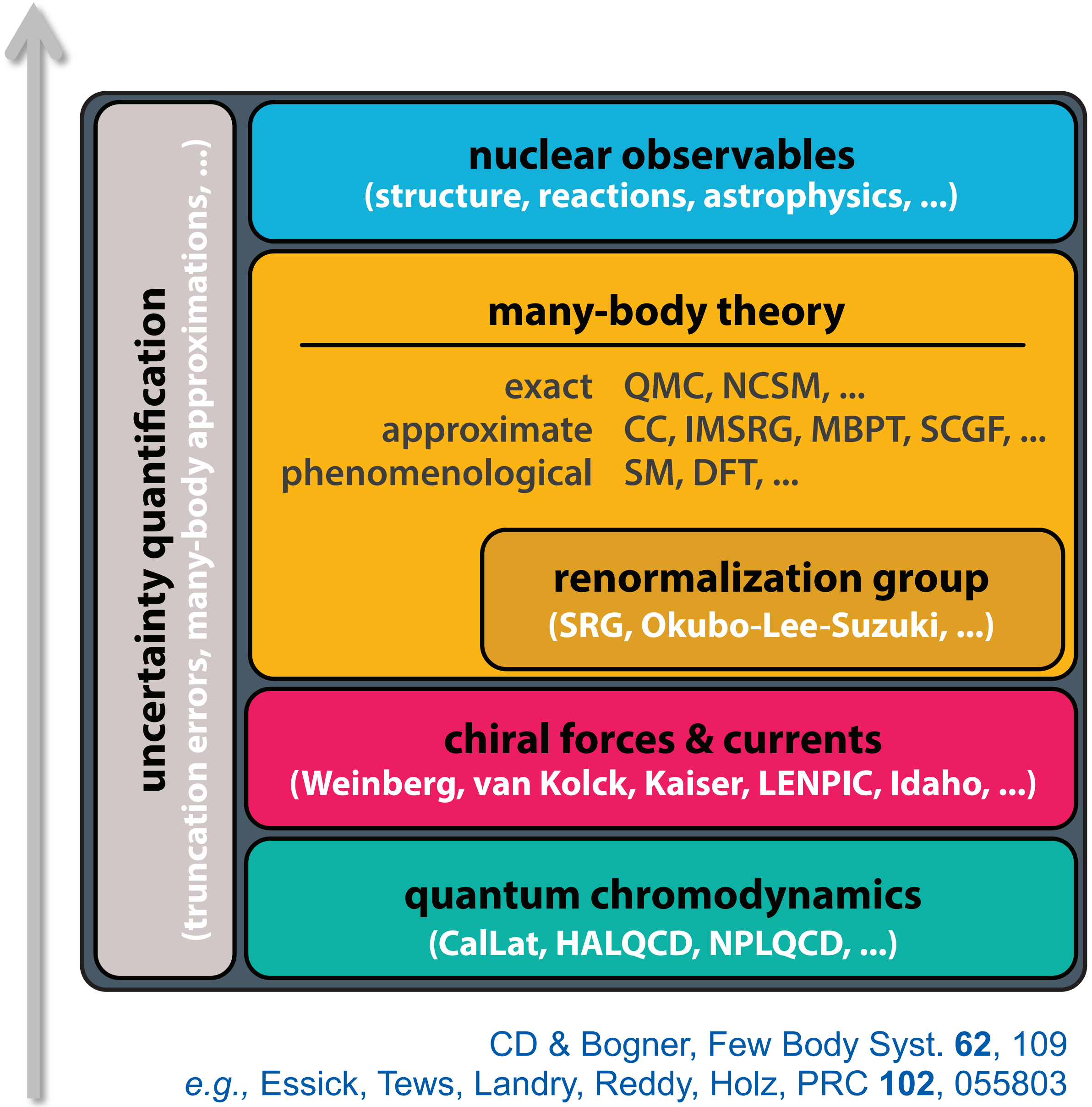

CD & Bogner, Few Body Syst. **62**, 109
e.g., Essick, Tews, Landry, Reddy, Holz, PRC **102**, 055803

Here: nuclear equation of state (EOS)

Pressure, *energy per particle*, or sound speed

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

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)

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

Low densities: *ab initio* workflow (idealized)

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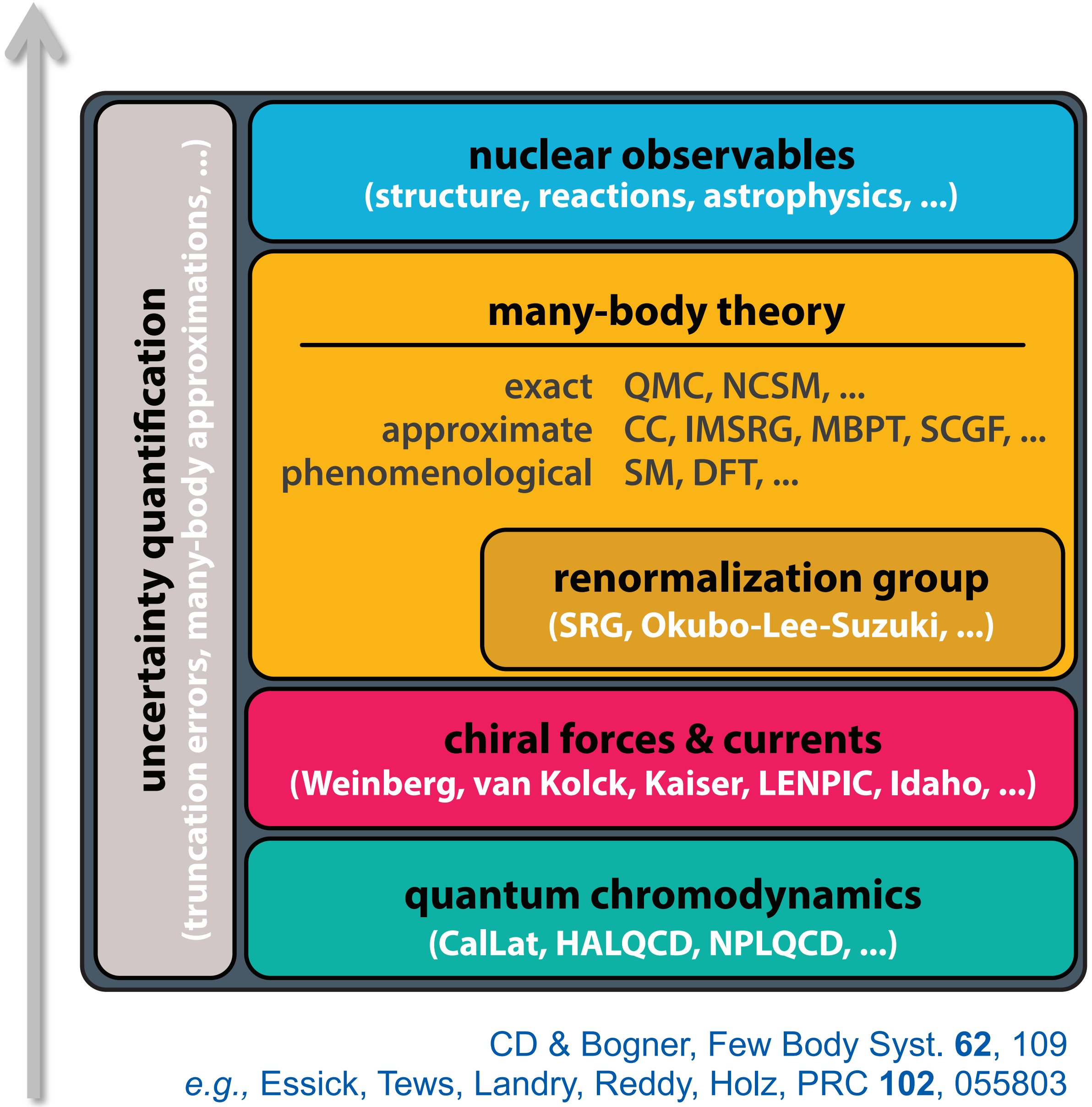

