

*Bridging the gap:*  
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:2404.06323

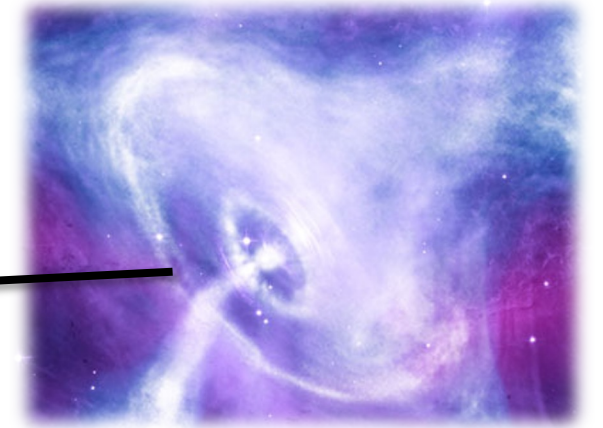
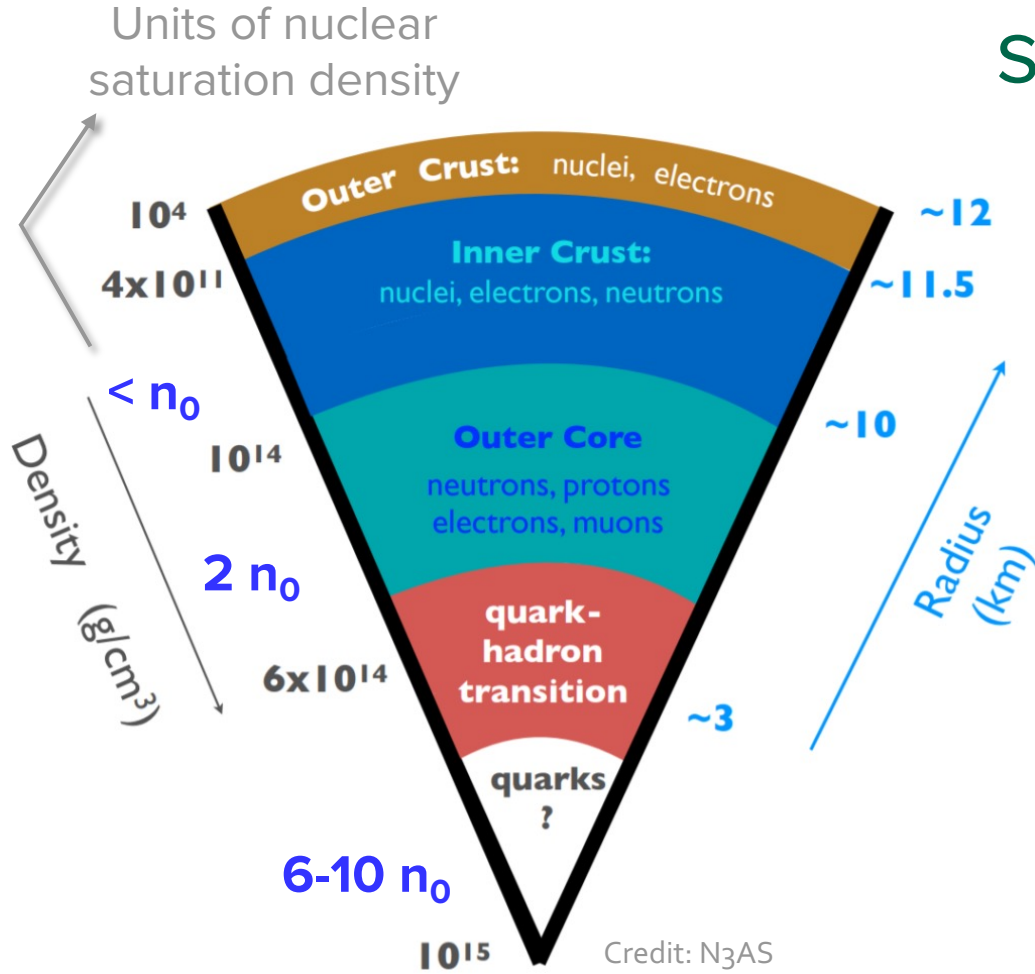


# Motivation: the equation of state (EOS)



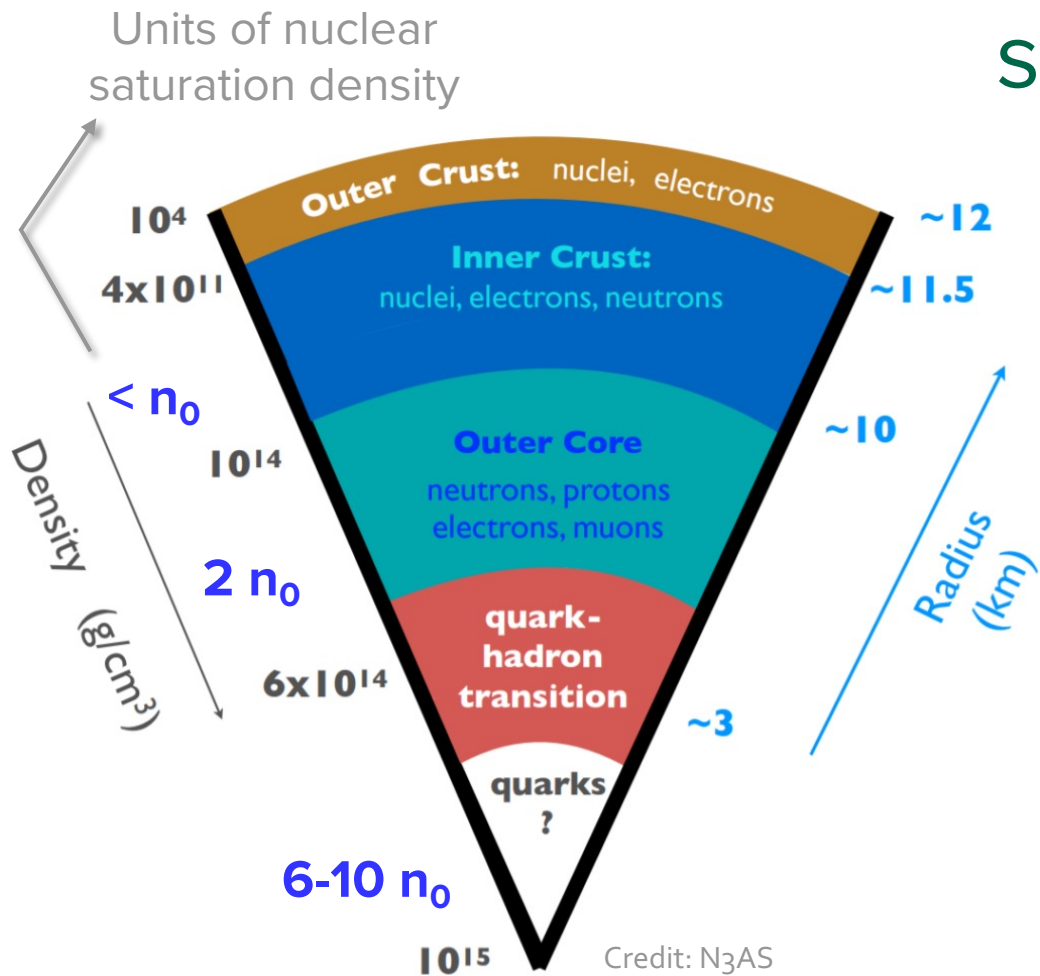
Credit: NASA

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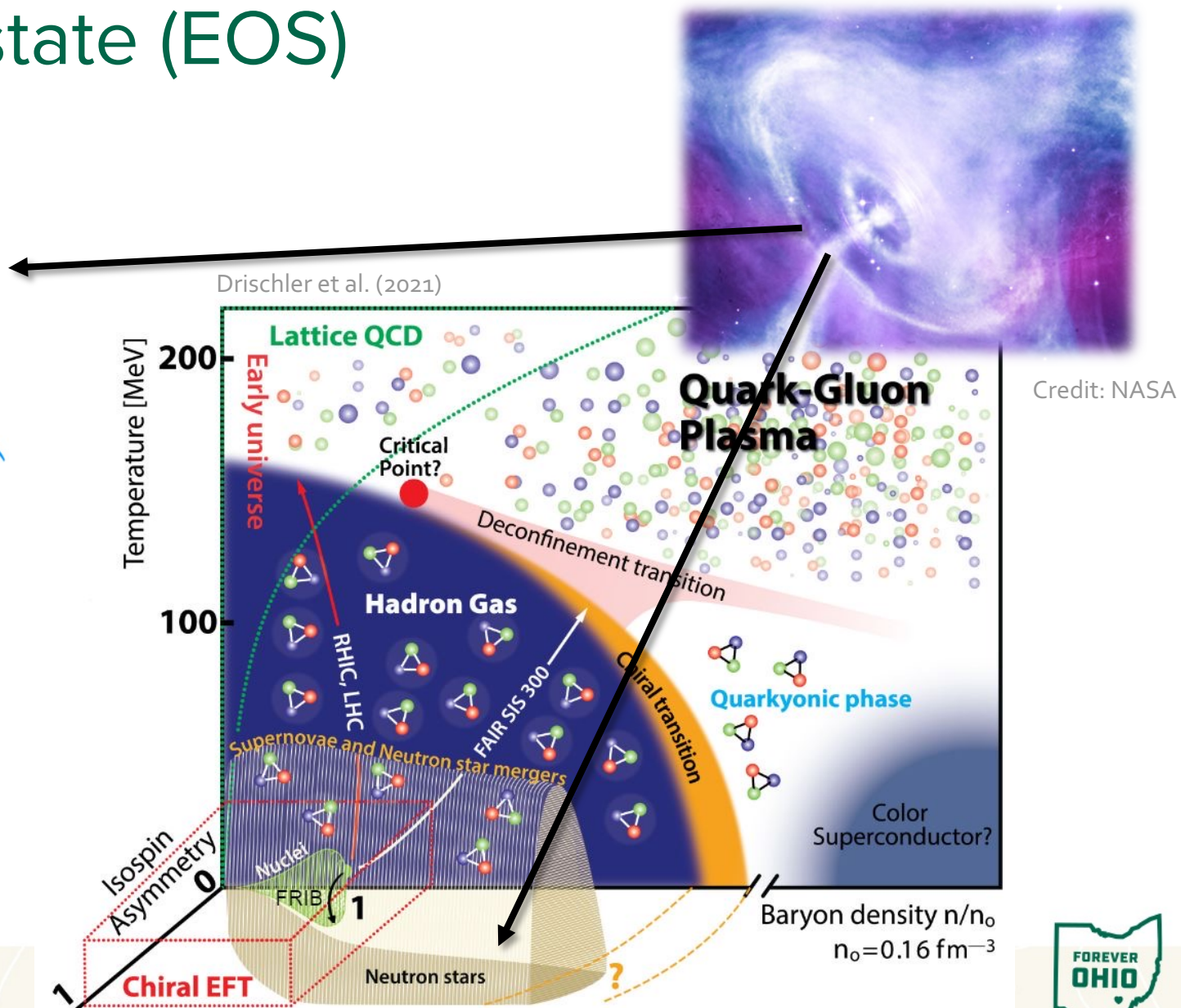


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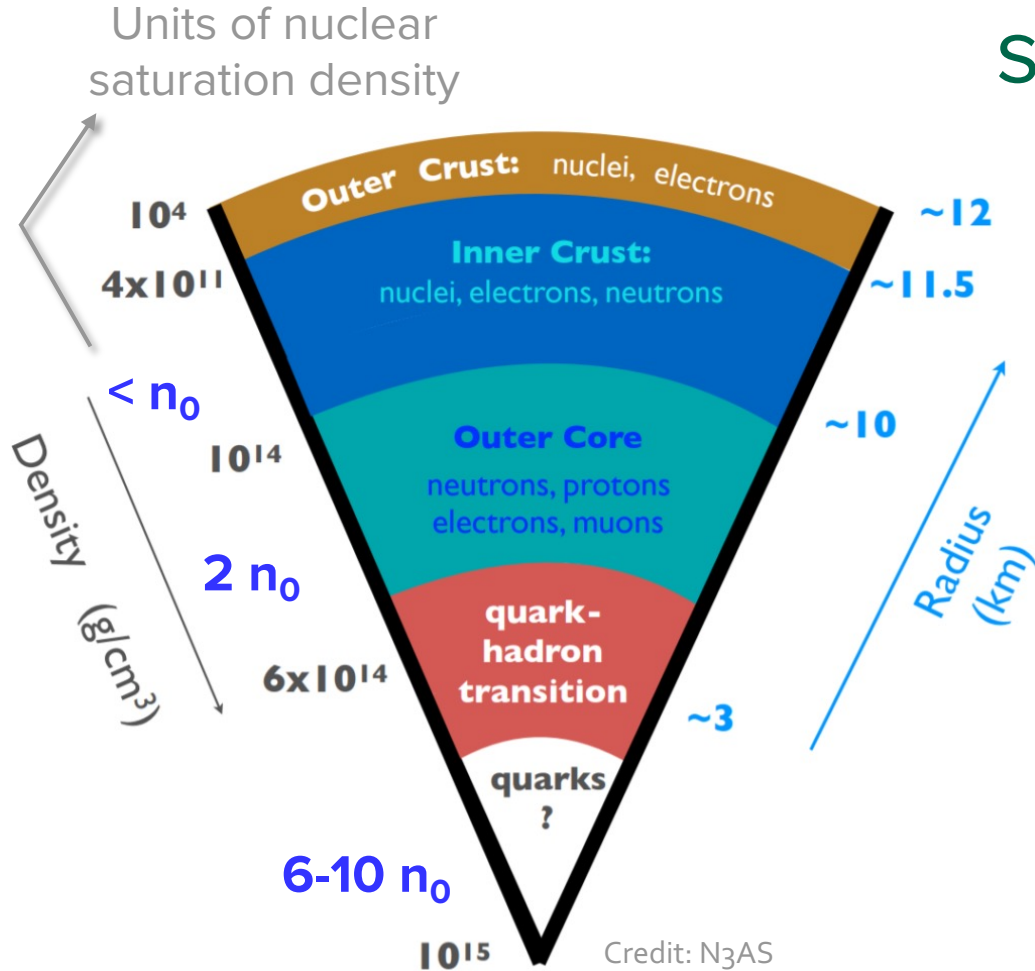
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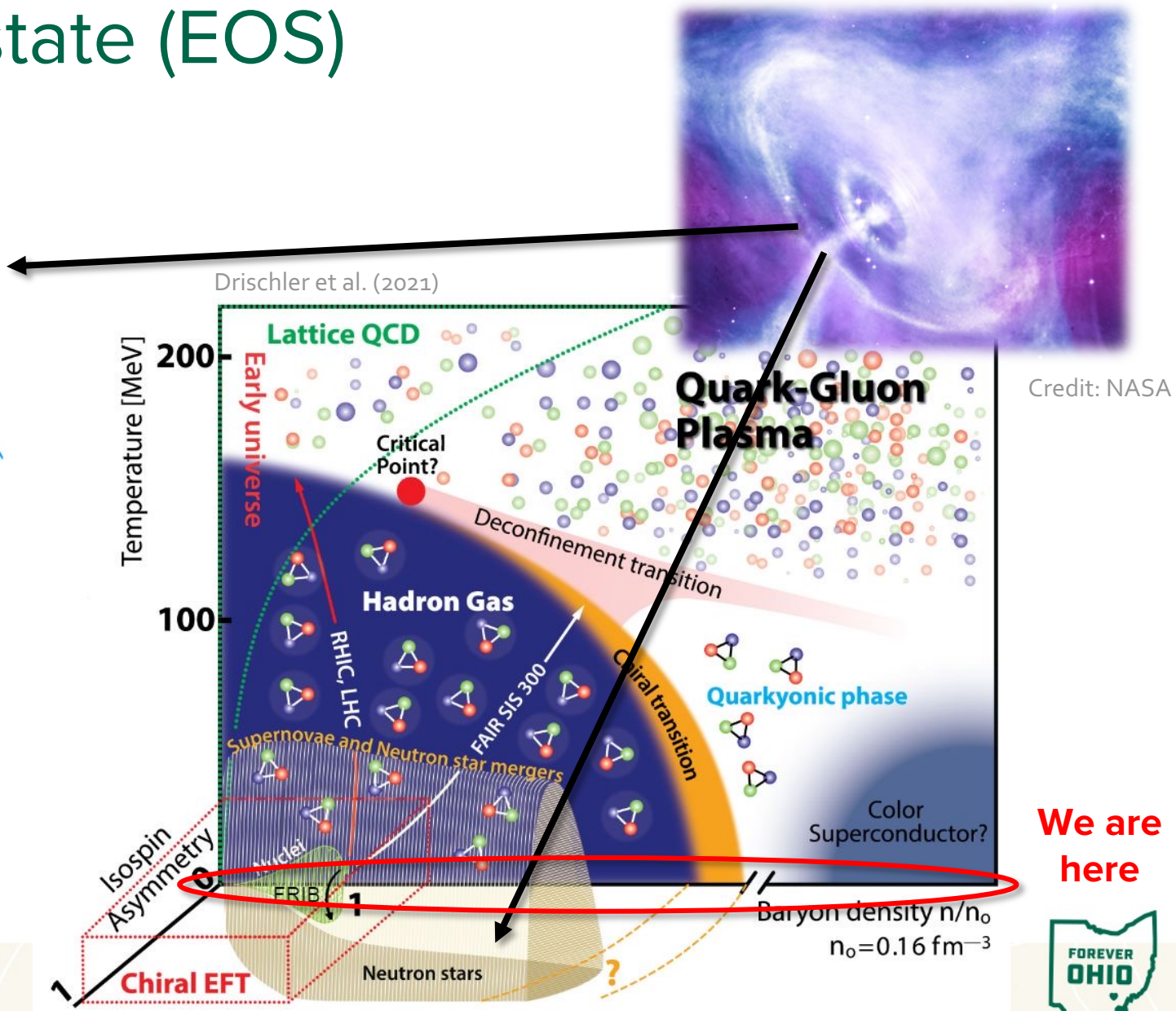
EOS describes the state of matter from nuclei to neutron stars to quarks and deconfinement



