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ASCSN

BAND
Bayesian Analysis of Nuclear Dynamics

From chiral EFT to perturbative QCD: a Bayesian model mixing approach to the dense matter equation of state

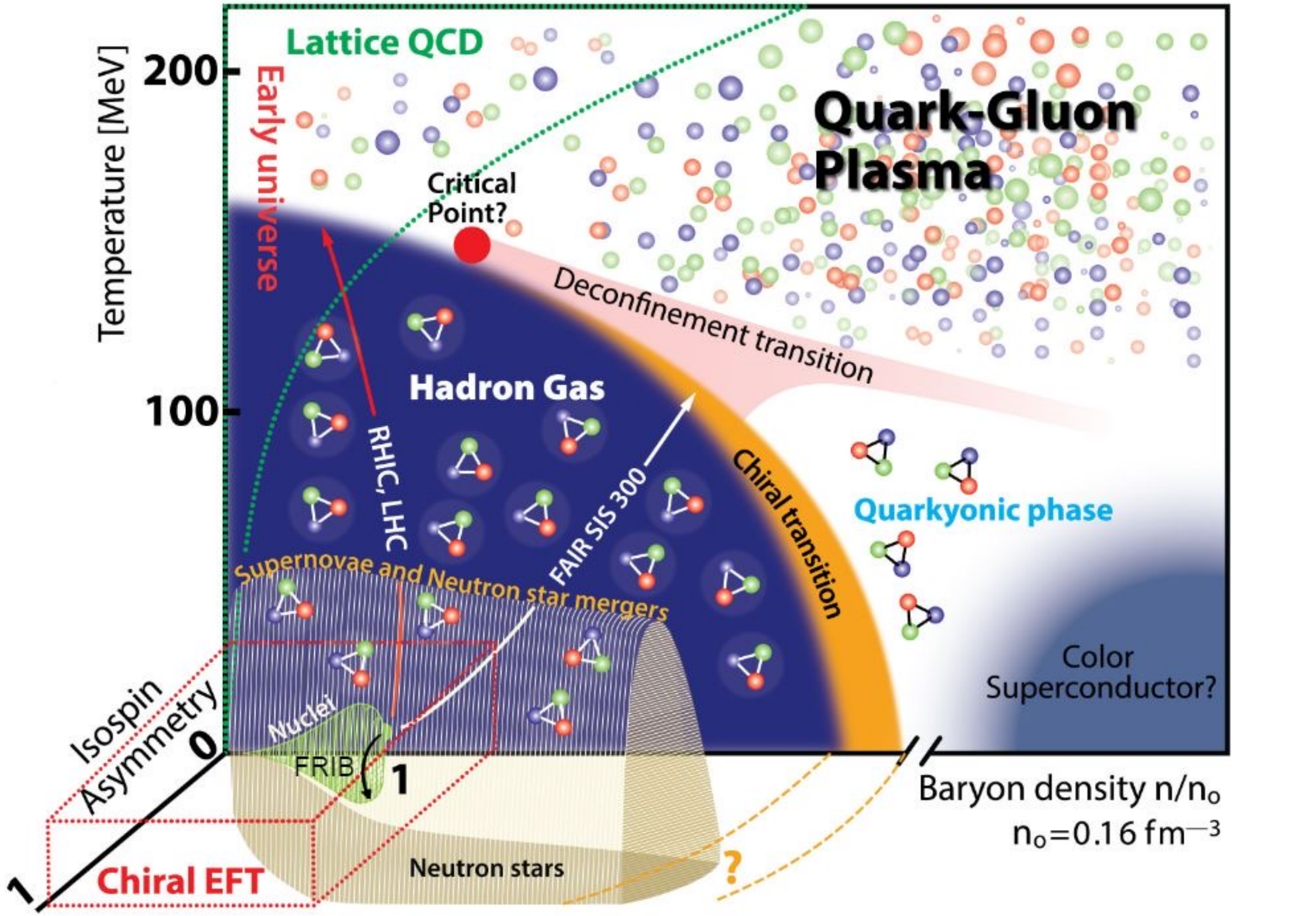
Alexandra C. Semposki

in collaboration with: C. Drischler, R. J. Furnstahl, J. A. Melendez, D. R. Phillips

arXiv:2404.06323v2

Motivation: a unified EOS

Drischler et al. (2021)



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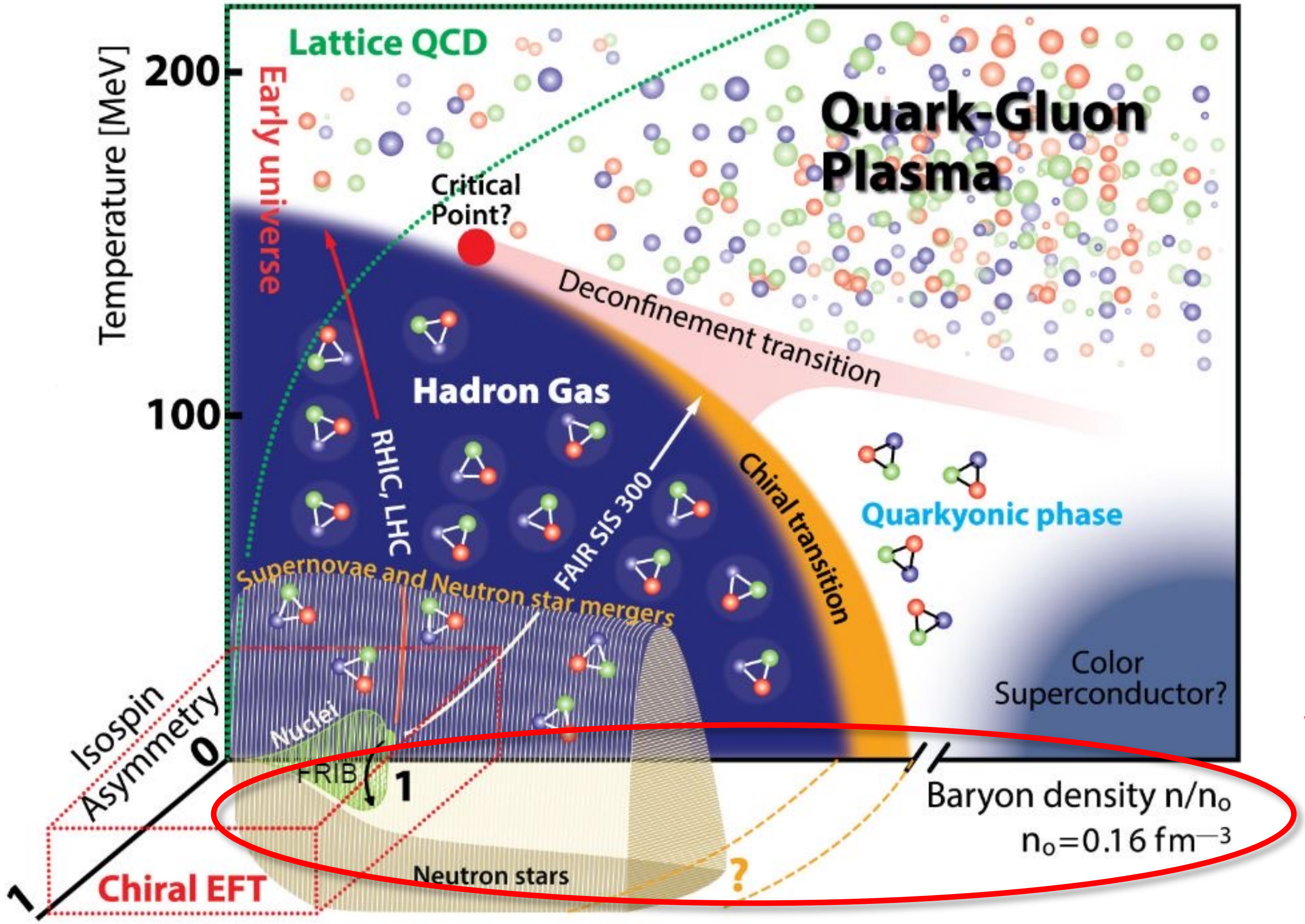

We are here

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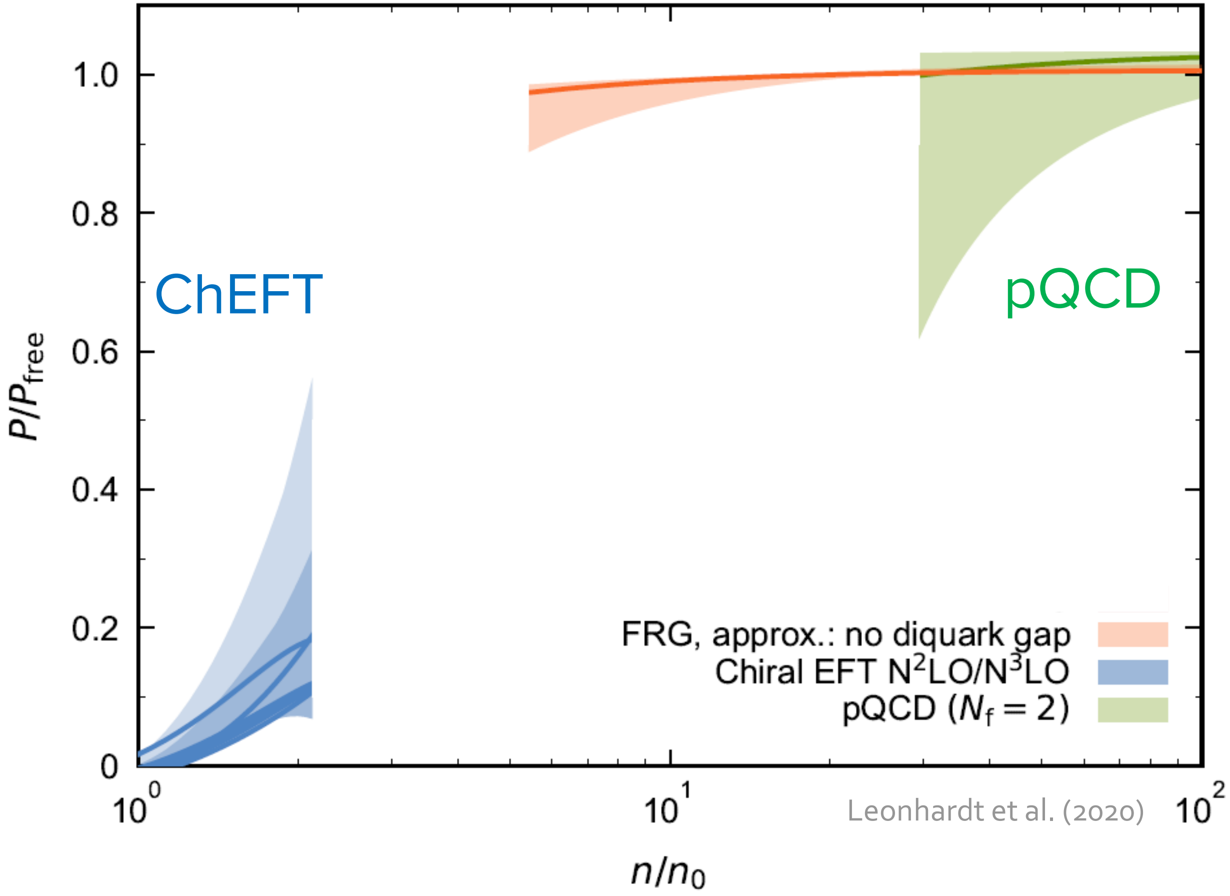
How to develop an overall model from several individual models for the EOS?

[Symmetric Nuclear Matter]

Our goal: improve current estimates & constrain the gap using UQ



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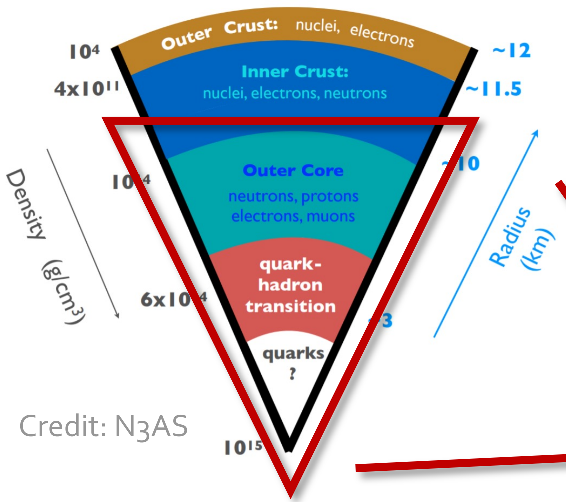

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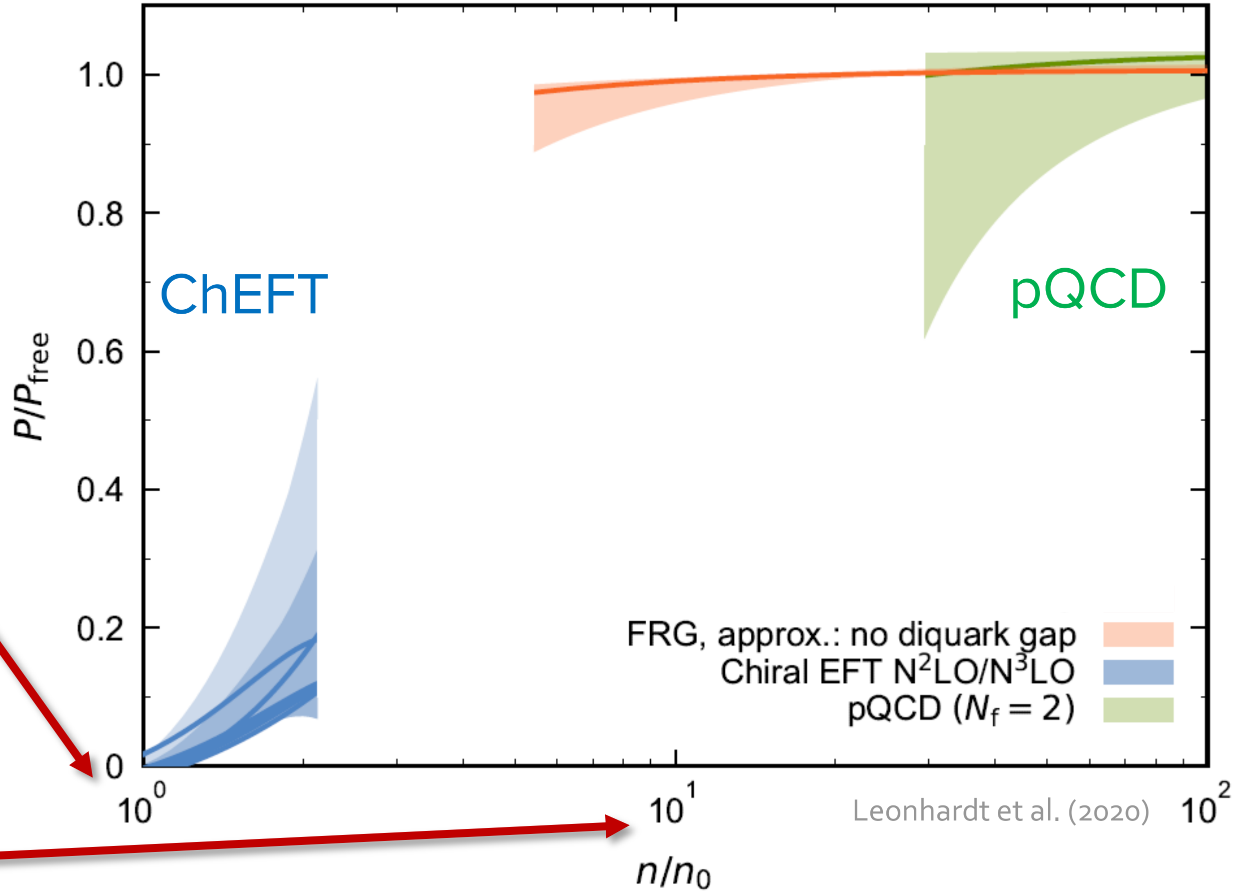

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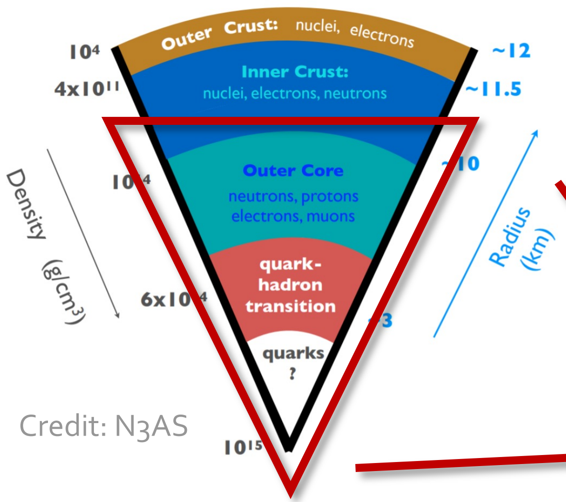

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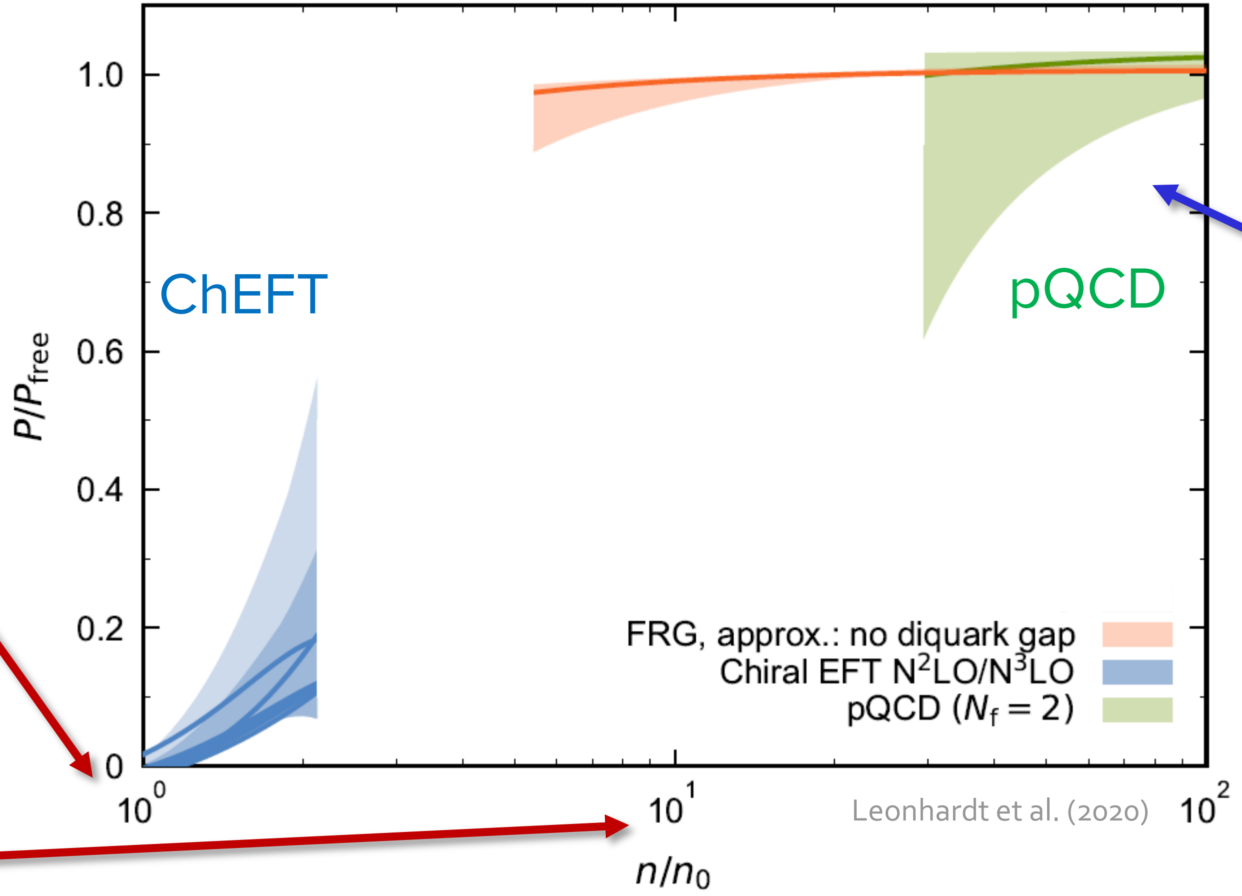

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High densities: perturbative QCD describes quark matter in the densest regions

FRG EOS in the gap, but uncertainties are not well-quantified (yet!) ...

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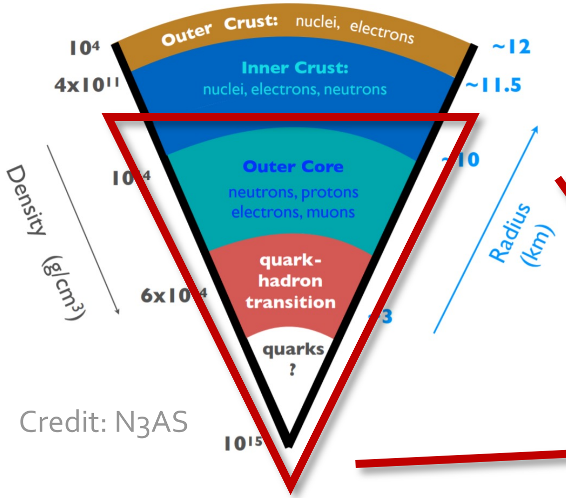

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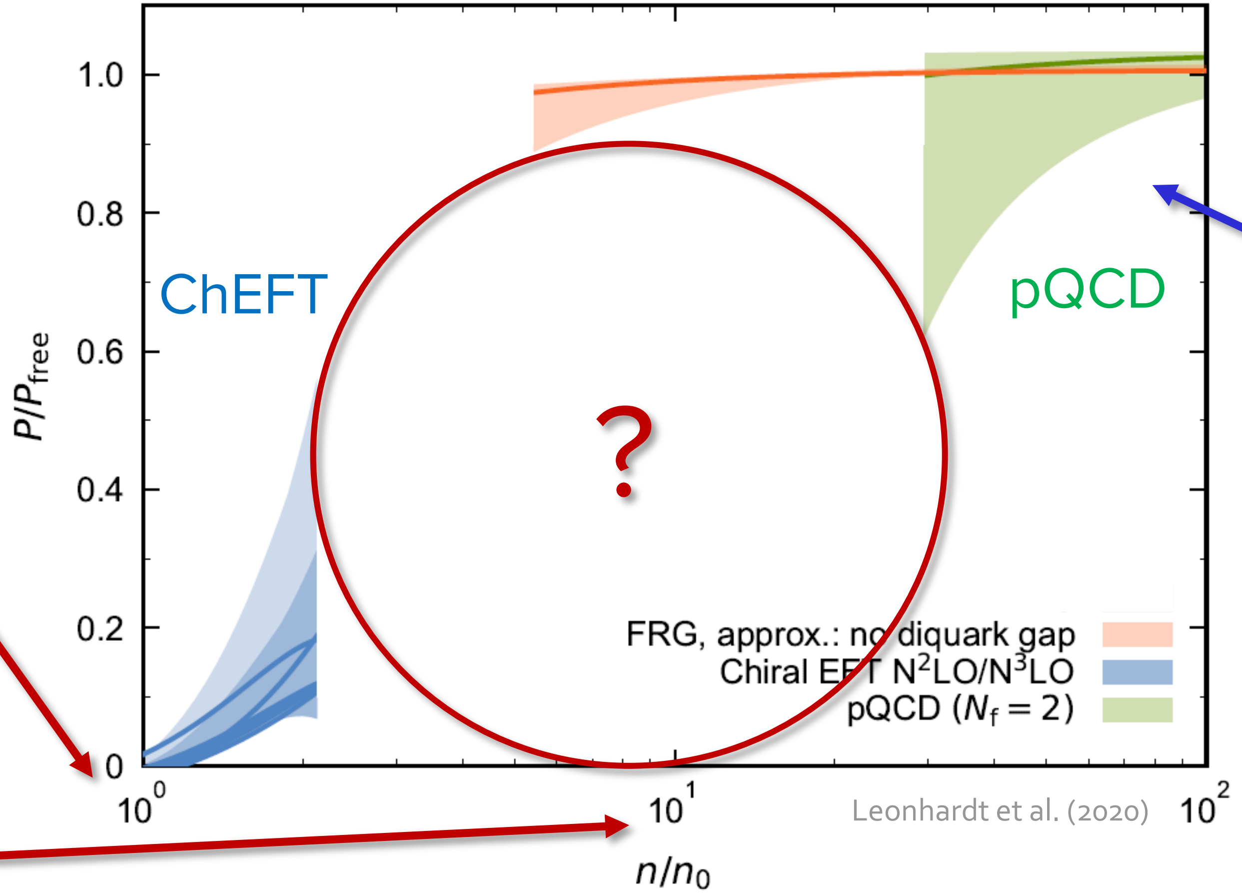

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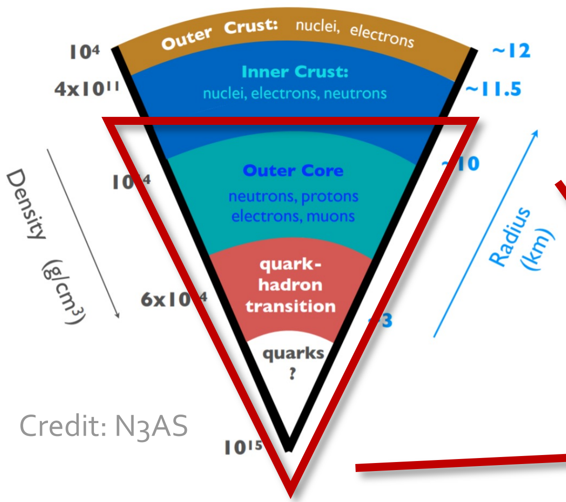

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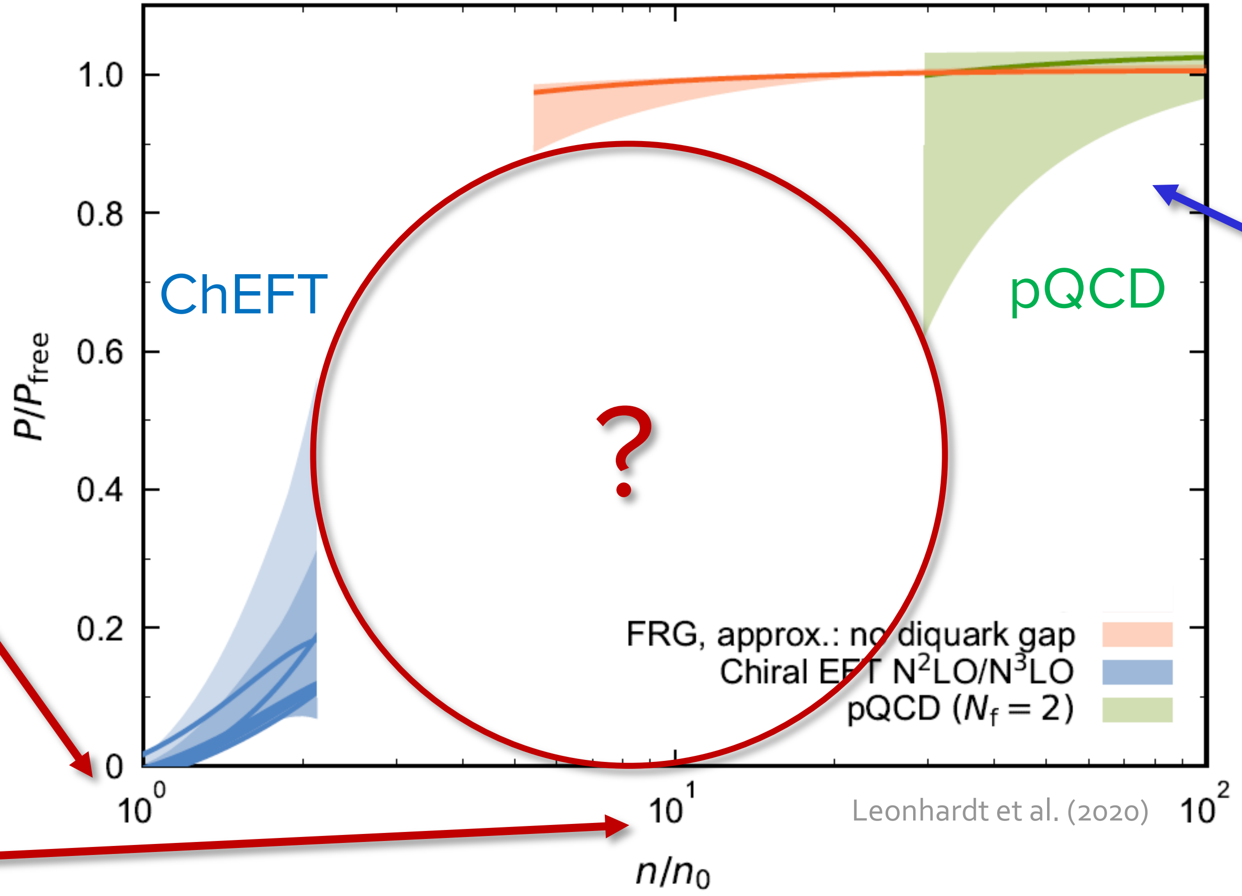

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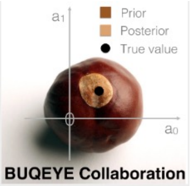
Bayes your way to victory!