CD & Bogner, Few Body Syst. **62**, 109
e.g., Essick, Tews, Landry, Reddy, Holz, PRC **102**, 055803

Here: nuclear equation of state (EOS)

Pressure, *energy per particle*, or sound speed

Exciting developments in *ab initio* many-body theory

new methods
emulators for UQ
new potentials (UQ)

e.g., Cook *et al.*, arXiv:2401.11694 (Parametric Matrix Models), Somasundaram *et al.*, arXiv:2404.11566

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

See also Kang Yu's talk in this session:
Nuclear Matter EOS from the IMSRG

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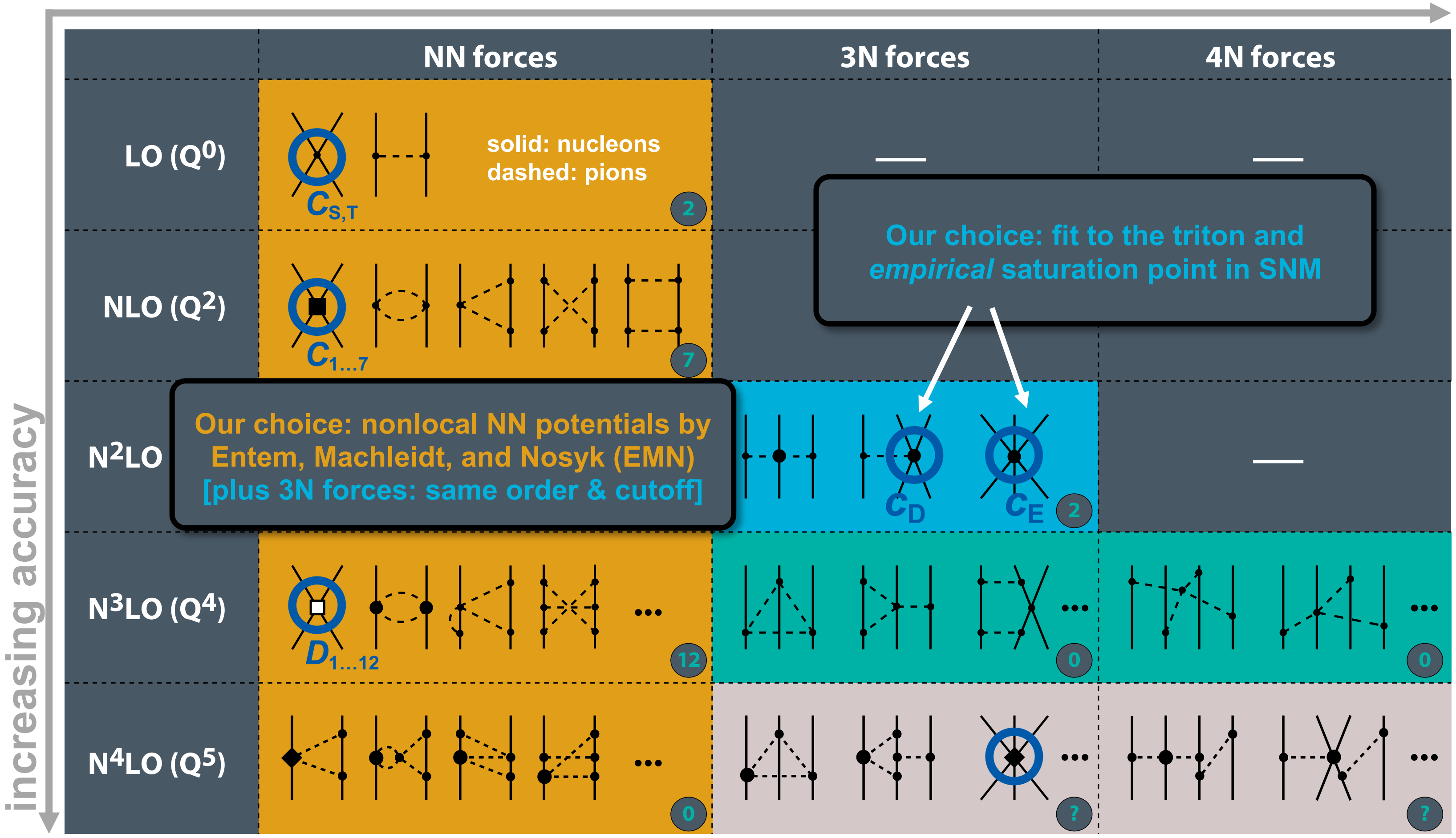
Hierarchy of chiral nuclear forces up to N^{4}LO

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

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



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

Chiral *effective* field theory

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

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

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

fit the unknown couplings to experimental (or lattice) data

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

Correlated EFT truncation error model

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

increasing accuracy

LO (Q^0)	y_0
NLO (Q^2)	y_1
N^{2}LO (Q^3)	y_2
N^{3}LO (Q^4)	y_3
N^{4}LO (Q^5)	y_4 (unknown)