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We are here

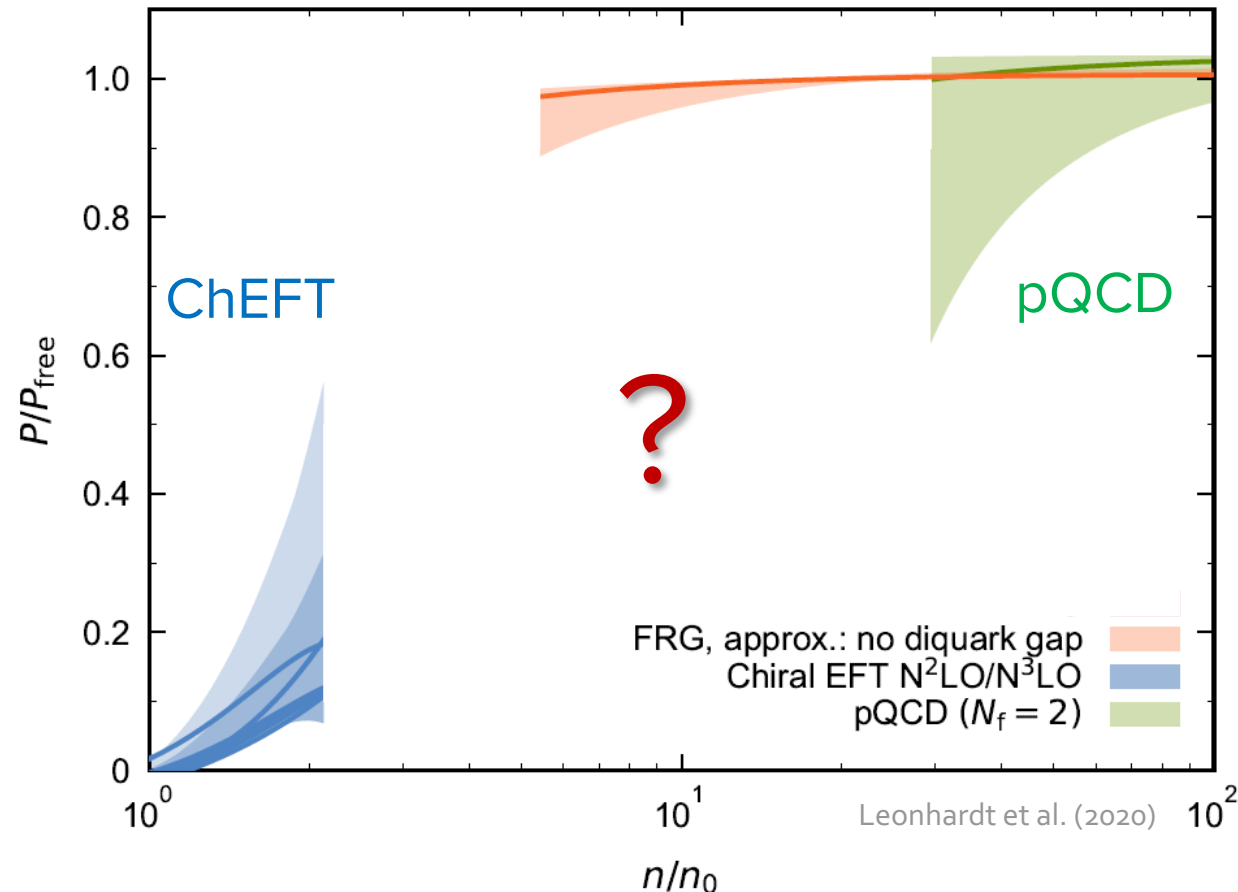


# Motivation: between two extremes

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

Symmetric Nuclear Matter  
(50% n, 50% p)

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



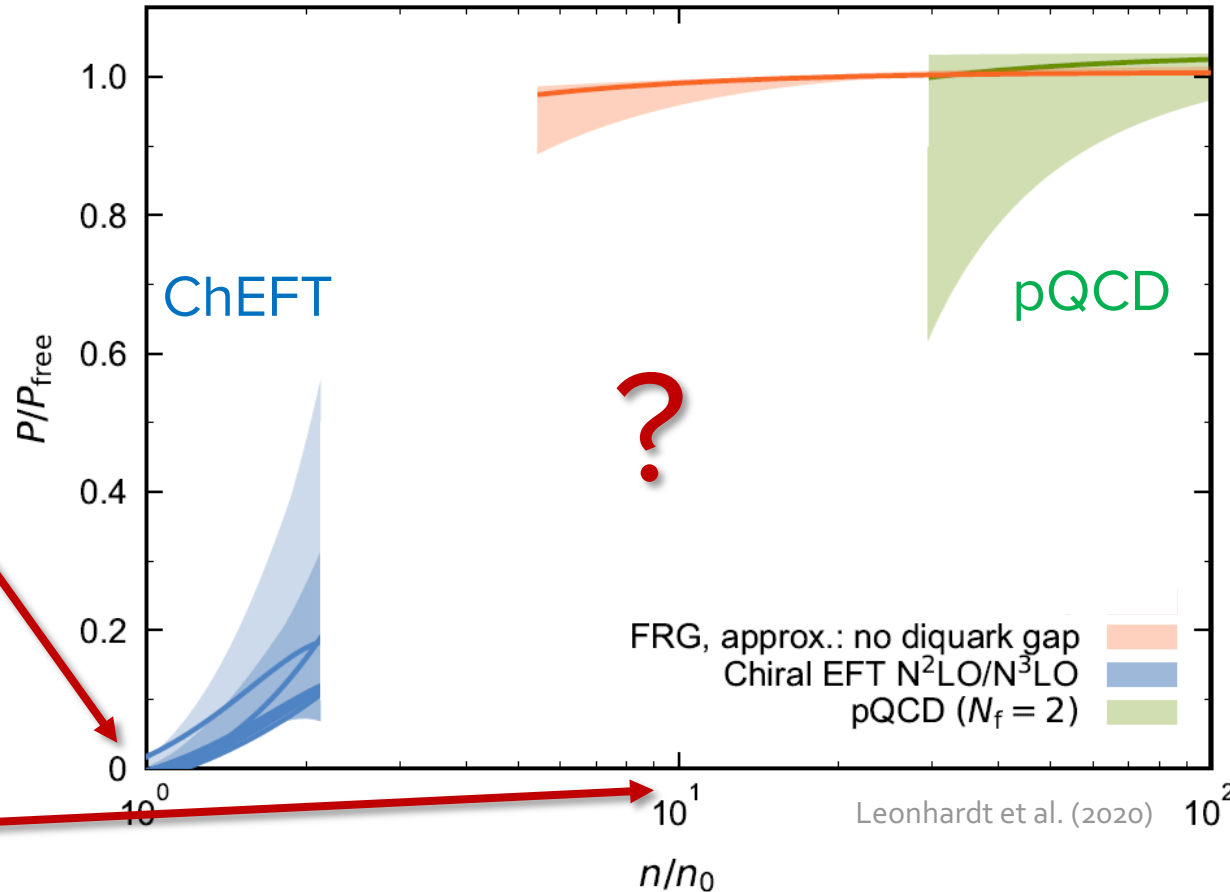
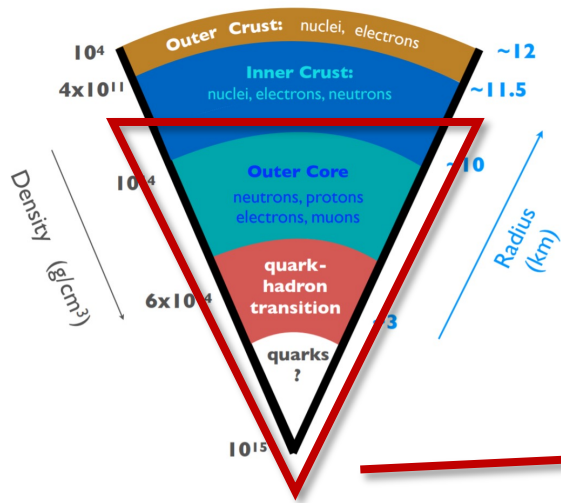
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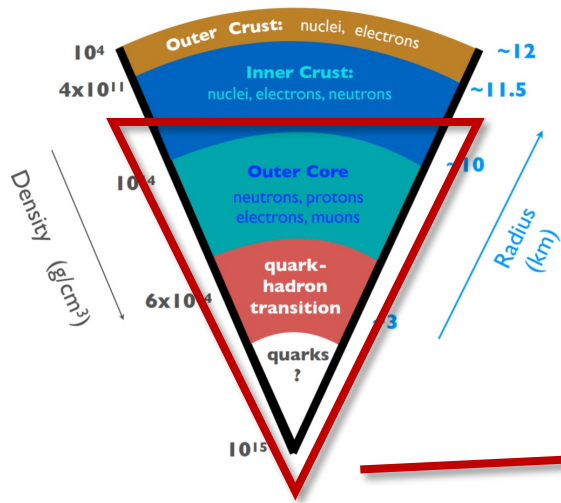
Low densities can be described by  $\chi$ EFT, constraints from heavy-ion collisions



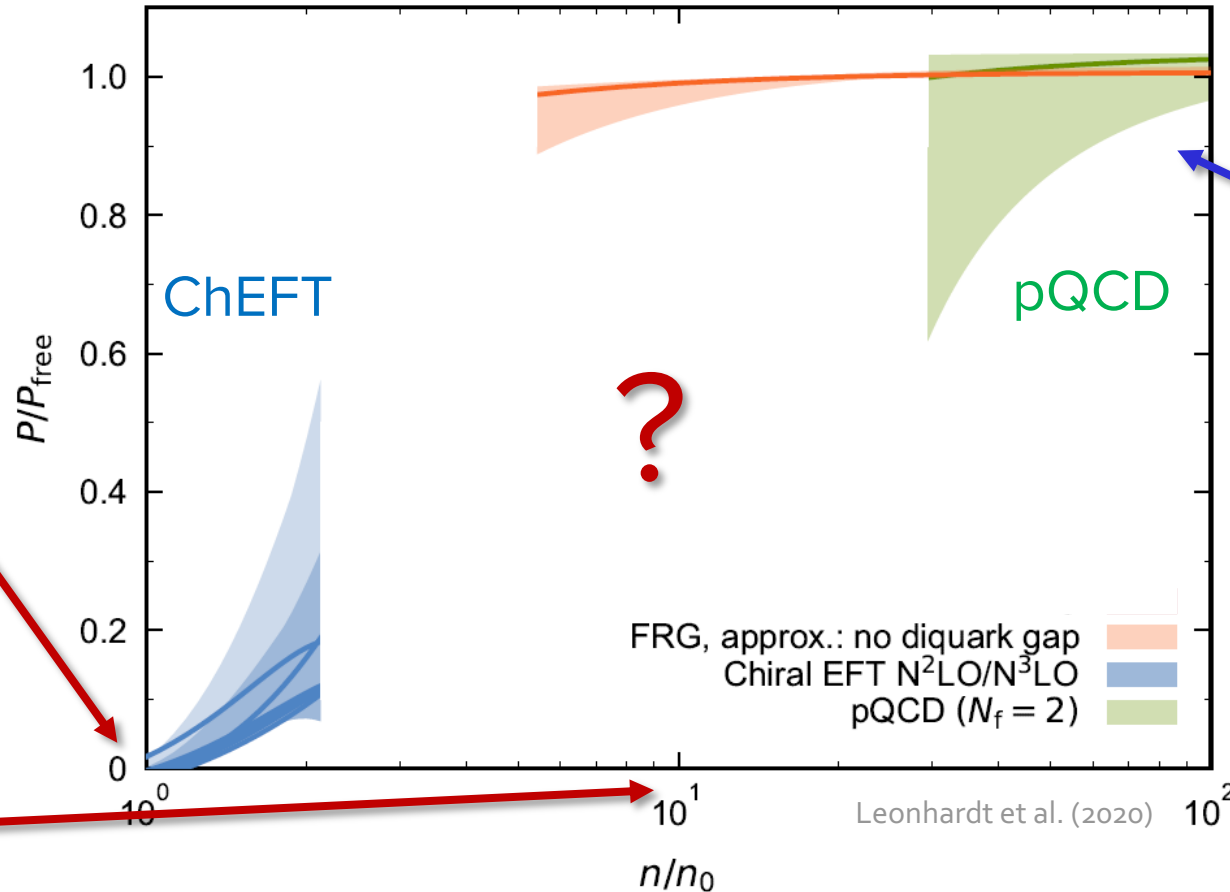
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FRG EOS in the gap, but uncertainties are not well-quantified (yet!) ...