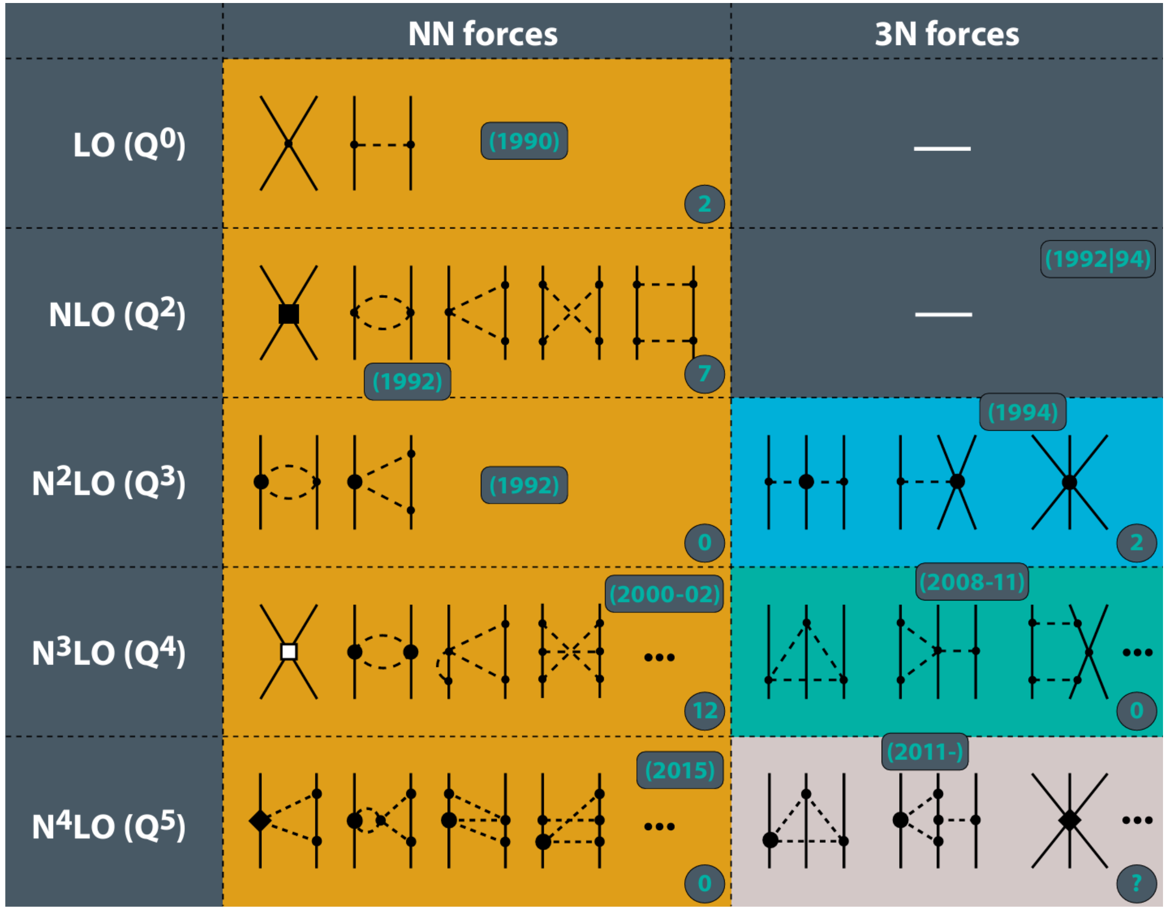
“Low” densities: EOS from chiral EFT



QCD non-perturbative at low energies, build *effective description* using nucleons, pions as degrees of freedom

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

Quantifiable truncation error, obeys all symmetries of QCD



C. Drischler, S. Bogner (2021)

Original calculations and ideas: C. Drischler, K. Hebeler, A. Schwenk, Phys. Rev. Lett. **122**, 042501 (2019)

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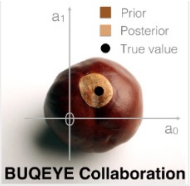

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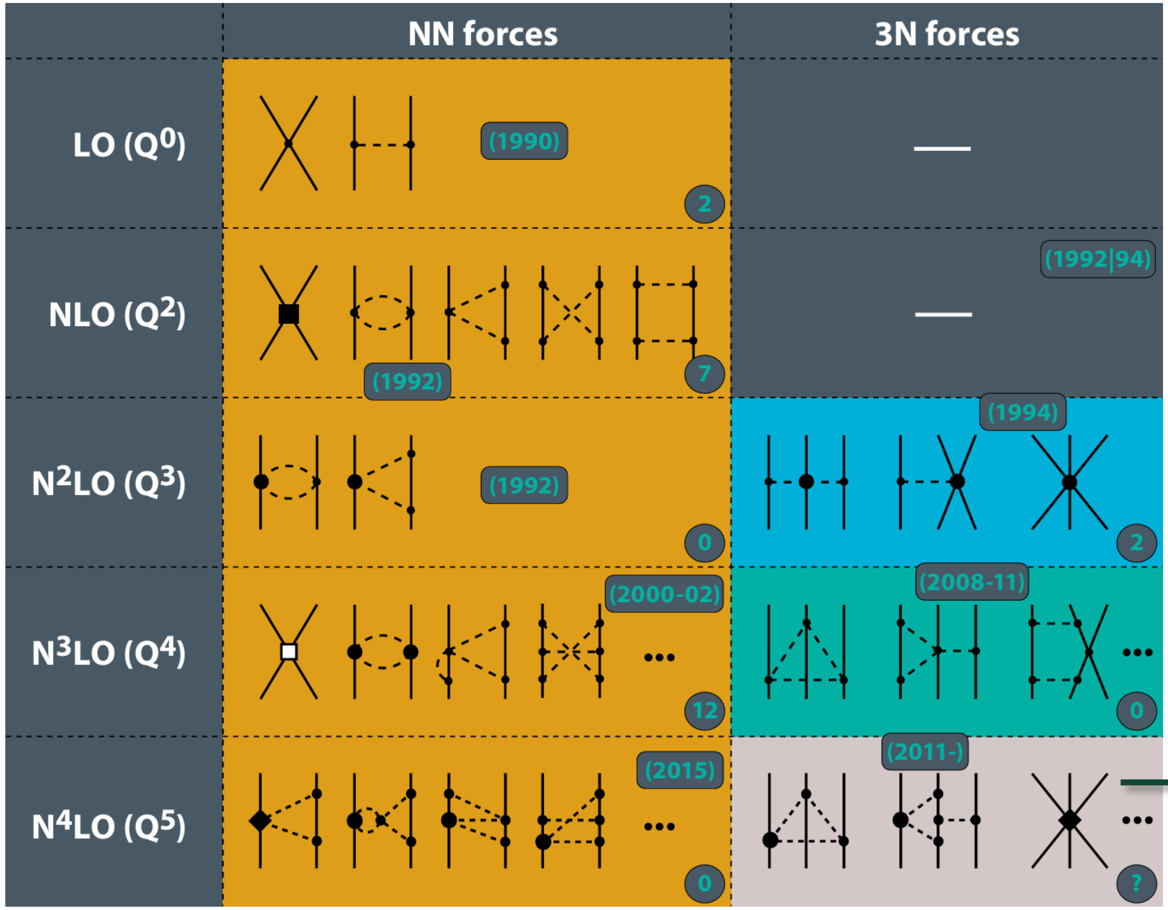

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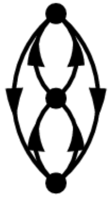
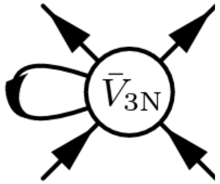
$\mathcal{E}_2(k_\mathrm{F}) =$  $= -\frac{1}{4}\sum_{ijab} V^{ij,ab} V^{ab,ij} f_{ij}\bar{f}_{ab}\frac{1}{D_{ab,ij}}$

$\mathcal{E}_{3,pp}(k_\mathrm{F}) =$ 

Use **MBPT*** for energy per particle (E/A) calculations

*A choice, not a necessity--- BMM framework is model-independent

$\left\langle \mathbf{2}'\mathbf{3}' \middle| V_\mathrm{NN}^\mathrm{med} \middle| \mathbf{23} \right\rangle =$ 

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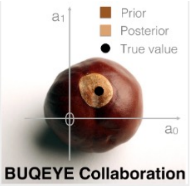

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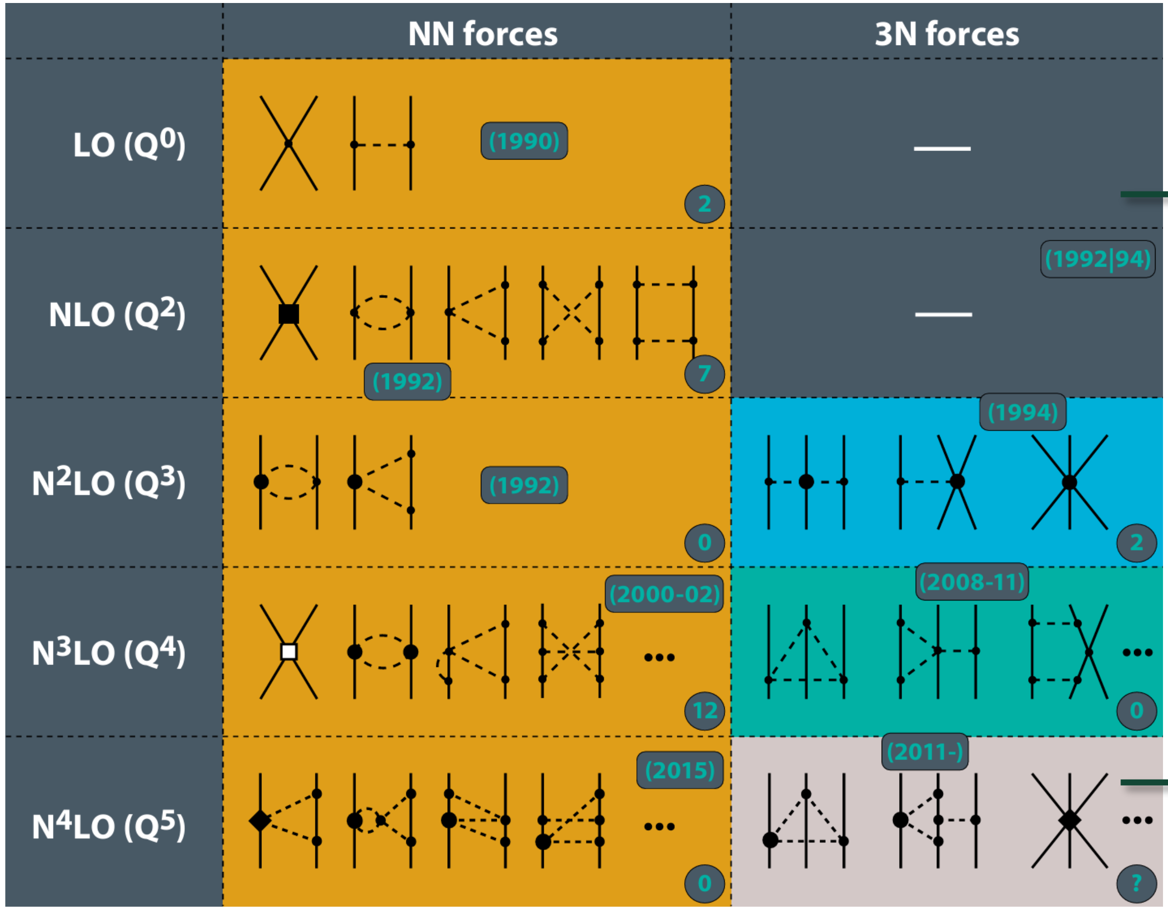

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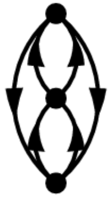
Using NN potential from **Entem, Machleidt, Nosyk** (2017) + **3N forces**
Fit **low-energy constants** (LECs) to experimental data, empirical saturation point of SNM
Employ momentum **cutoff** of 500 MeV

$$\mathcal{E}_2(k_\mathrm{F}) =$$  $$= -\frac{1}{4}\sum_{ijab} V^{ij,ab} V^{ab,ij} f_{ij}\bar{f}_{ab}\frac{1}{D_{ab,ij}}$$

$$\mathcal{E}_{3,pp}(k_\mathrm{F}) =$$ 

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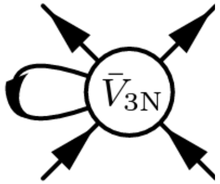
$$\left\langle 2'3' \middle| V_{\mathrm{NN}}^{\mathrm{med}} \middle| 23 \right\rangle =$$ 

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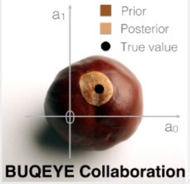
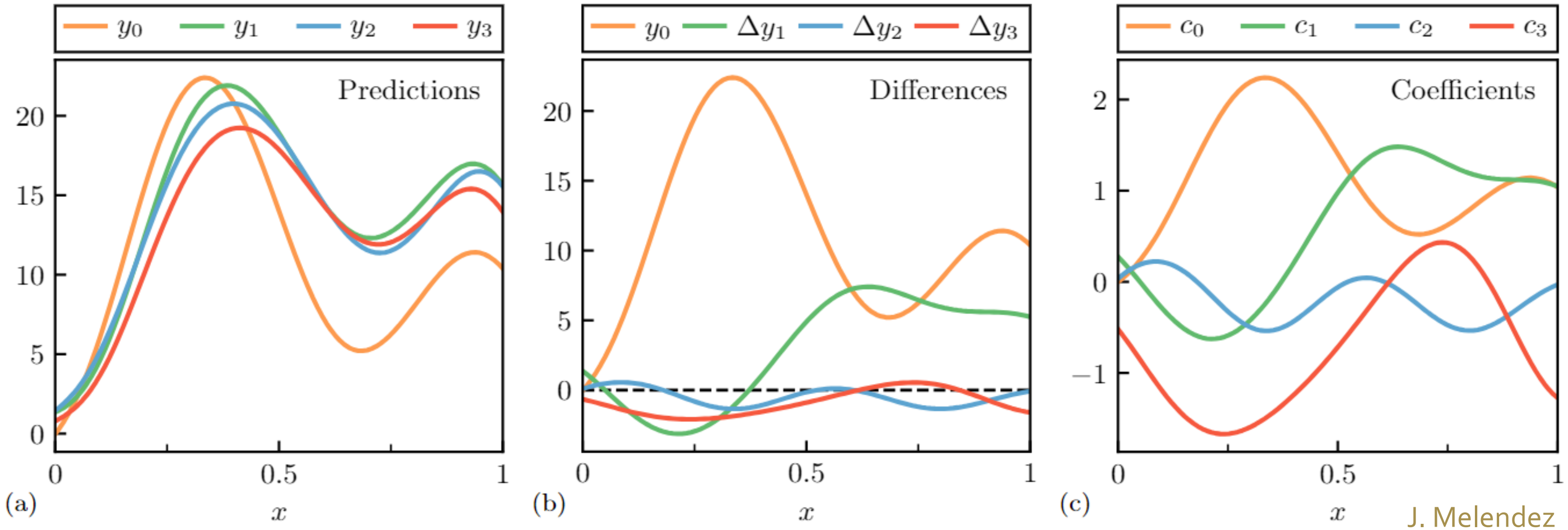
Uncertainty quantification for the EOS



Employ the BUQEYE truncation error model (**gsum**)

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

Known orders of expansion



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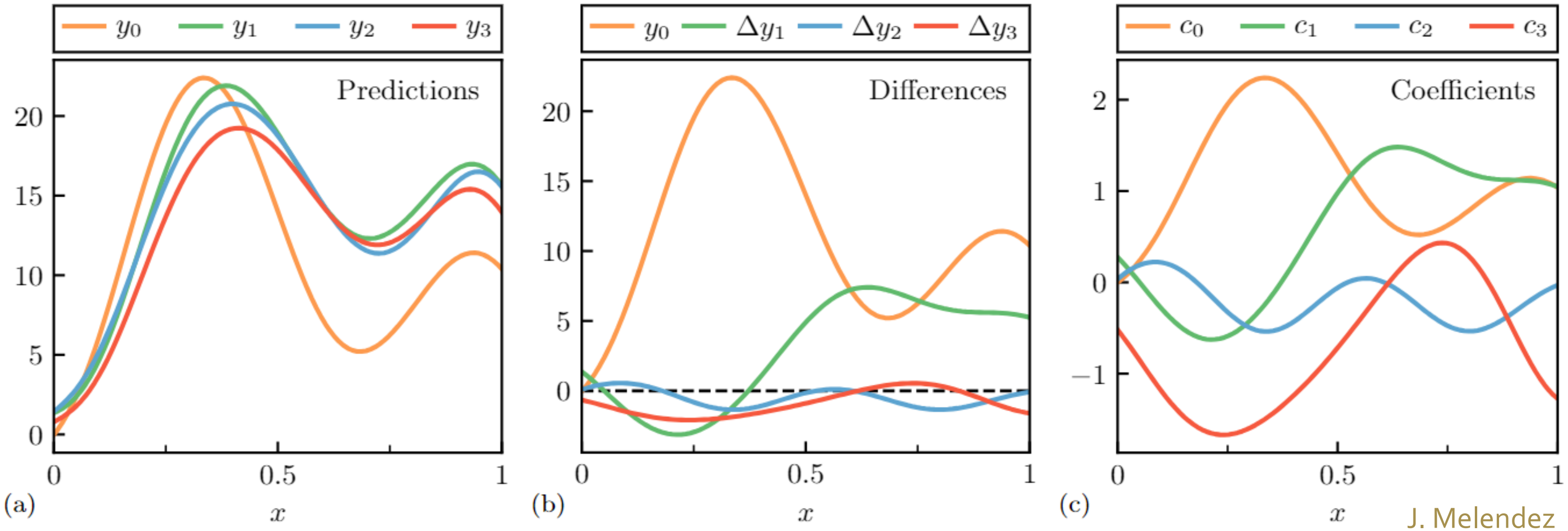

J. Melendez et al. (2019)

Estimations for unknown orders

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

Dimensional analysis

Natural i.i.d. curves

Expansion parameter (suppresses higher orders)

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BUQEYE Collaboration

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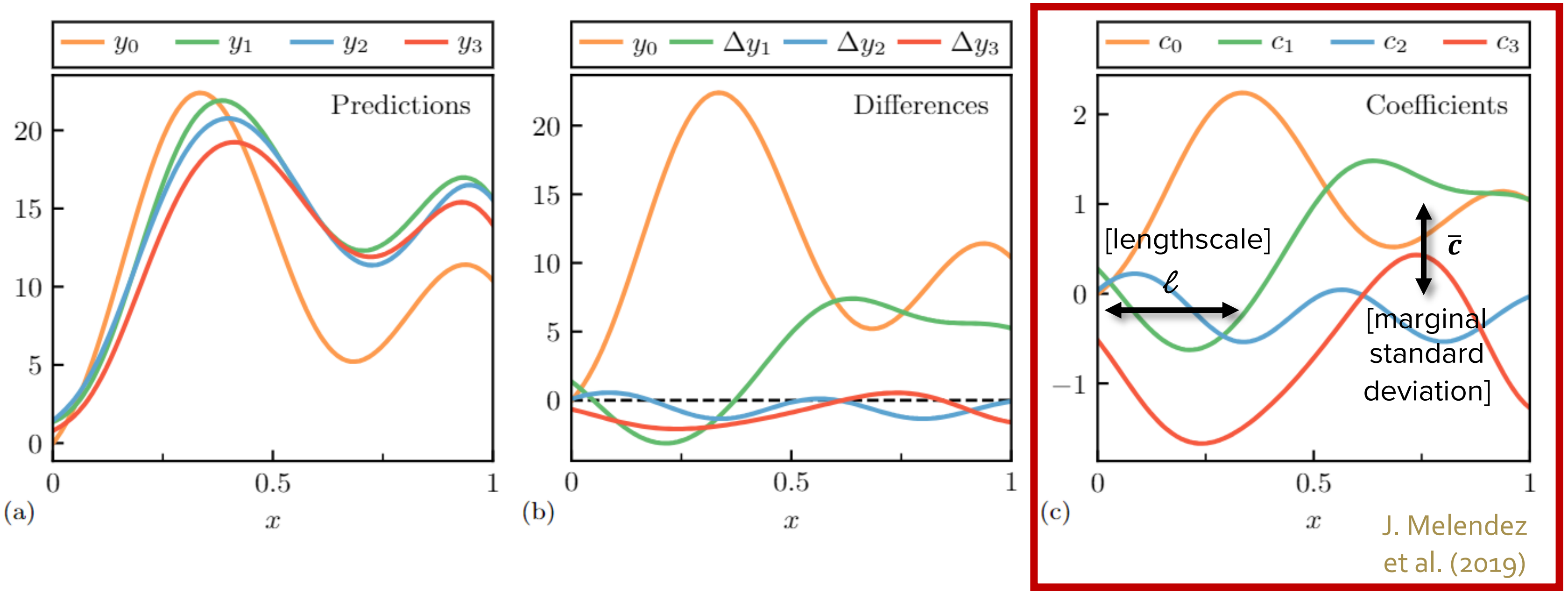


Gaussian Processes: learn coefficient distributions

Incorporates correlations in y(x), continuous model, priors constrain parameters of GP

Easily test with *diagnostics* (Mahalanobis distance, pivoted Cholesky decomposition,…)

Original work: Melendez, Wesolowski, Furnstahl, Phillips, Pratola, PRC (2019)

“Low” densities: EOS from chiral EFT

Obtain pressure as a function of number density, P(n), for model mixing calculations

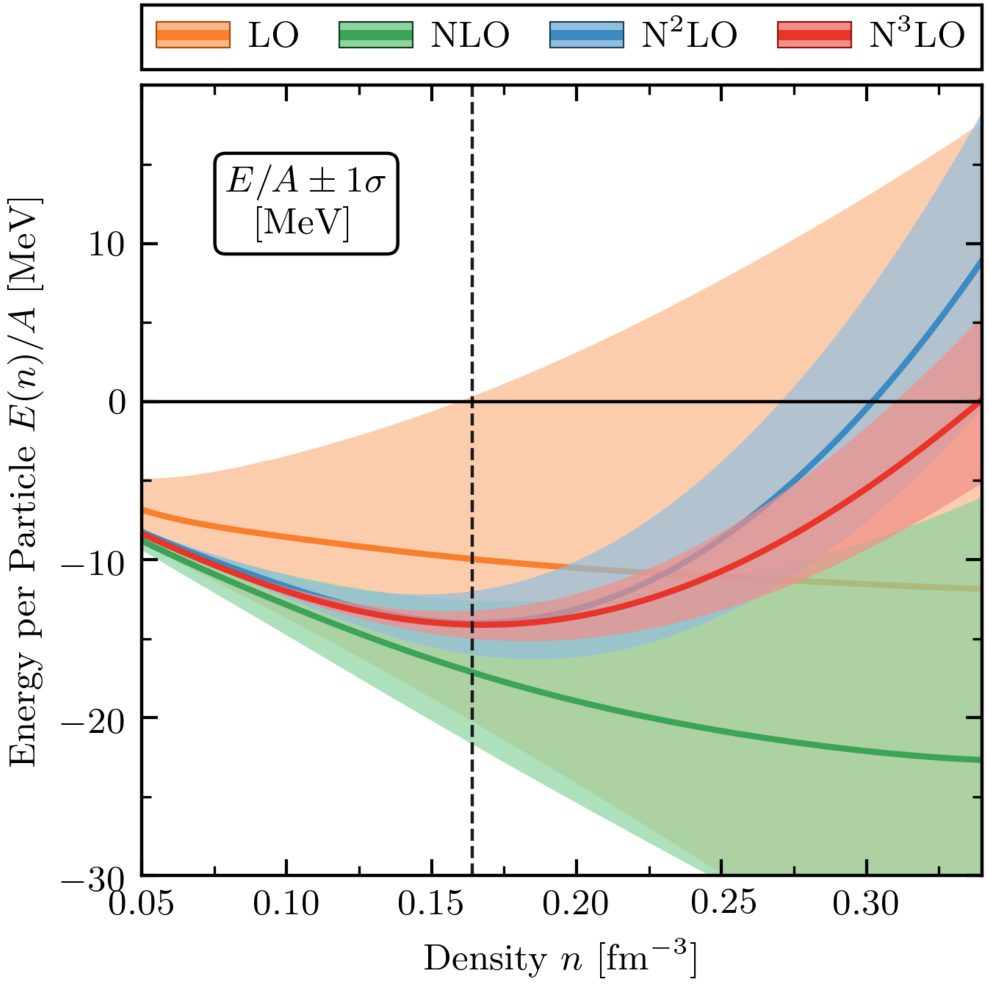
$$P(n) = n^2 \frac{\mathrm{d}}{\mathrm{d}n}\frac{E}{A}(n)$$

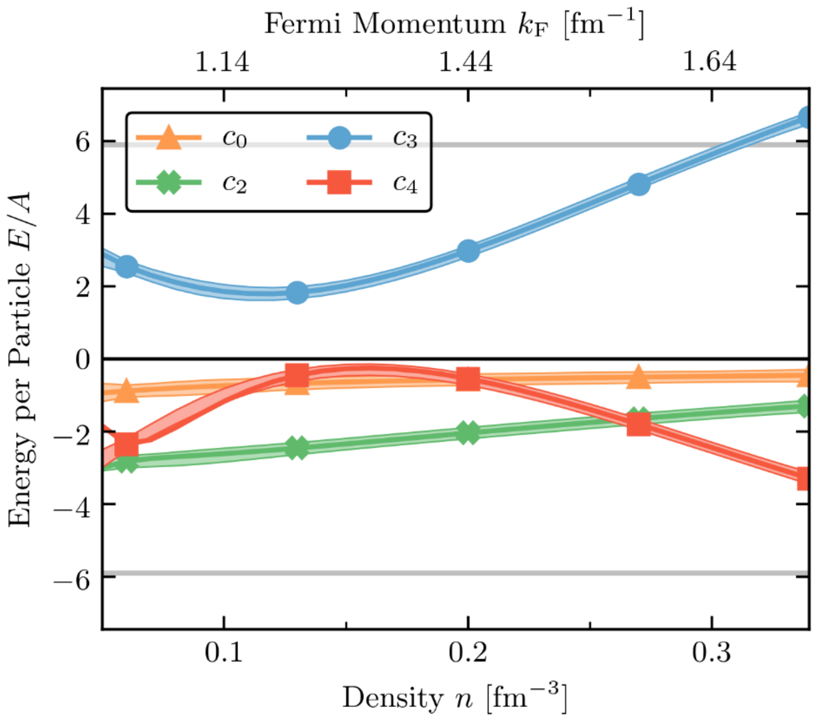
Coefficient extraction for truncation error estimation done via **gsum**

$$Q(k_F) = \frac{k_F}{\Lambda_b}$$ ≈ 600 MeV

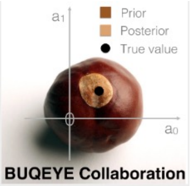
$$y_{\mathrm{ref}}(k_F) = 16\,\mathrm{MeV} \times \left(\frac{k_F}{k_{F,0}}\right)^2$$

Symmetric nuclear matter





Truncation error scheme yields natural-sized curves as expected



Truncation error analysis: C. Drischler, J. A. Melendez, R. J. Furnstahl, D. R. Phillips, Phys. Rev. C **102**, 054315 (2020)

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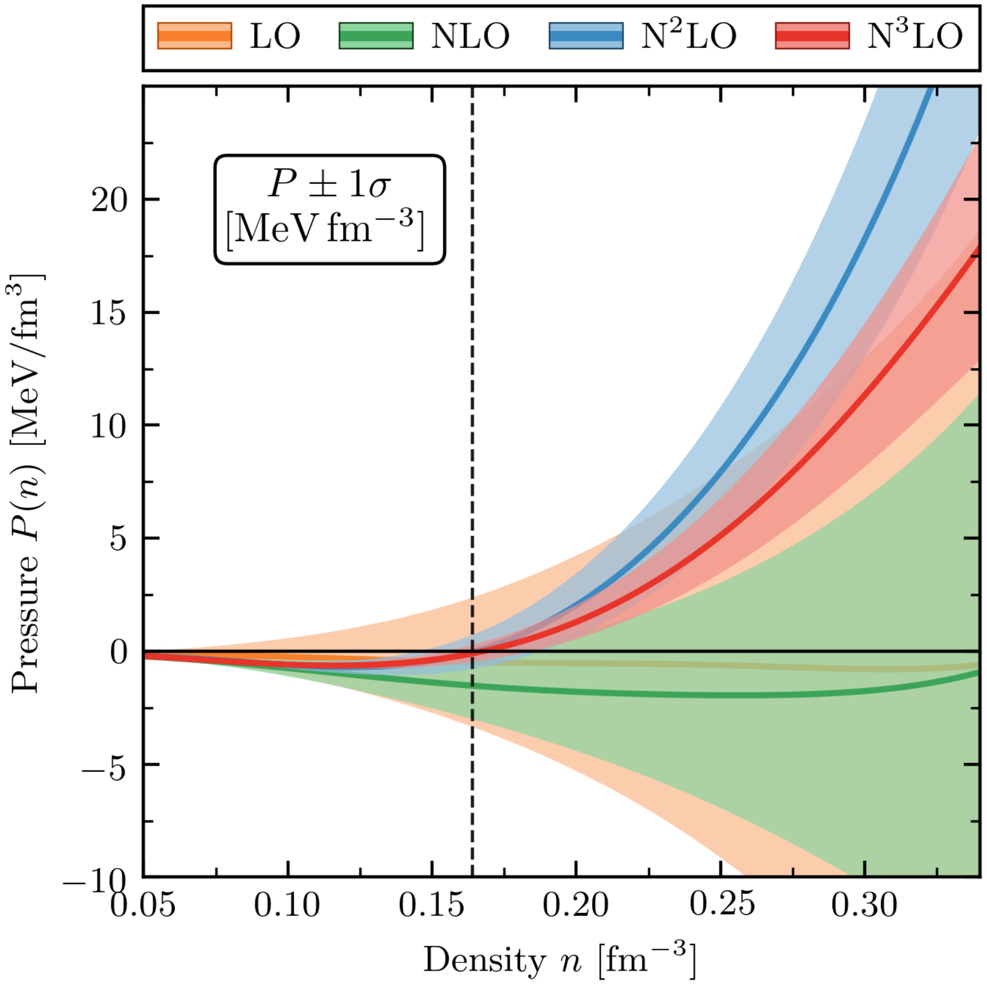