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

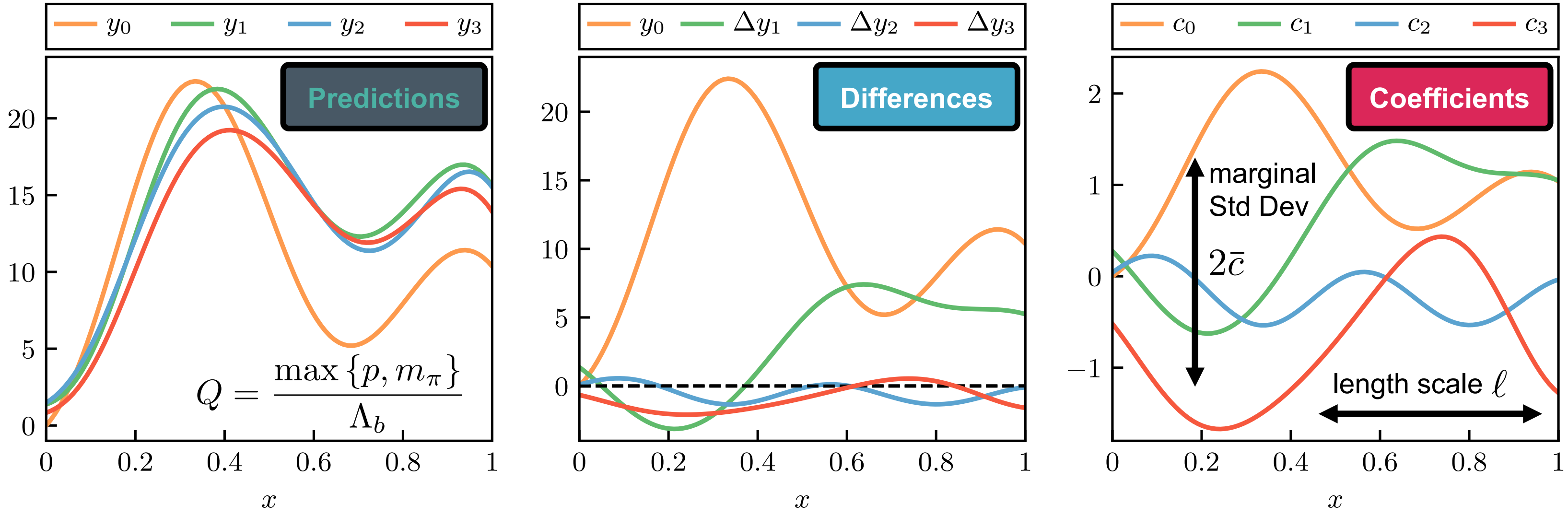
EFT prediction at $k^{\rm th}$ order

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

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

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

to-all-orders truncation error



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

***natural* coefficients**

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

Here: **RBF** (stationary)

predict observable y_k order by order in EFT

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

differences

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

Accounts for correlations in the observable $y(x)$
EFT breakdown scale estimation
Model checking diagnostics (*e.g.*, Mahalanobis distance)

many applications of this truncation error model

https://github.com/buqeye/gsum

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

MBPT in a nutshell

CD, Hebeler, Schwenk, PRL **122**, 042501
CD, Holt, and Wellenhofer, ARNPP **71**, 403
Arthuis *et al.*, Comput. Phys. **240**, 202

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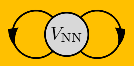
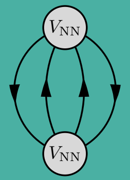


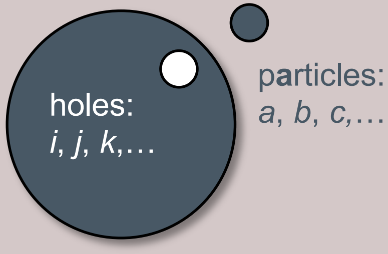
$$\frac{E^{(0)}}{V} = +\frac{1}{2}\sum_{ij} \langle ij \,|\, \overline{V}_{\rm NN} \,|\, ij \rangle$$

Hartree-Fock

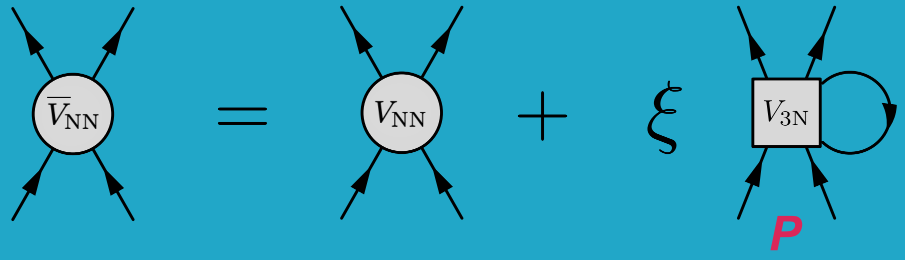


$$\frac{E^{(2)}}{V} = \frac{1}{4}\sum_{\substack{ij\\ab}} \frac{|\langle ij|\overline{V}_{\rm NN}|ab\rangle|^2}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}$$

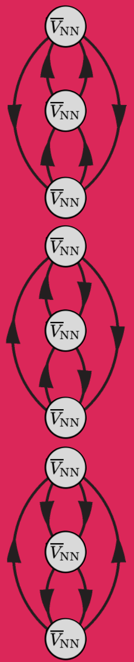
second order



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



Normal ordering 3N forces results in effective two-body potentials



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

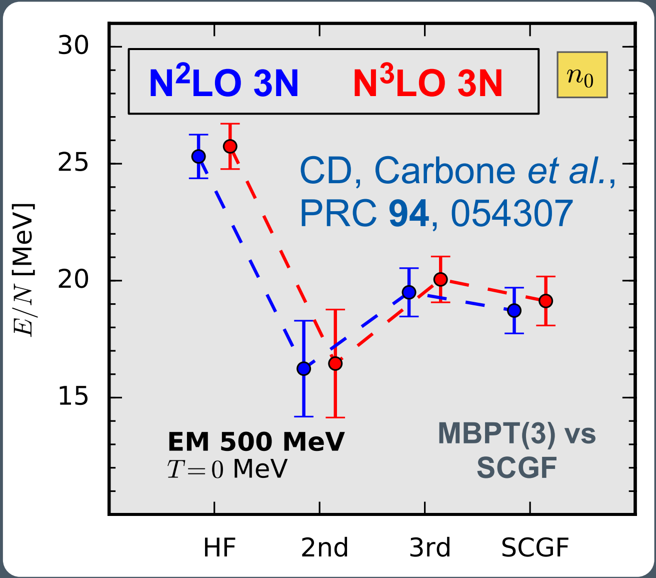
number of MBPT diagrams increases rapidly

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

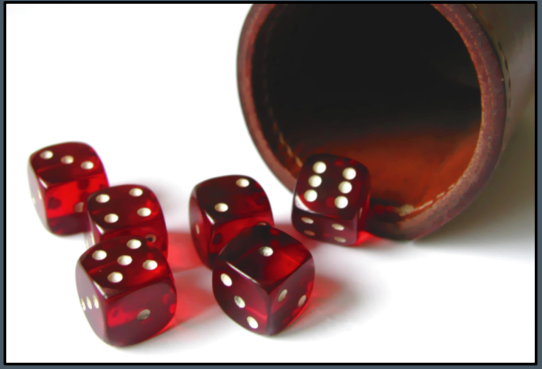
see Coraggio, Holt *et al.*, PRC **89**, 044321

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

third order



Controlled evaluation of multi-dimensional momentum integrals:
MC via improved VEGAS