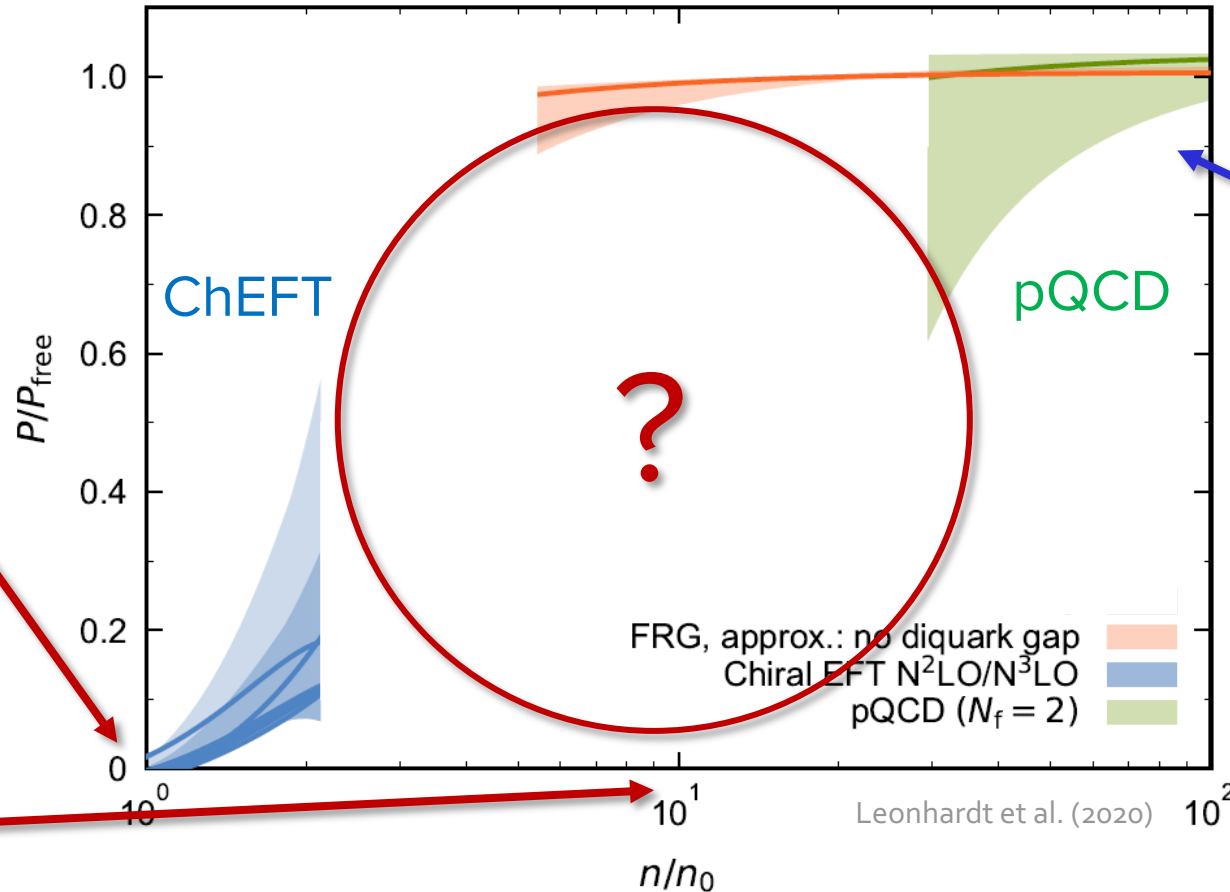
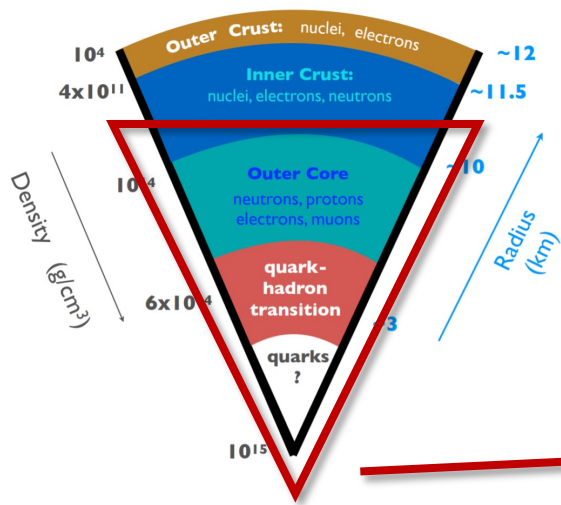
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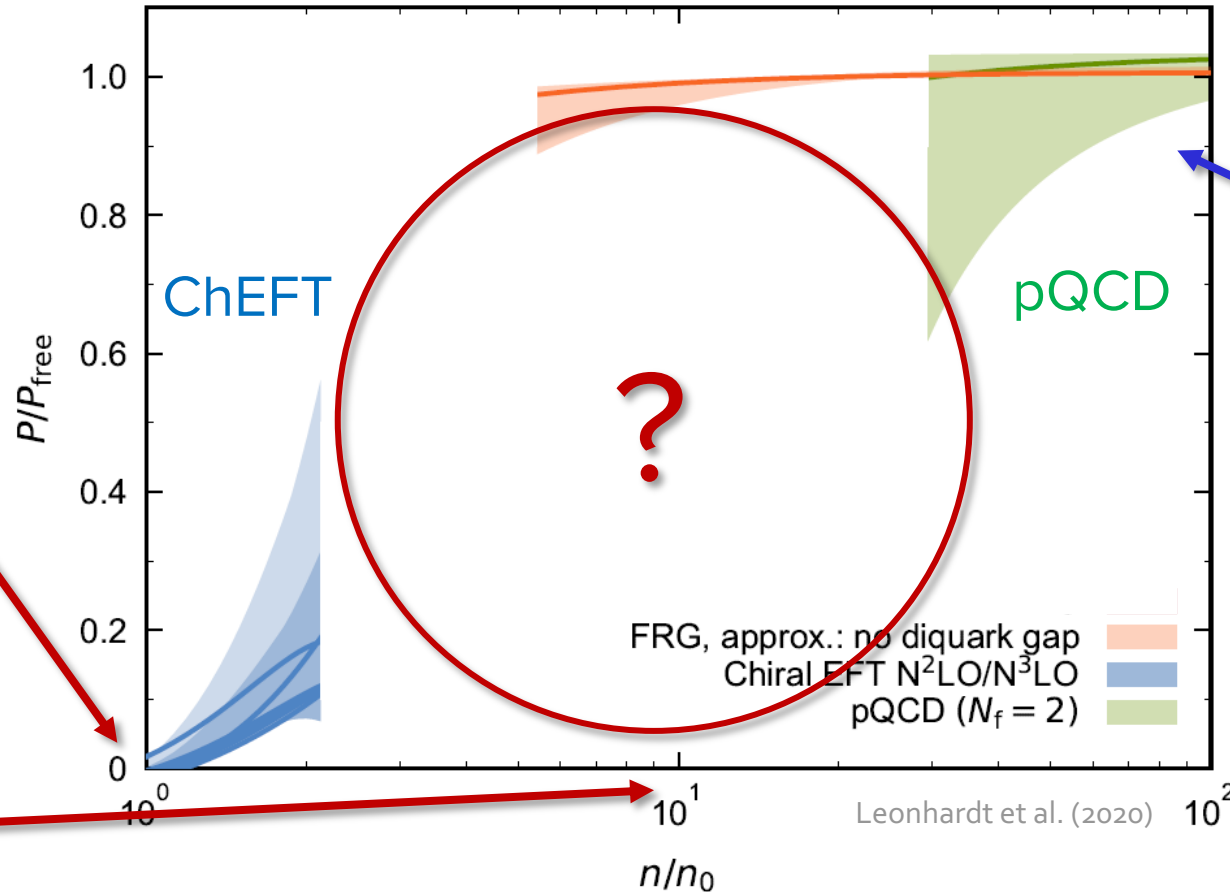
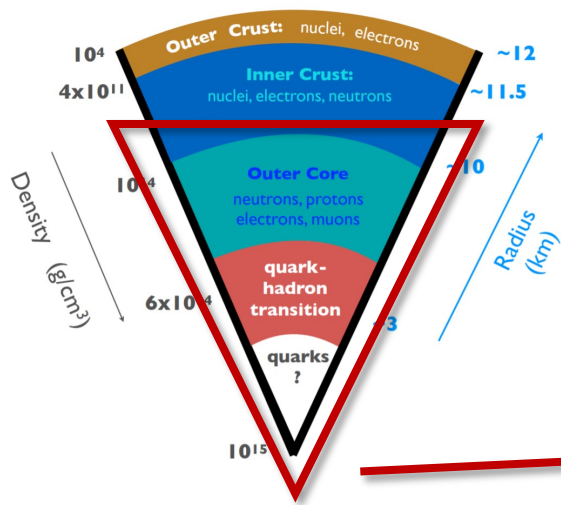
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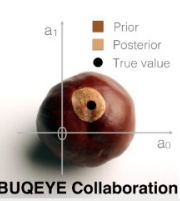
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Bayes your way to victory! Bayesian model mixing (BMM)!



# “Low” densities: EOS from chiral EFT



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

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

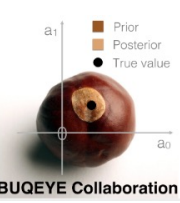
Quantifiable truncation error, obeys all symmetries of QCD

	NN forces	3N forces
LO ( $Q^0$ )	(1990) <span style="float: right;">2</span>	—
NLO ( $Q^2$ )	(1992) <span style="float: right;">7</span>	— (1992 94)
N <sup>2</sup> LO ( $Q^3$ )	(1992) <span style="float: right;">0</span>	(1994) <span style="float: right;">2</span>
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C. Drischler, S. Bogner (2021)

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

$$\mathcal{E}_{3,pp}(k_F) = \text{diagram}$$

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

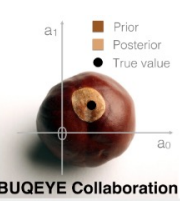
\*A choice, not a necessity--- BMM framework is model-independent

$$\langle \mathbf{2}' \mathbf{3}' | V_{NN}^{\text{med}} | \mathbf{23} \rangle = \text{diagram}$$

C. Drischler, J. Holt, C. Wellenhofer (2021)



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C. Drischler, S. Bogner (2021)

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

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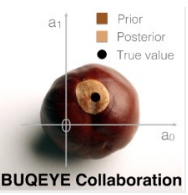
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# Uncertainty quantification for the EOS

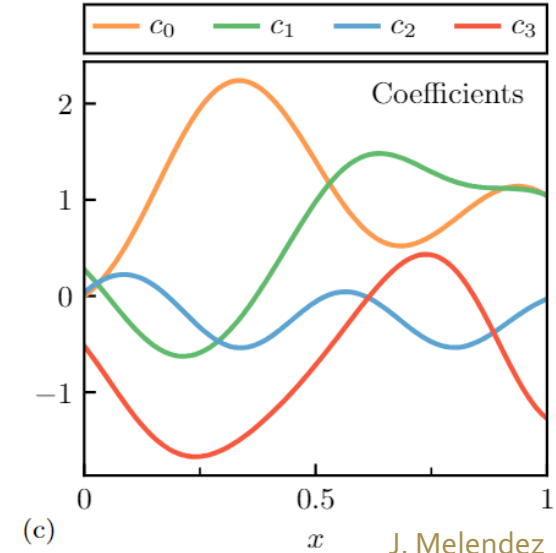
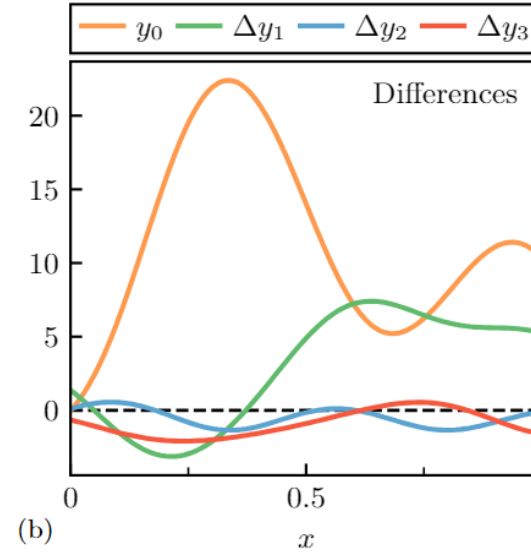
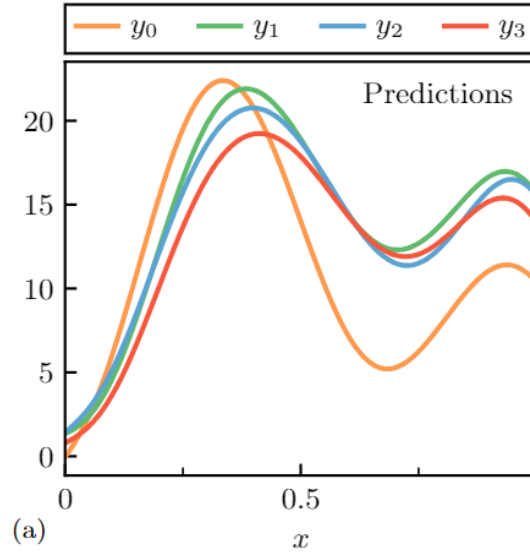


Employ the BUQEYE truncation error model (**gsum**)



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

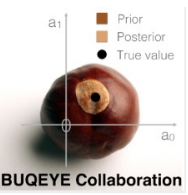
Known orders of expansion



J. Melendez et al. (2019)



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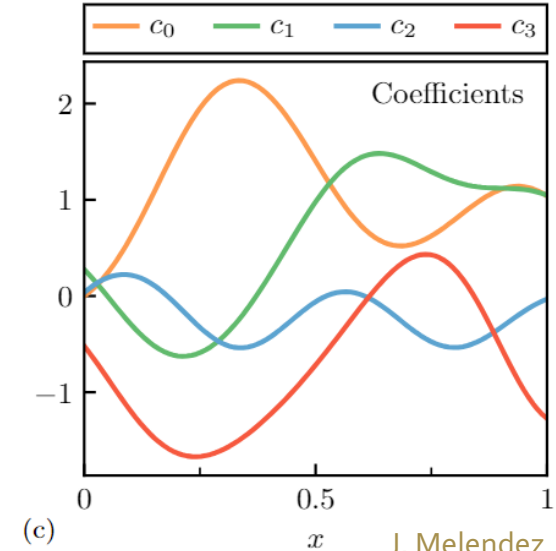
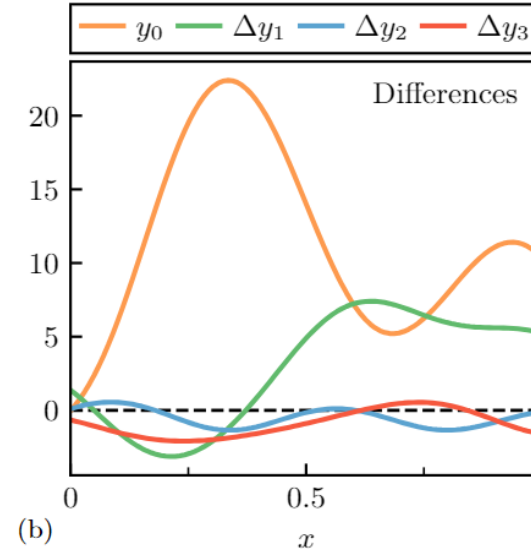
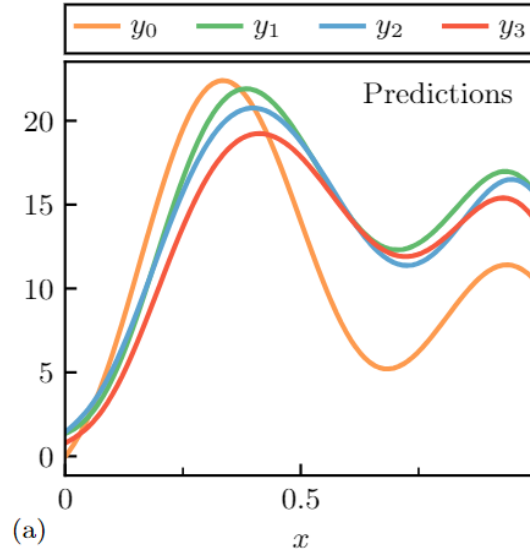


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Estimations for unknown orders

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

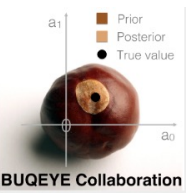
Dimensional analysis

Natural i.i.d. curves

Expansion parameter (suppresses higher orders)