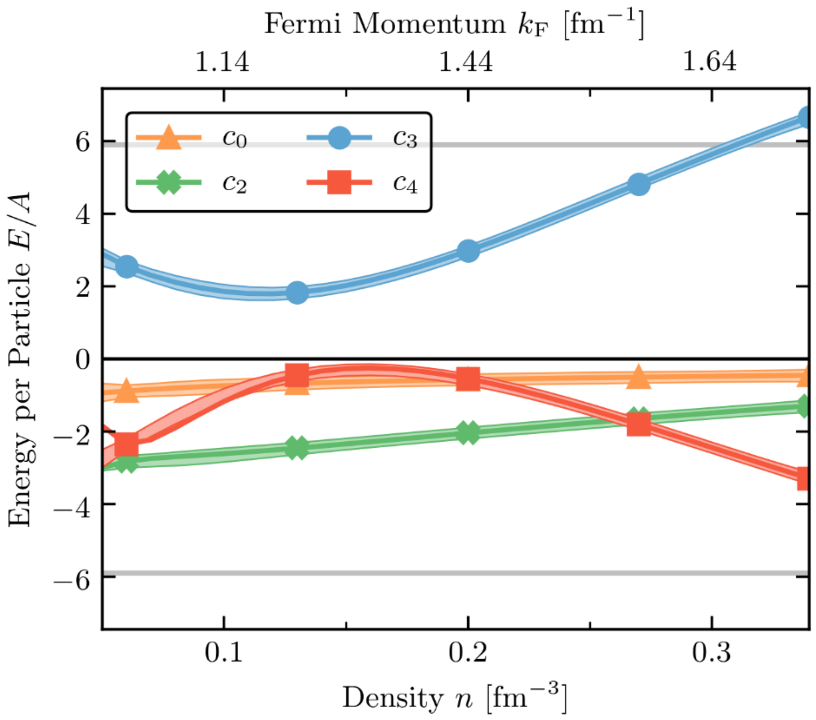

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High densities: pQCD EOS

QCD perturbative at high energies

Expansion in the strong coupling constant α_s

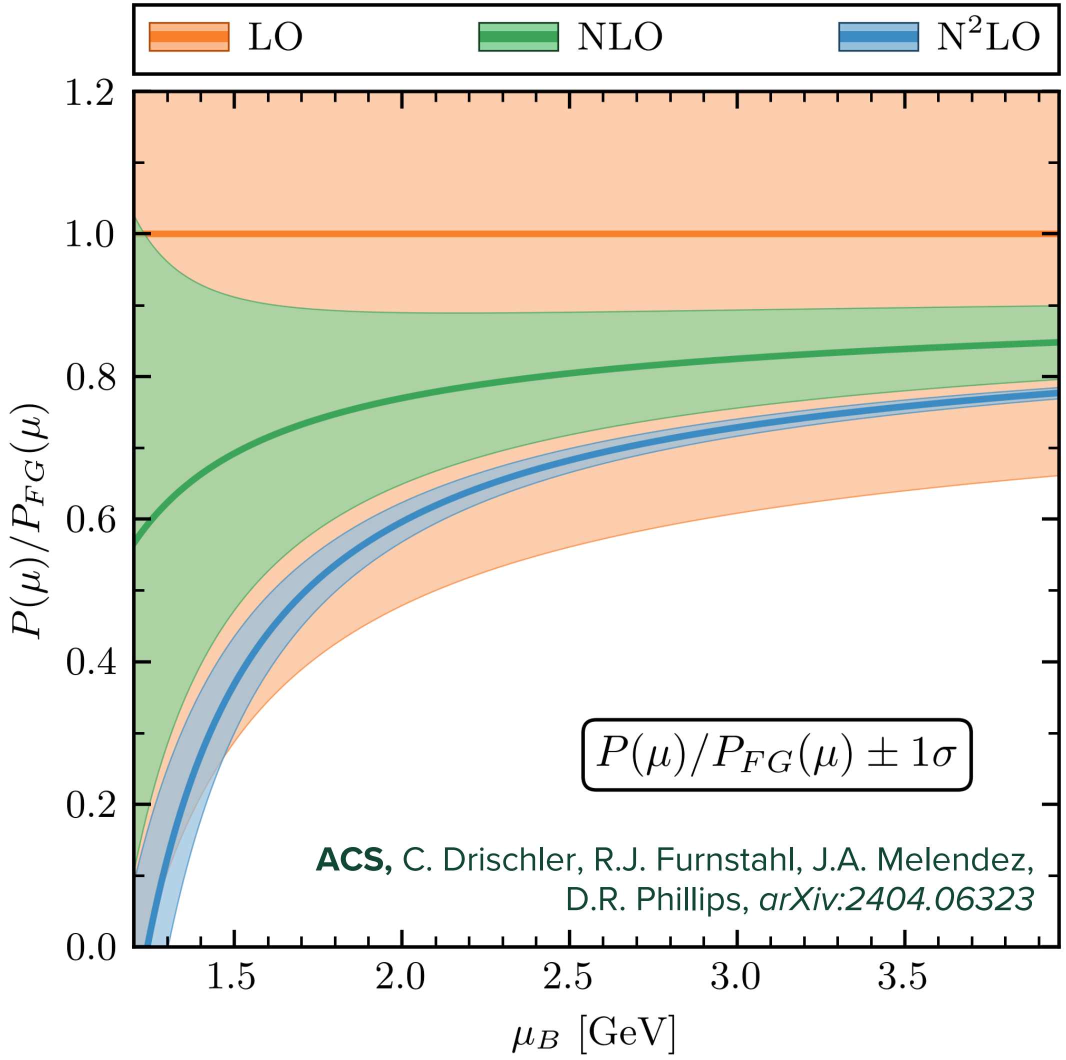
$$\frac{P(\mu)}{P_{FG}(\mu)} \simeq 1 + a_{1,1}\left(\frac{\alpha_s(\mu)}{\pi}\right) + N_f\left(\frac{\alpha_s(\mu)}{\pi}\right)^2\left[a_{2,1}\ln\left(\frac{N_f\alpha_s(\mu)}{\pi}\right) + a_{2,2}\ln\frac{\bar{\Lambda}}{2\mu} + a_{2,3}\right] + \mathcal{O}(\alpha_s^3),$$

Two-loop running:

$$\alpha_s(\bar{\Lambda}) = \frac{4\pi}{\beta_0 L}\left[1 - \frac{2\beta_1}{\beta_0^2}\frac{\ln L}{L}\right] \quad \begin{cases} L = \ln(\bar{\Lambda}^2/\Lambda_{\overline{MS}}^2), \\ \bar{\Lambda} = 2X\mu \end{cases}$$

Degrees of freedom: quarks and gluons

Massless u, d quarks with equal μ



ACS, C. Drischler, R.J. Furnstahl, J.A. Melendez, D.R. Phillips, *arXiv:2404.06323*

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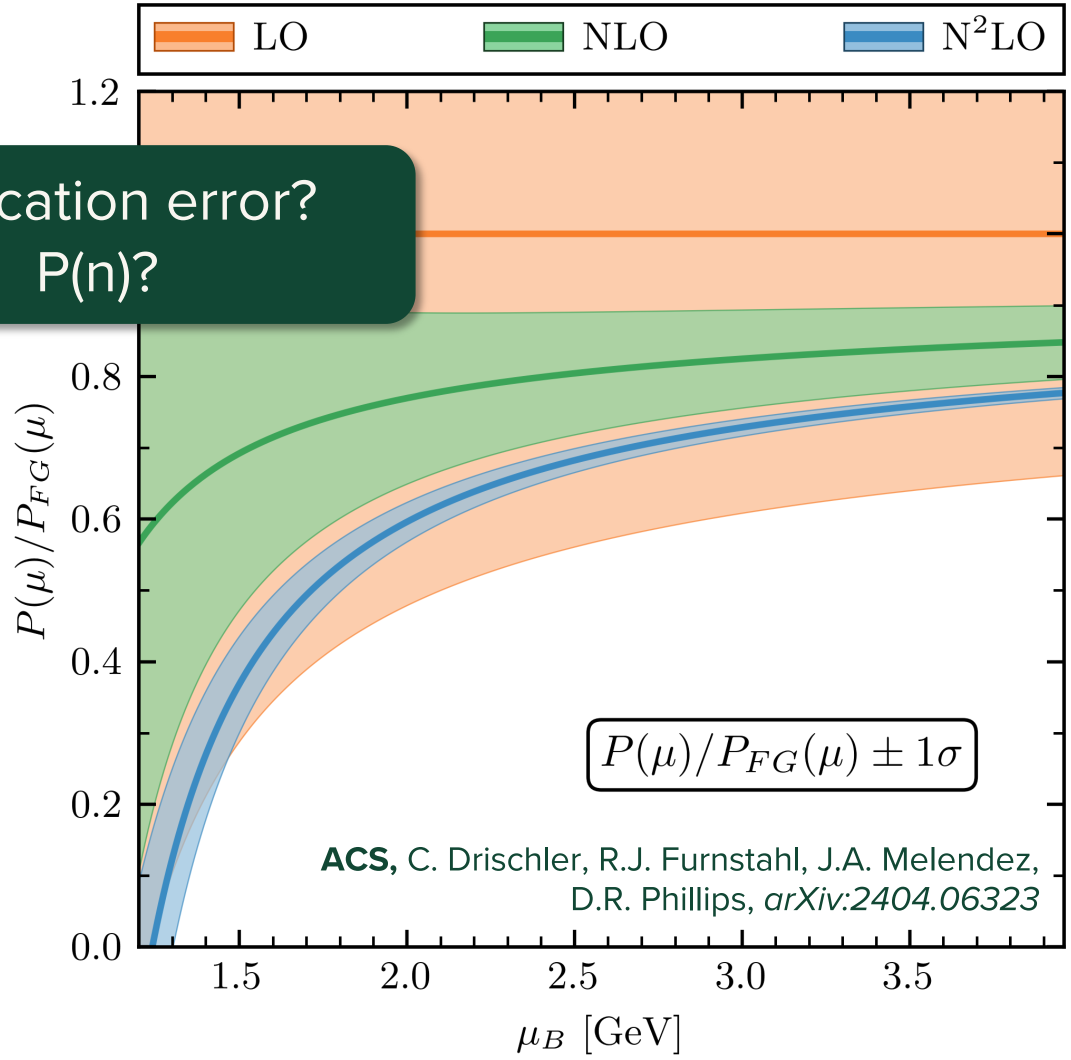

Truncation error?
P(n)?

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Apply **gsum** to **P(n)**

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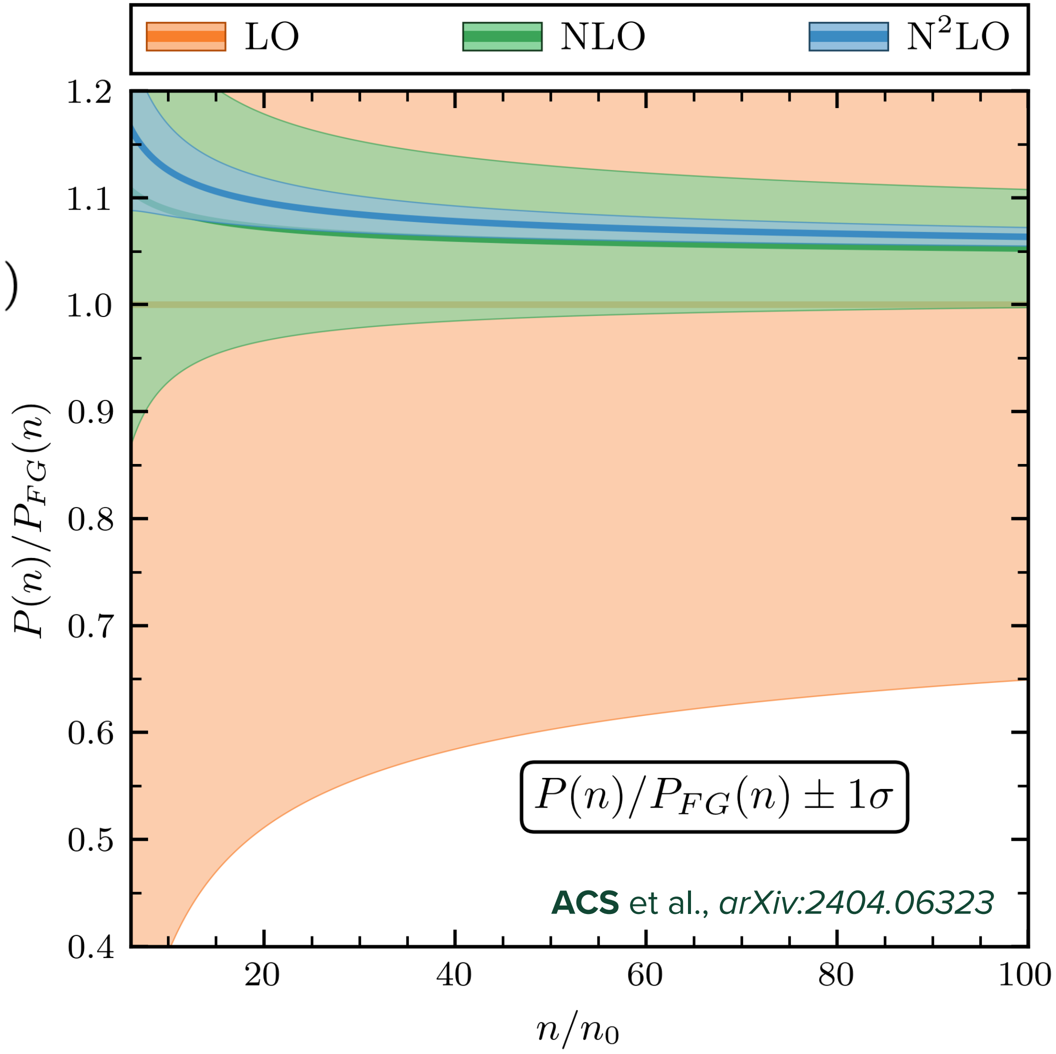

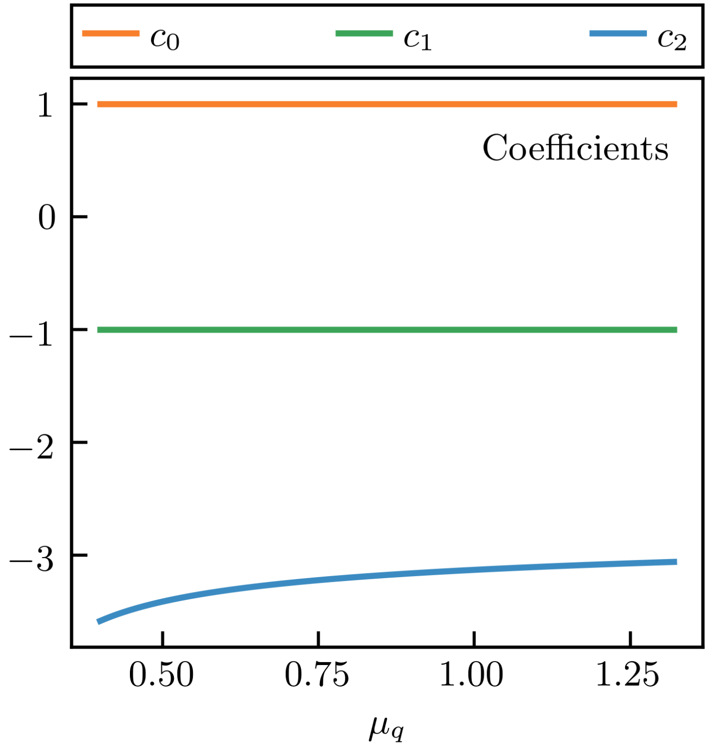

Truncation error often assessed by varying renormalization scale to obtain band---not statistically rigorous

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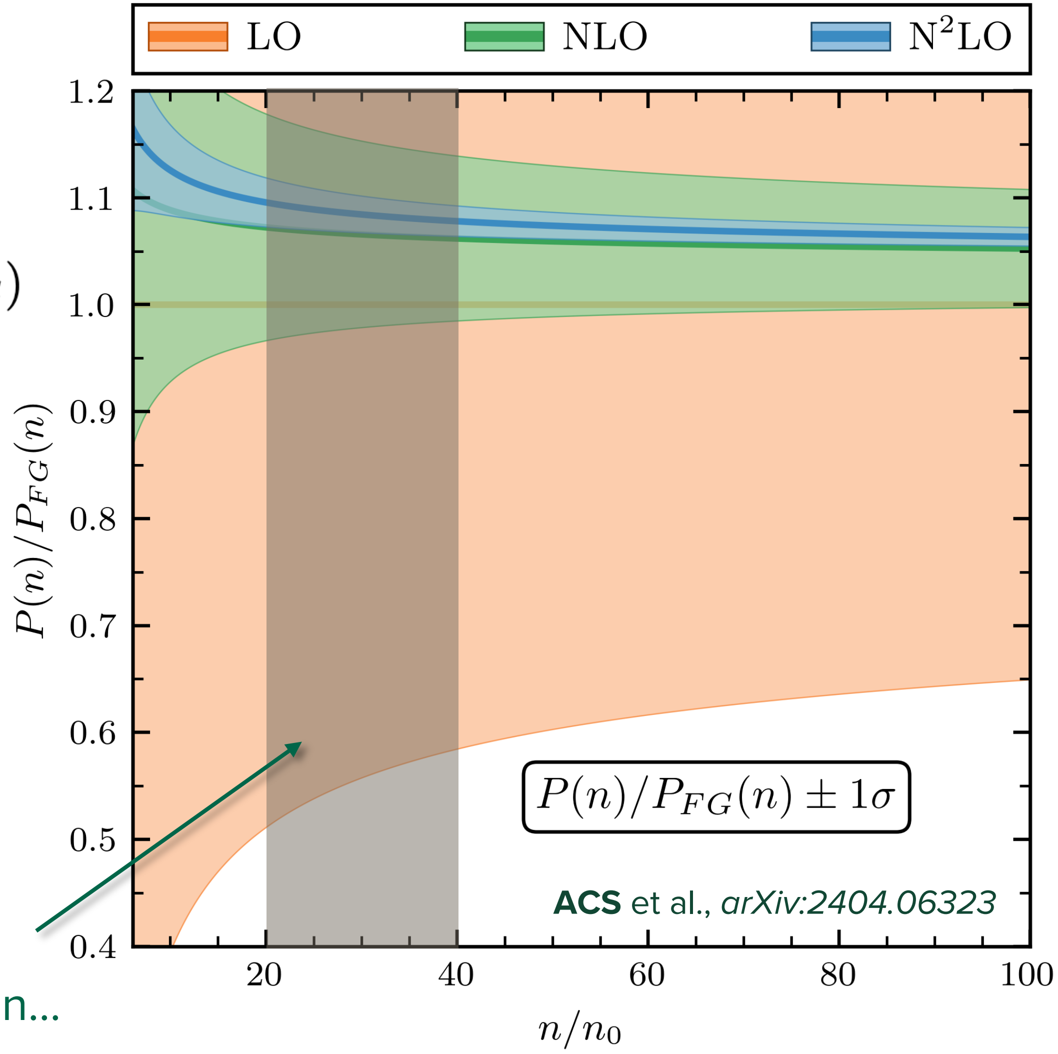
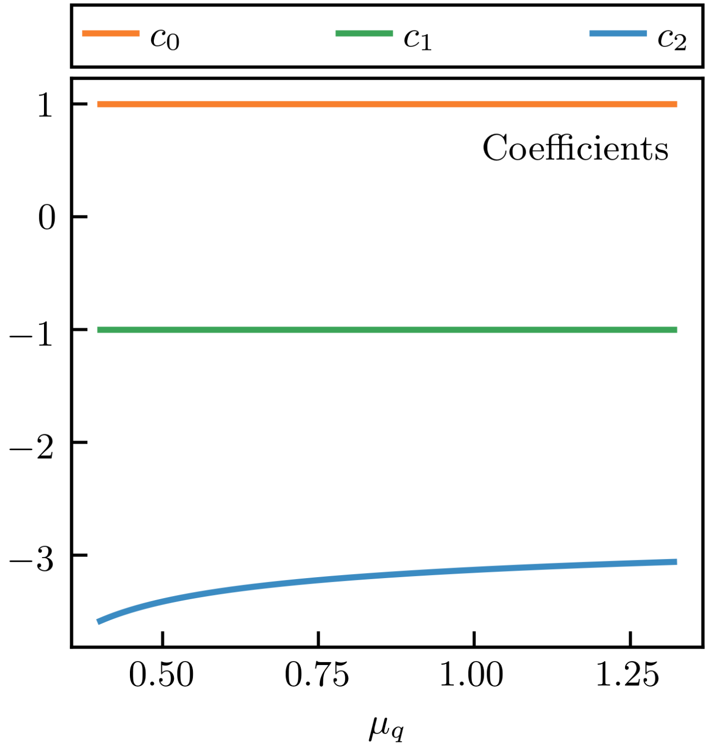


Nonperturbative effects under (20-40) n_0: pairing, hadronization...



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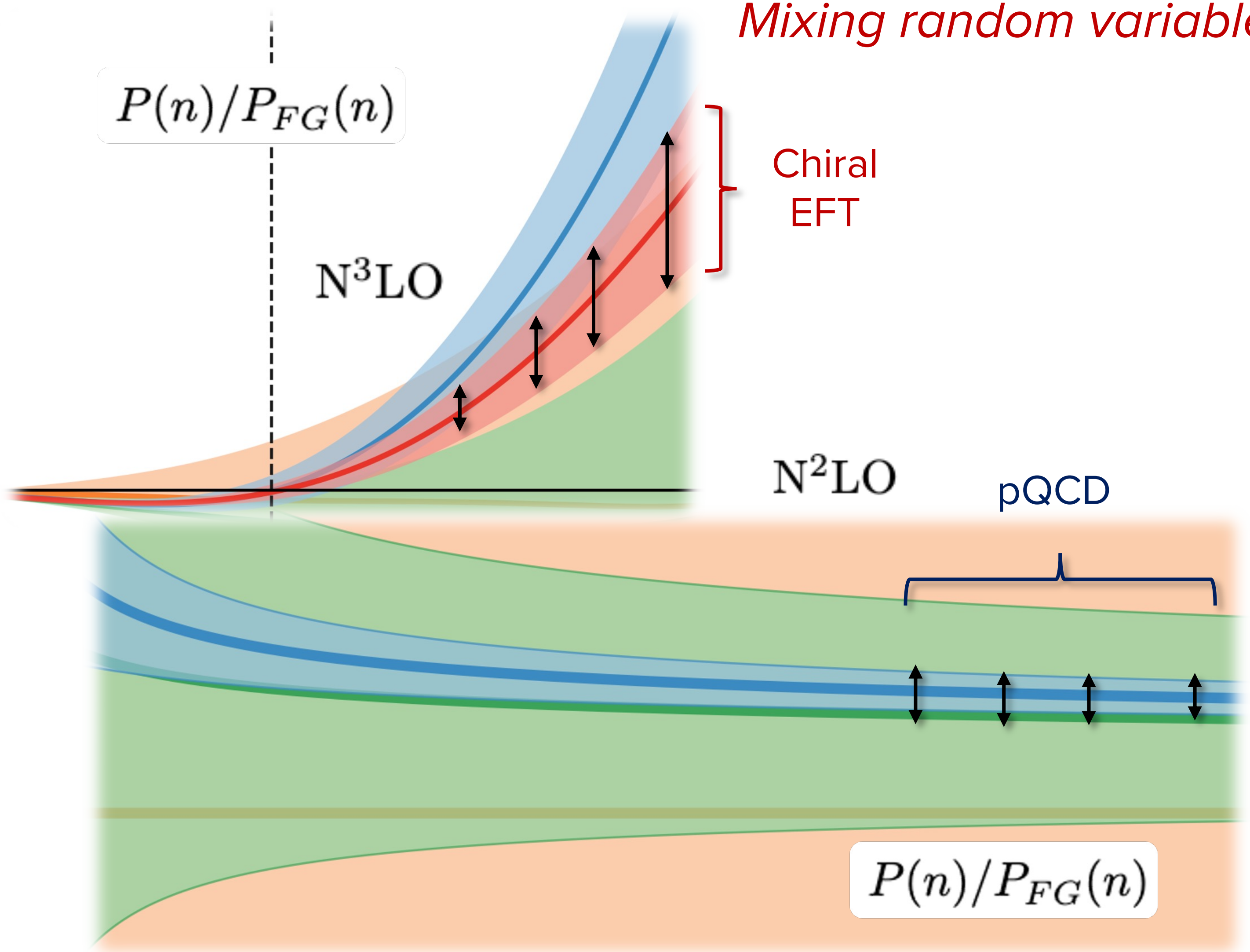
GPs: a correlated approach to BMM

Mixing random variables "curvewise"



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$$Y_i = F + \delta Y_i, \qquad i \in [0, M]$$

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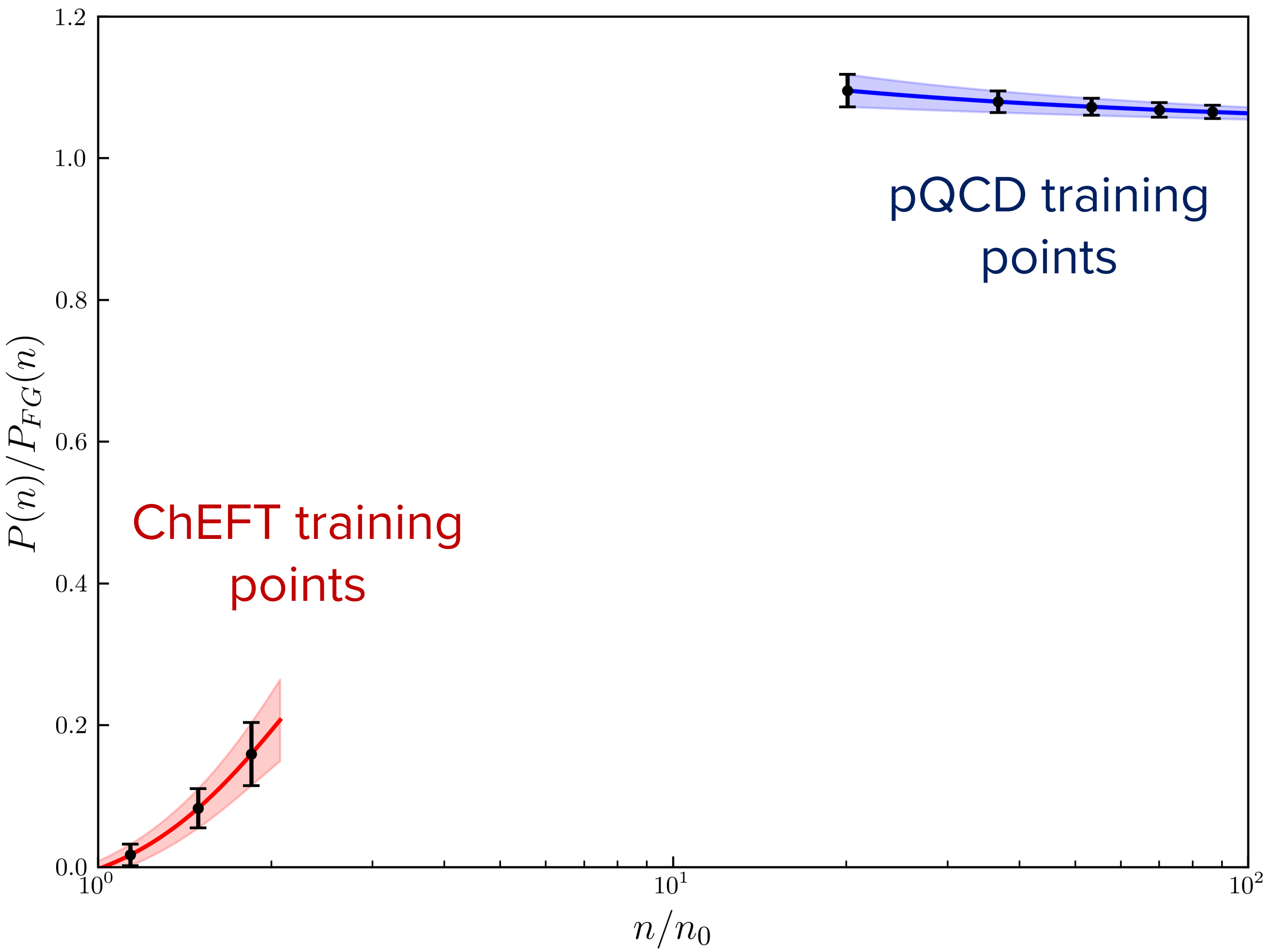

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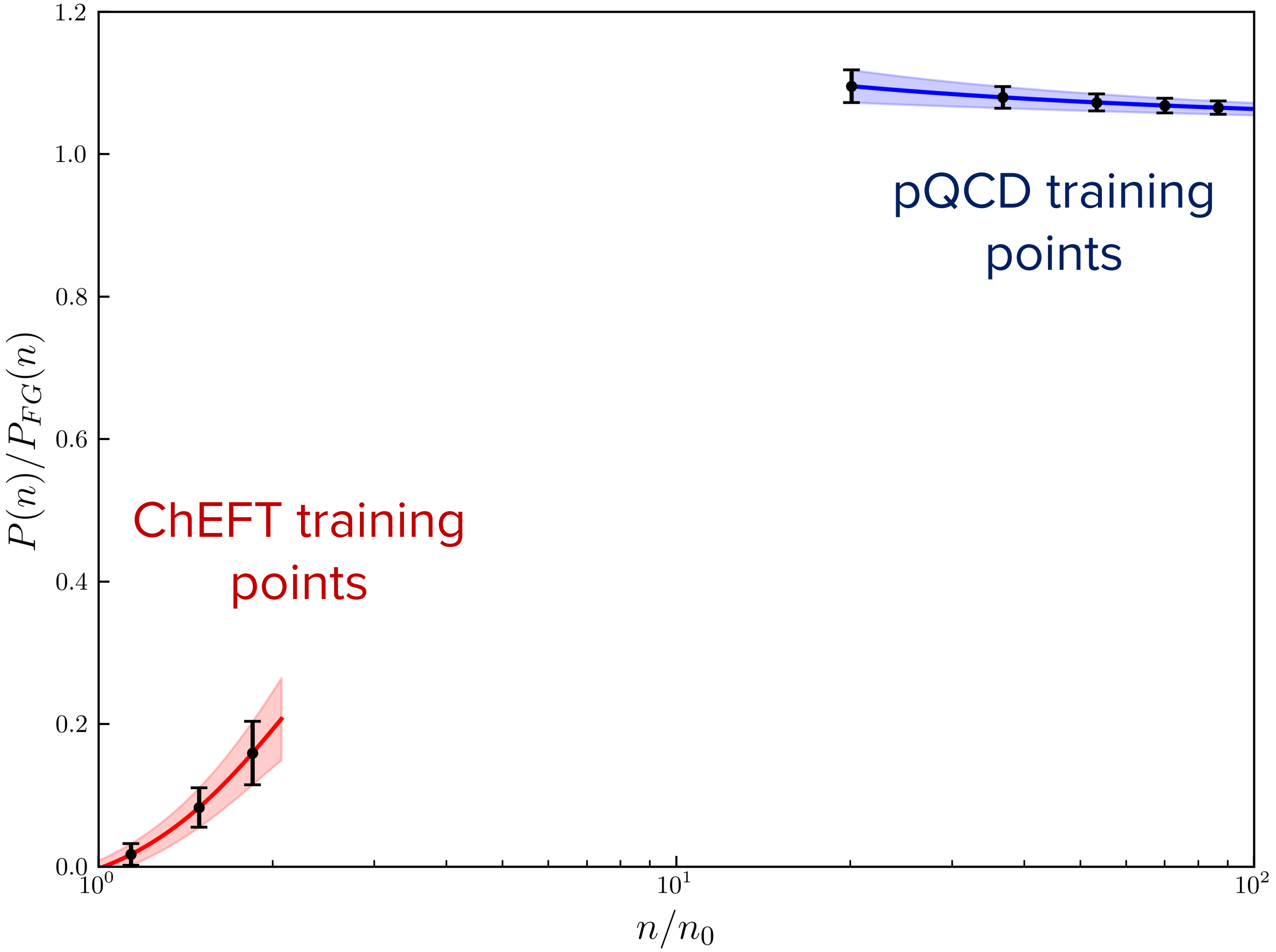