Automated derivation & evaluation of (thousands of) MBPT diagrams

Correlated EFT truncation error model (revisited)

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your EFT

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

Increasing accuracy

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

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

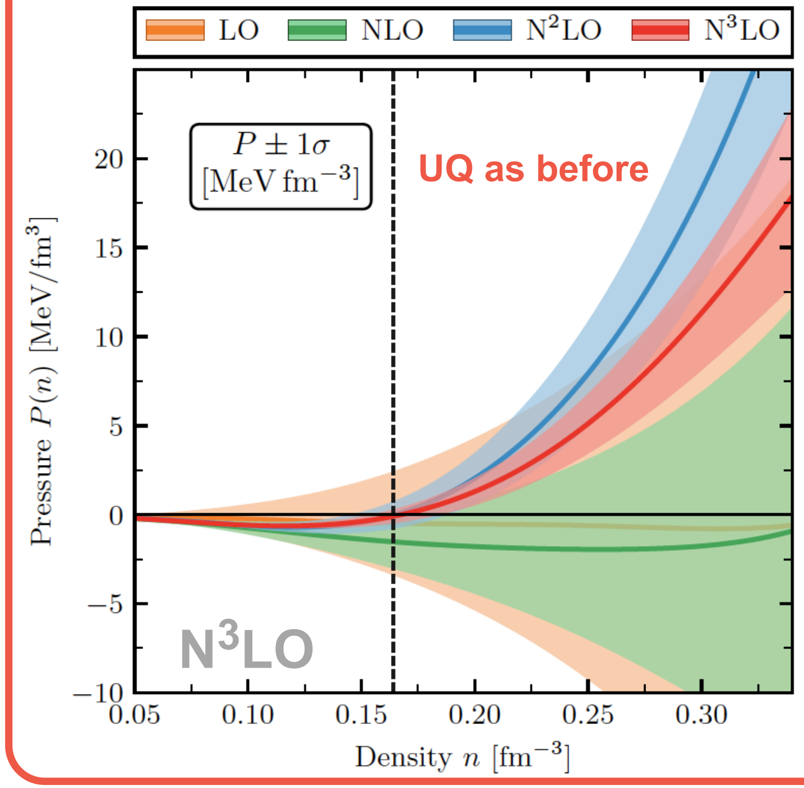
want full prediction: $y = y_k + \delta y_k$

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

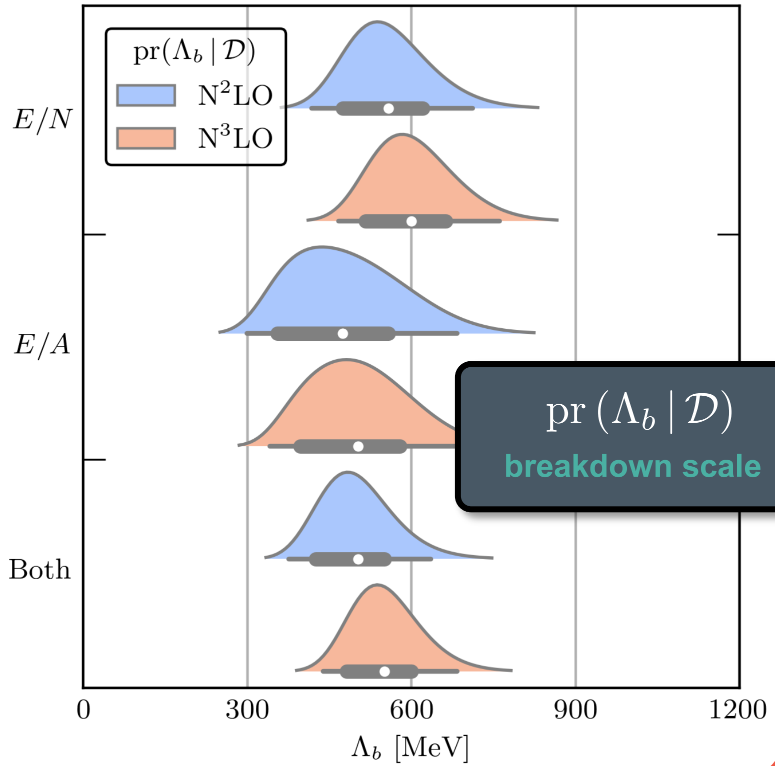
$$\delta y_k = y_{\rm ref} \sum_{n=k+1}^{\infty} c_n Q^n$$

to-all-orders truncation error

Chiral EFT



Bayesian inference of the in-medium breakdown scale



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

breakdown scale

$$Q(k_{\rm F}) = \frac{k_{\rm F}}{\Lambda_b}$$

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

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

Correlated EFT truncation errors (for pQCD)

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

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your EFT

Increasing accuracy

- LO (Q^0)
- NLO (Q^2)
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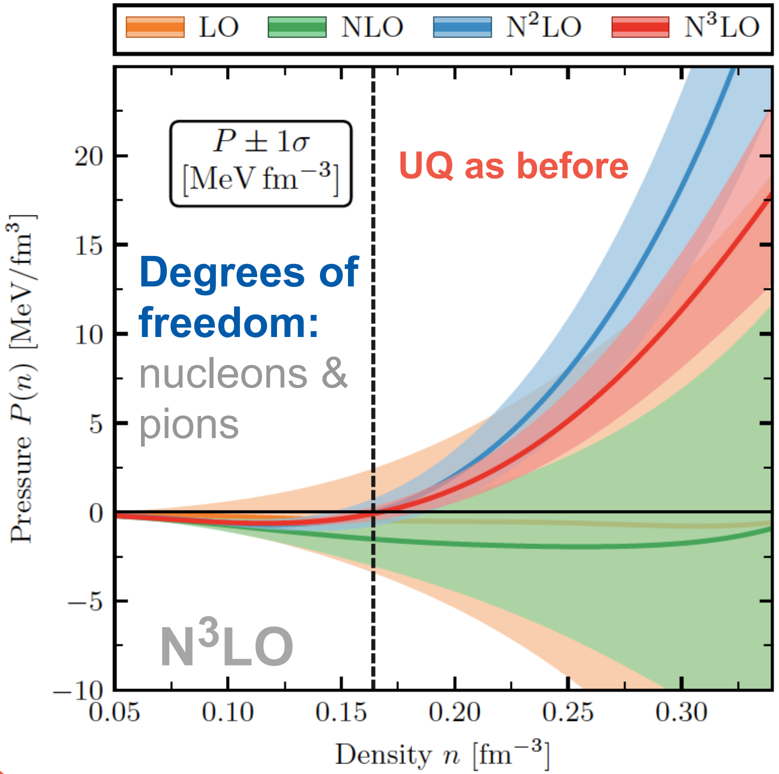

pQCD

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

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

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

$$\frac{P(\mu)}{P_{FG}(\mu)} \simeq 1 + a \ldots \left(\frac{\alpha_s(\bar{\Lambda})}{\pi}\right) \ldots$$

$$+ \; a_{2,2} \ln \frac{\bar{\Lambda}}{2\mu} + a_{2,3}\Big] + \mathcal{O}(\alpha_s^3),$$