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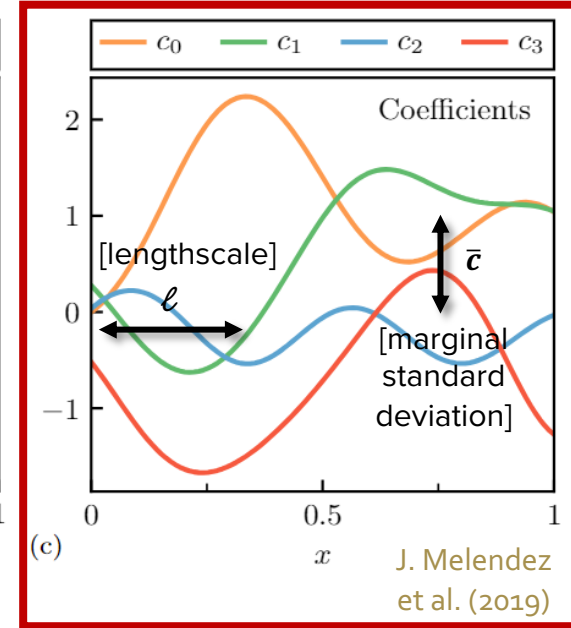
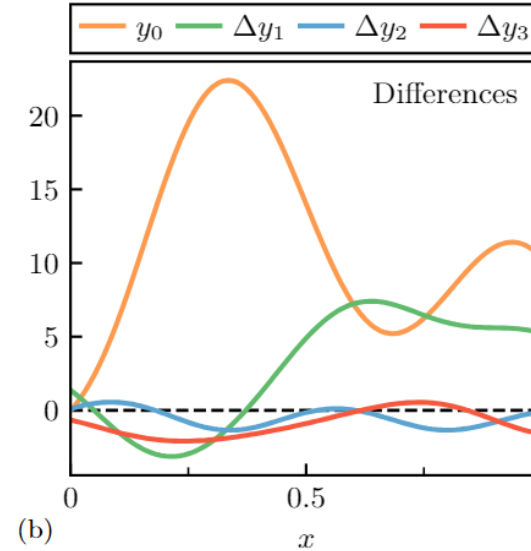
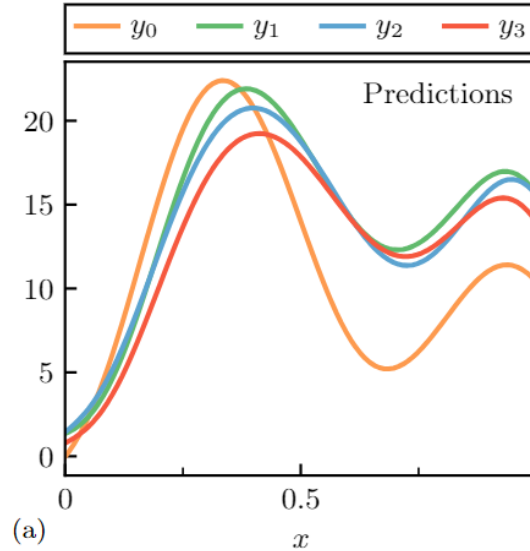


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**Gaussian Processes:** learn coefficient distributions

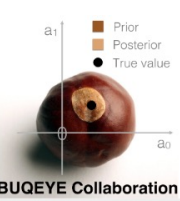
Incorporates correlations in  $y(x)$ , continuous model, priors constrain parameters of GP

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





# “Low” densities: EOS from chiral EFT



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

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

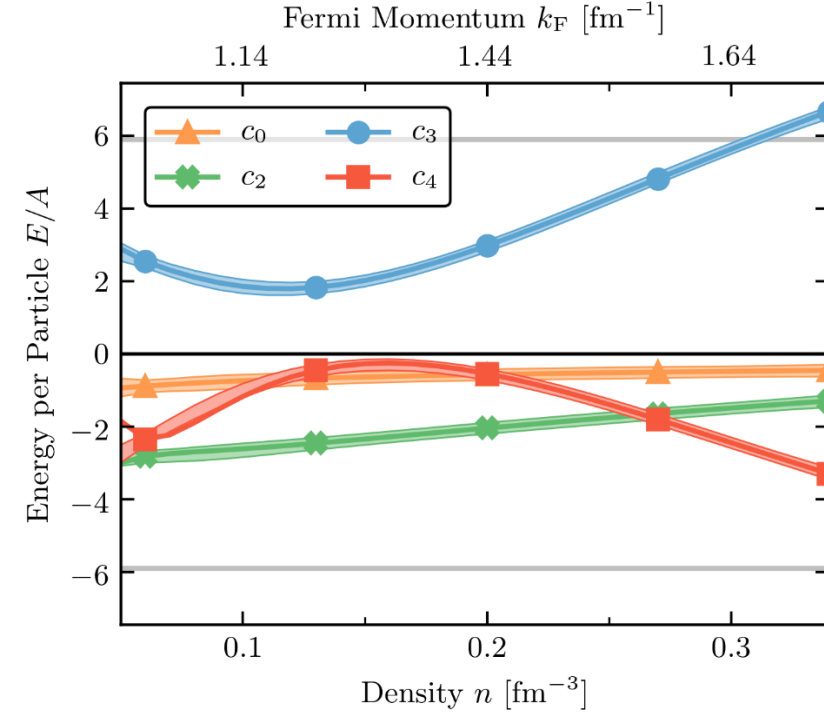
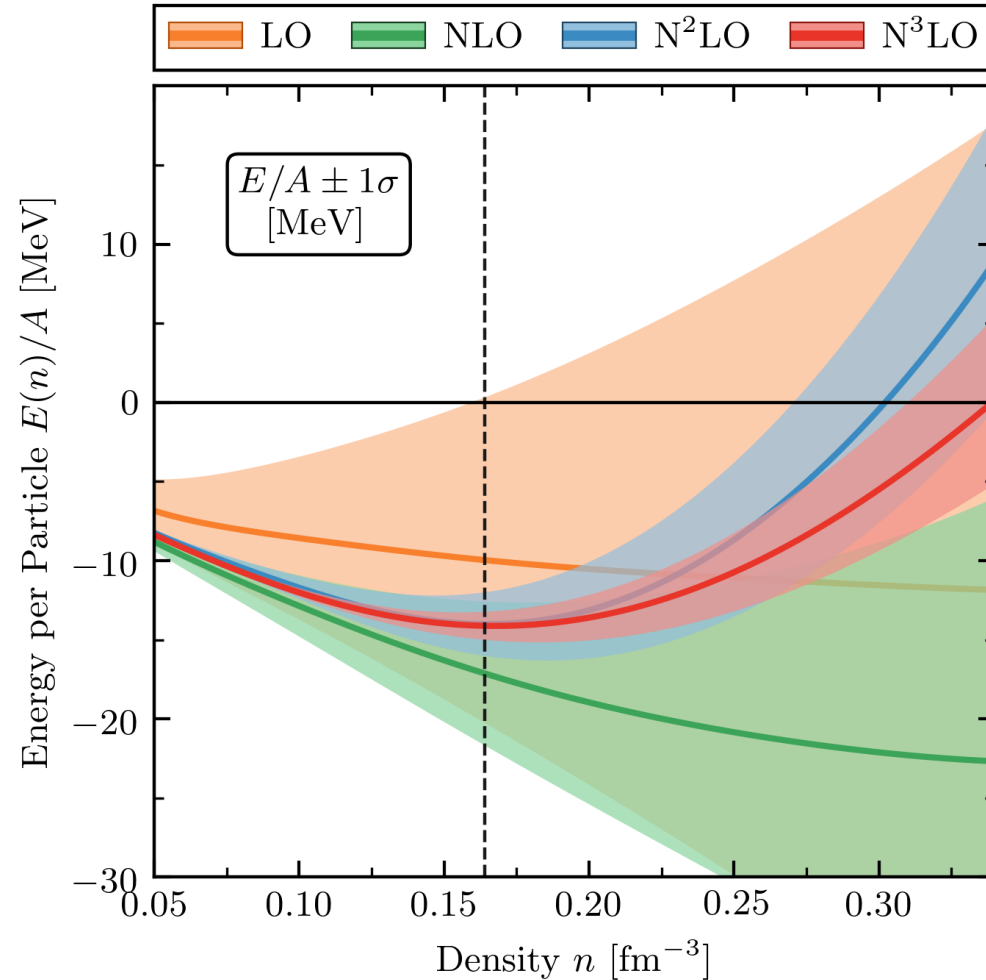


Coefficient extraction for truncation error estimation done via **gsum**

$$Q(k_F) = \frac{k_F}{\Lambda_b} \rightarrow \approx 600 \text{ MeV}$$

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

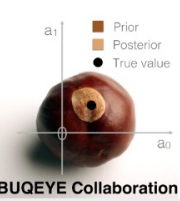
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Truncation error scheme yields natural-sized curves as expected



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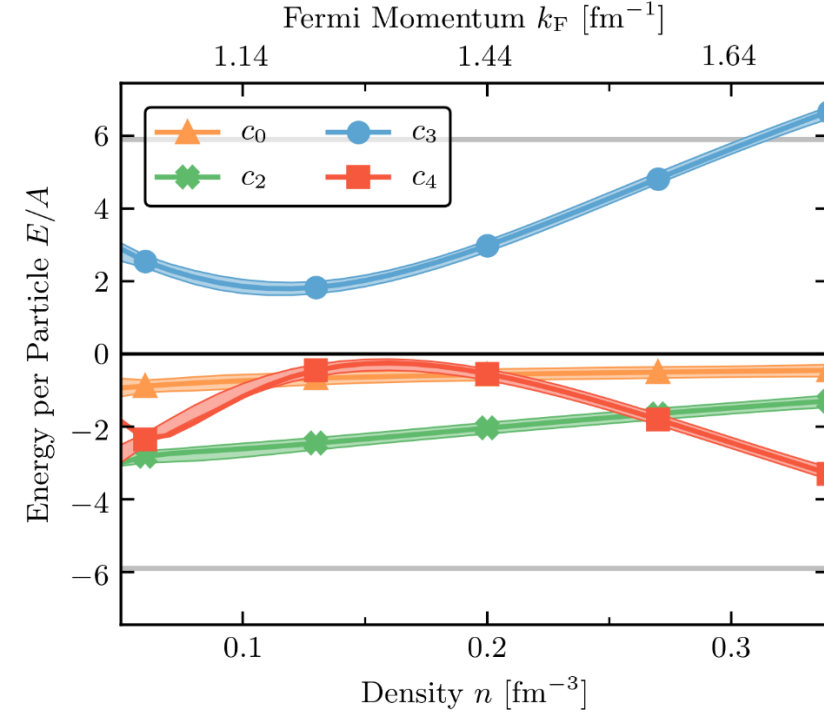
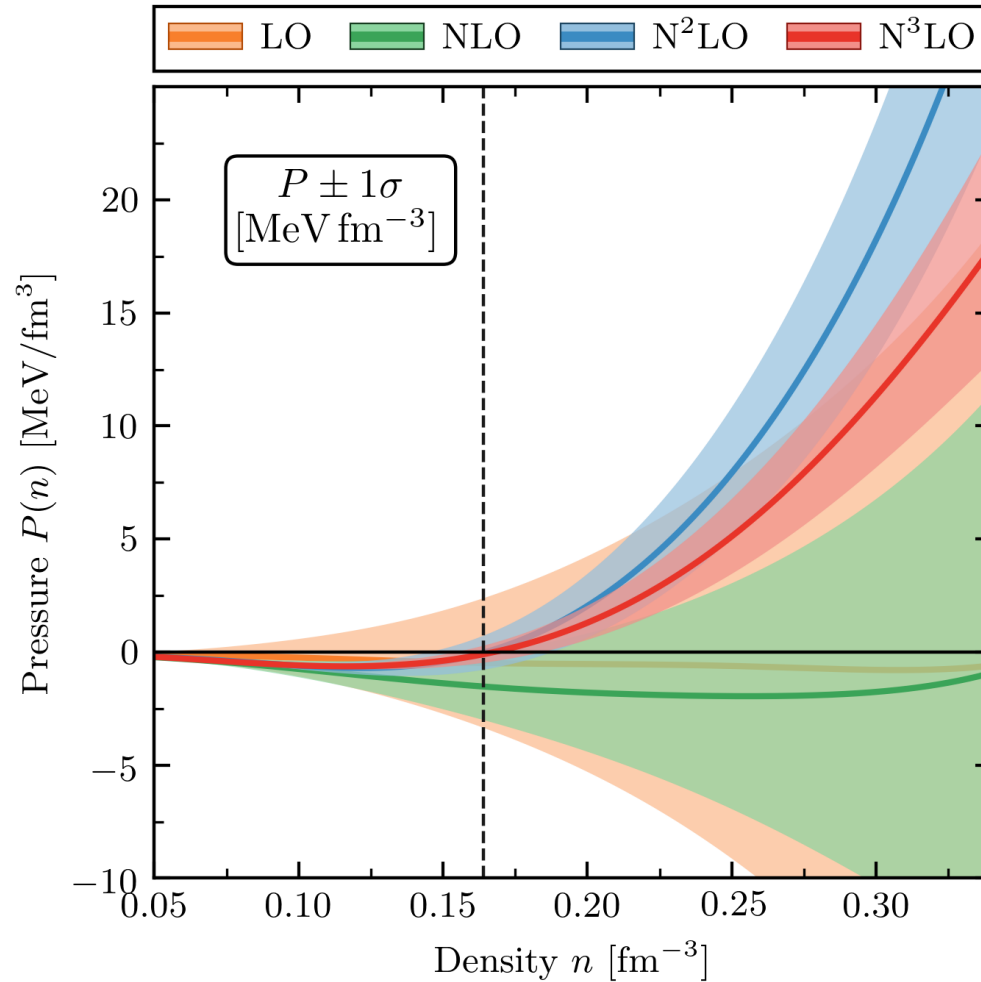


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# High densities: pQCD EOS

## QCD perturbative at high energies

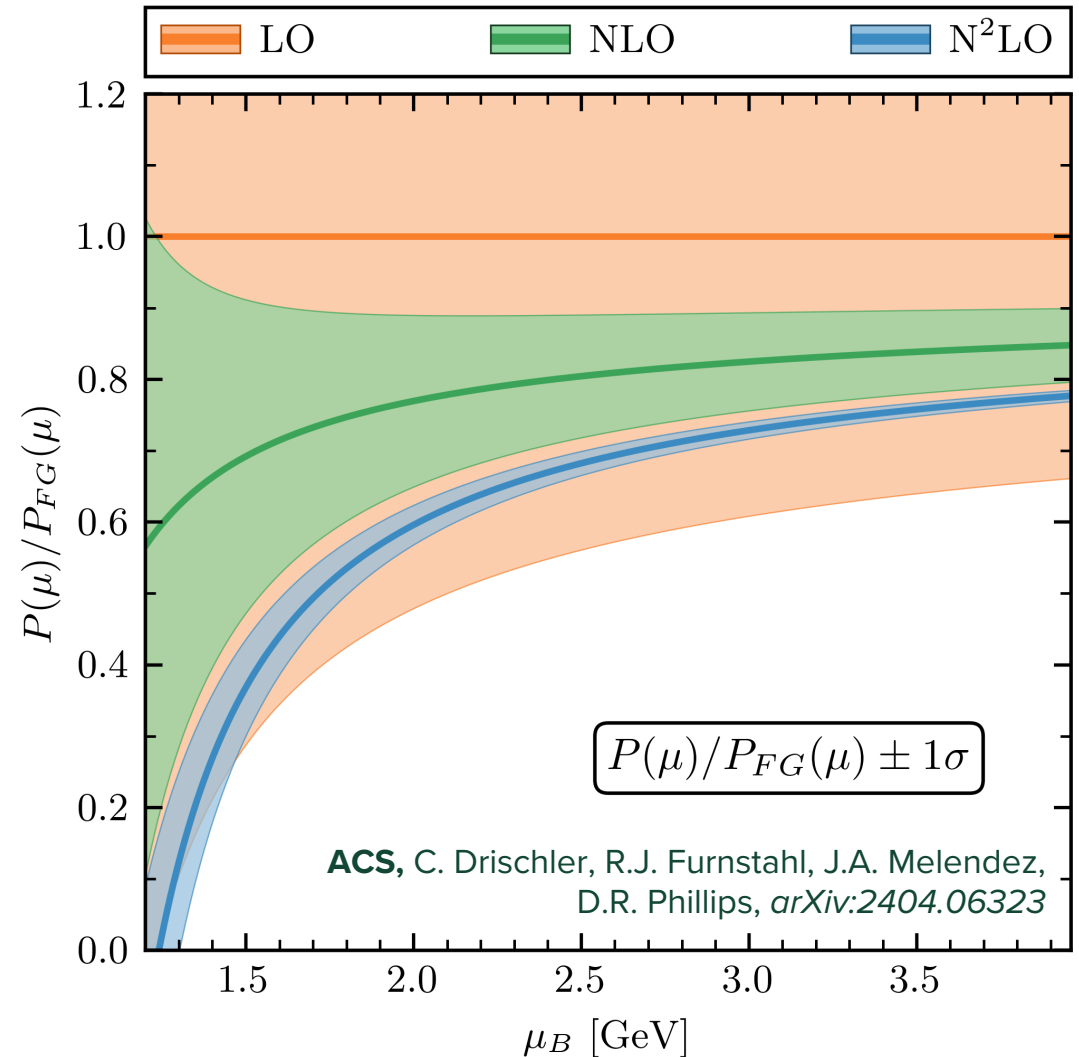
Expansion in the strong coupling constant  $\alpha_s$