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[Full covariance matrix]

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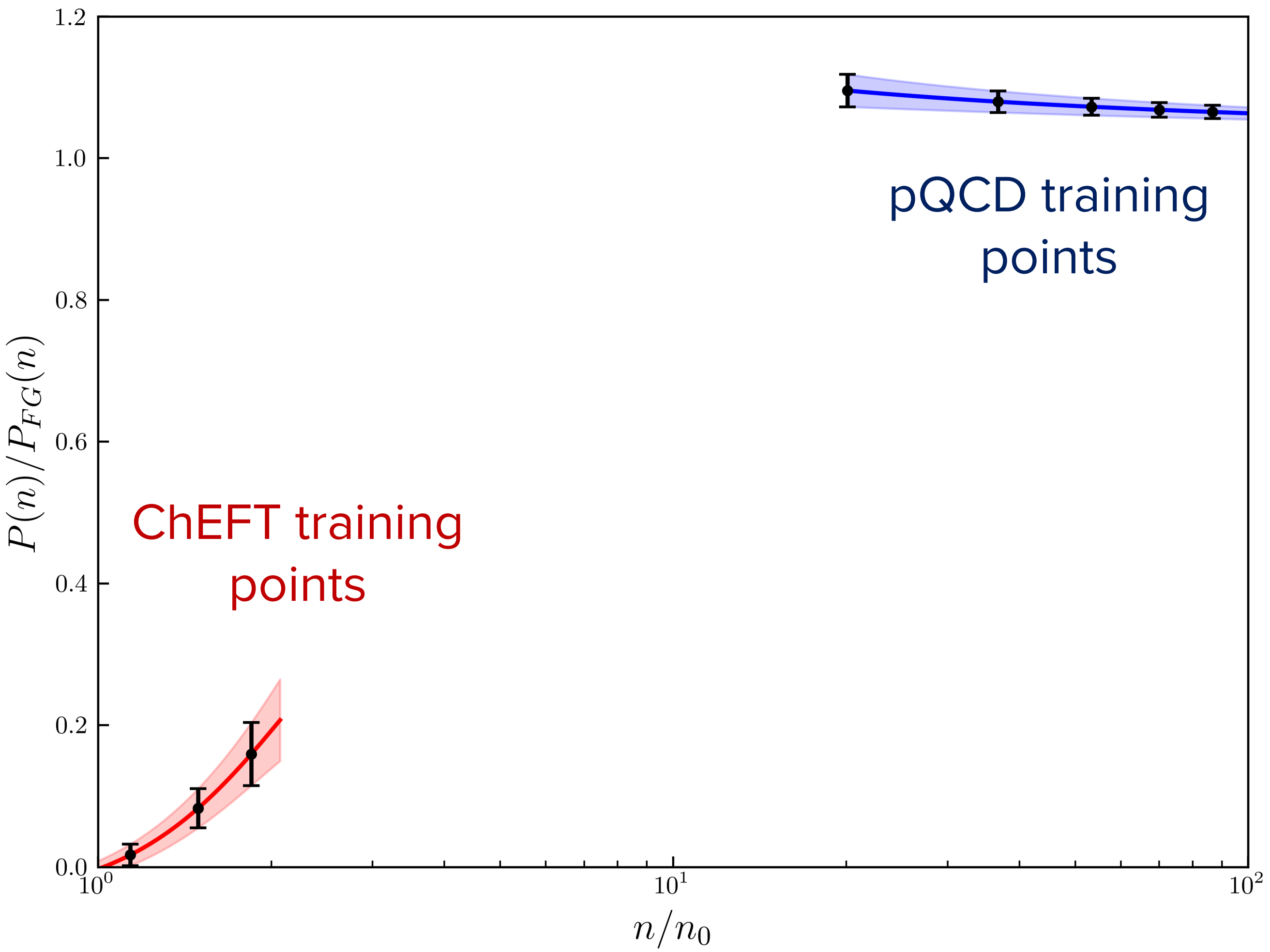

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$\sim \mathrm{GP}[0, \kappa_f(x, x')]$ [Kernel choice]

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

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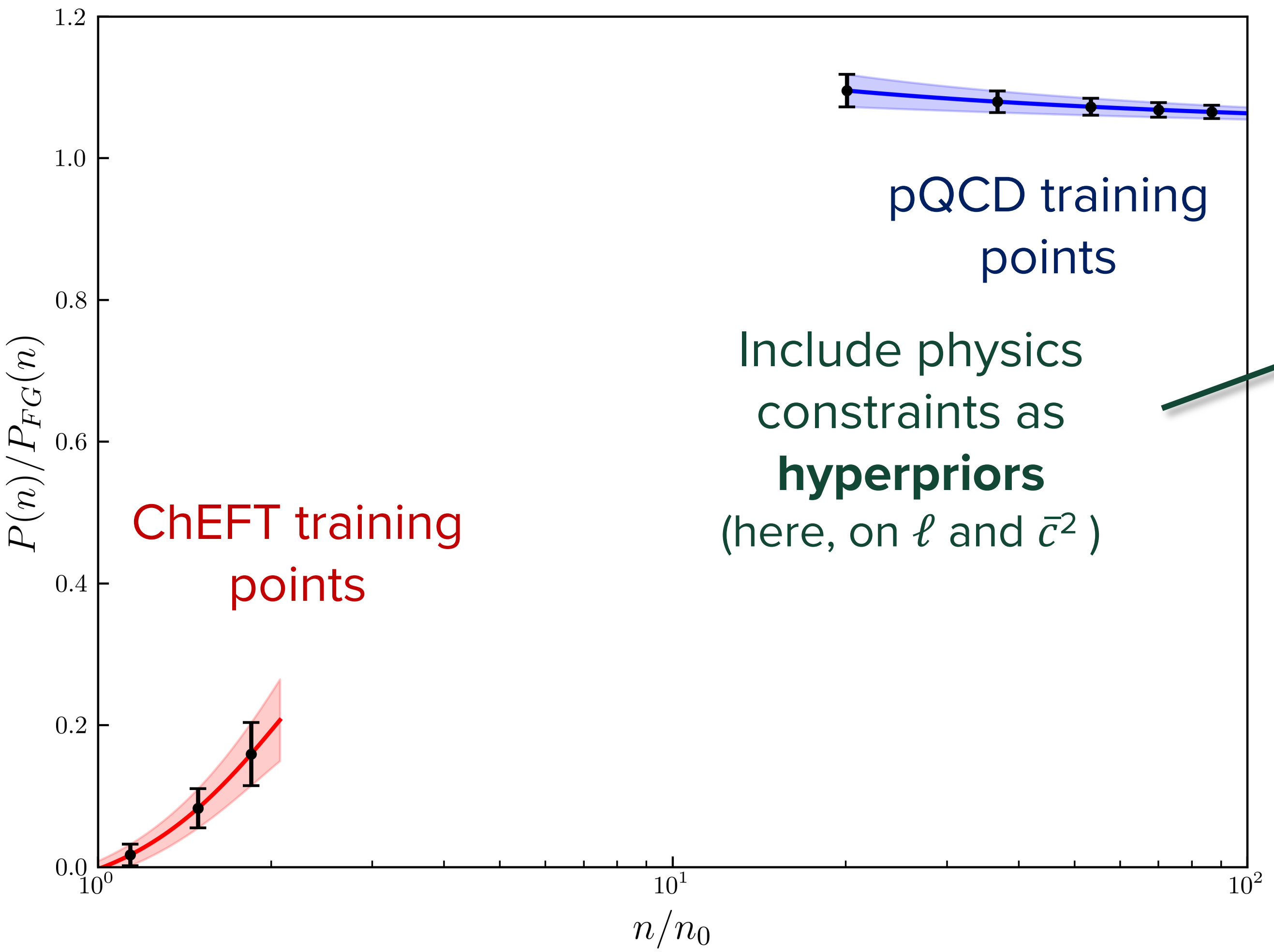

Include physics constraints as **hyperpriors** (here, on ℓ and $\bar{c}^2$)

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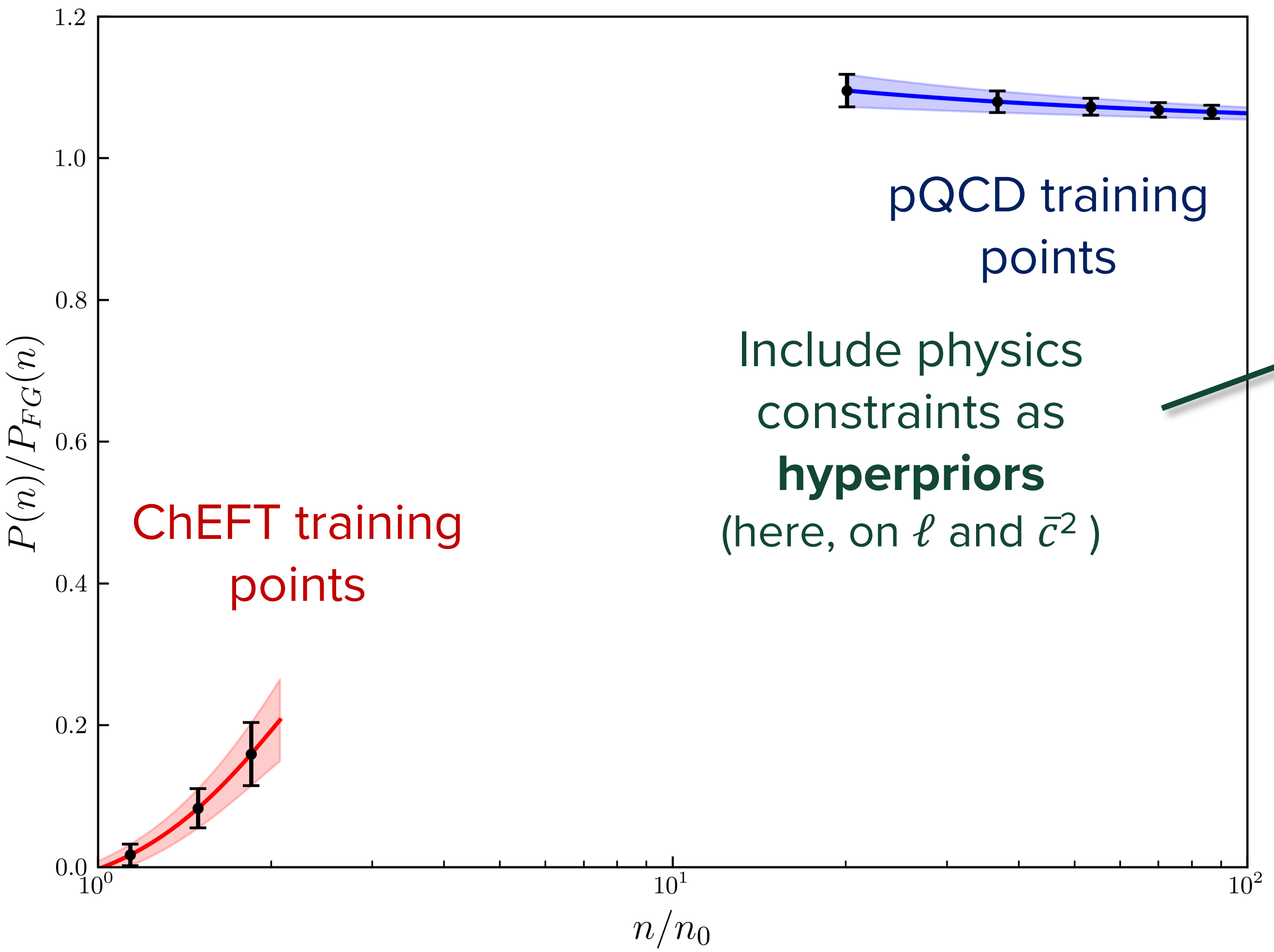
GPs: a correlated approach to BMM

Mixing random variables "curvewise"



Include physics constraints as **hyperpriors** (here, on ℓ and $\bar{c}^2$)

Underlying theory (QCD)

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Therefore, assuming a **Gaussian form** and using Bayes' theorem, again determine a **common mean**

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

$$\vec{\mu} \equiv \Sigma B_t^T K_y^{-1} \vec{y}$$

$$\Sigma \equiv (K_f^{-1} + B_t^T K_y^{-1} B_t)^{-1}$$

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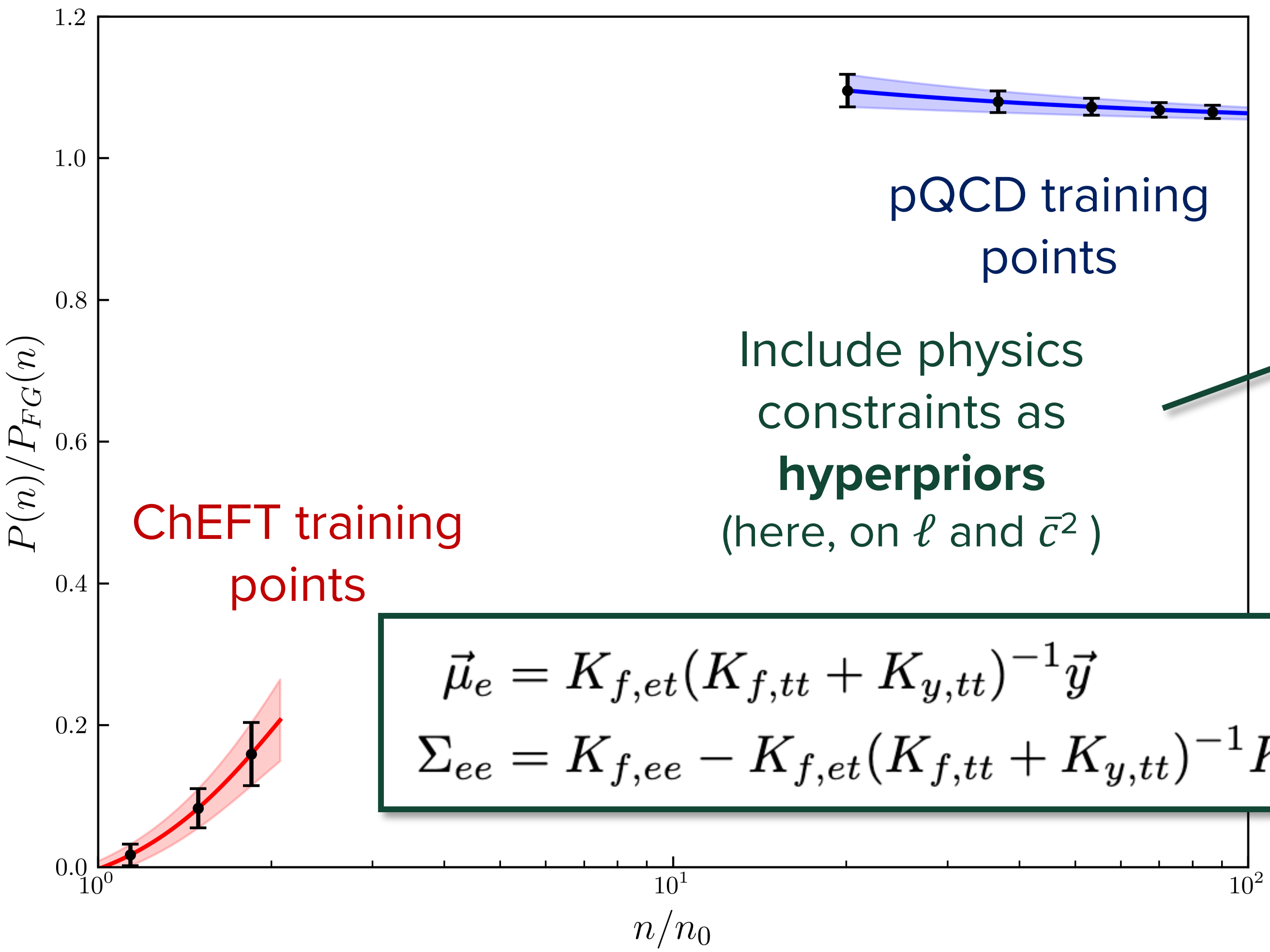

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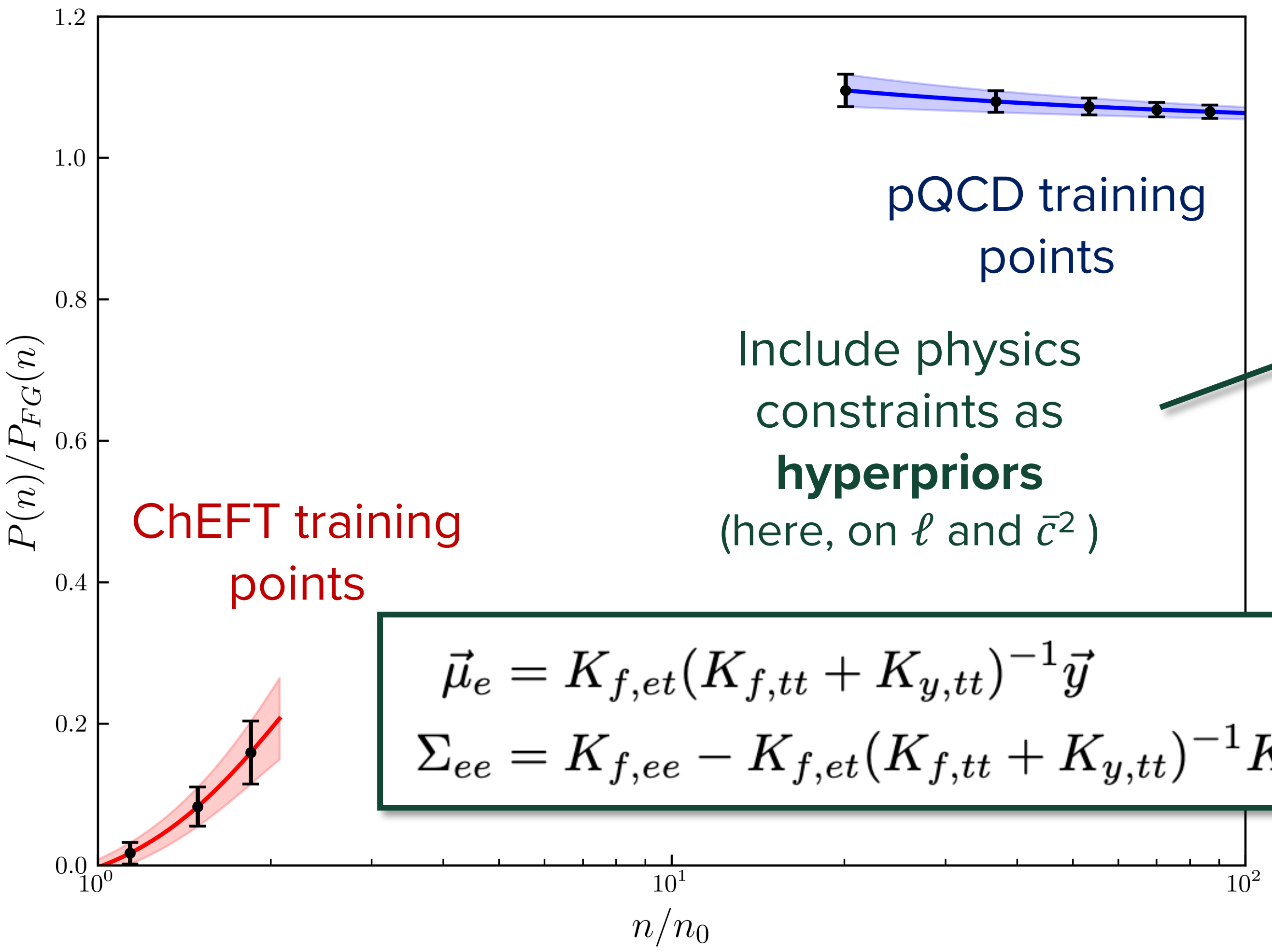

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GP equations are the mixed model result!

Results: pressure of SNM

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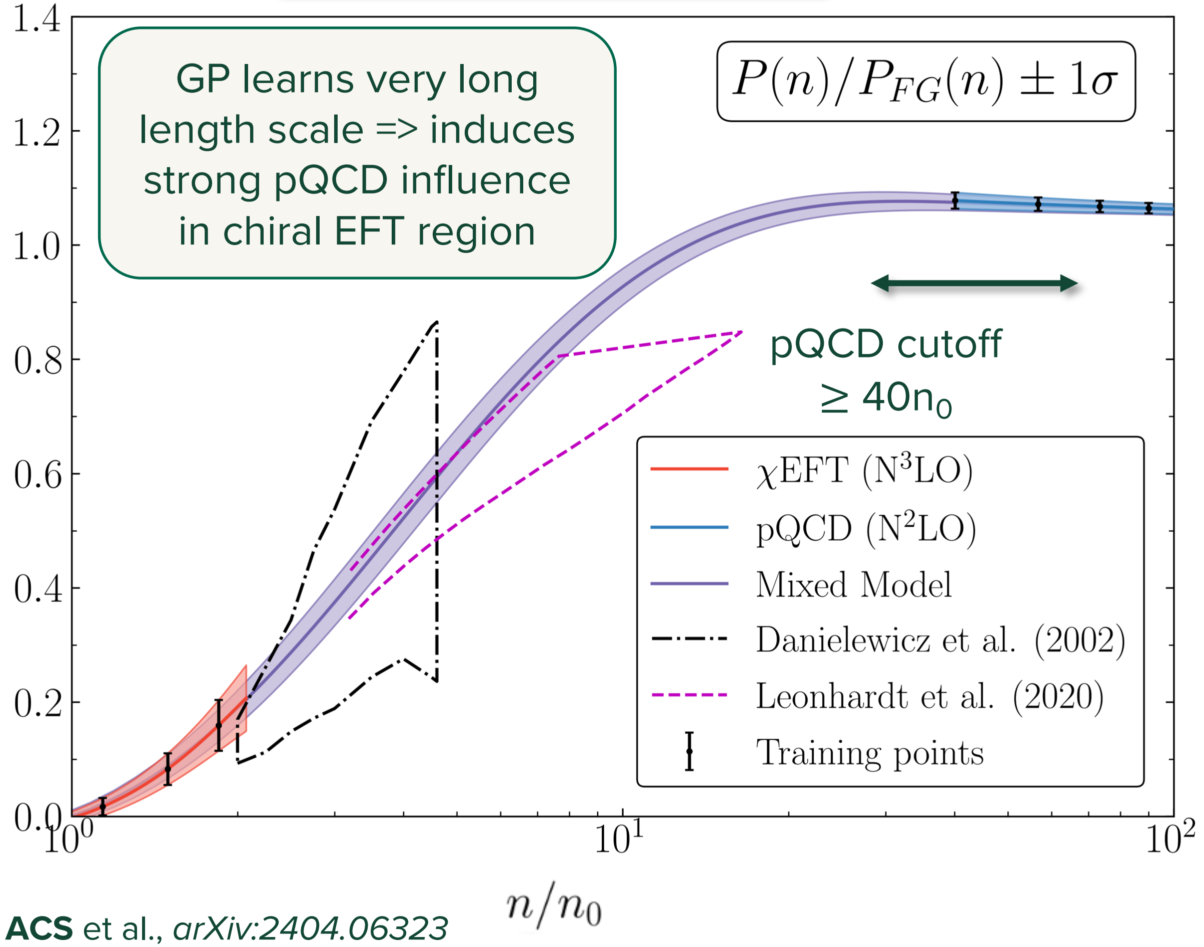
Unconstrained prior



ACS et al., *arXiv:2404.06323*

Results: pressure of SNM

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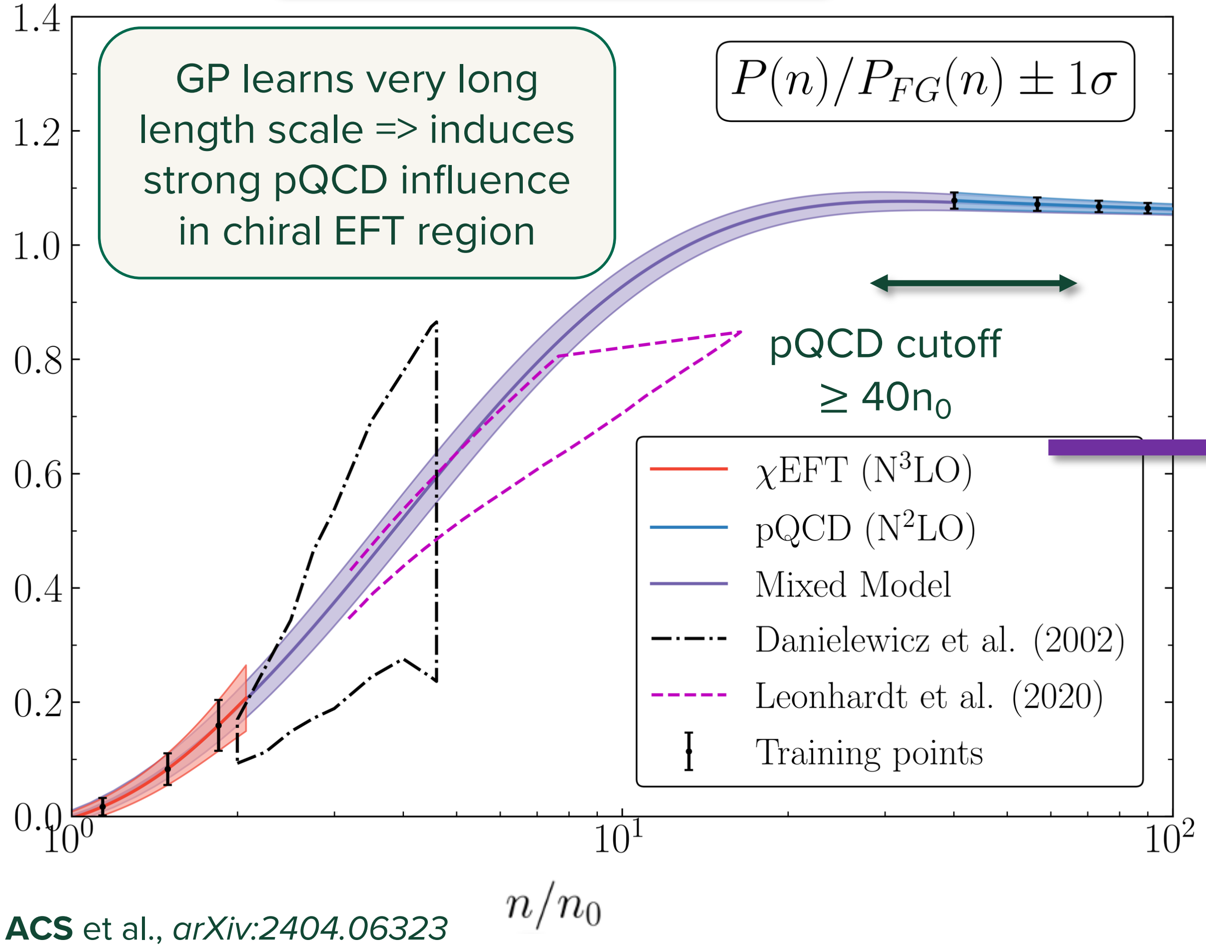
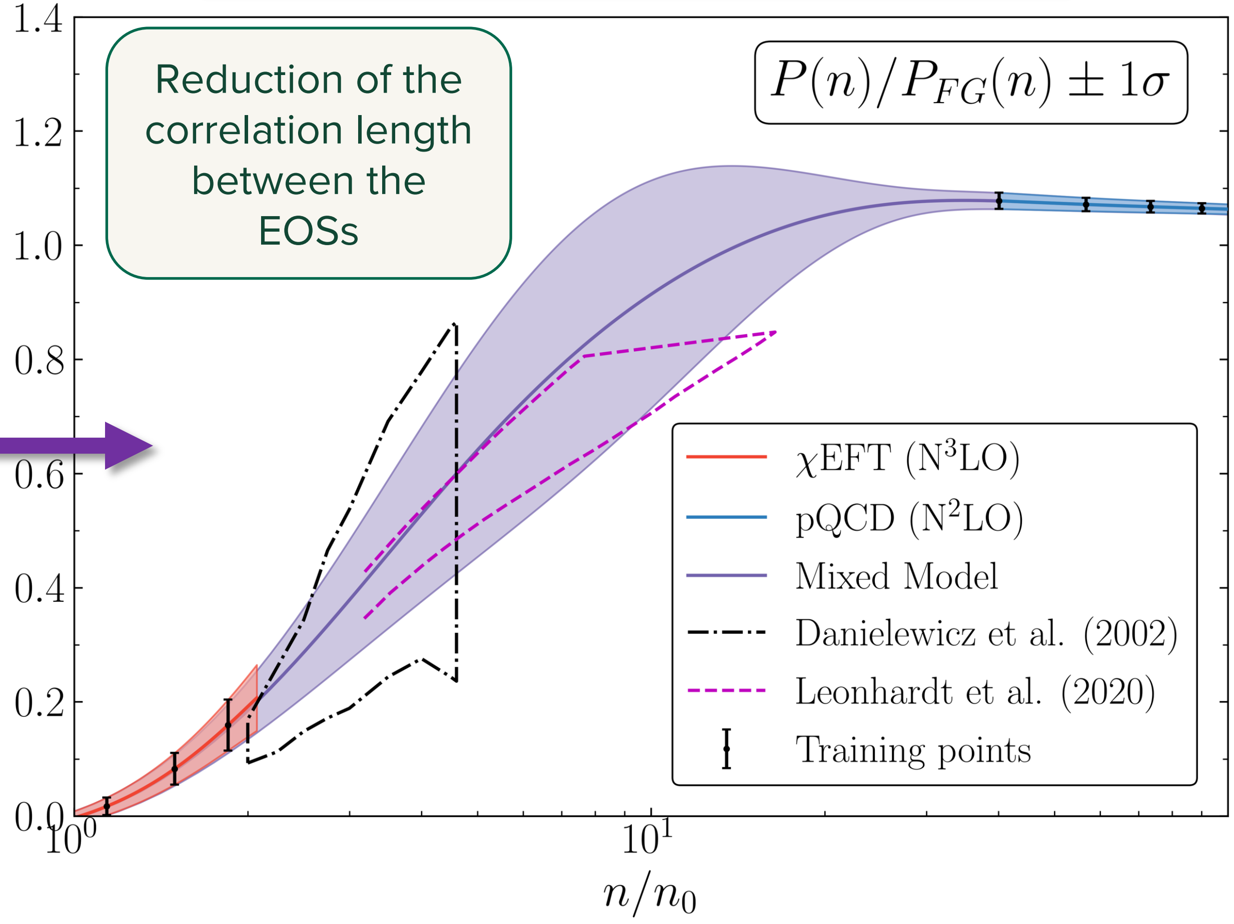