−2

−1

−4.8333

−8.0021

See also talks by Aleksi Vuorinen and Tyler Gorda next Monday

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)

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

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your EFT

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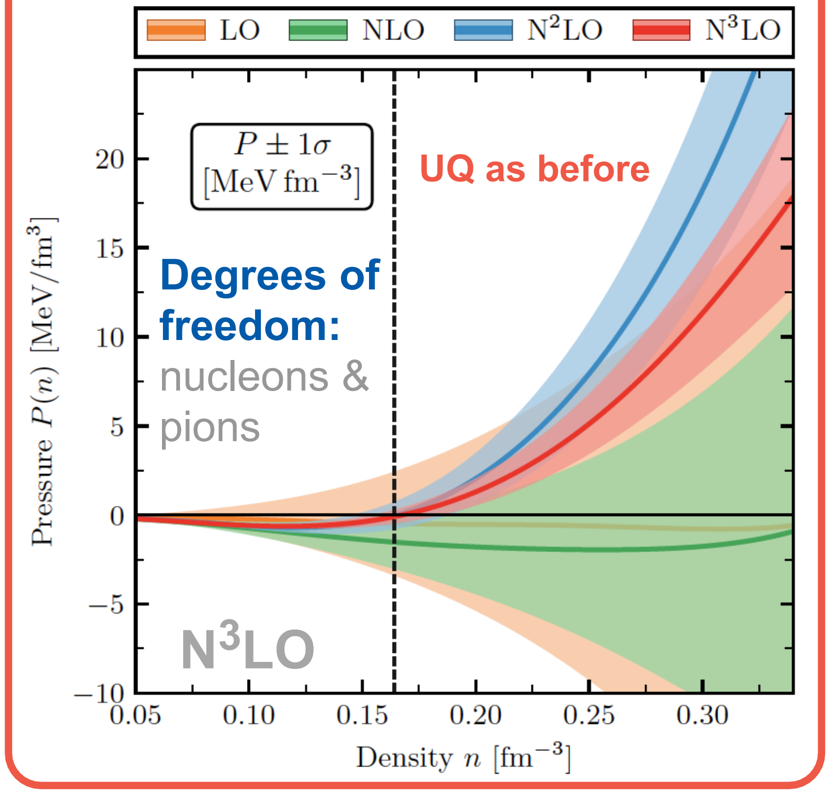
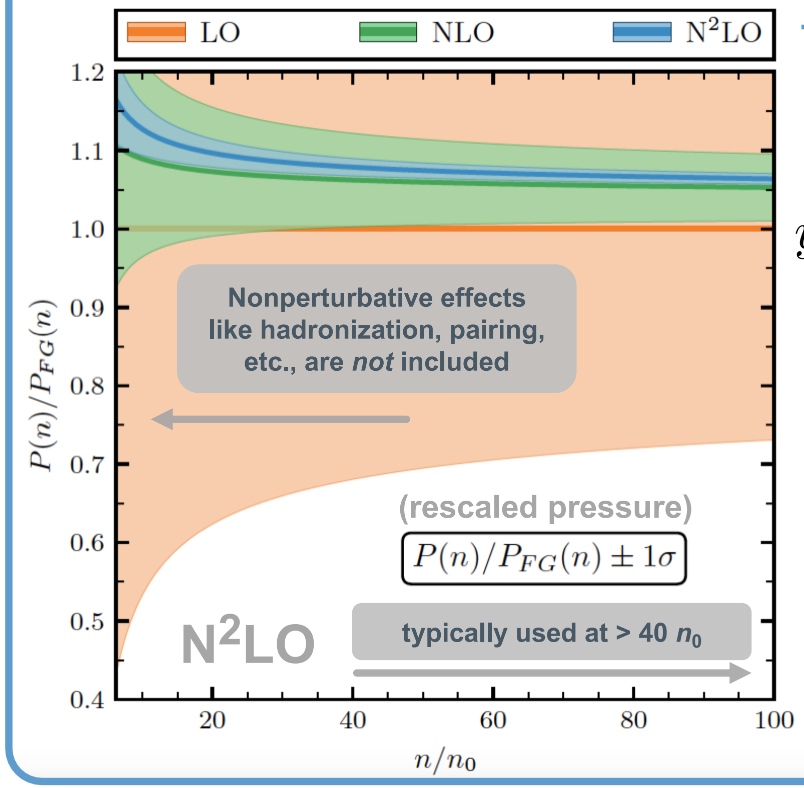
to-all-orders truncation error

Chiral EFT



pQCD



Truncation error estimation:

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

$$y_{\rm ref} = P_{\rm FG}(n)$$

(two-loop level)

Kohn-Luttinger-Ward inversion:

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

(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)