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

Two-loop running:

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

Degrees of freedom: quarks and gluons  
Massless u, d quarks with equal  $\mu$



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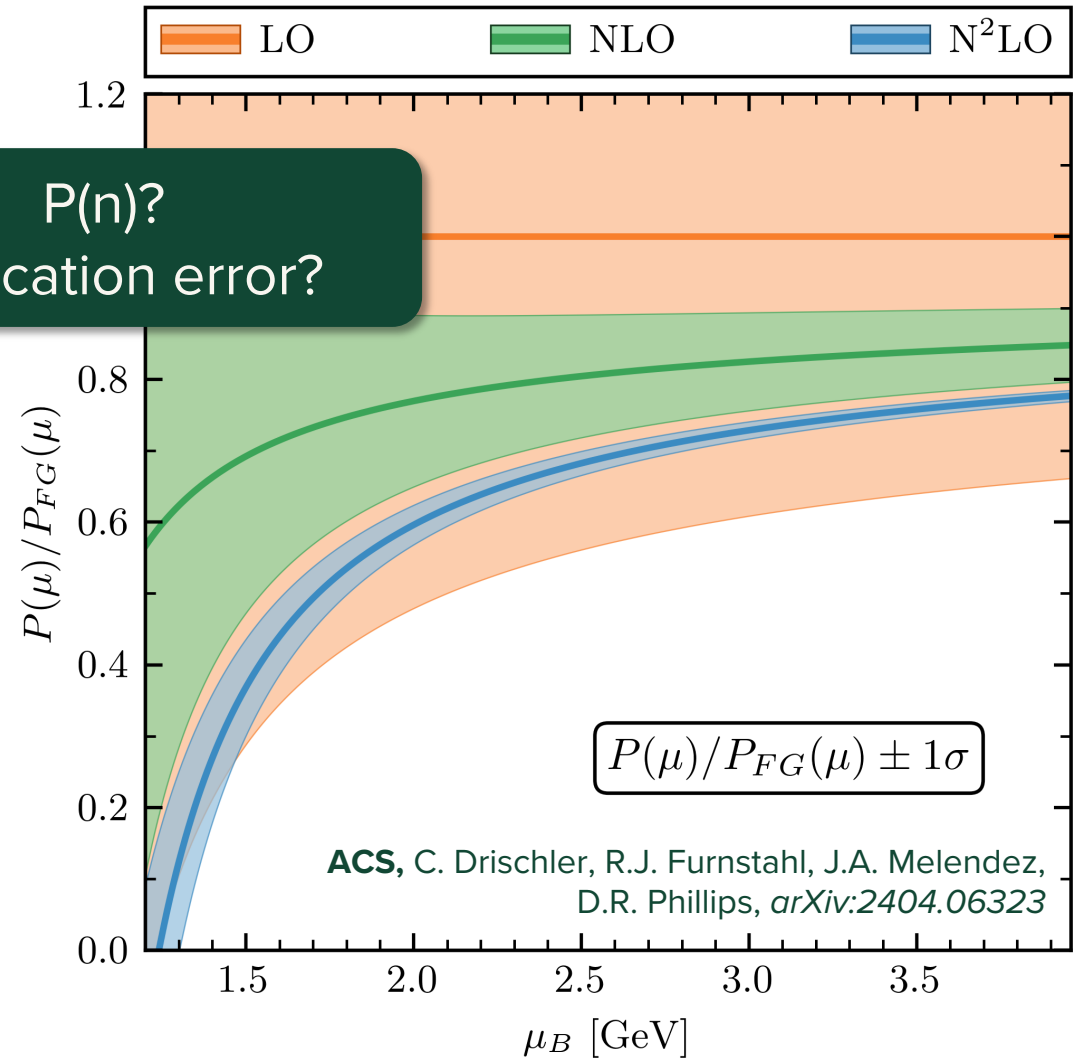
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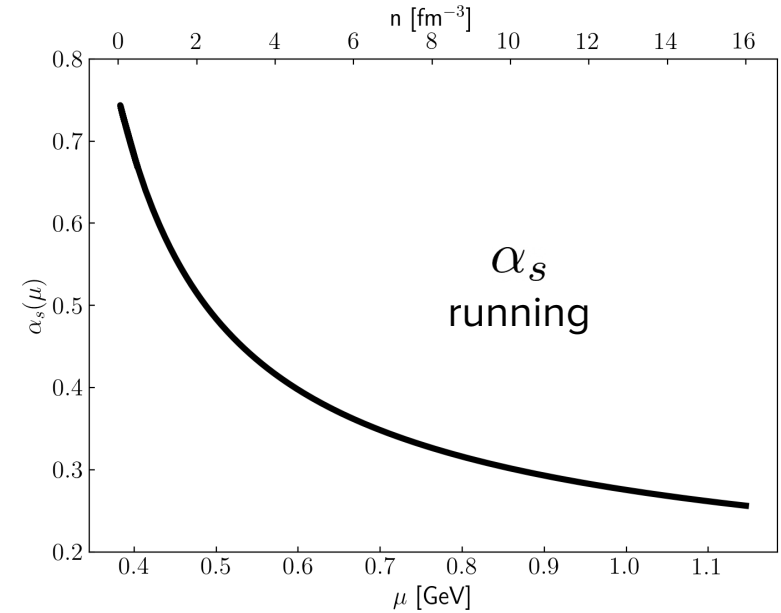
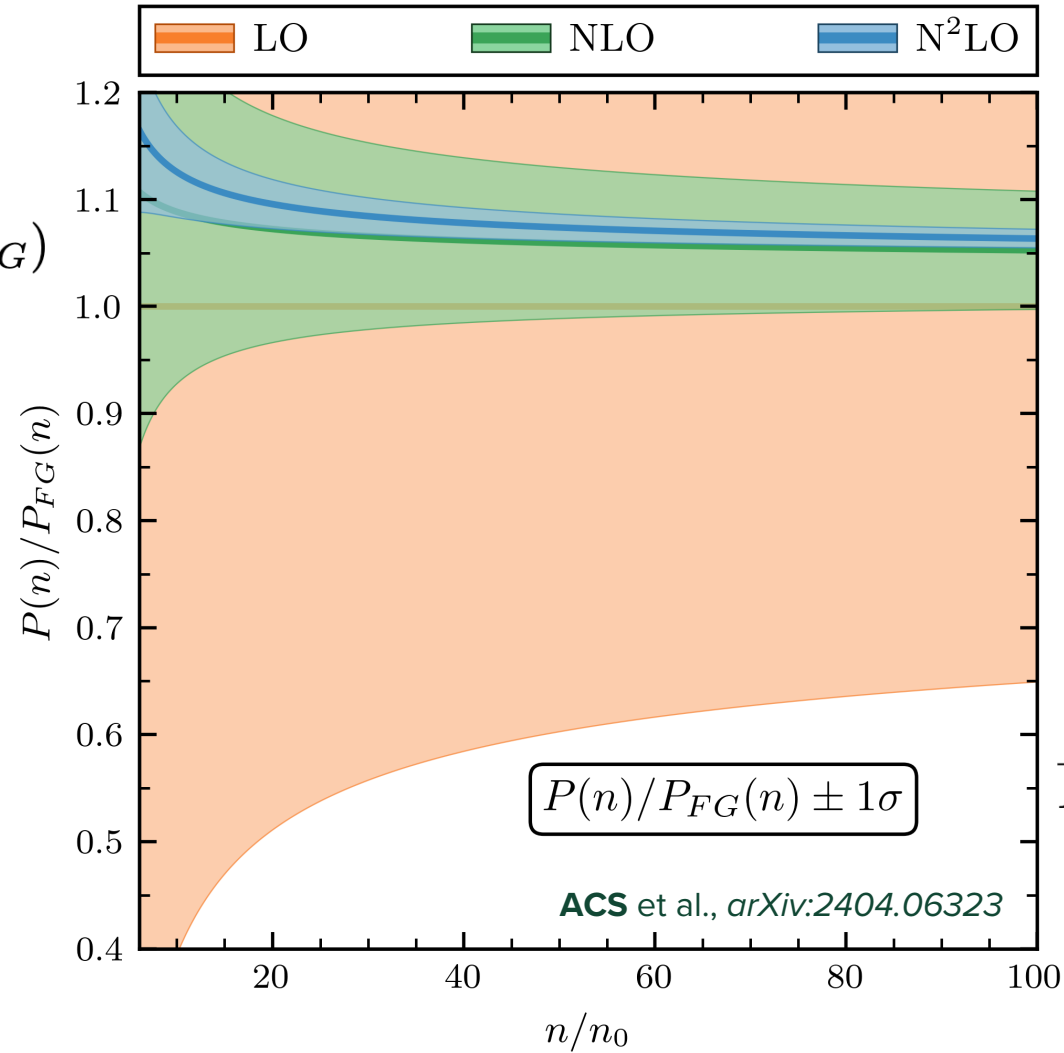
P(n)?  
Truncation error?



# High densities: pQCD EOS

Invoke the Kohn-Luttinger-Ward inversion theorem

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



$P(n)$  scaled by FG pressure:

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

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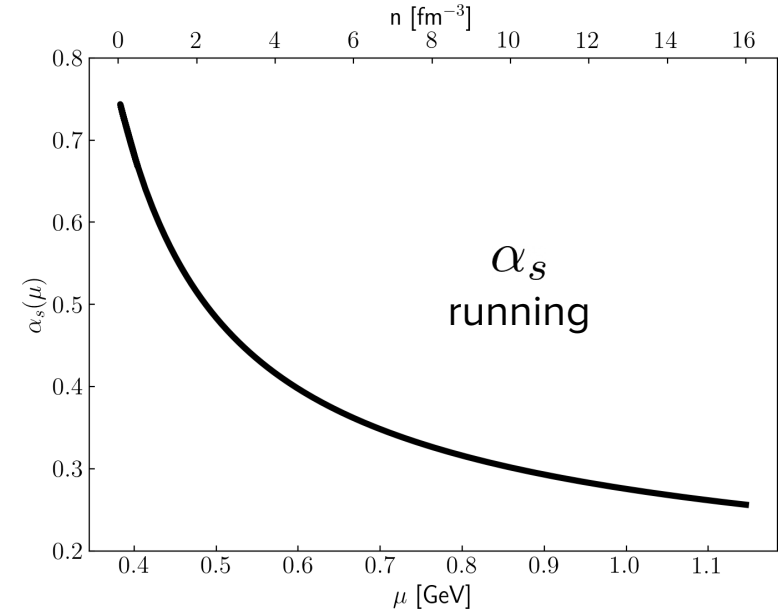
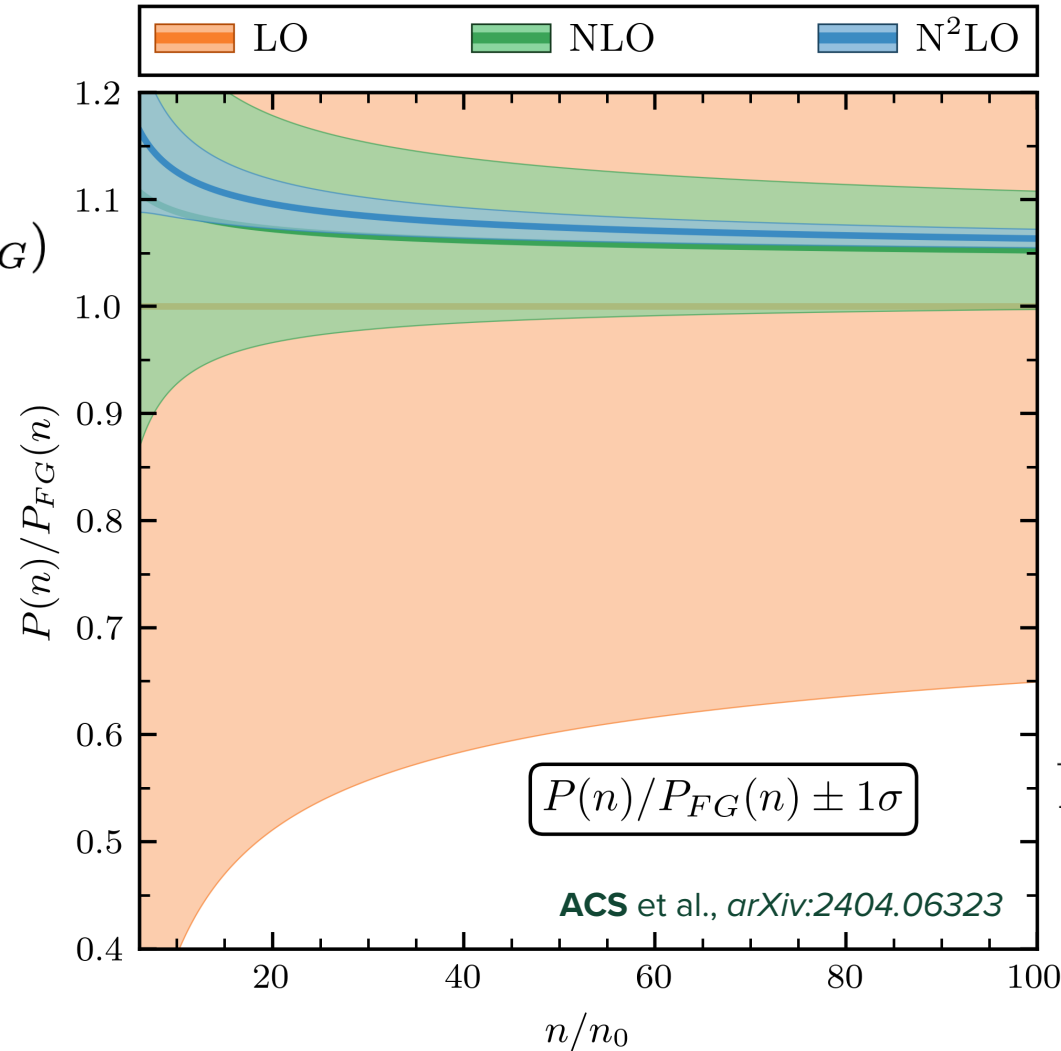
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Apply **gsum** to **P(n)**