ACS et al., *arXiv:2404.06323*

Constrained prior on lengthscale



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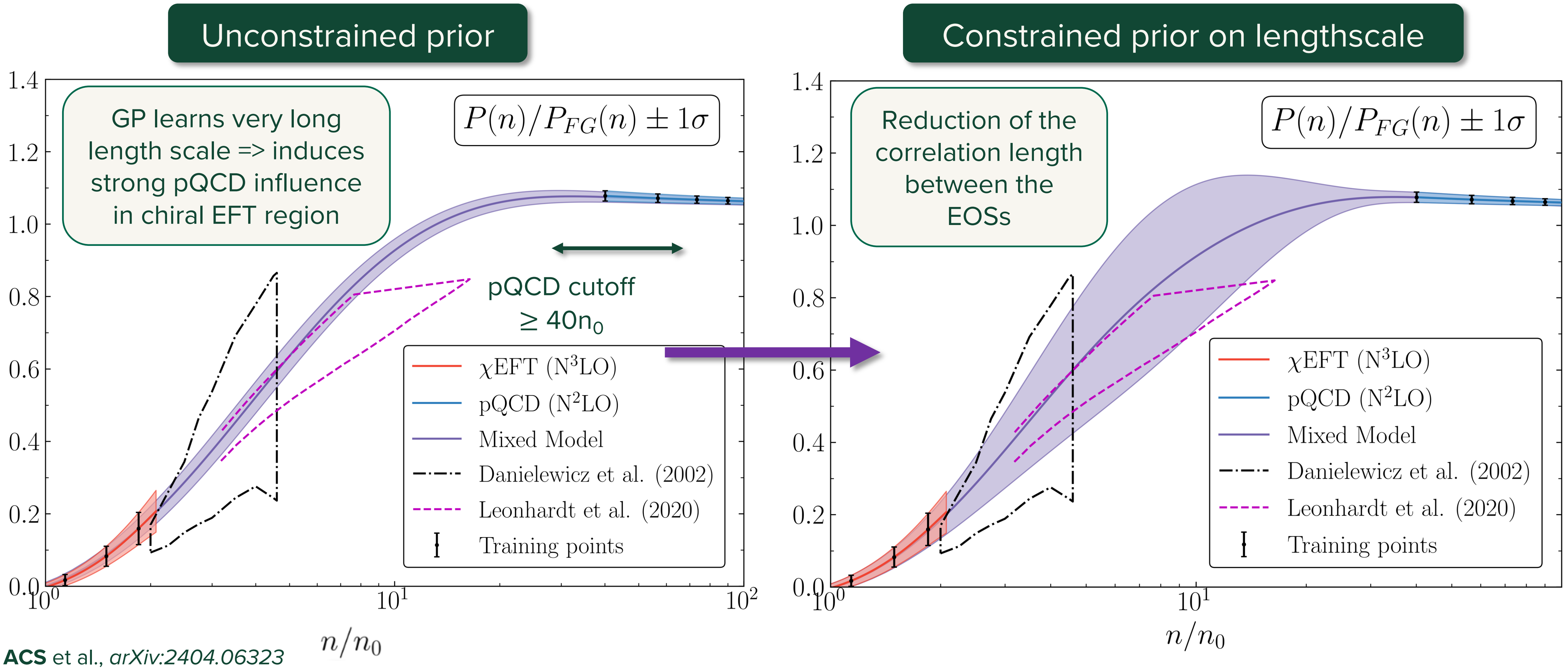


ACS et al., *arXiv:2404.06323*

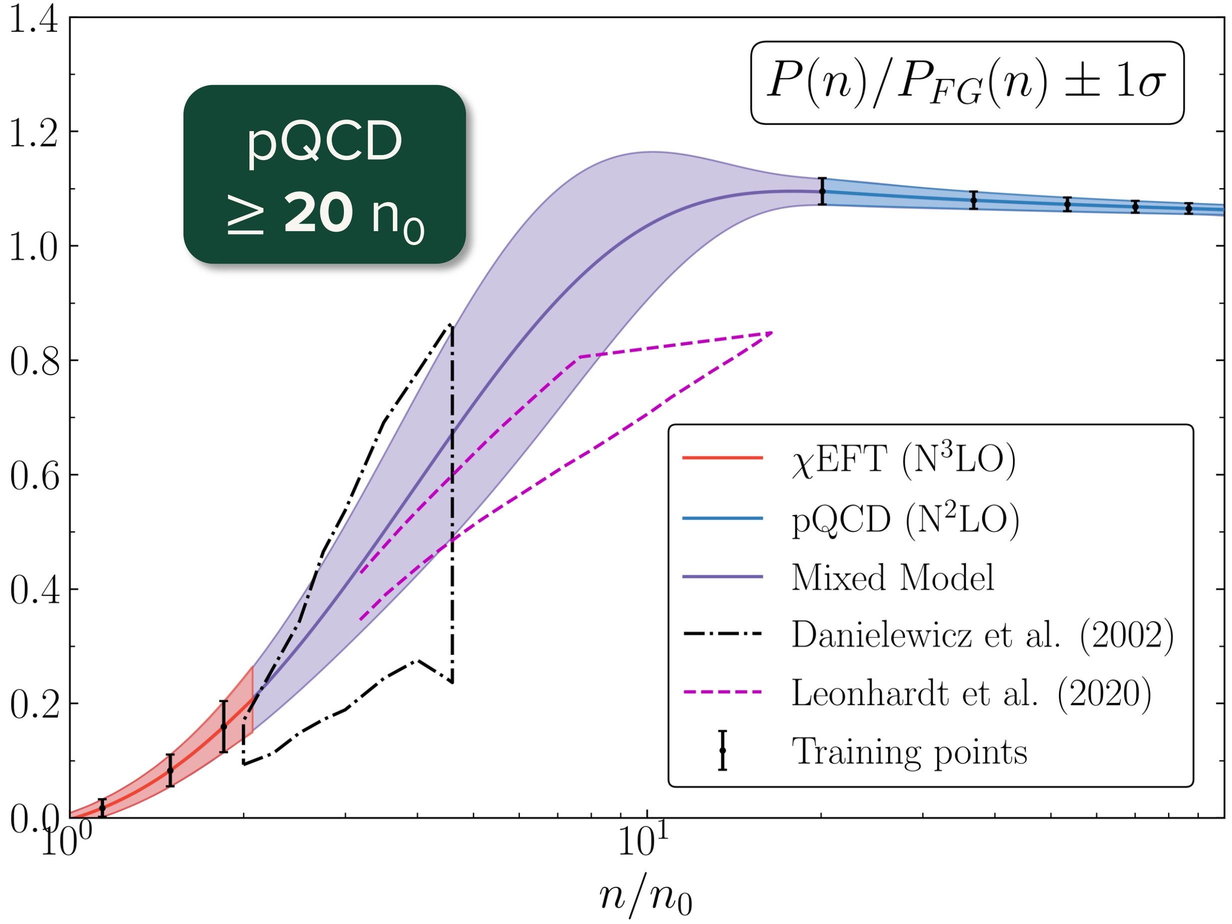
Physics-informed priors on the mixed model GP have a very large influence on the uncertainties obtained

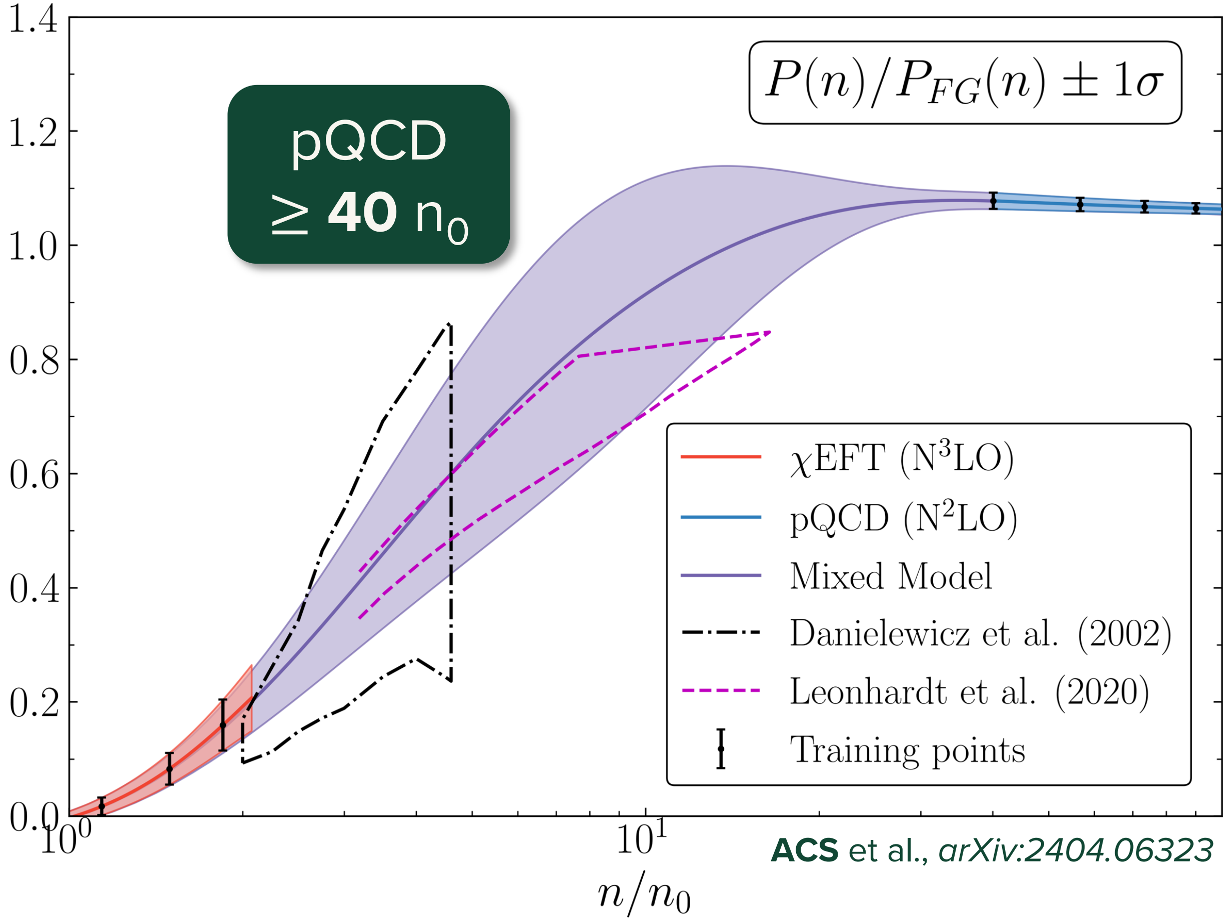
Results: pressure

Unknown cutoff of pQCD validity = testing with **two cases**: pQCD cutoffs for ≥ **20 n_0** & ≥ **40 n_0**

$$p(\vec{\theta}) = \prod_i \mathcal{U}(\theta_i \in [a_i, b_i]) \mathcal{N}(\theta_i, \mu_i, \sigma_i^2)$$

Hyperpriors
truncated normal distributions





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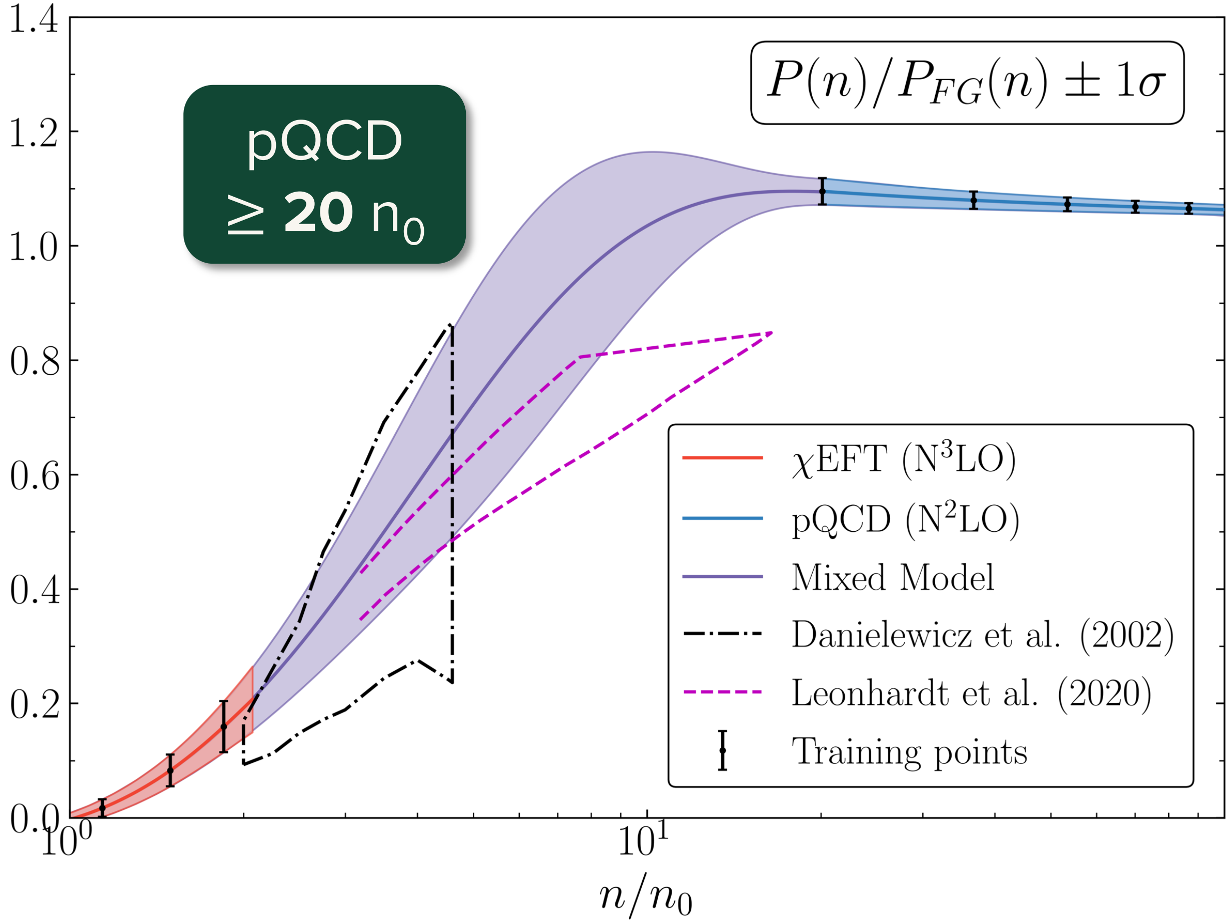
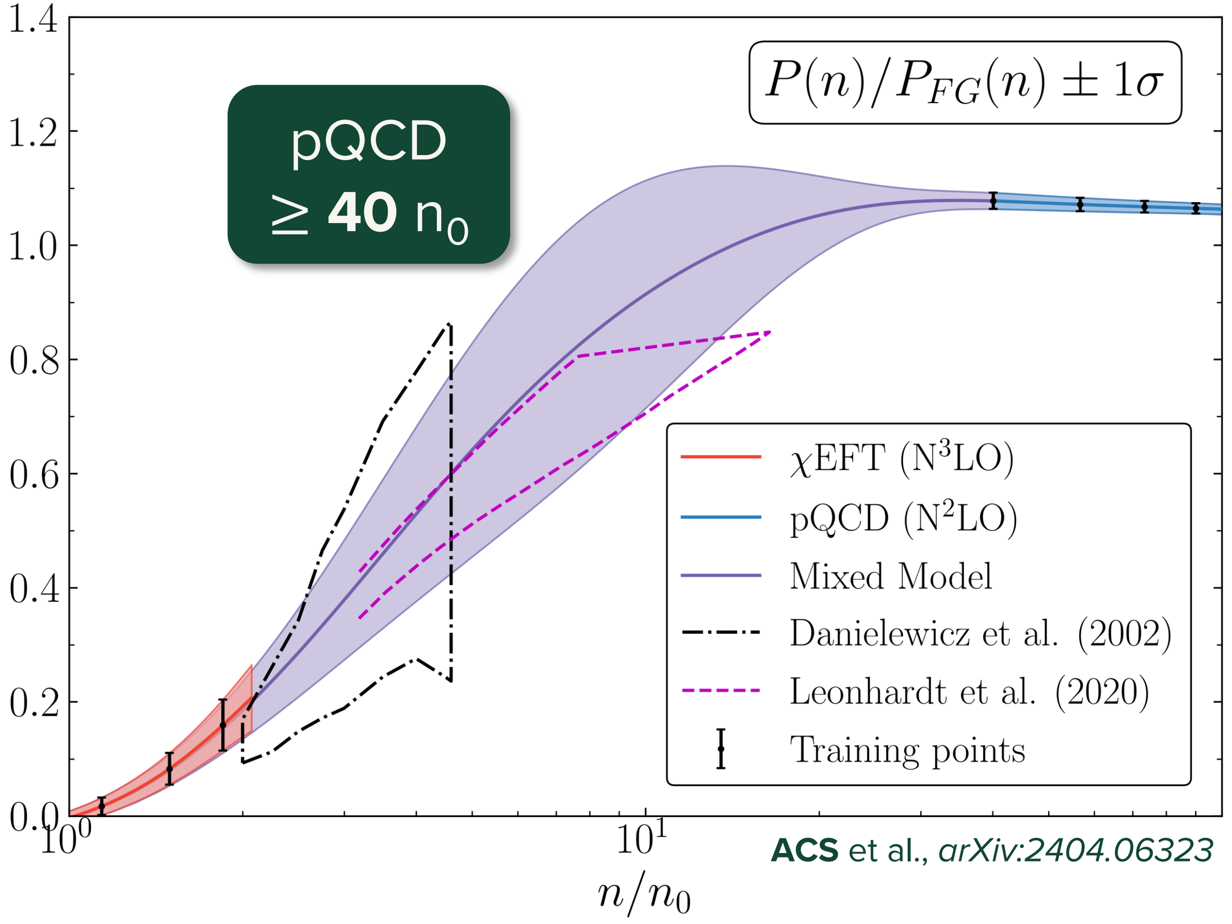




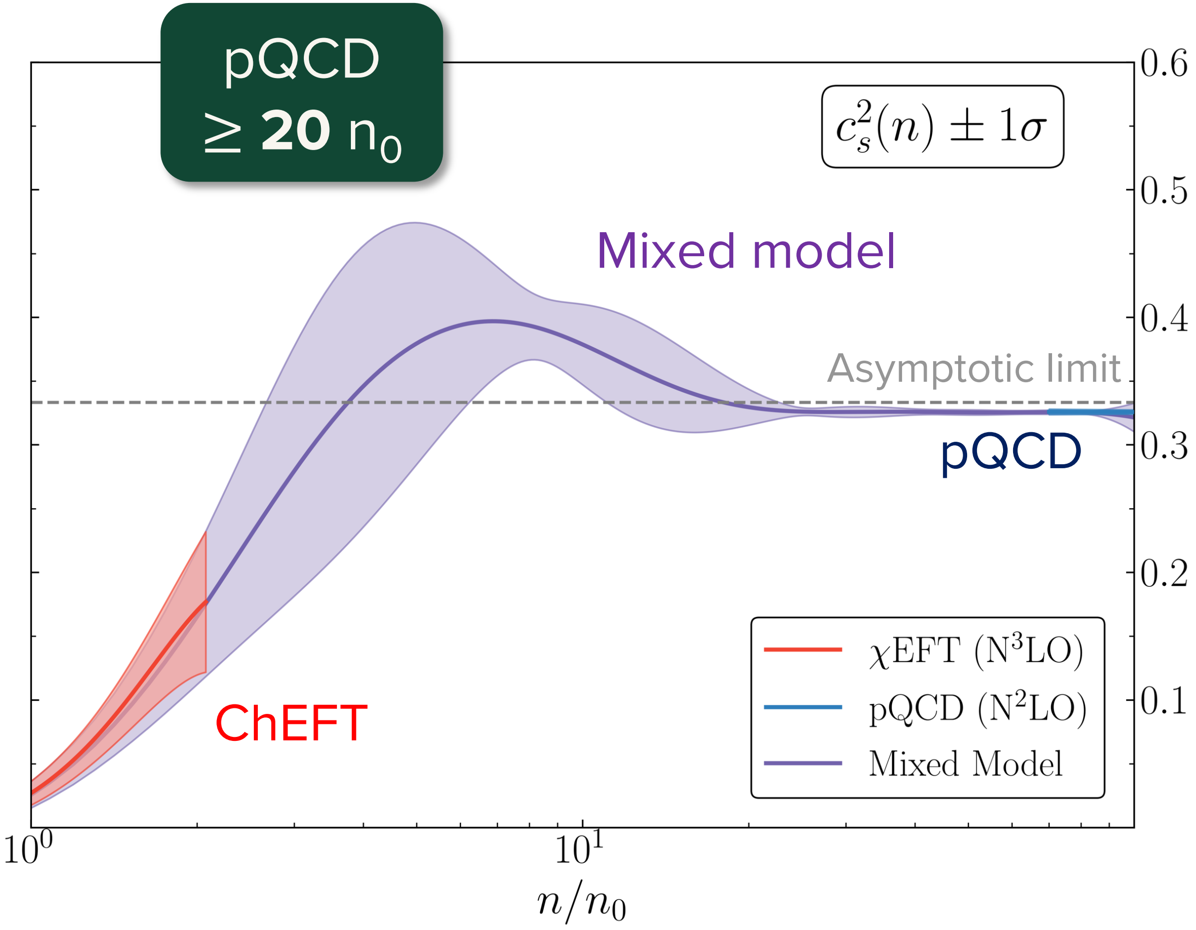
ACS et al., *arXiv:2404.06323*

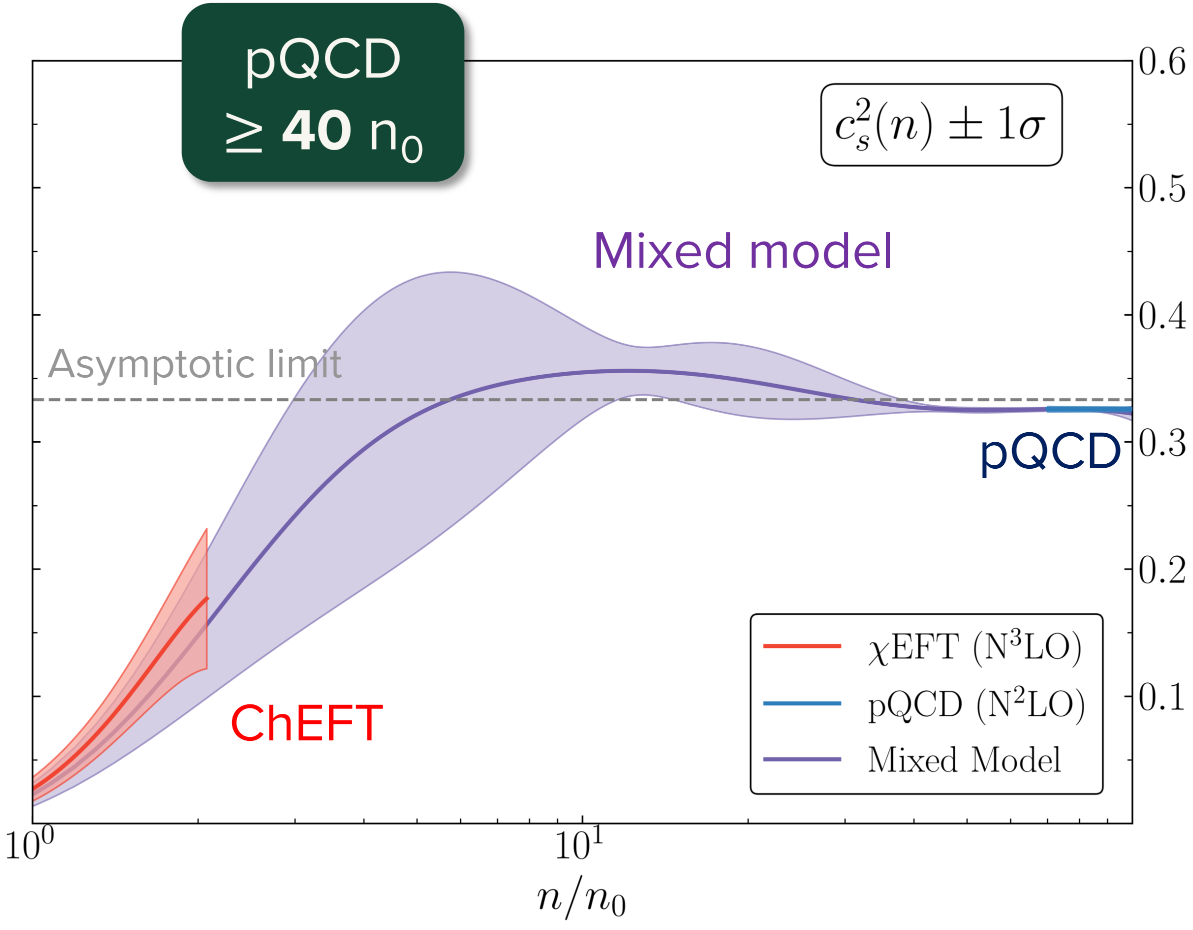
Constraining the correlation length between chiral EFT & pQCD is crucial to avoid unphysical model correlations at low densities

Results: speed of sound

Mixed models both approaching 0.33 asymptotically (from below)

$$c_s^2(n) = \frac{1}{\mu}\frac{\partial P}{\partial n}$$





ACS et al., *arXiv:2404.06323*

Causal, stable EOS

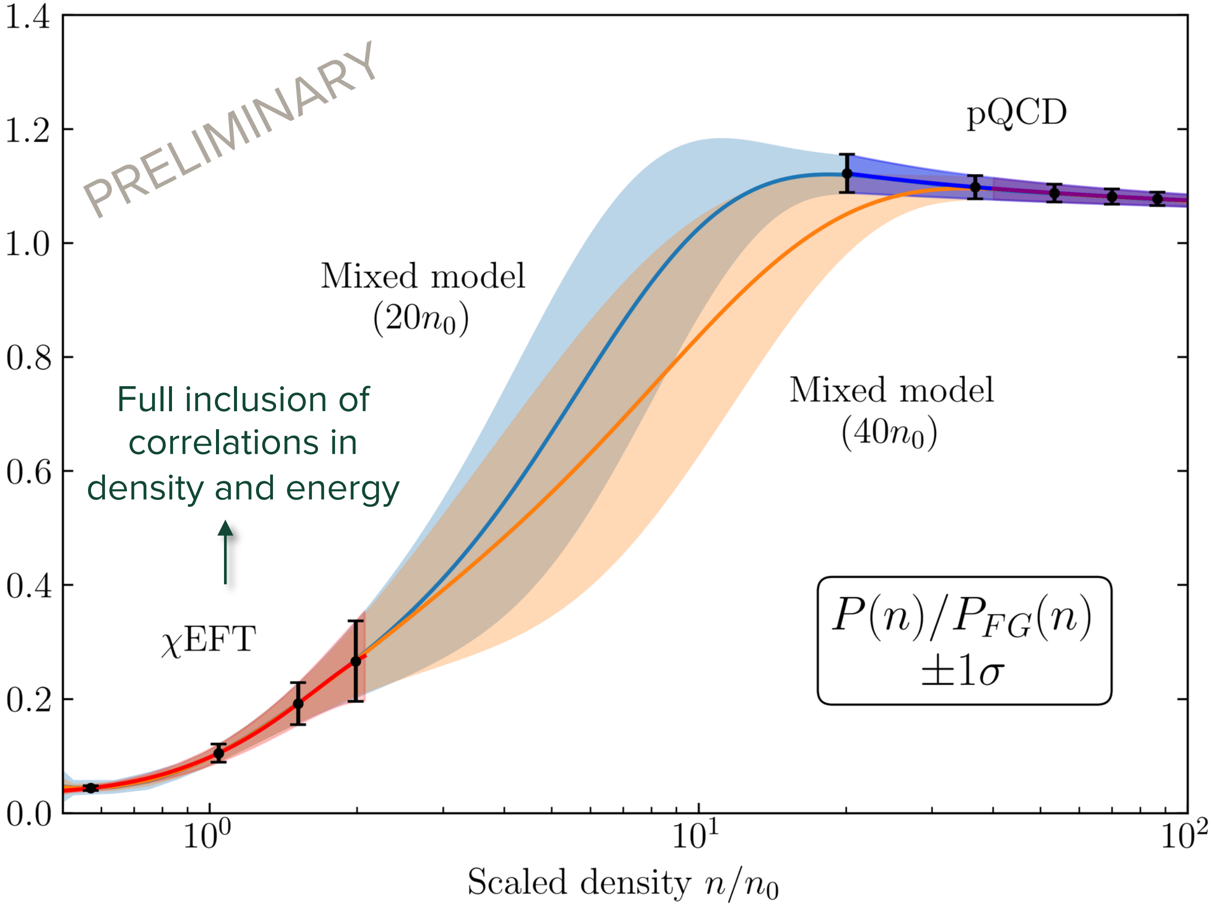
Results: asymmetric matter

GP kernel: stationary, smooth RBF (as with SNM)
[Other stationary kernels give similar results]