Curvewise mixing of random variables

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

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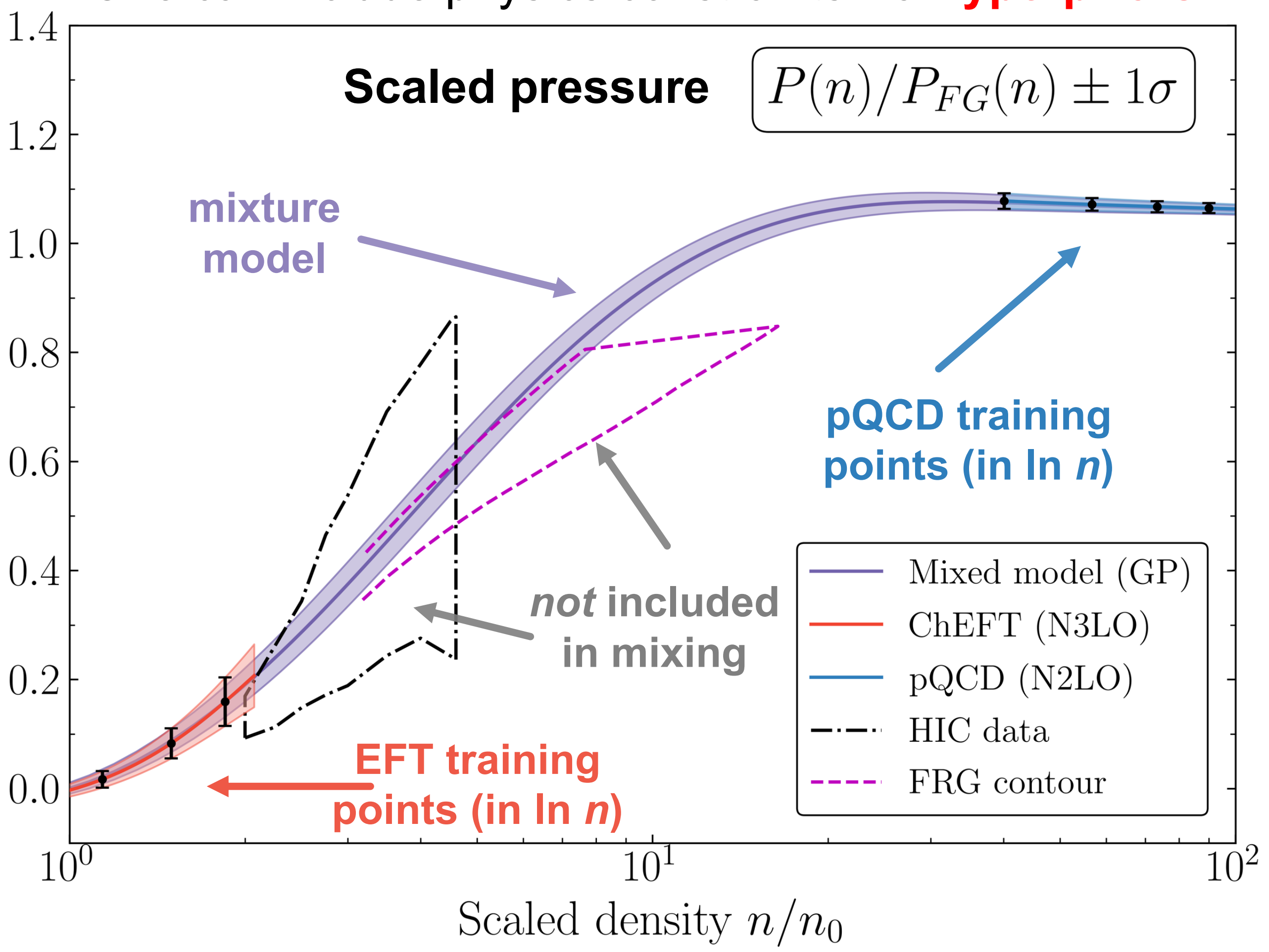
One can include physics constraints via **hyperpriors**



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:

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

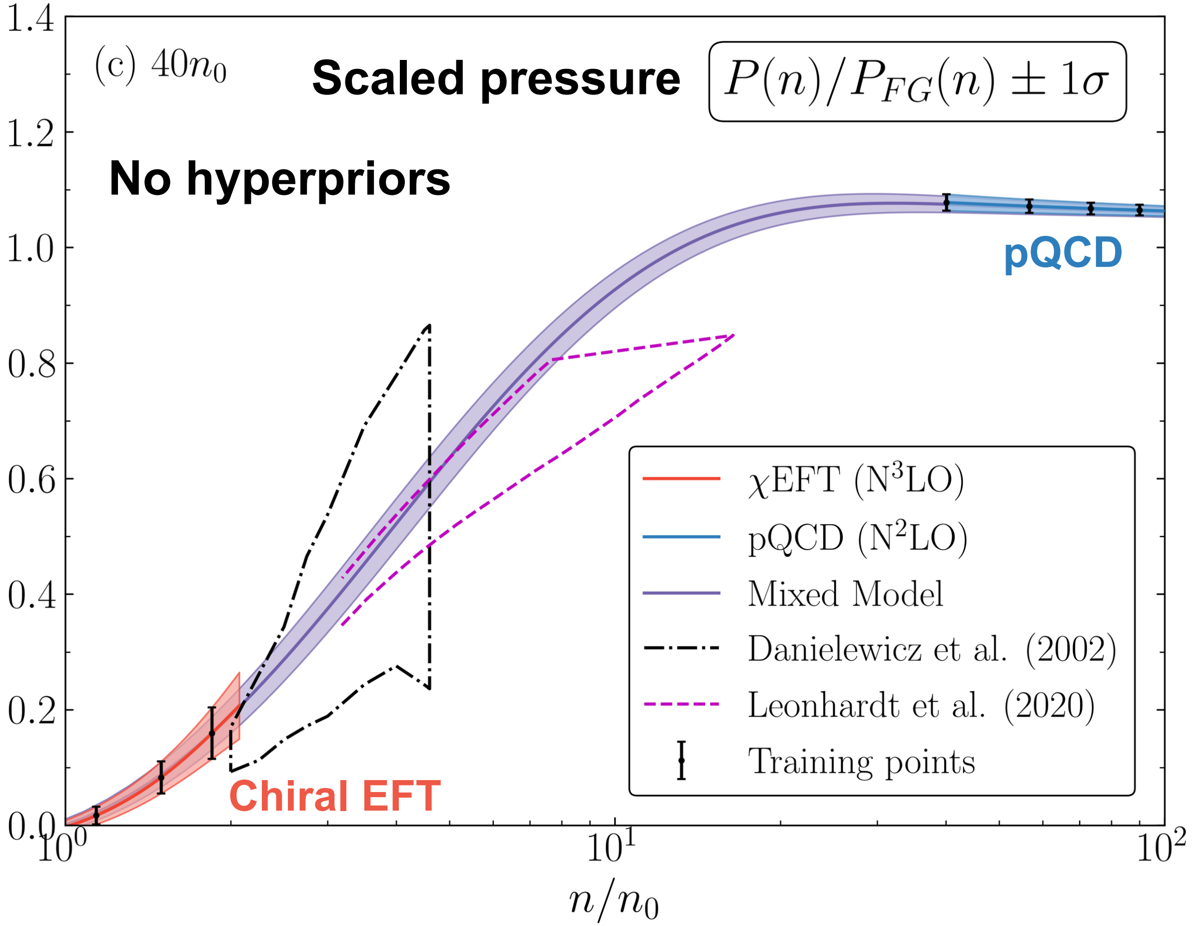
$$\vec{\mu} \equiv \Sigma B_t^T K_y^{-1} \vec{y}, \qquad \Sigma \equiv (K_f^{-1} + B_t^T K_y^{-1} B_t)^{-1}$$