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

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



**P(n) scaled by FG pressure:**

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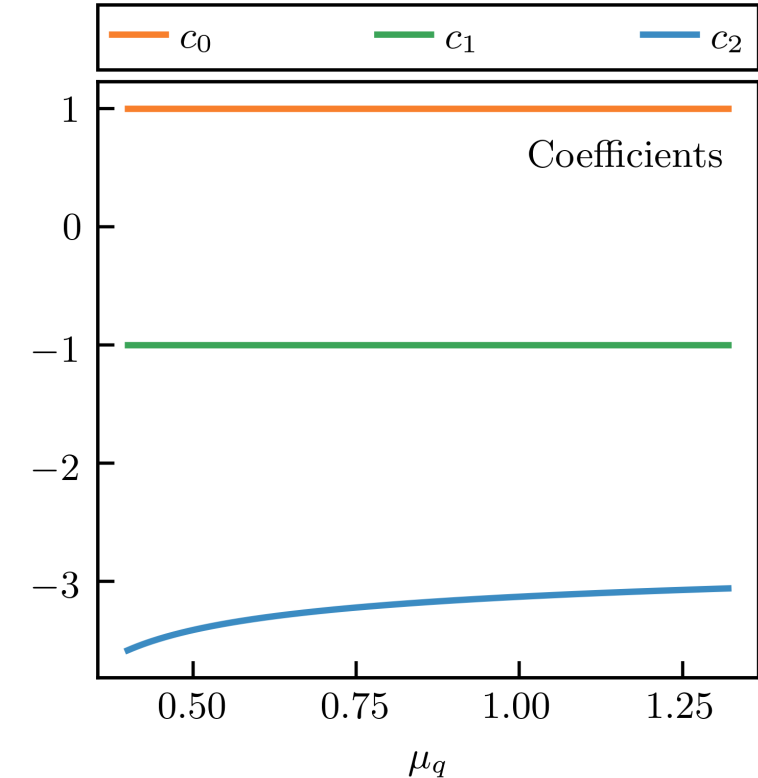
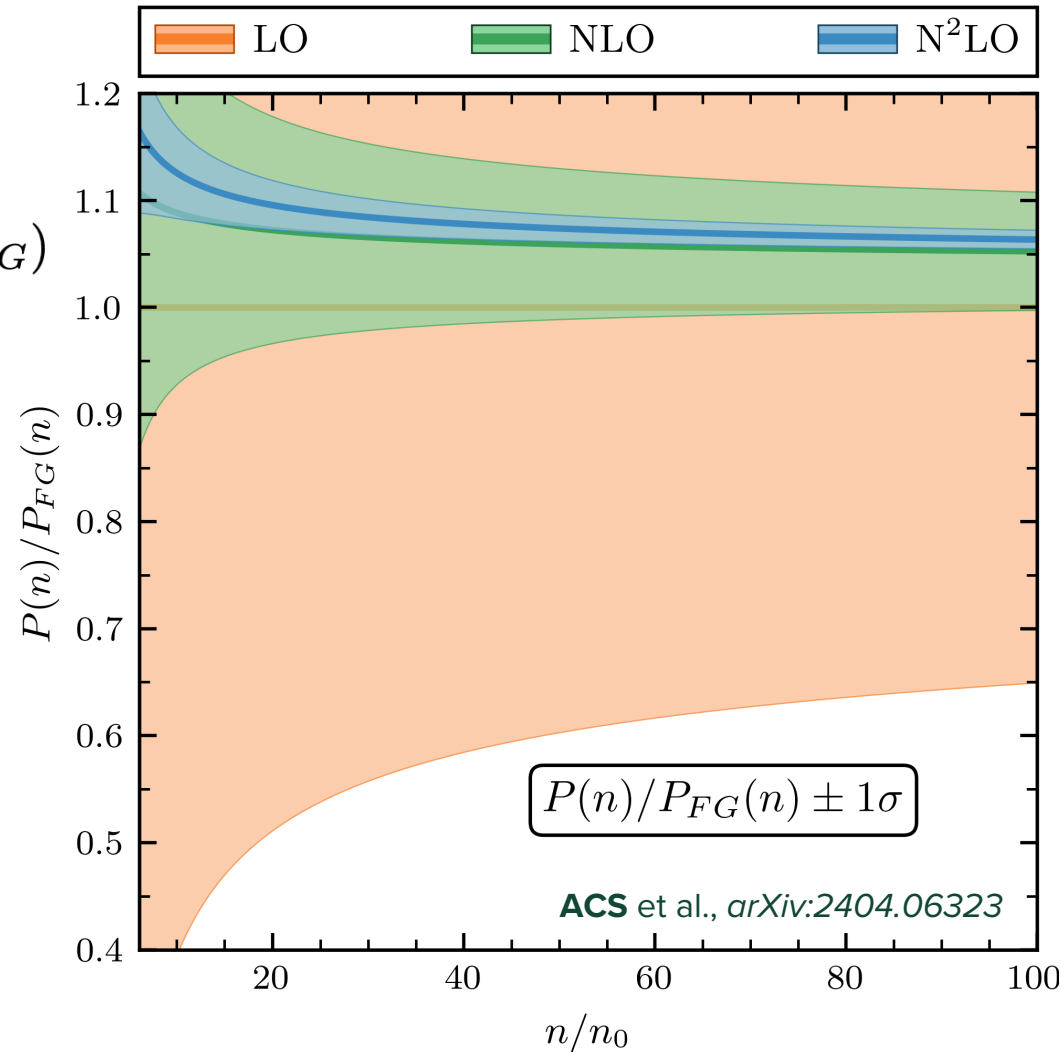
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**Truncation error** often assessed by varying renormalization scale to obtain band---not statistically rigorous

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

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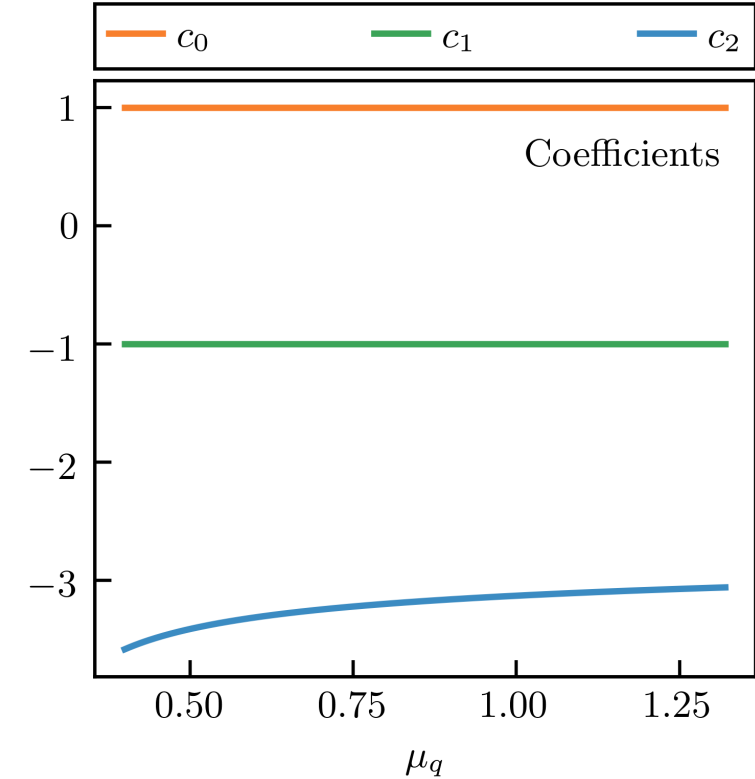
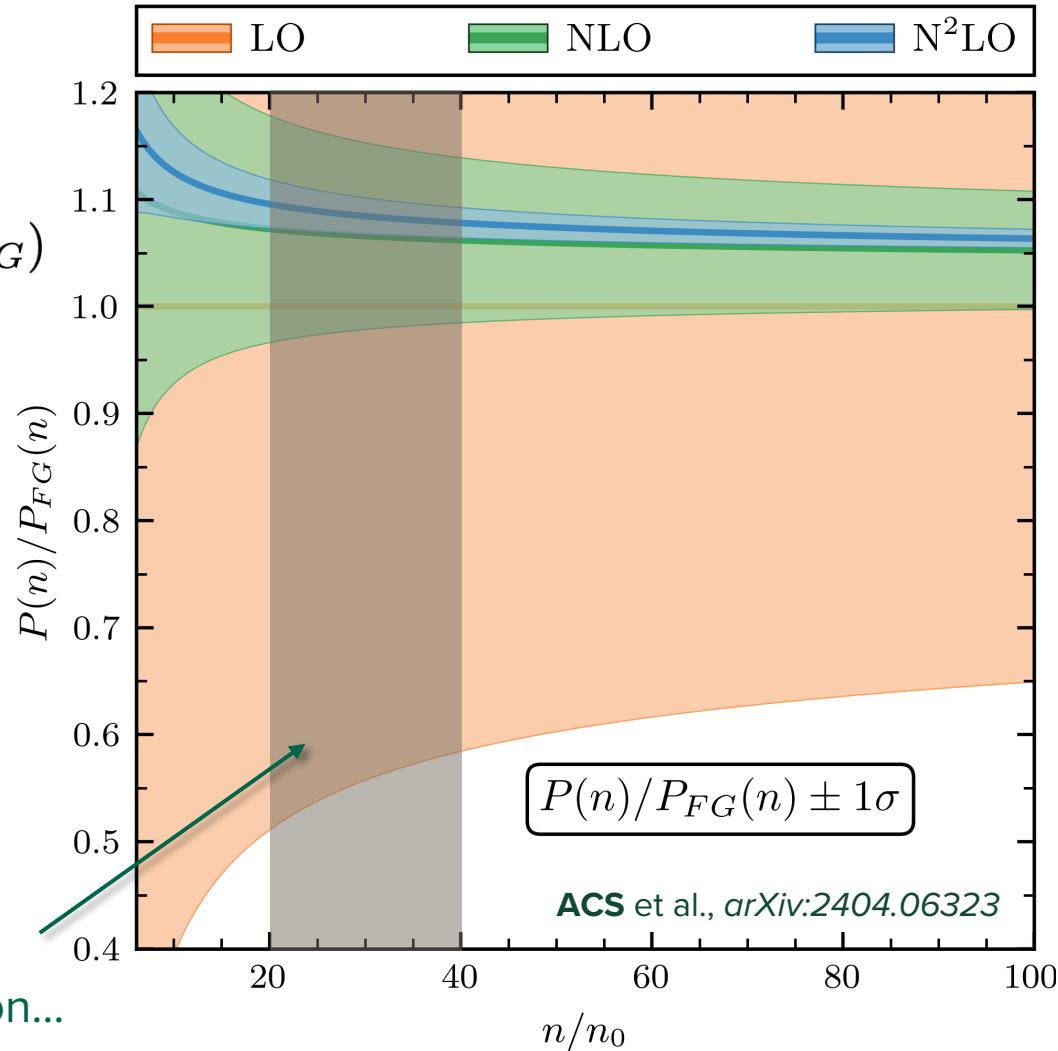
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\* See newer works by Gorda et al. (2022, 2023), MiHO model for higher orders



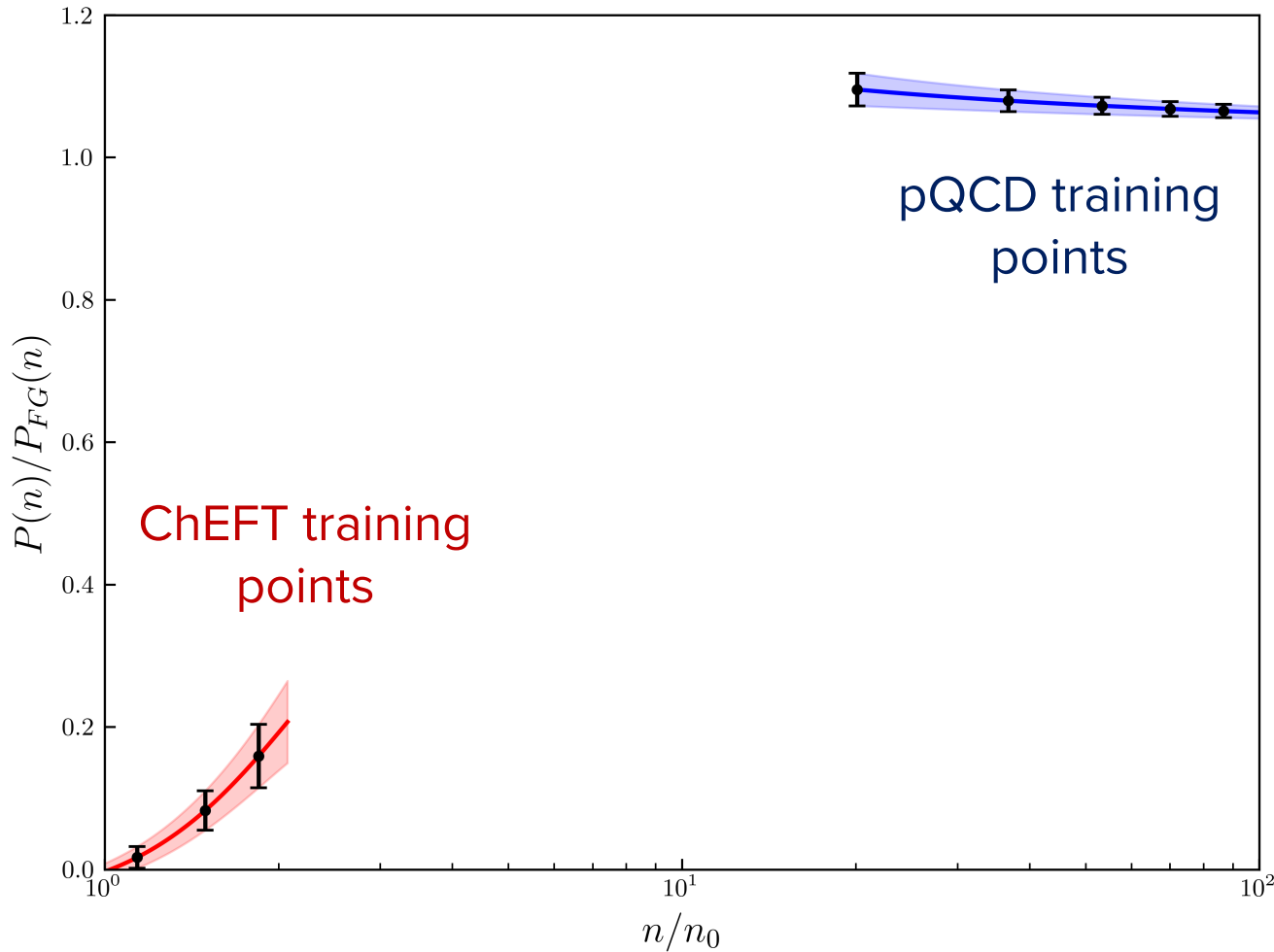


# GPs: a correlated approach to BMM

*Mixing random variables “curvewise”*

Underlying theory (QCD)