Hyperpriors

$$p(\vec{\theta}) = \prod_i \mathcal{U}(\theta_i \in [a_i, b_i]) \mathcal{N}(\theta_i, \mu_i, \sigma_i^2)$$

truncated normal distributions



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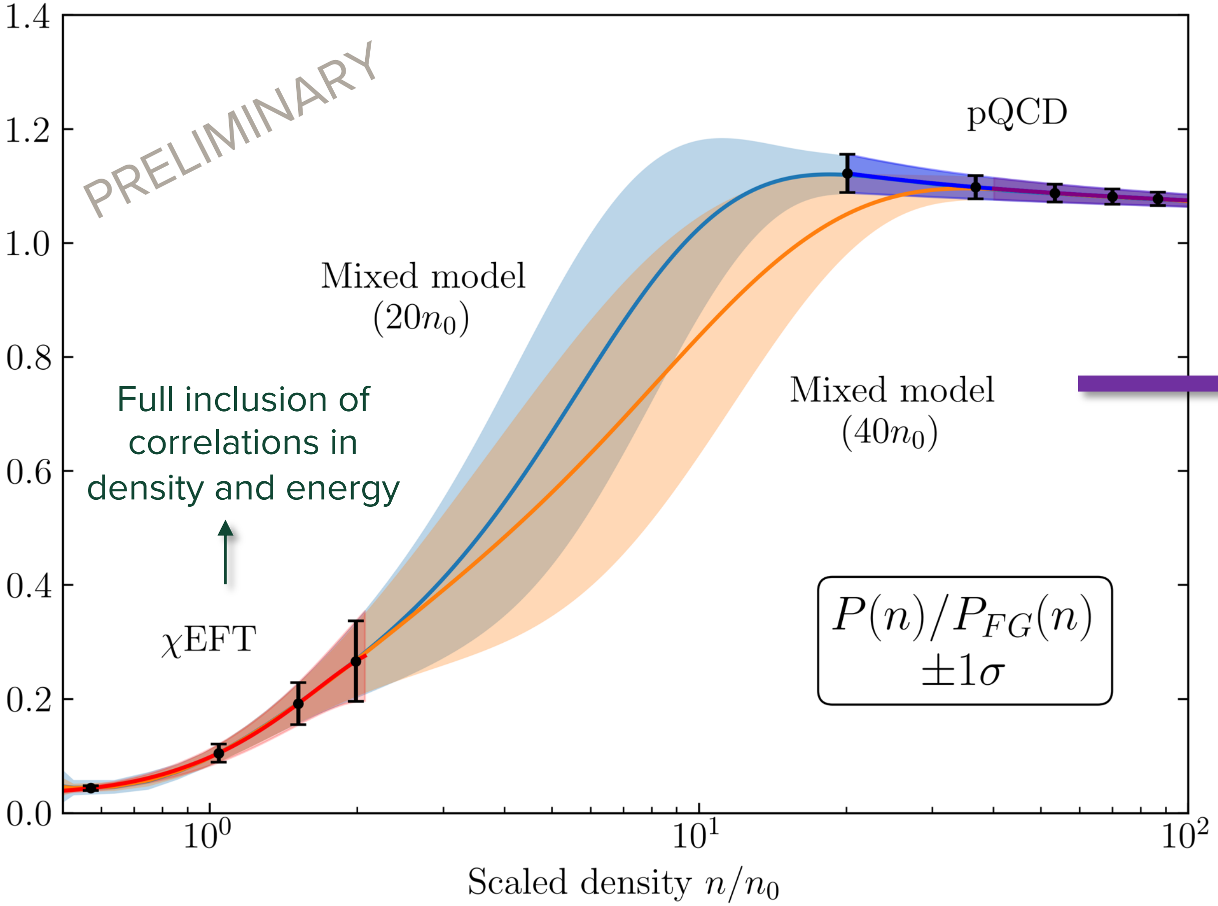

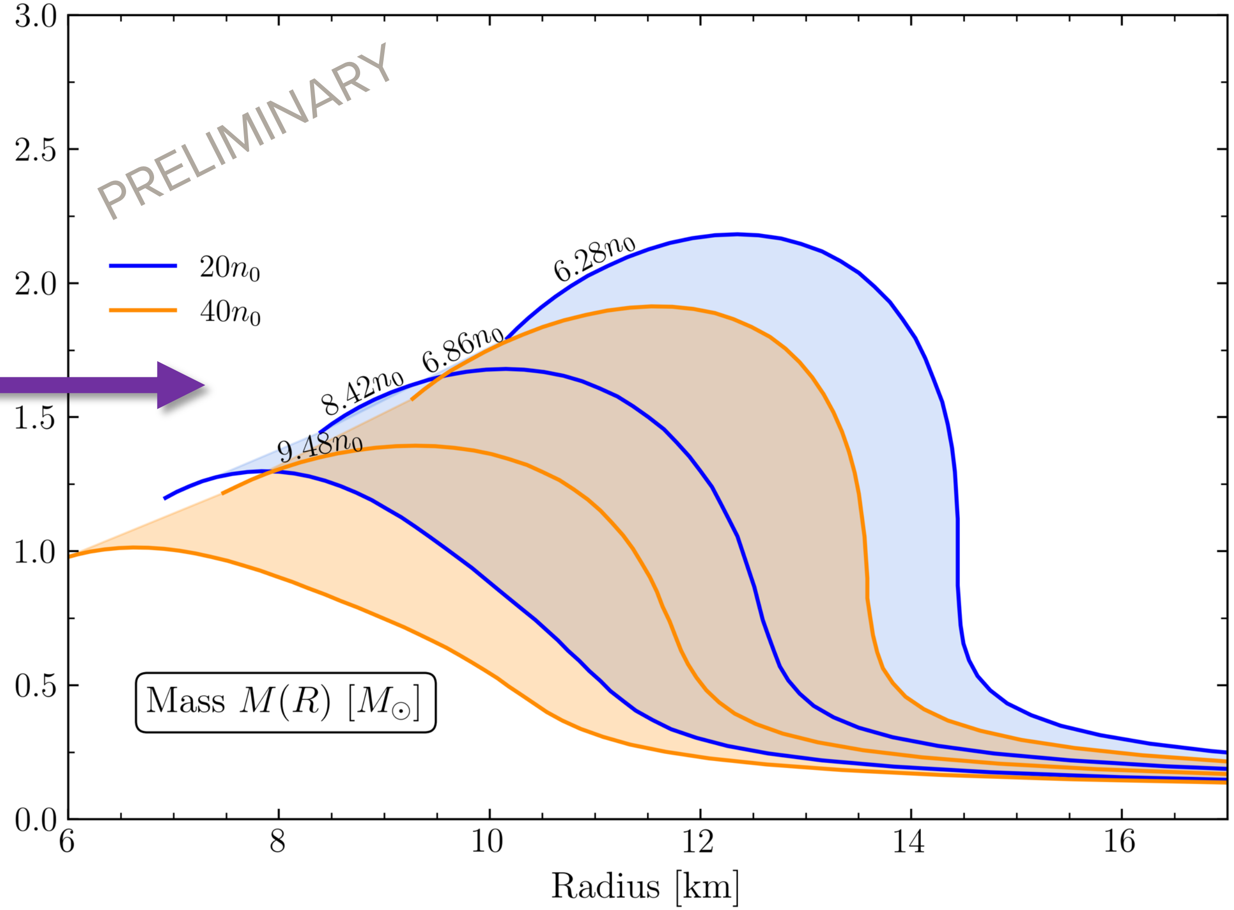

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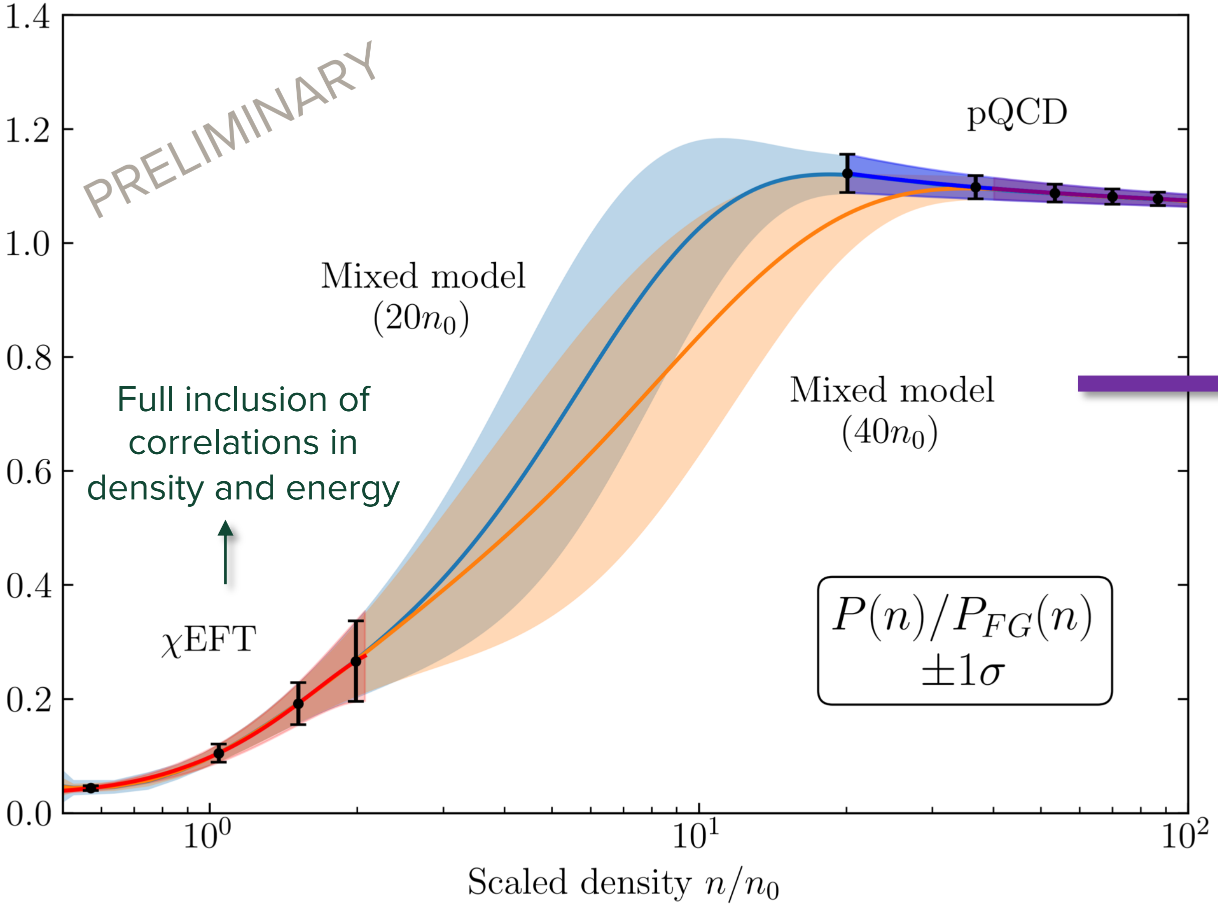
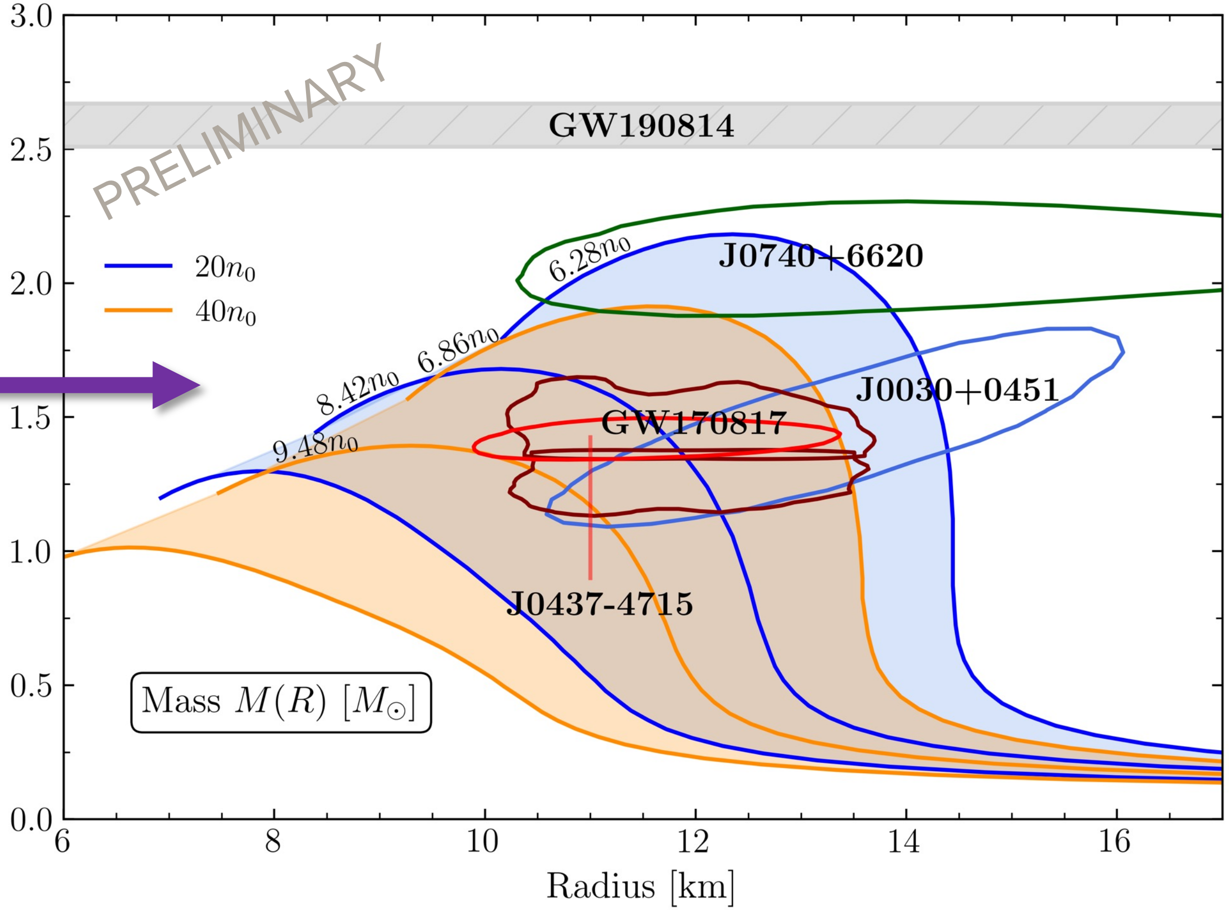


Full inclusion of correlations in density and energy



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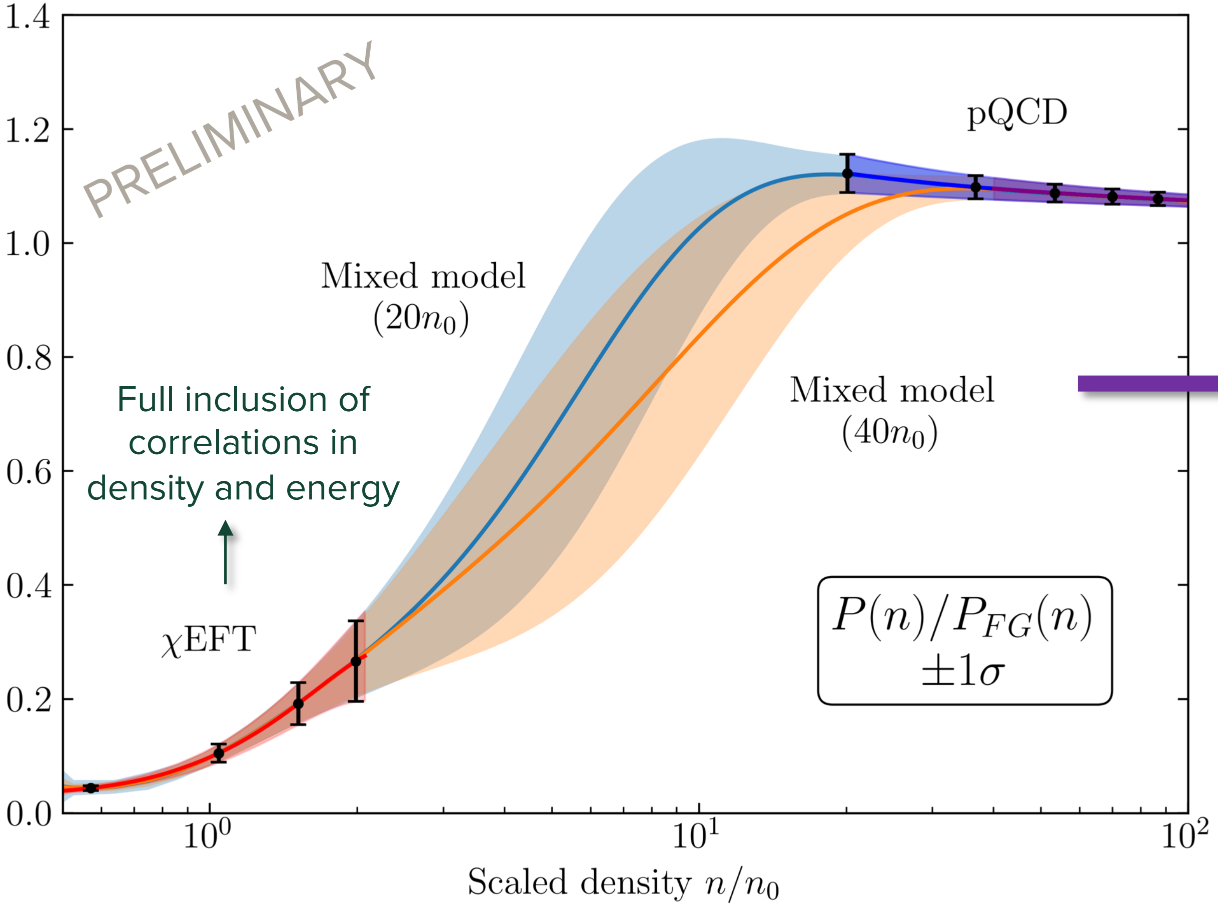

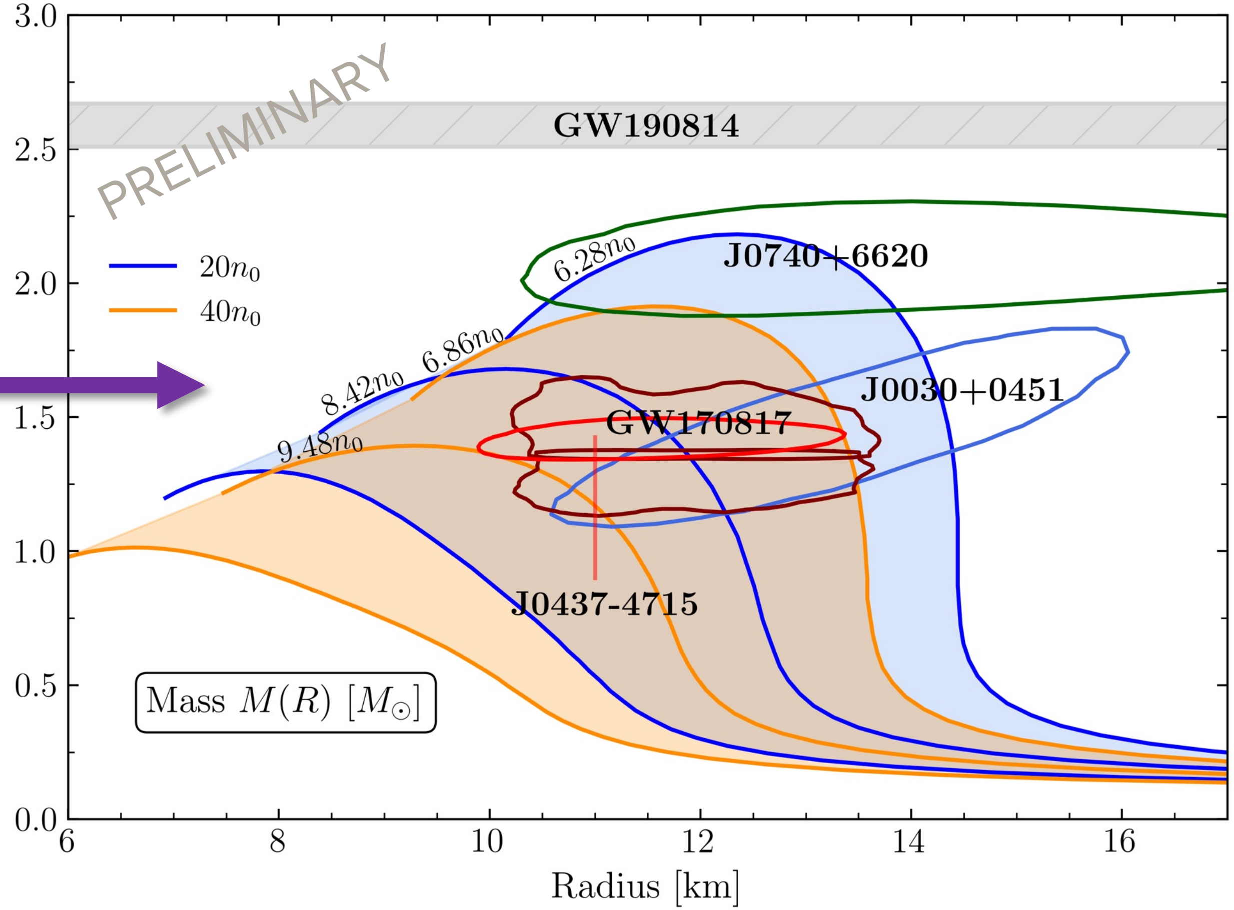

Microscopic input for a Bayesian framework

Summary & discussion

Summary

Applied Bayesian model mixing to ChEFT and pQCD in **pressure** for **SNM** and **ANM**

Examined the **speed of sound** results for the mixed EOS

Quantified the **truncation error** in pQCD using BUQEYE methods and consistently obtained **P(n)**

Goals: multi-dimensional extension of BMM to finite T, δ; integration with **MUSES** framework

Current adventures

Exploring phase transitions
Inclusion of discontinuous phase transitions through non-stationary GP kernels

Confronting the mixed model with data
Implementing the Bayesian framework to further constrain the posterior of the EOS with astrophysical and heavy-ion results

… and stuff we left out

Including a microscopic crust
Use results from neural-network quantum states (includes clusters), learn crust-core transition

Full UQ of chiral EFT
Low energy constant (LEC) uncertainties not included, many-body uncertainties may be underestimated

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Confronting the mixed model with data
Implementing the Bayesian framework to further constrain the posterior of the EOS with astrophysical and heavy-ion results

Our end goal: global, microscopic, QCD-based EOSs for merger simulations, but…

… and stuff we left out

Including a microscopic crust
Use results from neural-network quantum states (includes clusters), learn crust-core transition

Full UQ of chiral EFT
Low energy constant (LEC) uncertainties not included, many-body uncertainties may be underestimated

!

BMM is generally applicable to problems in dense matter

OHIO UNIVERSITY

DOI: 10.21105/joss.06175

Taweret: BMM software

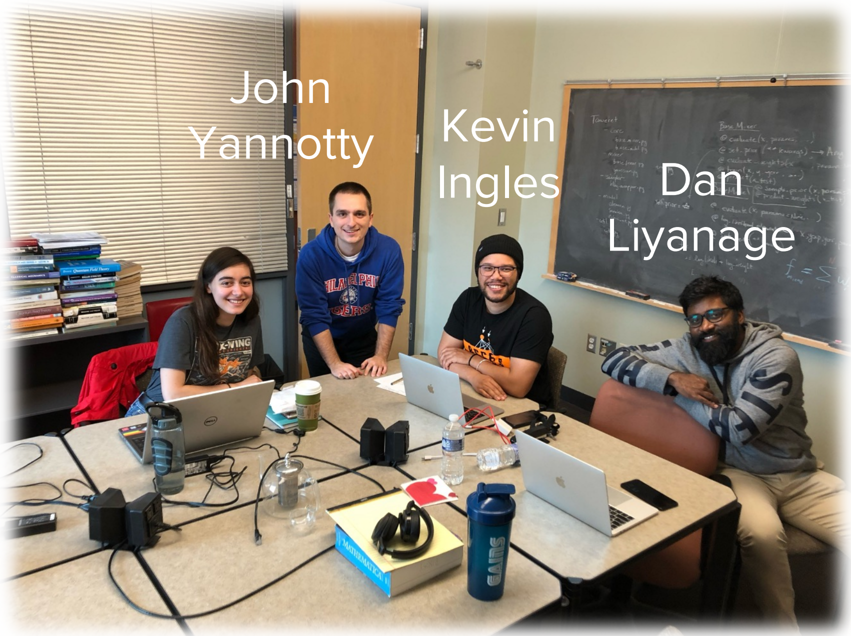
Open-source repository:
https://github.com/bandframework/Taweret

Python interface for user to use BMM methods on **their own models**

Present: our 3 methods + toy models

Near future: *add your own BMM method!*

Published in JOSS The Journal of Open Source Software



Picture credit: Dick Furnstahl

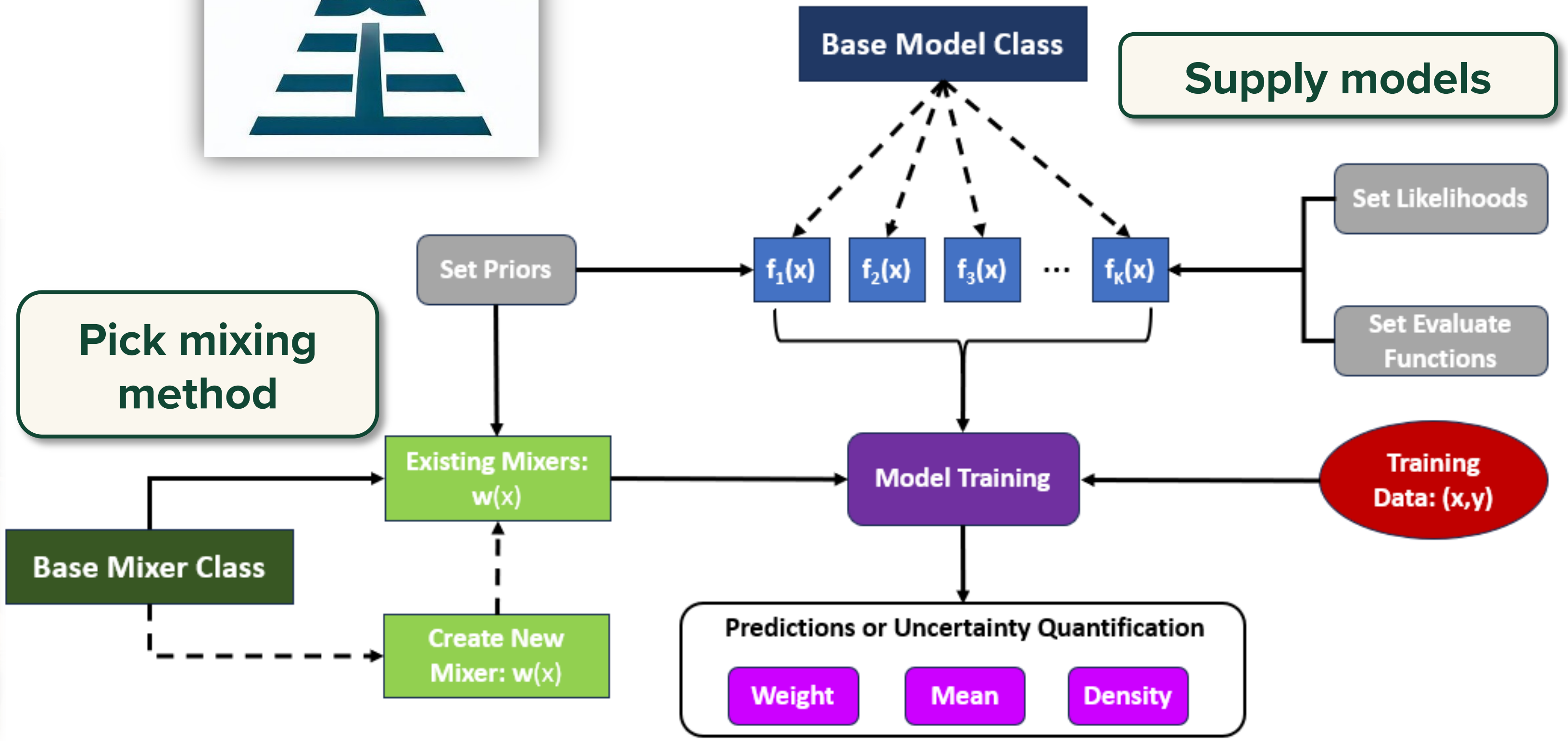


Figure credit: John Yannotty

Open-source repository for the EOS coming soon!

FOREVER OHIO

OHIO UNIVERSITY

Thank you!