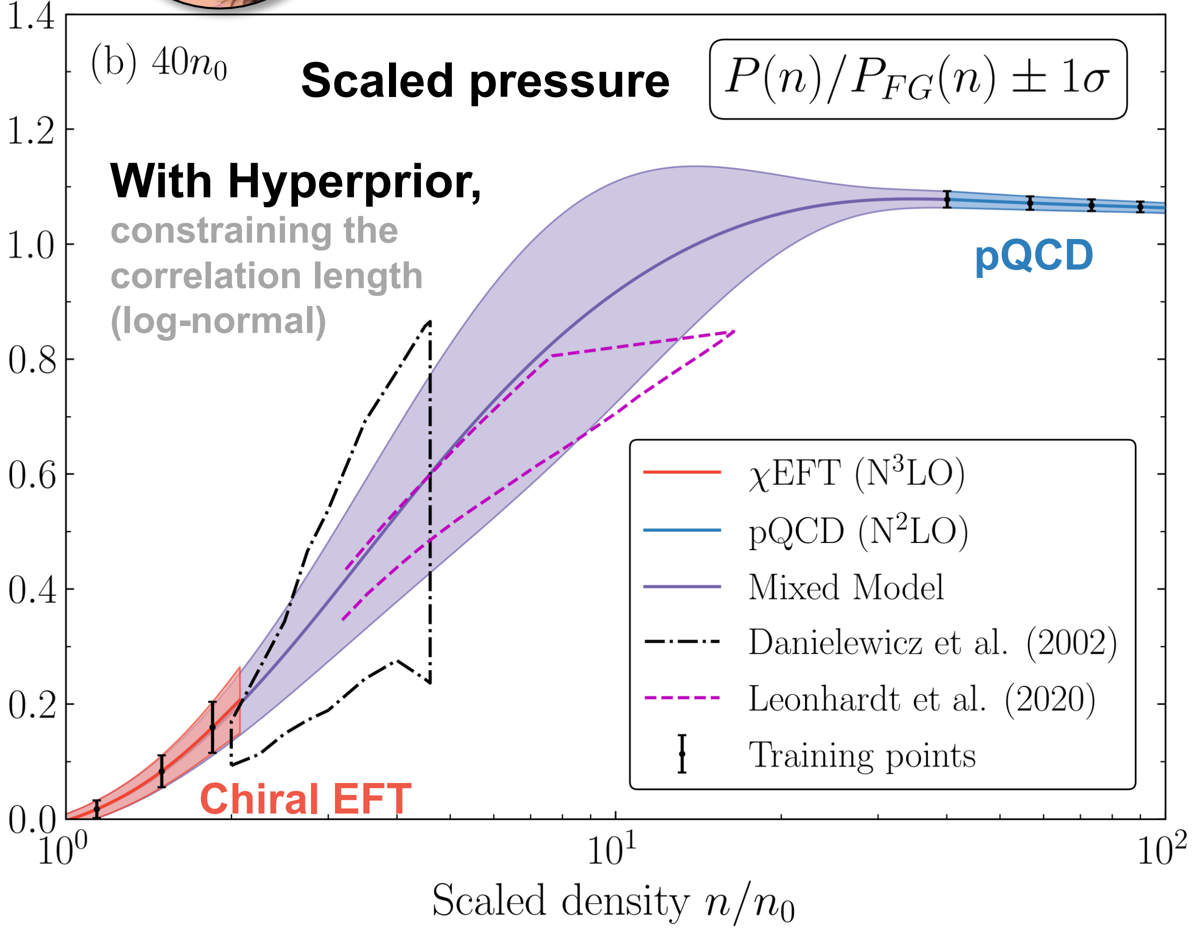
Assumptions (*not* necessarily satisfied, validation needed):

- *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





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)

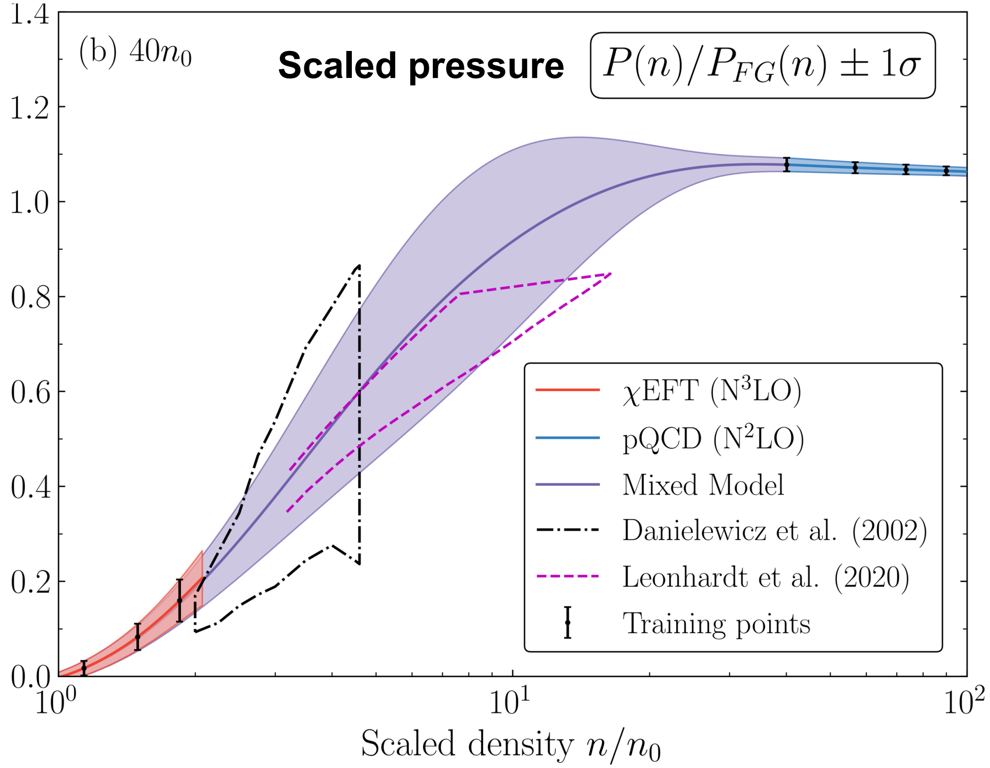
These effects become more important as the density is lowered

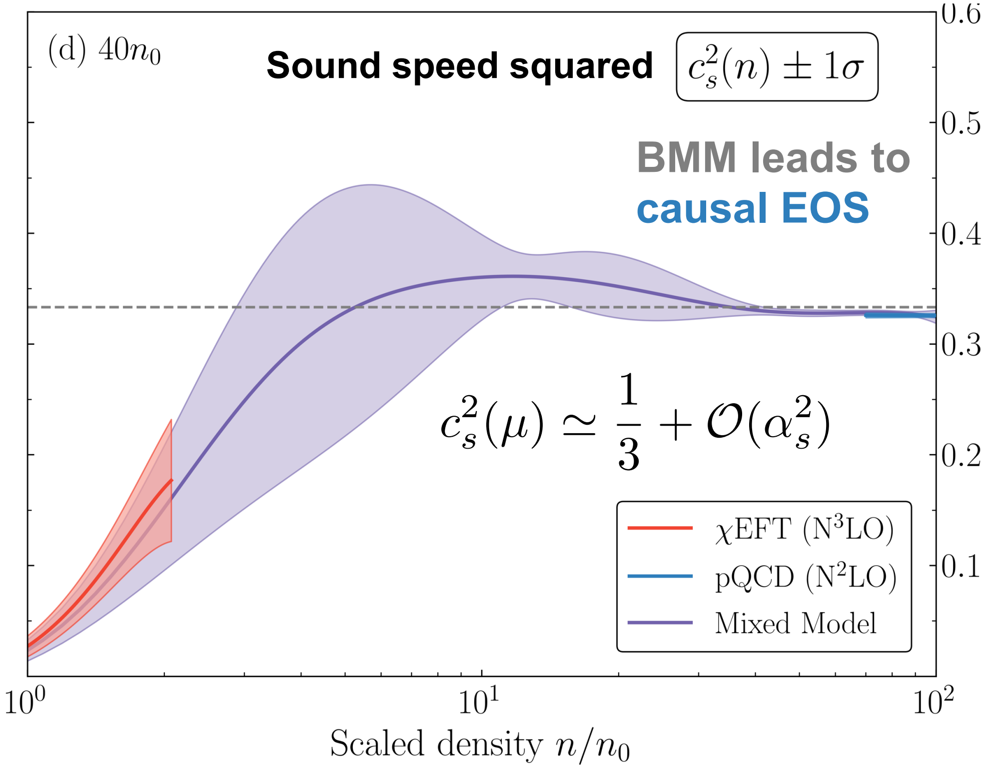
What is the lowest density for including pQCD constraints?