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



# GPs: a correlated approach to BMM

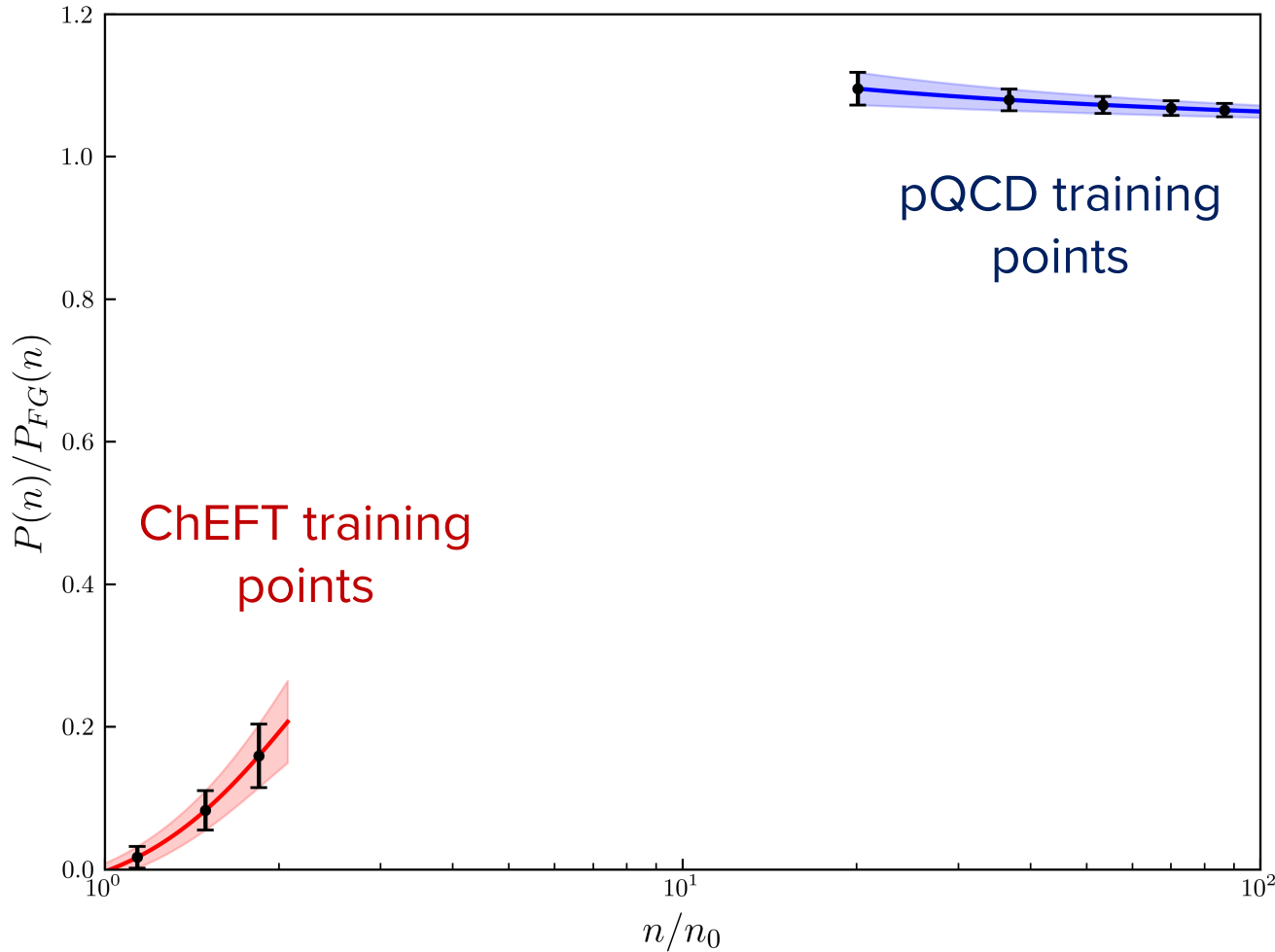
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$$\sim \text{GP}[0, \kappa_y^{(i)}(x, x')]$$

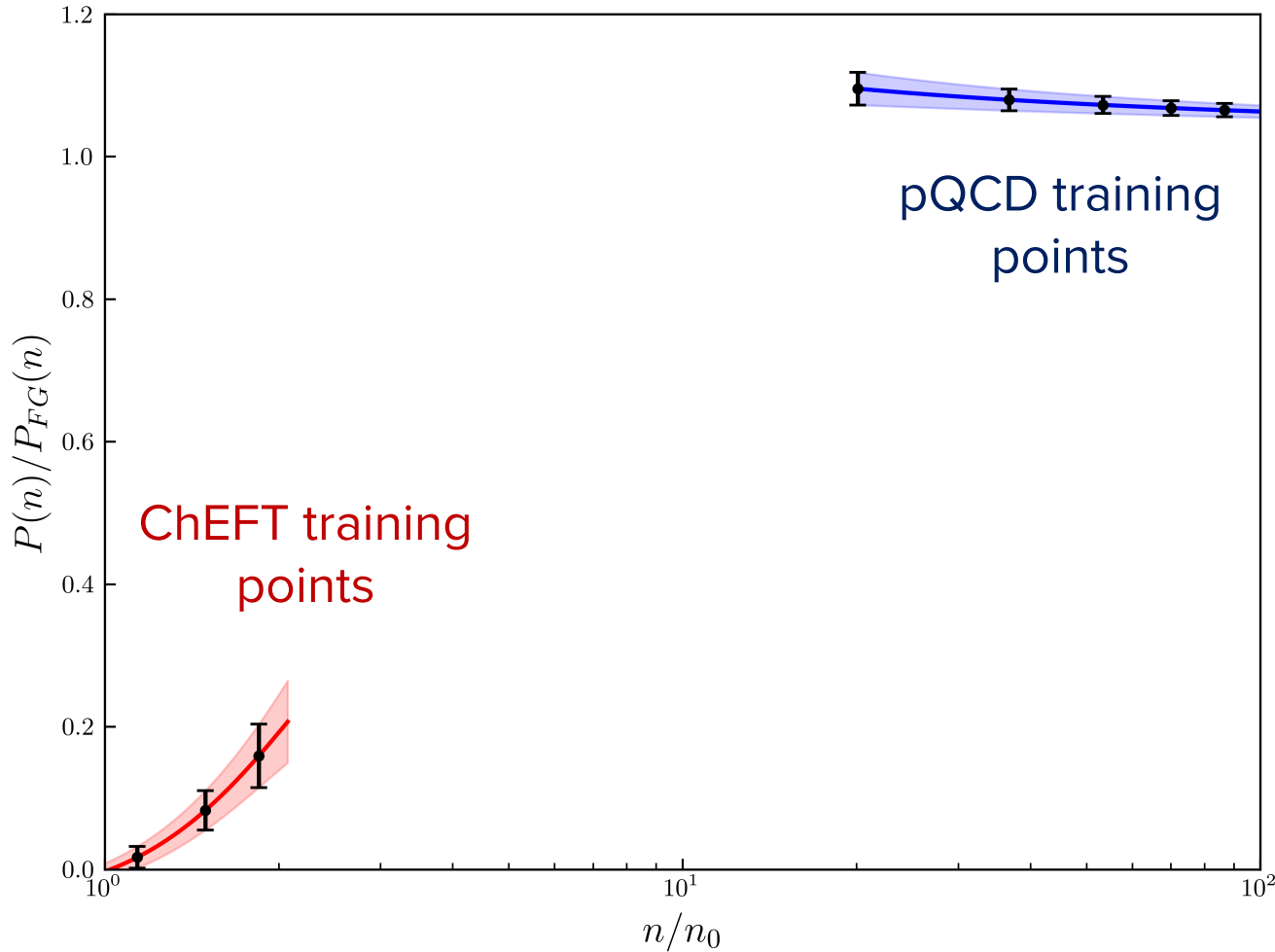
[Full covariance matrix]



# GPs: a correlated approach to BMM

Mixing random variables “curvewise”

Underlying theory (QCD)



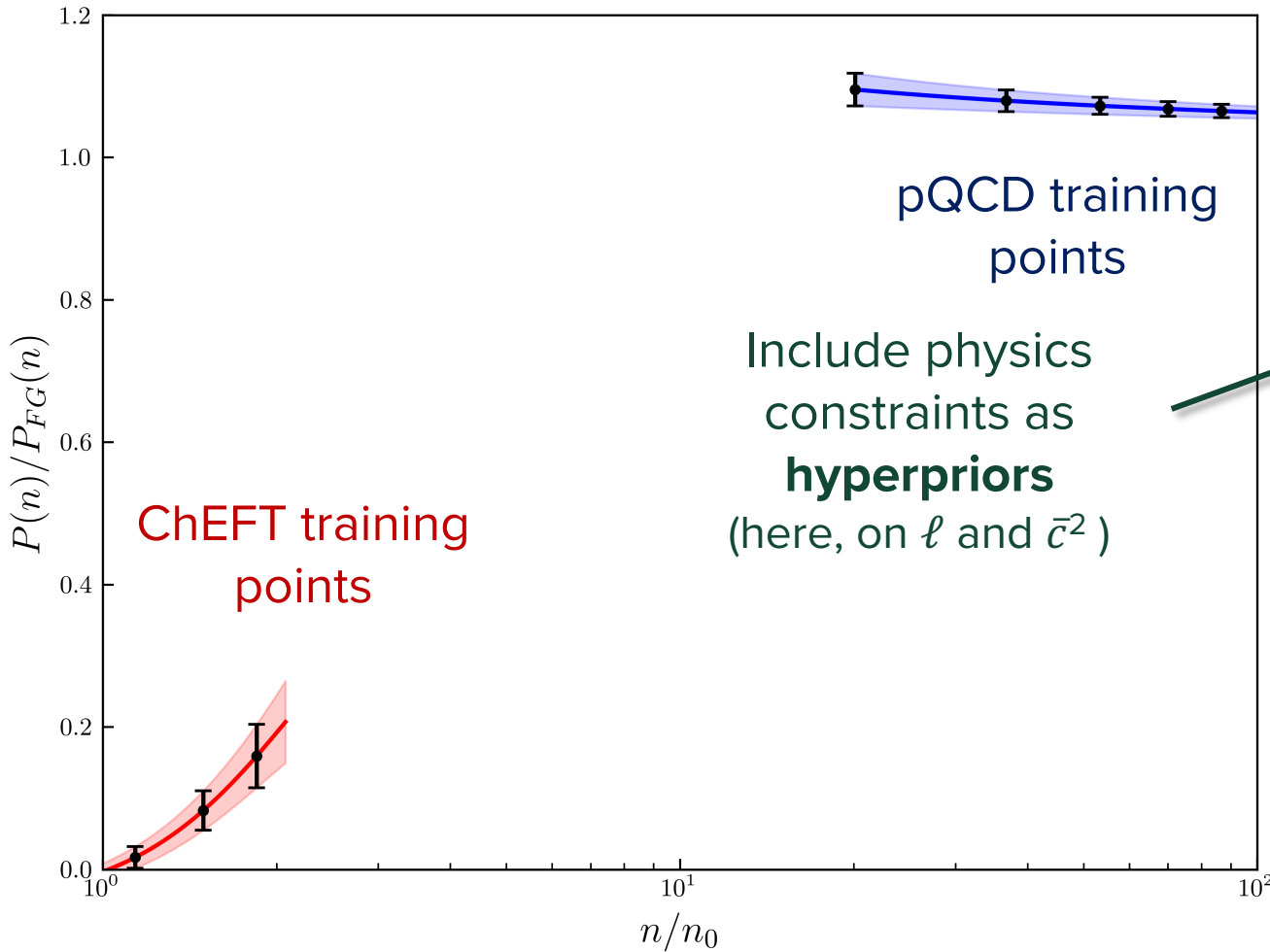
$$Y_i = F + \delta Y_i, \quad i \in [0, M]$$

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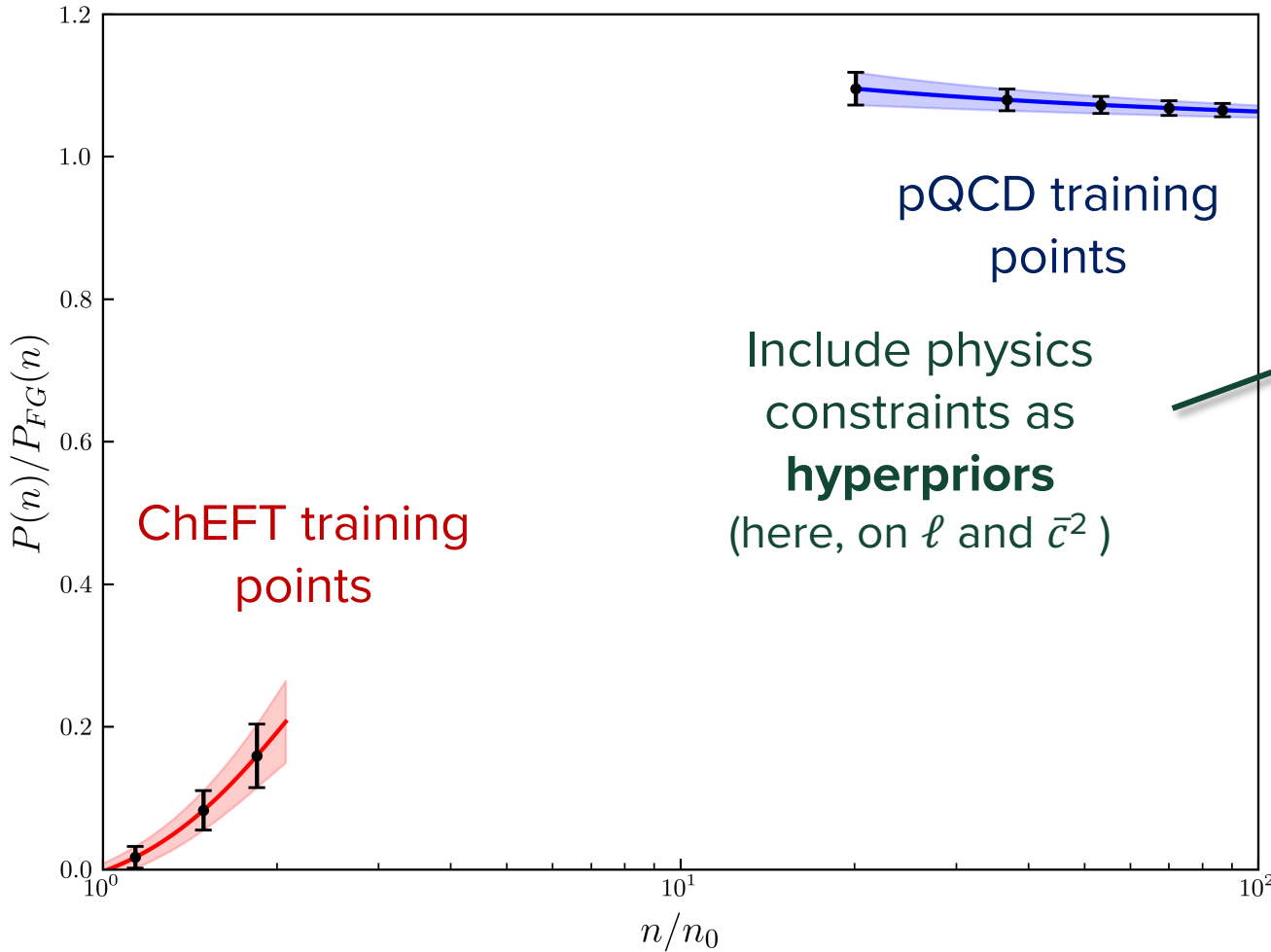
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Therefore, assuming a **Gaussian form** and using Bayes’ theorem, again determine a **common mean**

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

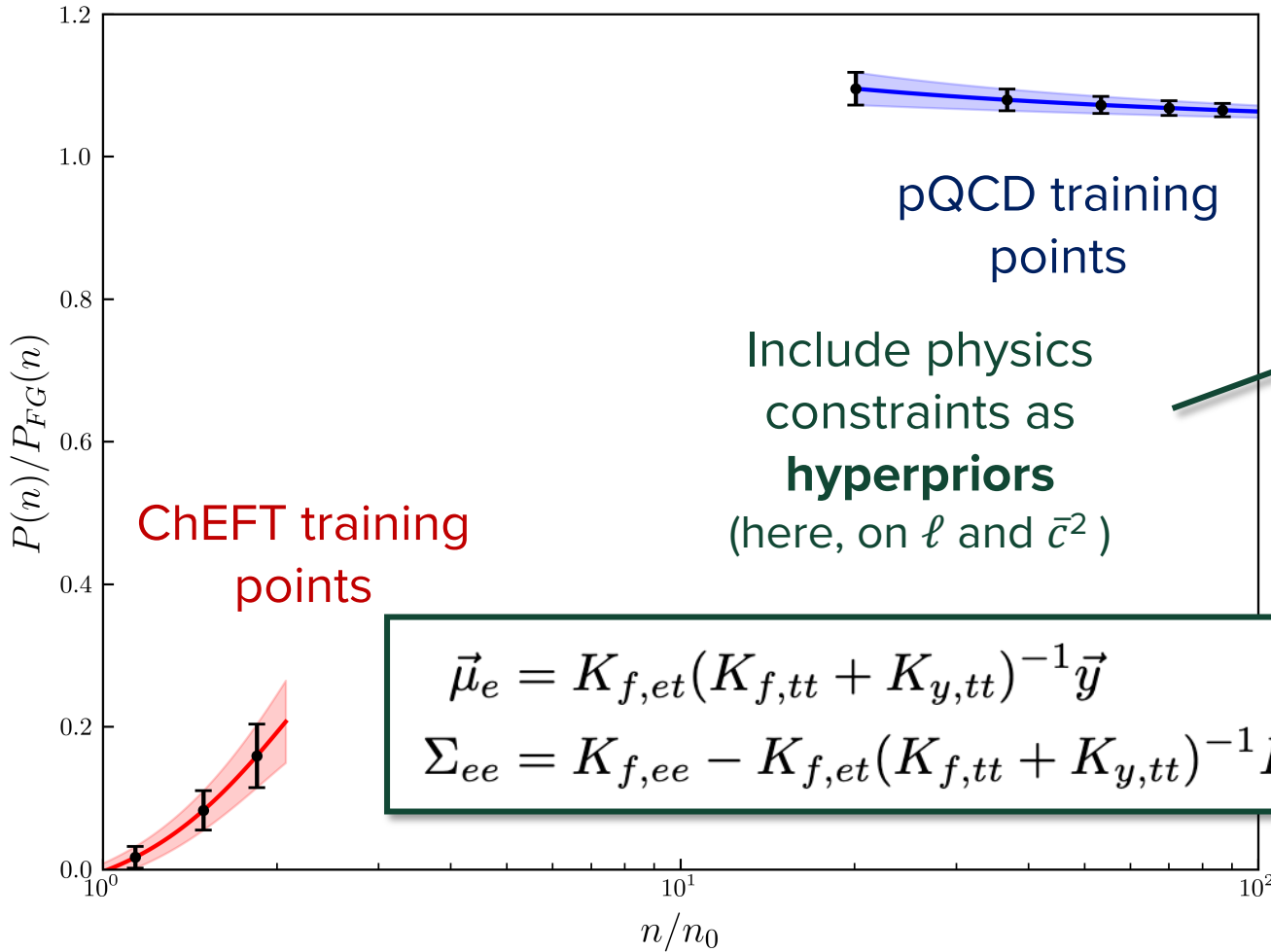
$$\vec{\mu} \equiv \Sigma B_t^T K_y^{-1} \vec{y}$$