Daniel Phillips (OU)

Dick Furnstahl (OSU)

Christian Drischler (OU)

Jordan Melendez

BAND Bayesian Analysis of Nuclear Dynamics

U.S. DEPARTMENT OF ENERGY

NSF

ASCSN

BUQEYE Collaboration

INSTITUTE OF NUCLEAR & PARTICLE PHYSICS INPP @OHIO UNIVERSITY

ACS supported by: US DOE, contract DE-FG02-93ER-40756, NSF CSSI program, award number OAC-2004601

Backup slides

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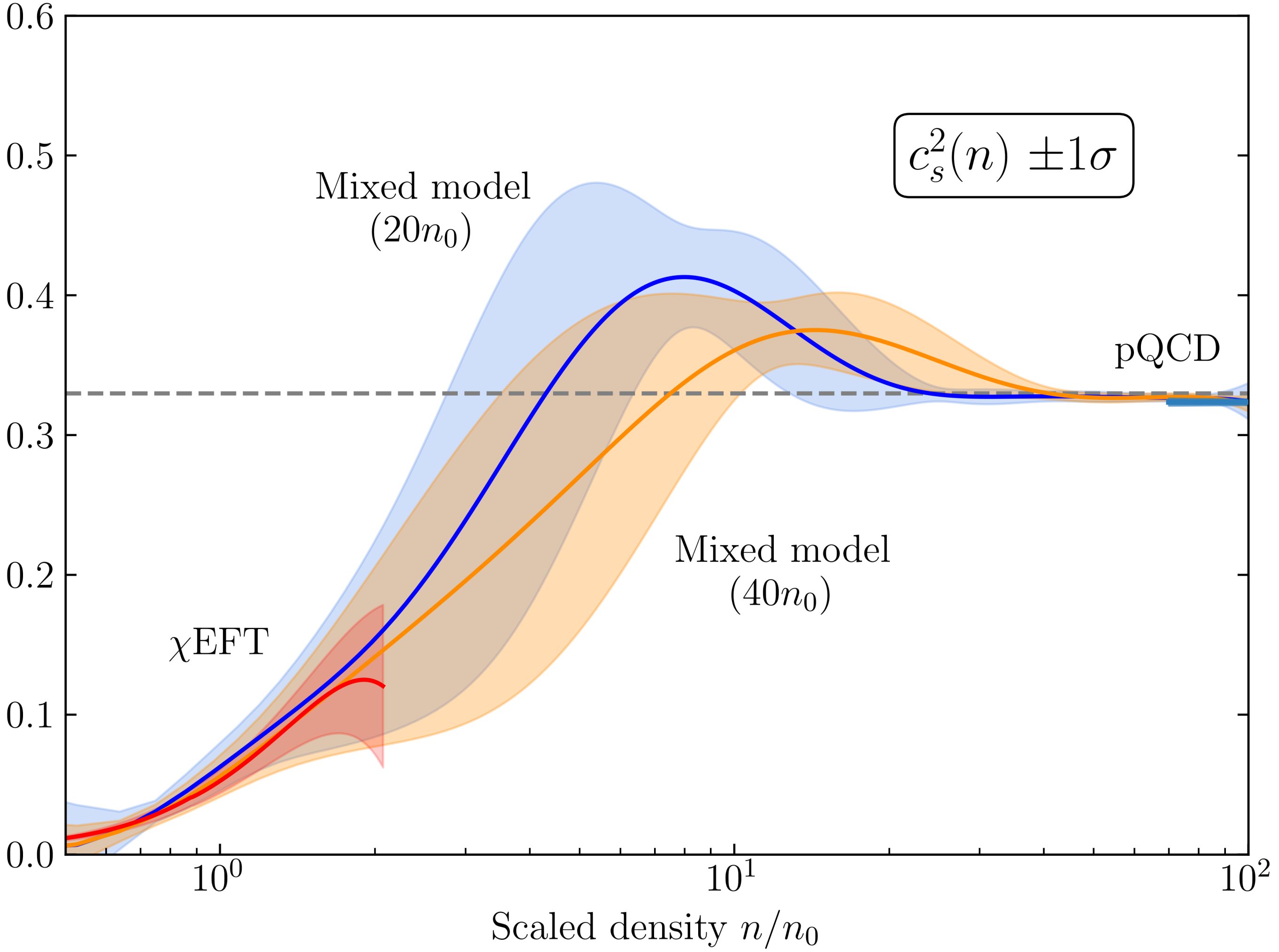
Speed of sound



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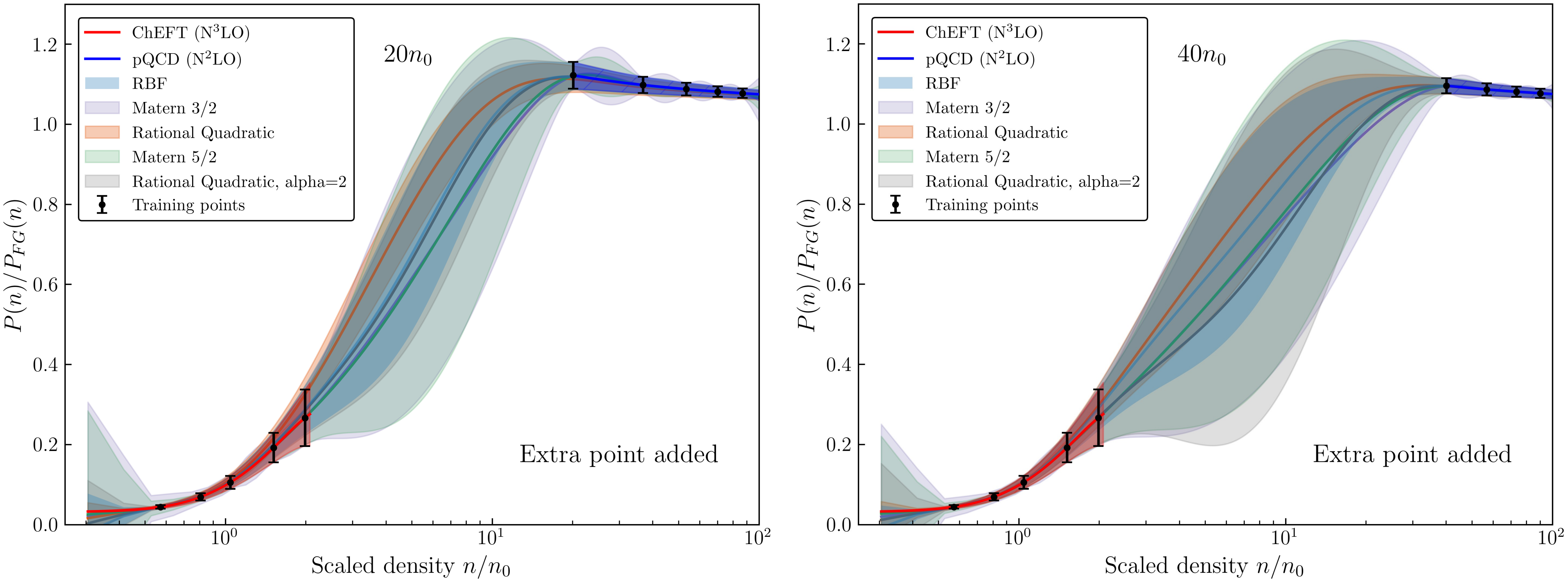
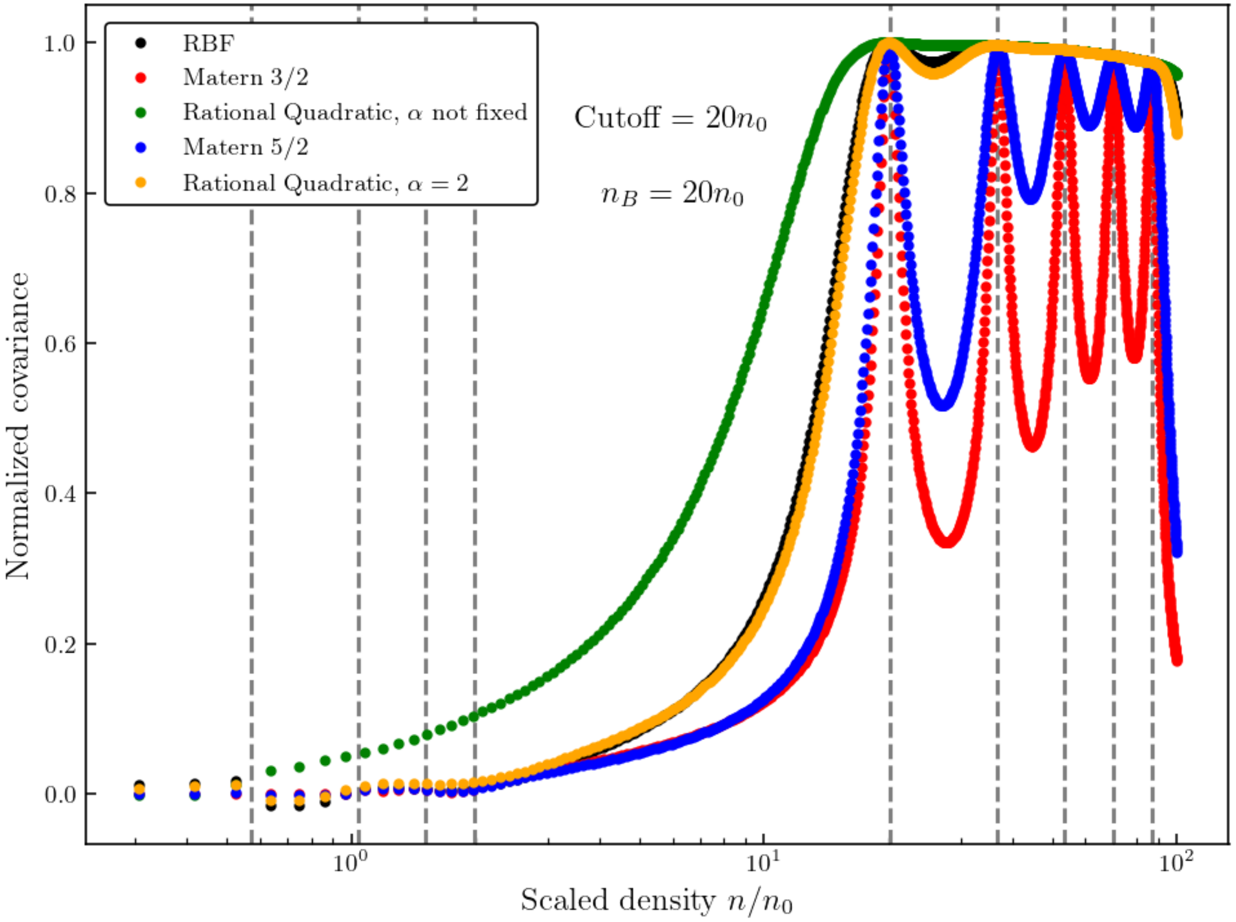
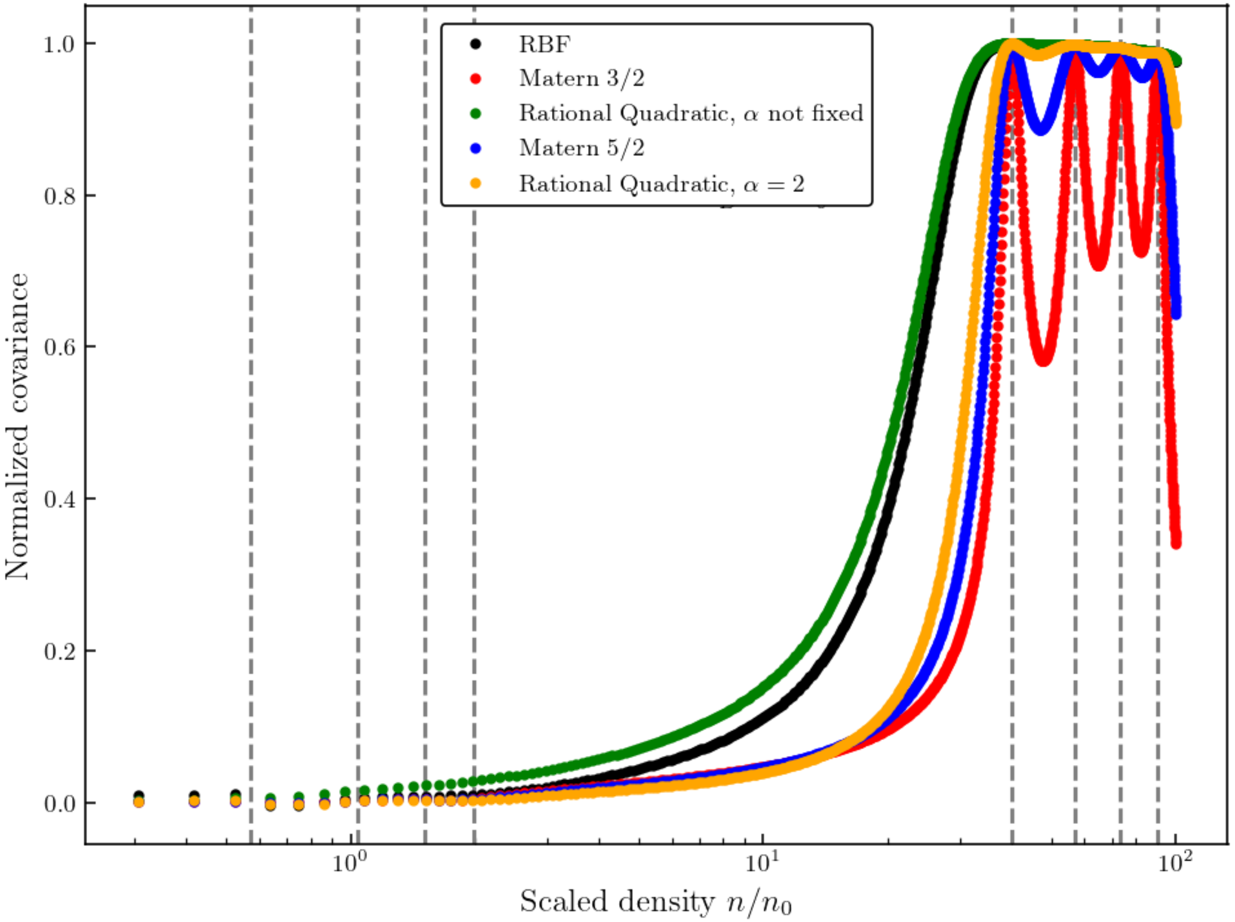
Stationary kernel investigation



Covariance investigation





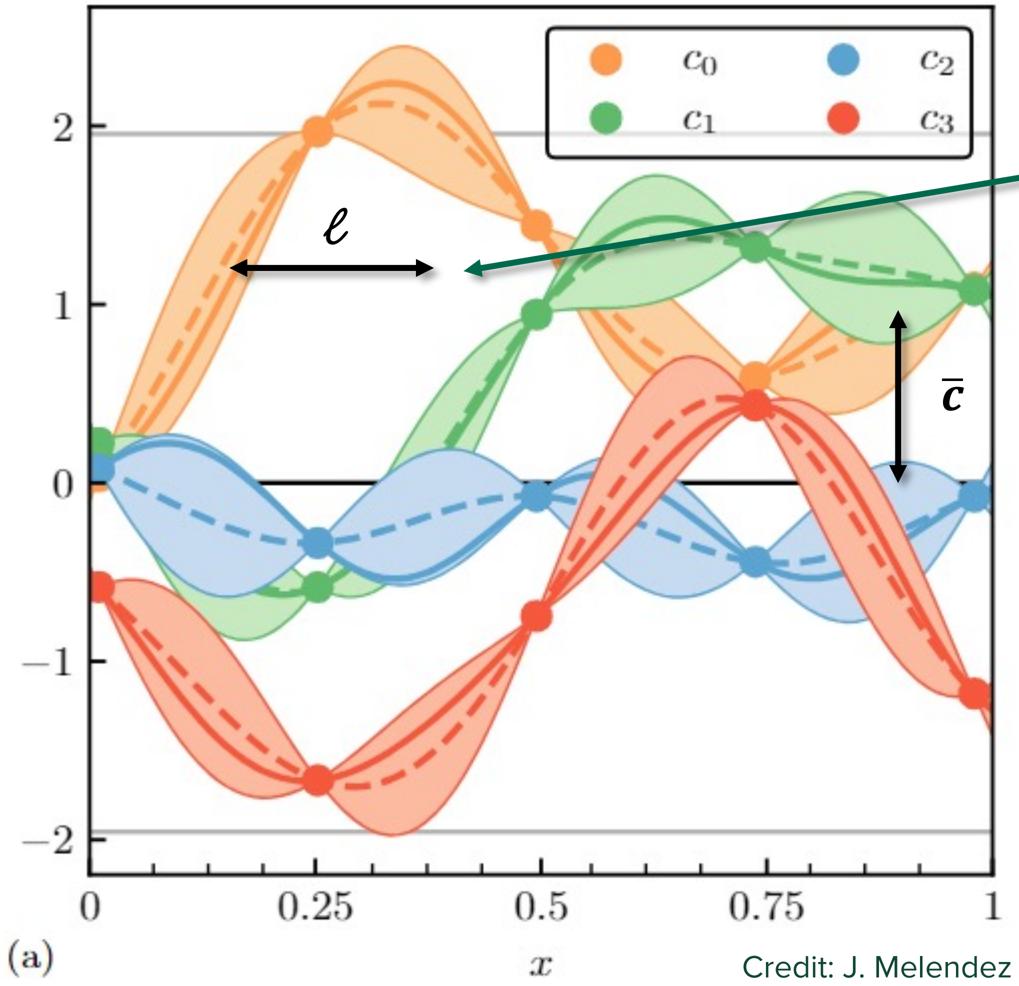
Crash course: Gaussian Processes (GPs)

"Set of random variables, any subset of which possesses a Gaussian distribution"

Less abstract:
Defined by mean function and covariance function (*kernel*)

$$f(x) \sim \mathcal{GP}[m(x), \kappa(x, x')]$$

Contains dependence on variance and lengthscale (RBF, Matérn, etc.)



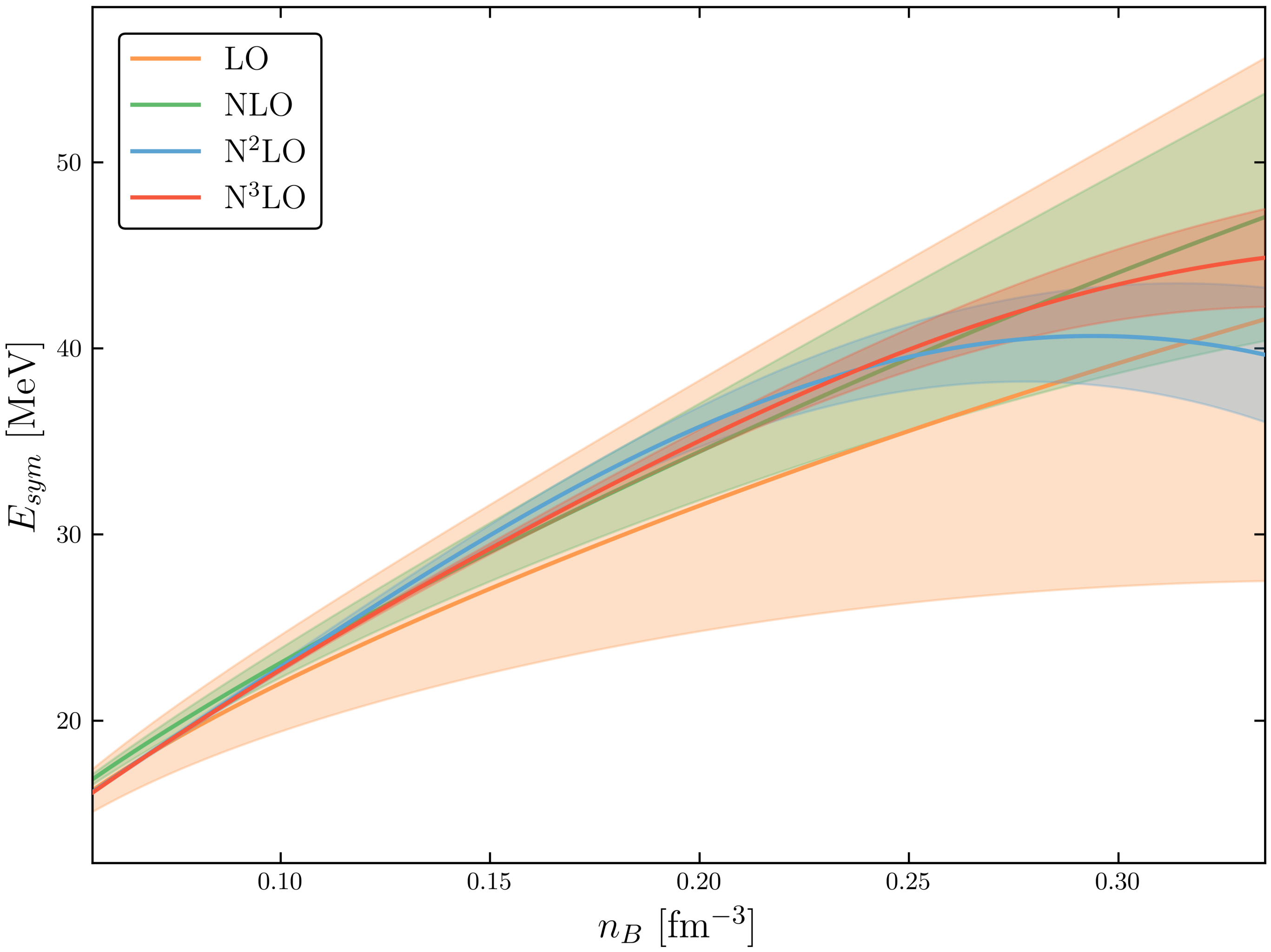
Credit: J. Melendez et al. (2019)

Correlation structure parameterized by a lengthscale and variance

Hyperparameters that *can* be determined by Bayesian parameter estimation

Can be fitted to **data + uncertainties** and used to predict at new points

Symmetry energy from chiral EFT



High densities: pQCD EOS

Invoking the Kohn-Luttinger-Ward inversion theorem

$$P(\mu) = P_{FG}(\mu)\left[c_0 + c_1 Q(\bar{\Lambda}) + c_2(\mu) Q^2(\bar{\Lambda})\right]$$

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

1 $\mu = \mu_{FG} + \mu_1 + \mu_2$ ← Perturbative expansion

2 Taylor expand => $n(\mu) = \frac{\partial P(\mu)}{\partial \mu}$ → $n(\mu_{FG}) \equiv n(\mu_{FG} + \mu_1 + \mu_2) \equiv \bar{n}$ Input number density

3 Equate terms by counting powers of α_s

$$\bar{n}(\mu) = c_0(\mu) \frac{\partial P_{FG}(\mu)}{\partial \mu}\bigg|_{\mu=\mu_{FG}}, \quad \mu_1 = -\frac{c_1 Q(\bar{\Lambda}) \frac{\partial P_{FG}(\mu)}{\partial \mu}}{c_0 \frac{\partial^2 P_{FG}(\mu)}{\partial \mu^2}}\Bigg|_{\mu=\mu_{FG}}$$

+ μ_2 expression

4 Expand P(μ), insert terms, keep up to second order in α_s

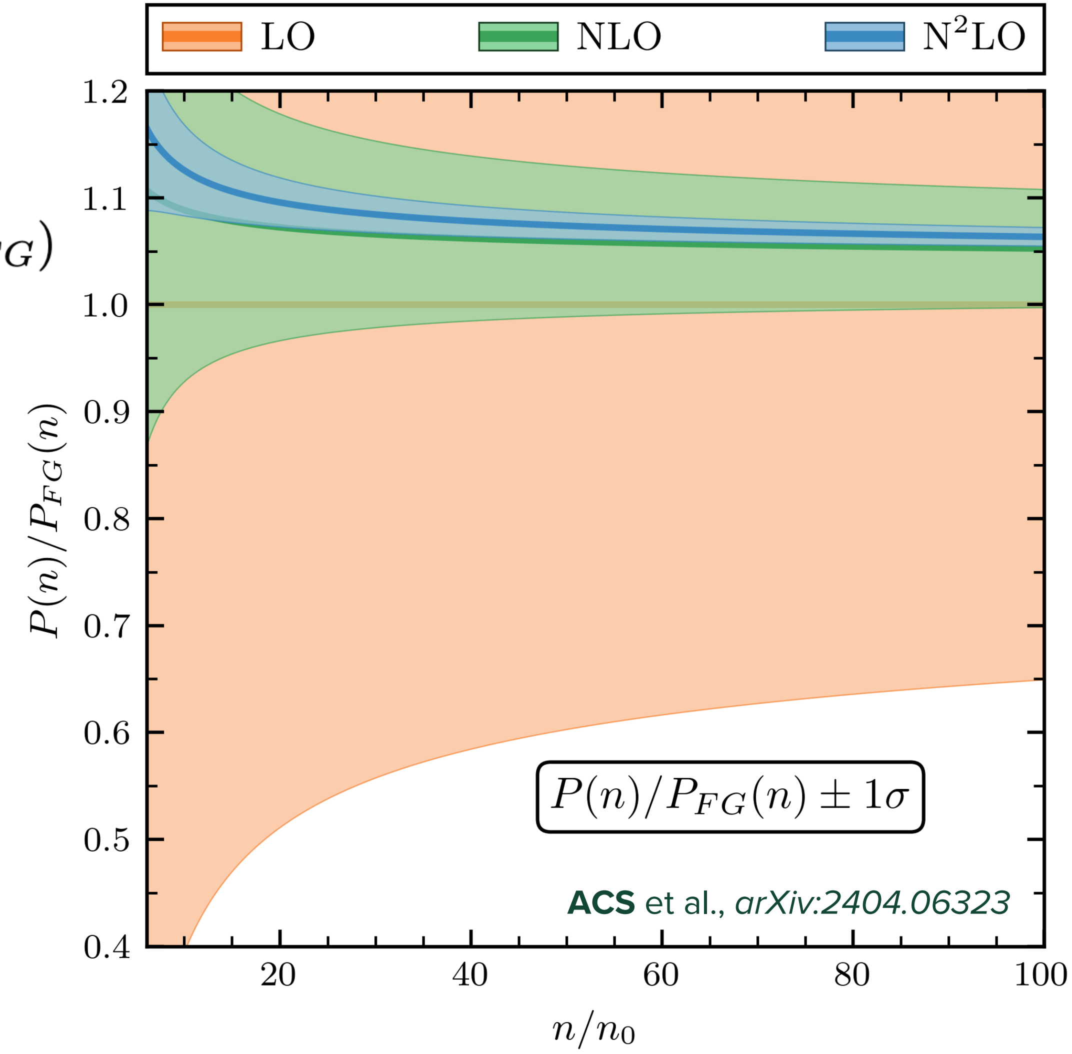
$$\frac{P(n)}{P_{FG}(n)} = 1 + \frac{2}{3\pi}\alpha_s(\bar{\Lambda}_{FG}) + \frac{8}{9\pi^2}\alpha_s^2(\bar{\Lambda}_{FG}) - \frac{N_f^2}{3\pi^2} c_2(\mu_{FG})\alpha_s^2(\bar{\Lambda}_{FG}) - \frac{\beta_0}{3\pi^2}\alpha_s^2(\bar{\Lambda}_{FG})$$

Directly *n*-dependent

High densities: pQCD EOS

Expansion in the strong coupling constant α_s

$$P(n) = P_{FG}(n)\left[c_0 + c_1 Q(\bar{\Lambda}_{FG}) + c_2(n) Q^2(\bar{\Lambda}_{FG}) + \ldots\right]$$



Original model: Tyler Gorda, Risto Paatelainen, Saga Säppi, and Kaapo Seppänen, Phys. Rev. Lett. **131**, 181902

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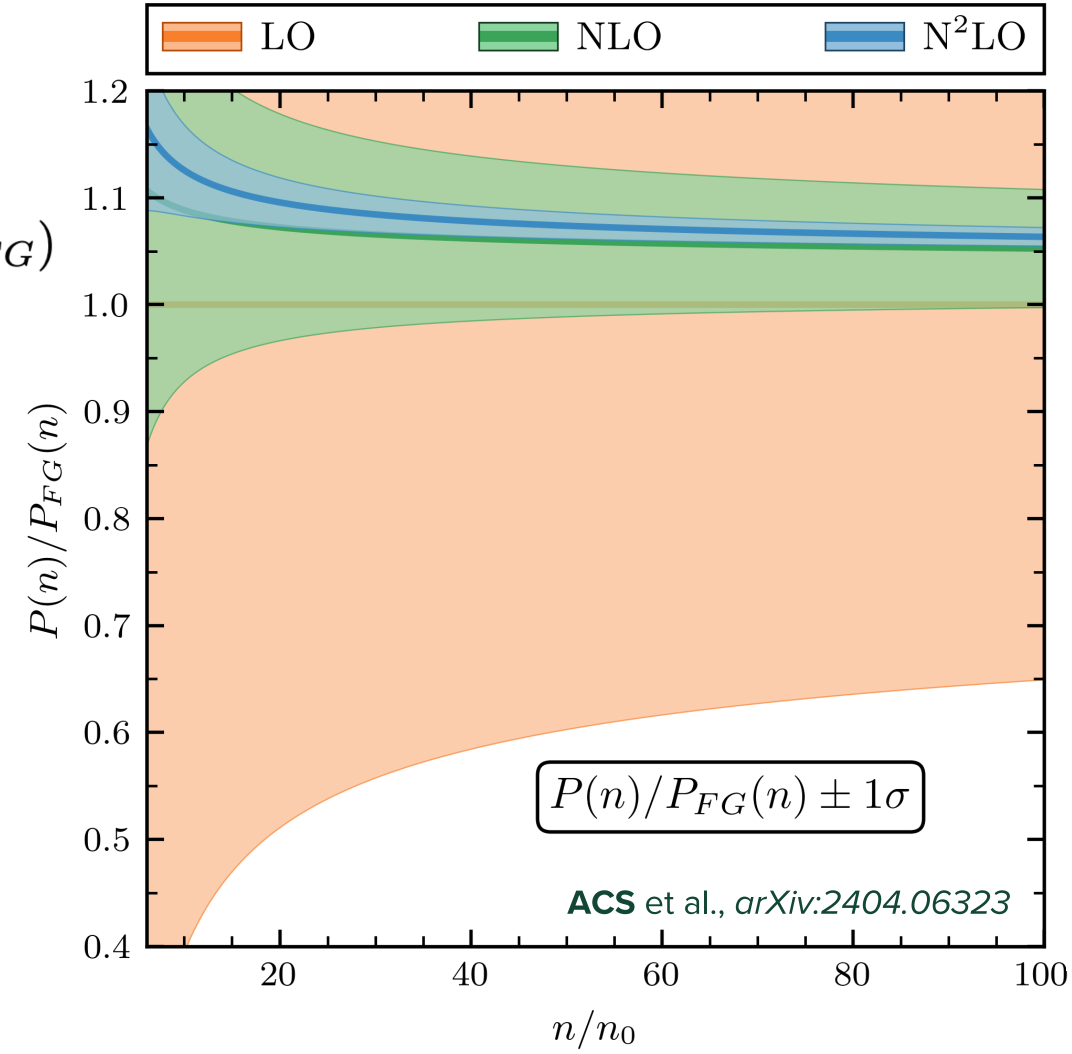
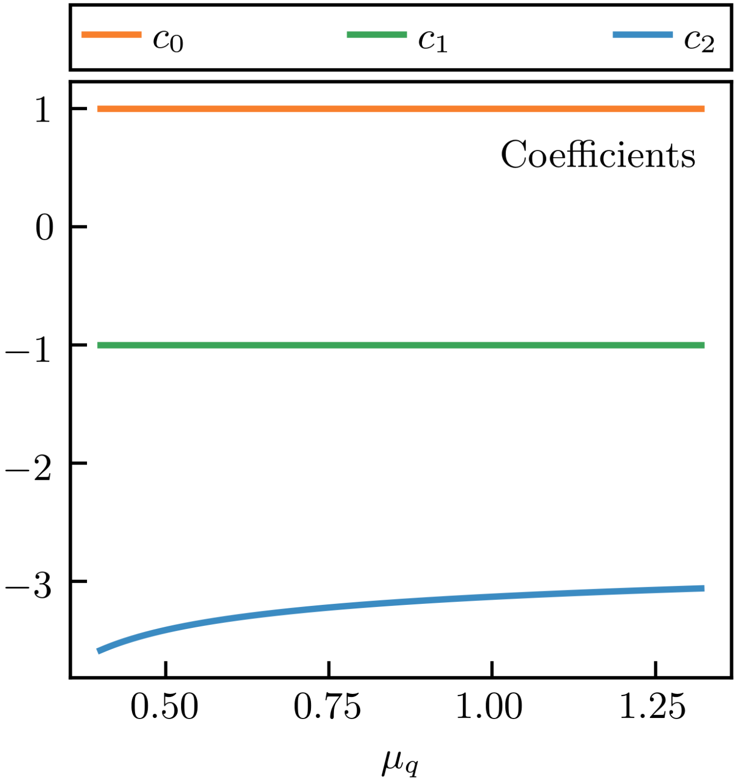
Apply **gsum** to **P(n)**

$$Q = \frac{N_f}{\pi}\alpha_s(\bar{\Lambda})$$

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





Truncation error often assessed by varying renormalization scale to obtain band---not as statistically rigorous