$$n \geqslant 40n_0$$

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

BAND Bayesian Analysis of Nuclear Dynamics





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

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

pQCD: two massless quark flavors

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

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

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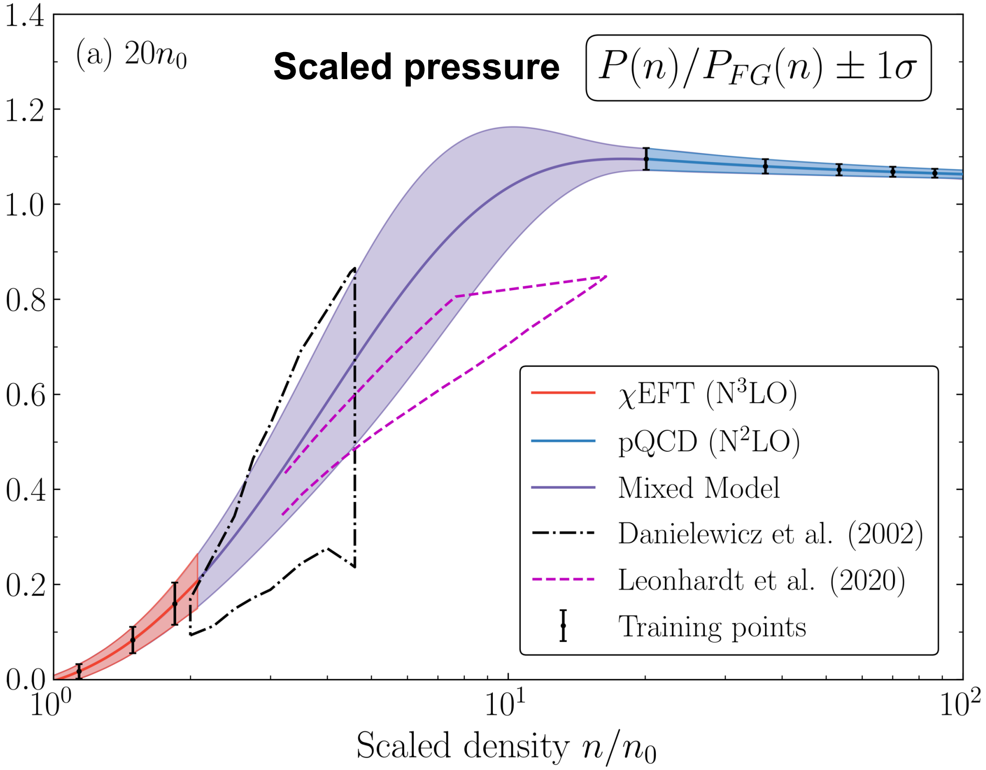
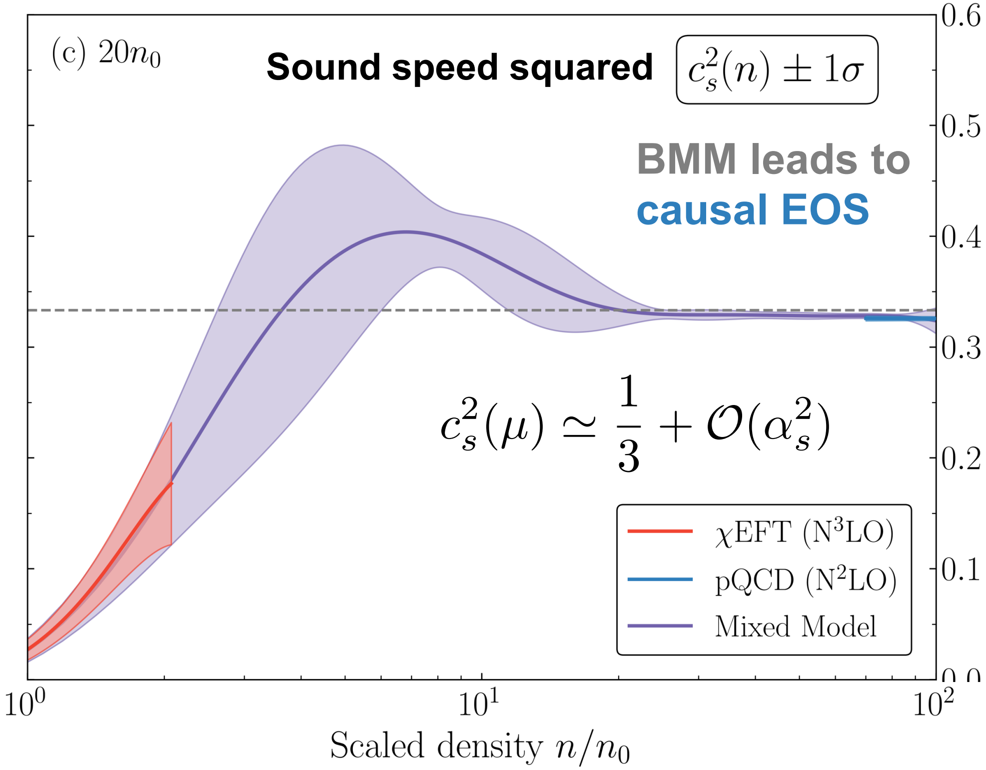
BAND Bayesian Analysis of Nuclear Dynamics

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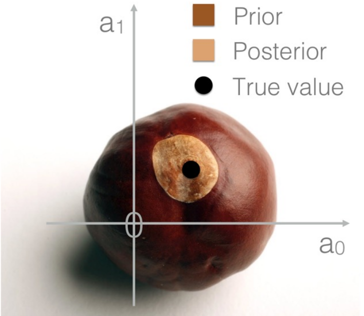
1. **Chiral EFT enables microscopic calculations of nuclei and infinite matter at n $\lesssim 2n_0$ (and finite temperature) with quantified uncertainties**

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**



BUQEYE Collaboration

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