* See newer works by Gorda et al. (2022, 2023), MiHO model for higher orders

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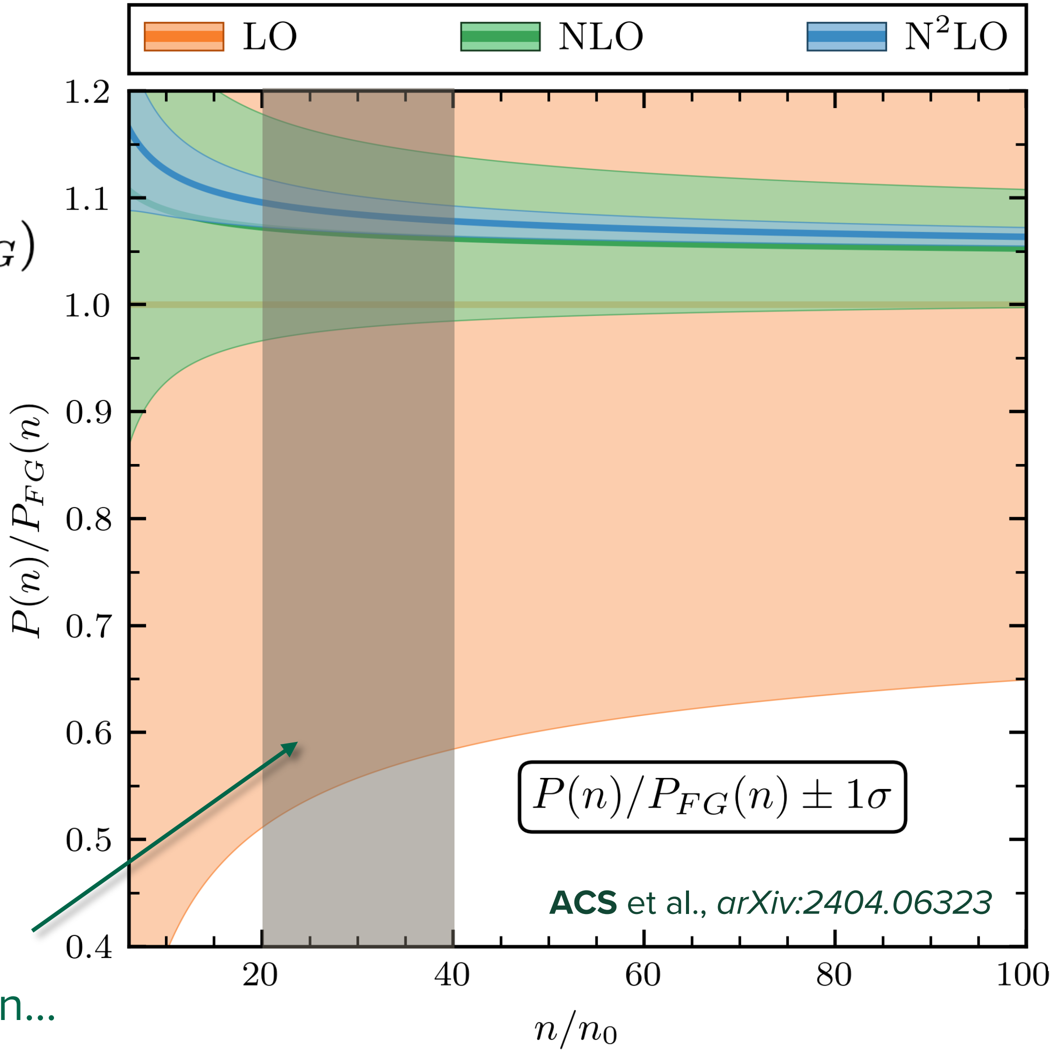
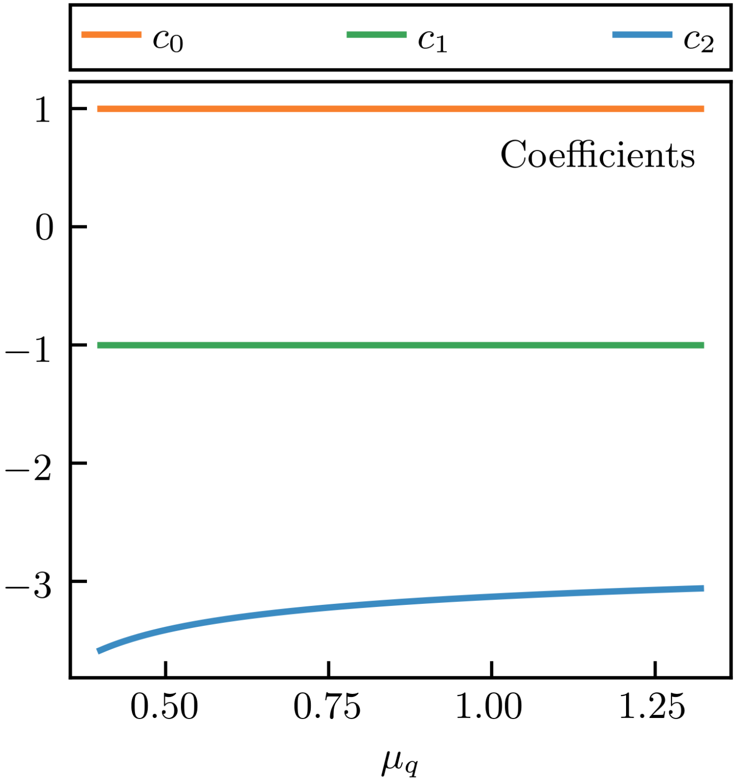
Nonperturbative effects under (20-40) n_0: pairing, hadronization...





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High densities: pQCD EOS

Calculate **speed of sound** squared:

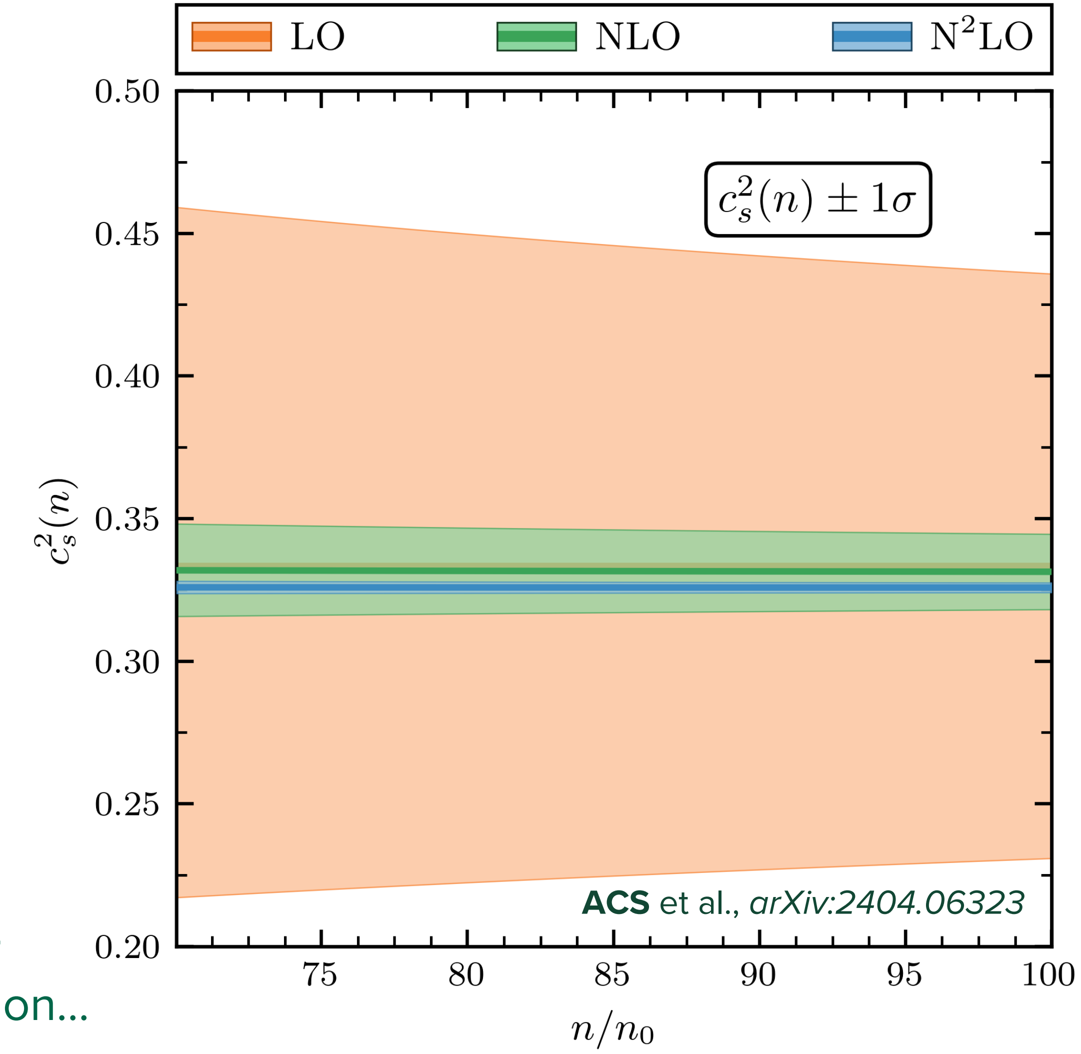
$$c_s^2(n) = n\frac{\partial \ln(\mu(n))}{\partial n}$$

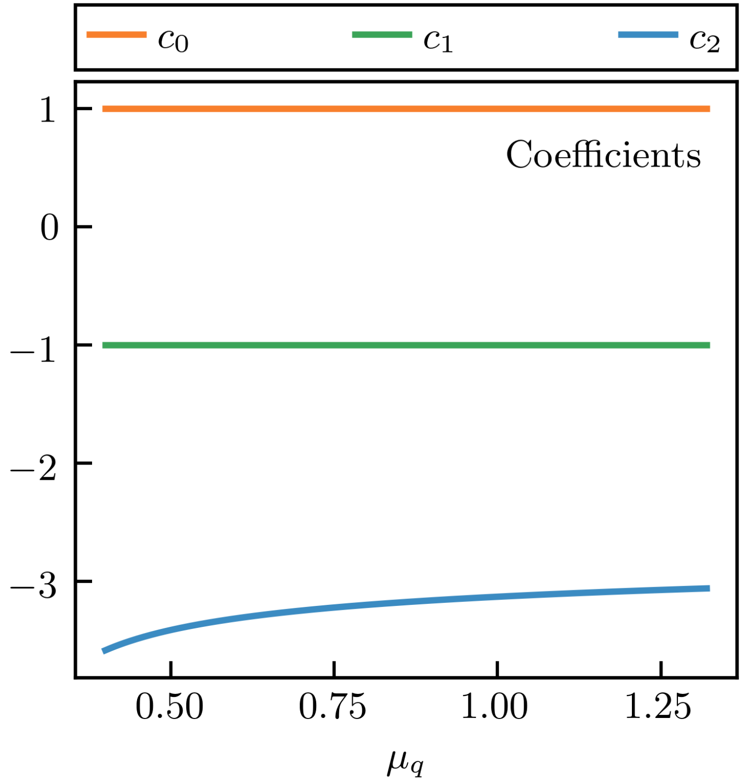
[**Equal** at N^{2}LO to the calculation of $c_s^2(\mu)$ using the pressure directly]

Q = $\frac{N_f}{\pi}\alpha_s(\bar{\Lambda})$

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

Nonperturbative effects under (20-40) n_0: pairing, hadronization...





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BAND collaboration: efforts

Bayesian Analysis of Nuclear Dynamics

v0.4 coming soon!

https://github.com/bandframework/bandframework

Cyber-infrastructure

Develop tools for nuclear physics community

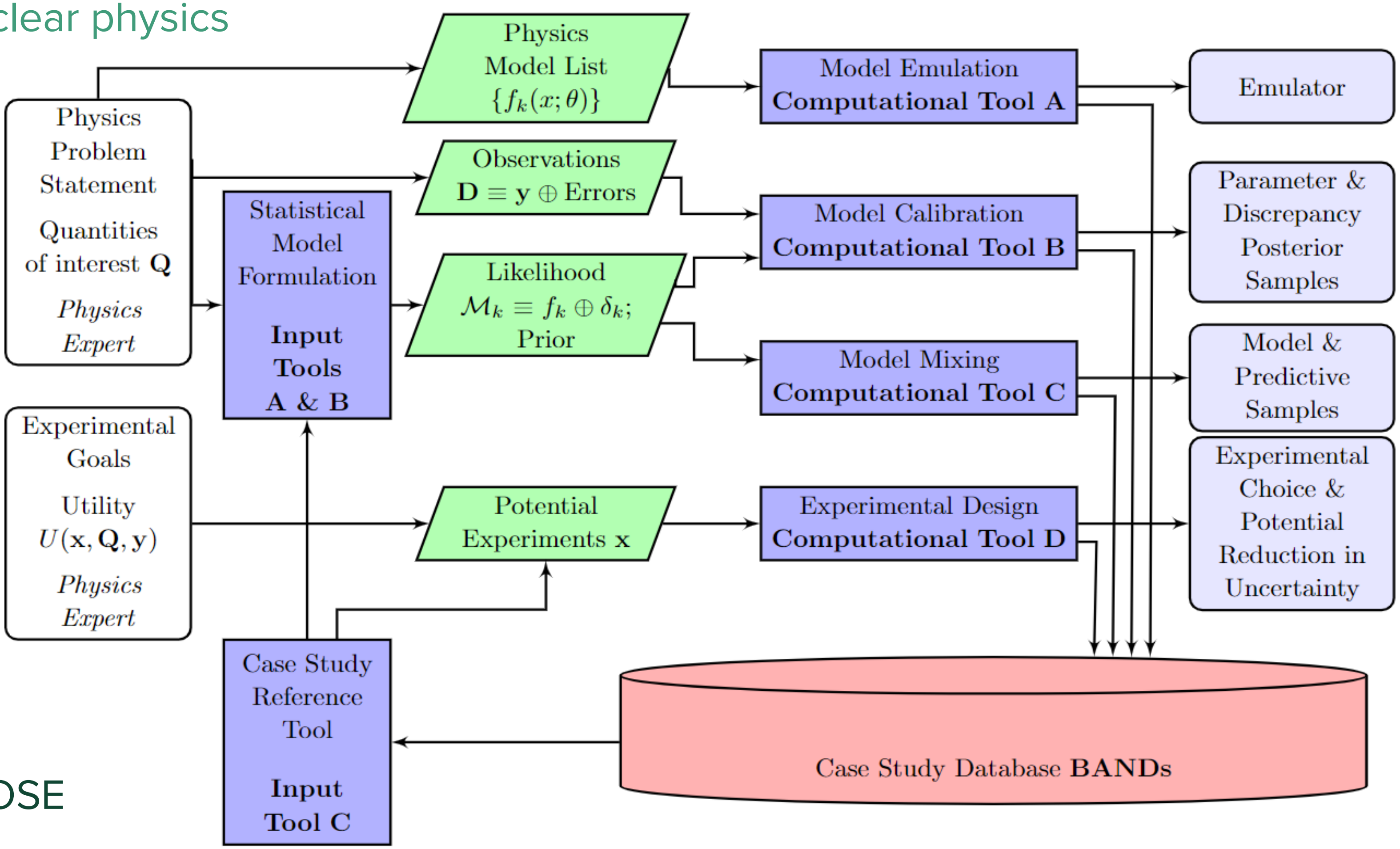
Test on toy models and real-world applications

ParMOO

BMEX

surmise

ROSE



Our model mixing software!

SAMBA

Taweret

Truncation error: gsum and GPs

GP: governed by mean function and covariance function

$$\delta y_k(x) \,|\, \boldsymbol{\theta}, Q \sim \mathcal{GP}[m_{\delta k}(x), \bar{c}^2 R_{\delta k}(x, x'; \ell)] \longleftarrow \begin{array}{c} c_n(x) \,|\, \boldsymbol{\theta} \overset{\text{iid}}{\sim} \mathcal{GP}[\mu, \bar{c}^2 r(x, x'; \ell)], \\ \boldsymbol{\theta} \equiv \{\mu, \bar{c}^2, \ell\}. \end{array} \longrightarrow$$

$$m_{\delta k}(x) \equiv y_{\text{ref}}(x) \frac{Q(x)^{k+1}}{1 - Q(x)} \mu \equiv b_{\delta k}(x) \mu$$

$$R_{\delta k}(x, x'; \ell) \equiv y_{\text{ref}}(x) y_{\text{ref}}(x') \frac{[Q(x)Q(x')]^{k+1}}{1 - Q(x)Q(x')} r(x, x'; \ell)$$

Hyperparameter estimation

Results insensitive to exact form, so use conjugate priors $\mu, \bar{c}^2 \sim \mathrm{N}\chi^{-2}(\eta_0, V_0, \nu_0, \tau_0^2)$

Diagnostic tests for assessing the calibration of the GP

Squared Mahalanobis distance: multi-dimensional sum of squared residuals

$$\mathrm{D}^2_{\mathrm{MD}}(\mathbf{f}_{\text{val}}) = (\mathbf{f}_{\text{val}} - \mathbf{m})^\intercal K^{-1} (\mathbf{f}_{\text{val}} - \mathbf{m})$$

Pivoted Cholesky decomposition: pinpoints data that is yielding a failing MD

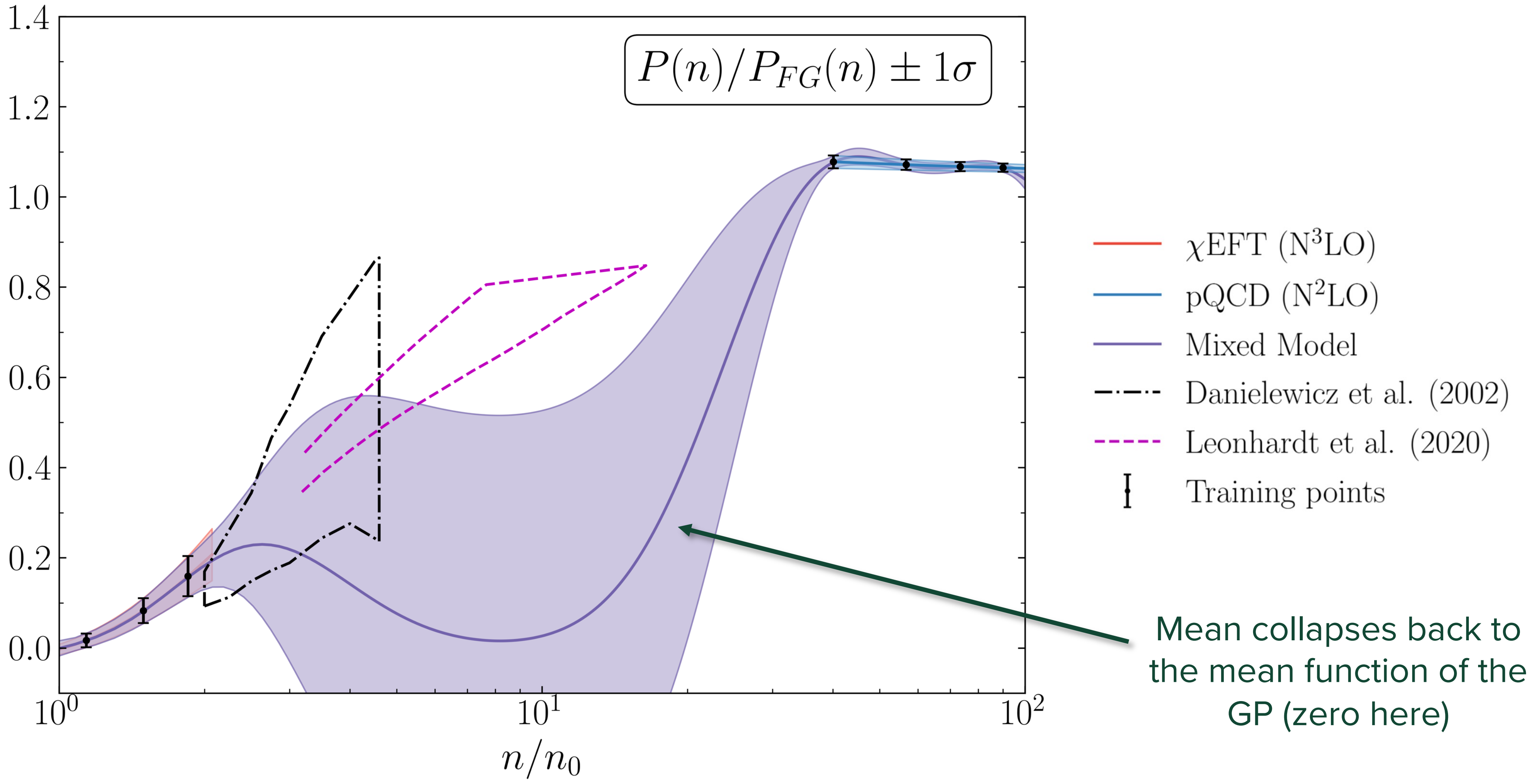
$$K = GG^\intercal \longrightarrow \mathbf{D}_G = G^{-1}(\mathbf{f}_{\text{val}} - \mathbf{m})$$

Credible interval diagnostic: testing accuracy of the emulator

$$\mathrm{D}_{\mathrm{CI}}(\alpha, \mathbf{f}_{\text{val}}) = \frac{1}{M} \sum_{i=1}^{M} \mathbf{1}[f_i \in \mathrm{CI}_i(\alpha)]$$

All equations from J. Melendez et al. (2020)

Extreme case: very short lengthscale



Mean collapses back to the mean function of the GP (zero here)

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Results: pointwise approach

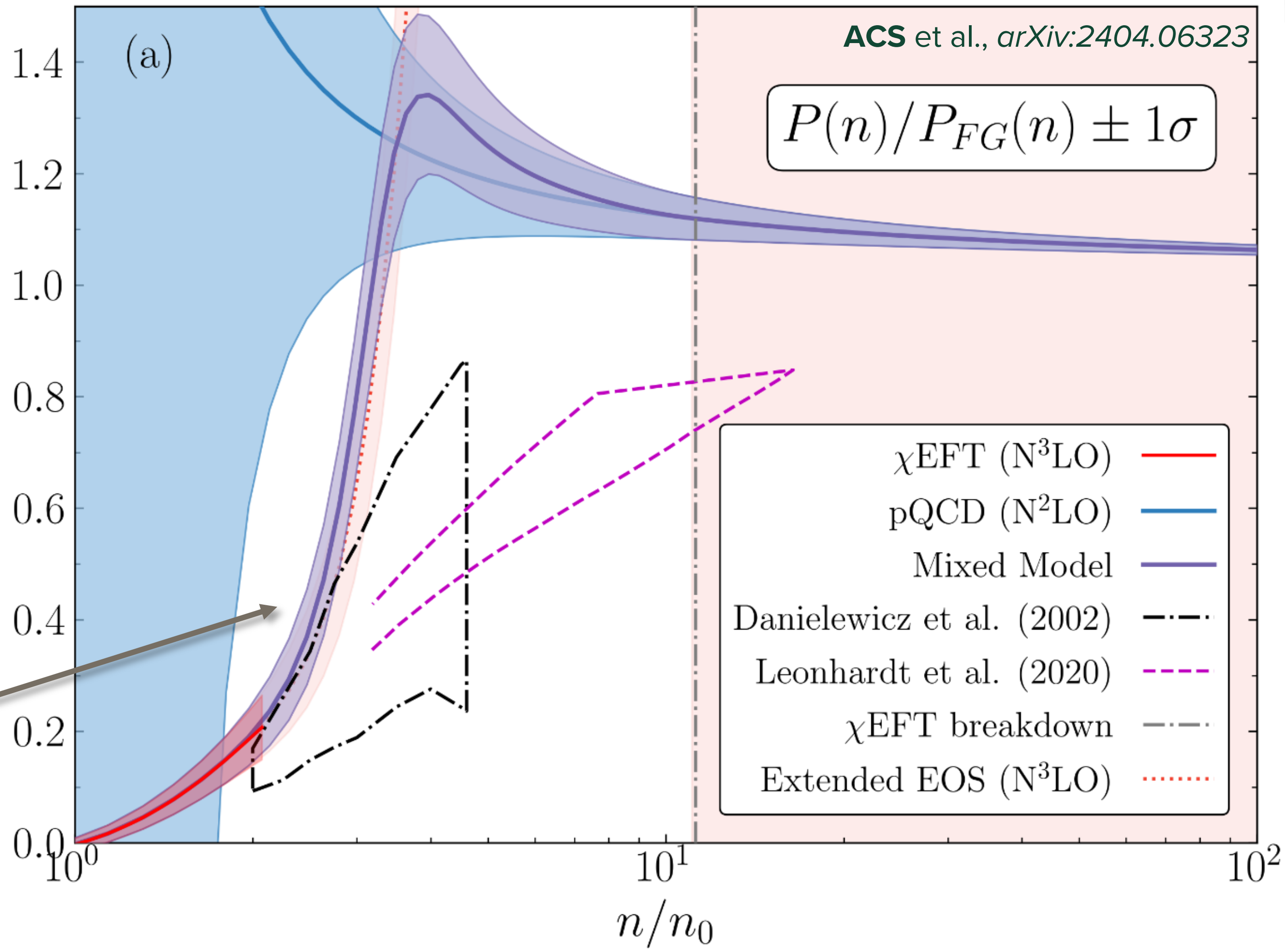
BMM using the pointwise approach

$$\mu = \frac{1}{Z_P}\sum_{i=1}^{M}\frac{1}{\sigma_i^2}y_i,$$

$$\Sigma^{-1} \equiv \sum_{i=1}^{M}\frac{1}{\sigma_i^2}$$

Extended EOS from chiral EFT with PAL EOS to have estimates across total density region

Prakash, Ainsworth, Lattimer (1988)



BAND Bayesian Analysis of Nuclear Dynamics

Performed using ***Taweret***

Taweret arXiv: 2310.20549

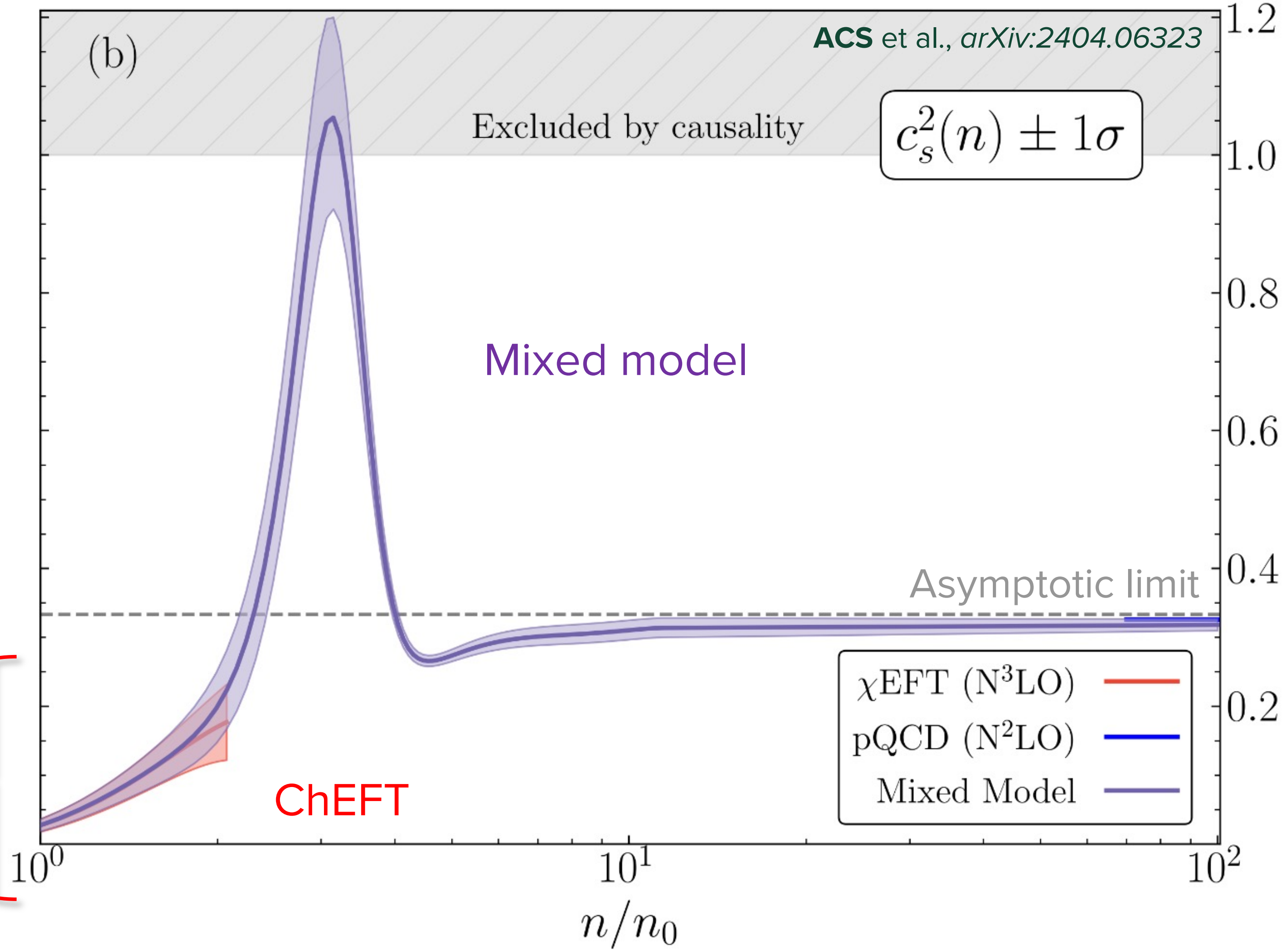
Rapidly increasing EOS from crossover to pQCD

Complete agreement with chiral EFT and pQCD uncertainties in the two limits

Some agreement with heavy-ion data, no overlap with FRG contour

Requires information at all densities from both theories!

Results: speed of sound



Good agreement with ChEFT EOS

pQCD

Mixed model approaching 0.33 asymptotically from below (expected)

Acausal EOS