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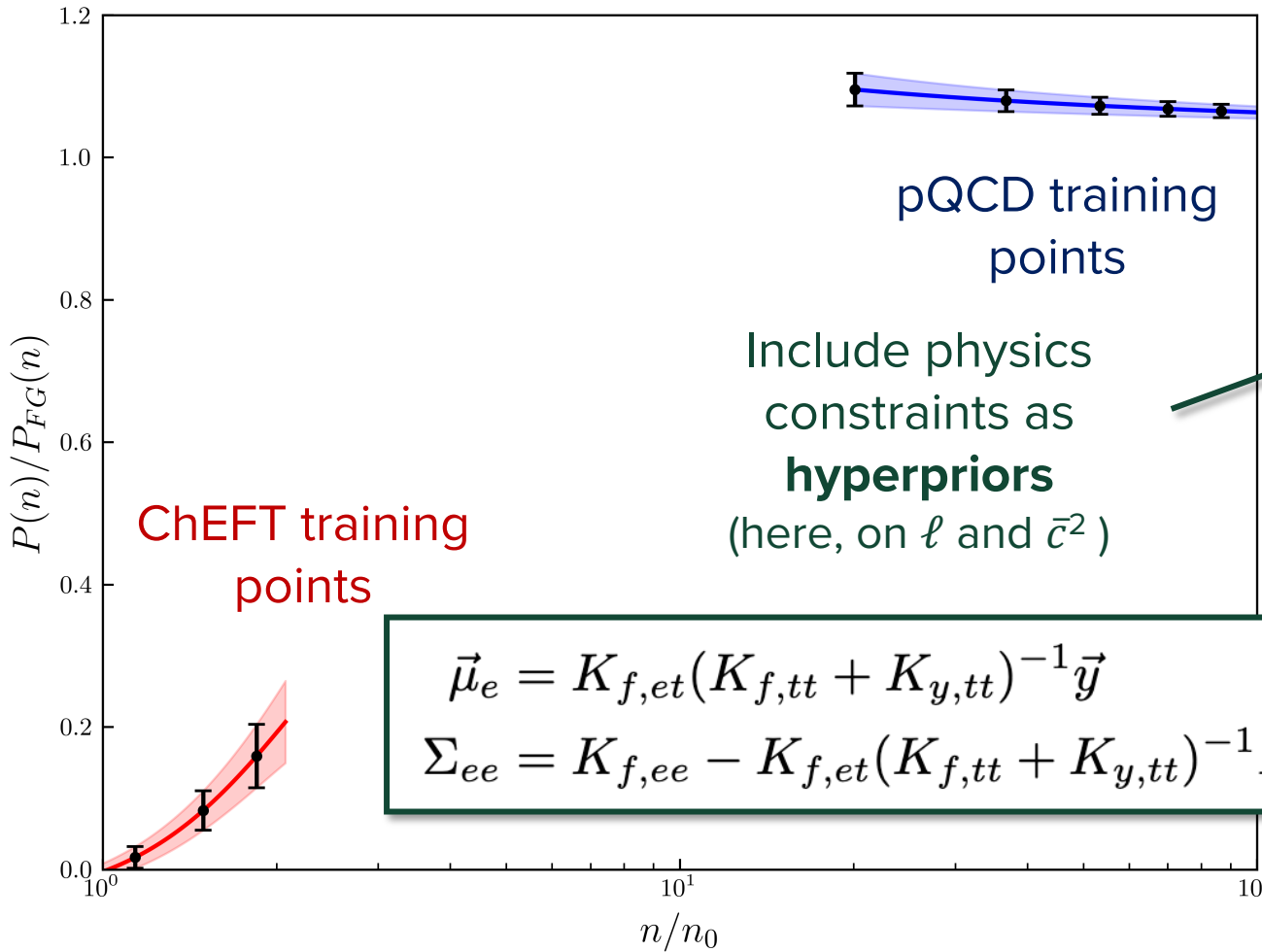
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$$\vec{\mu}_e = K_{f,et}(K_{f,tt} + K_{y,tt})^{-1}\vec{y}$$

$$\Sigma_{ee} = K_{f,ee} - K_{f,et}(K_{f,tt} + K_{y,tt})^{-1}K_{f,te}$$

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

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

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**GP equations are the mixed model result!**

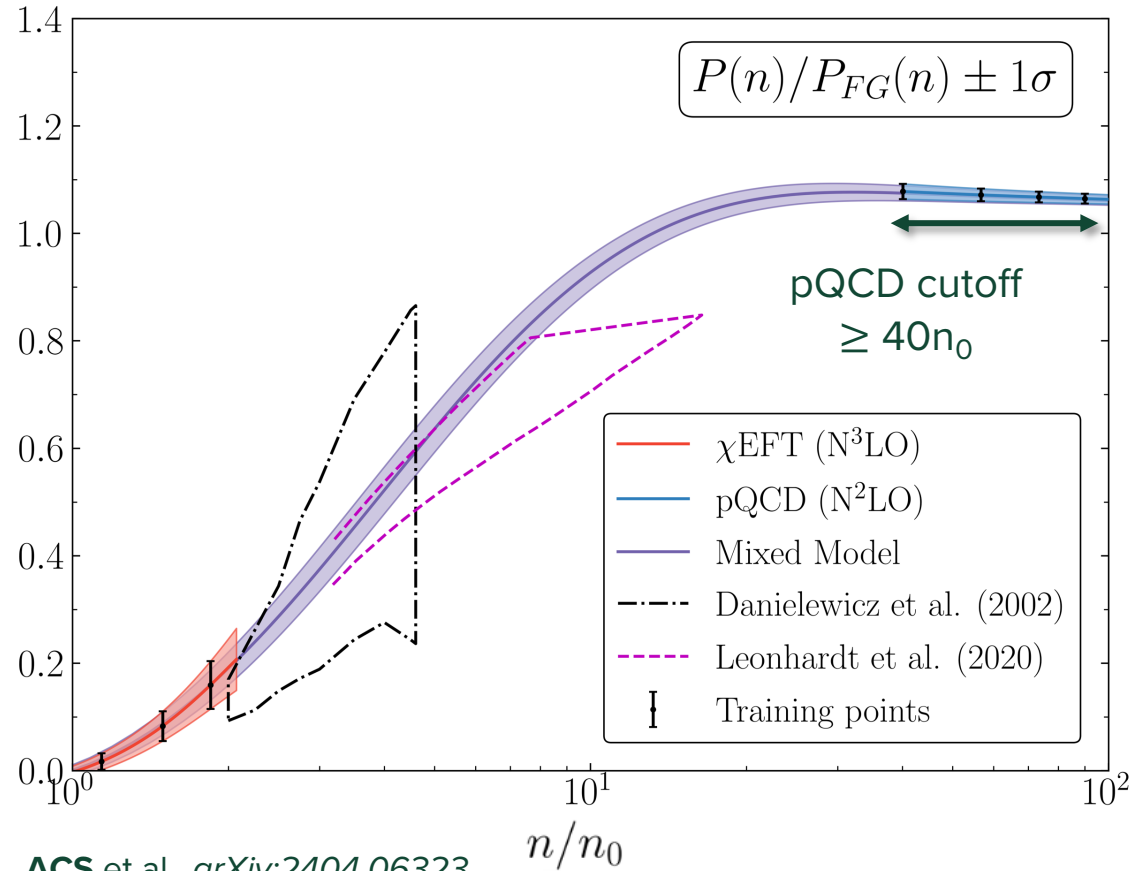


# Results: pressure



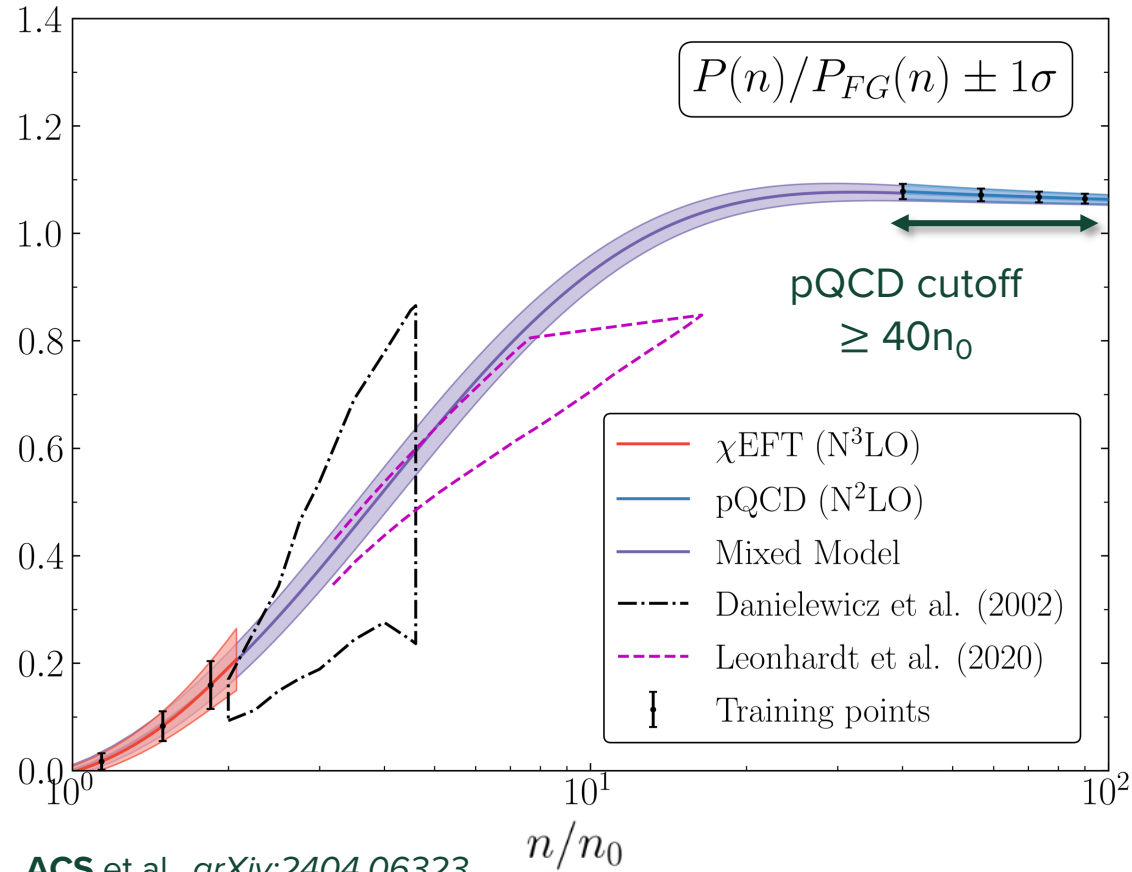
## Unconstrained prior

GP learns very long lengthscale ( $\sim 1.9$  in  $\ln(n)$  space)  $\Rightarrow$  induces strong pQCD influence in chiral EFT region  $\Rightarrow$  **small bands**

ACS et al., *arXiv:2404.06323*

## Unconstrained prior

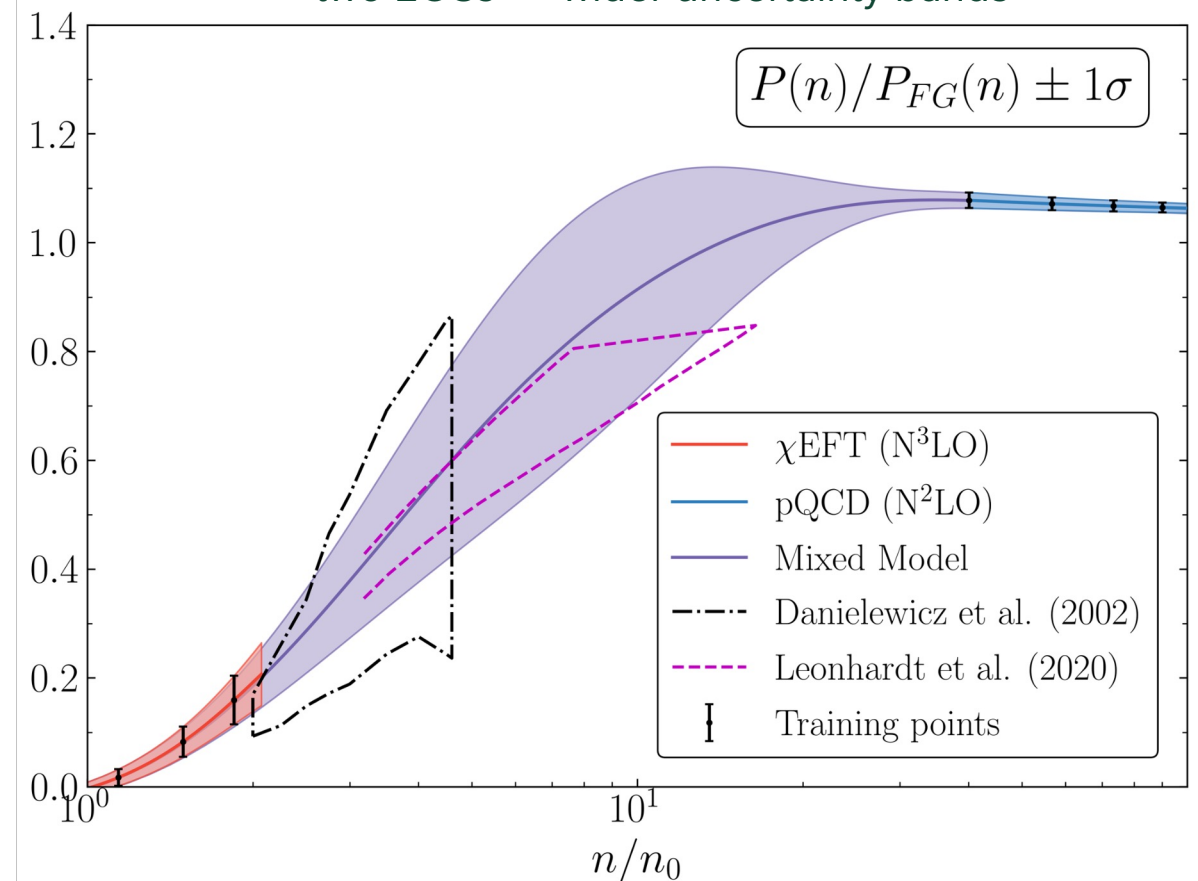
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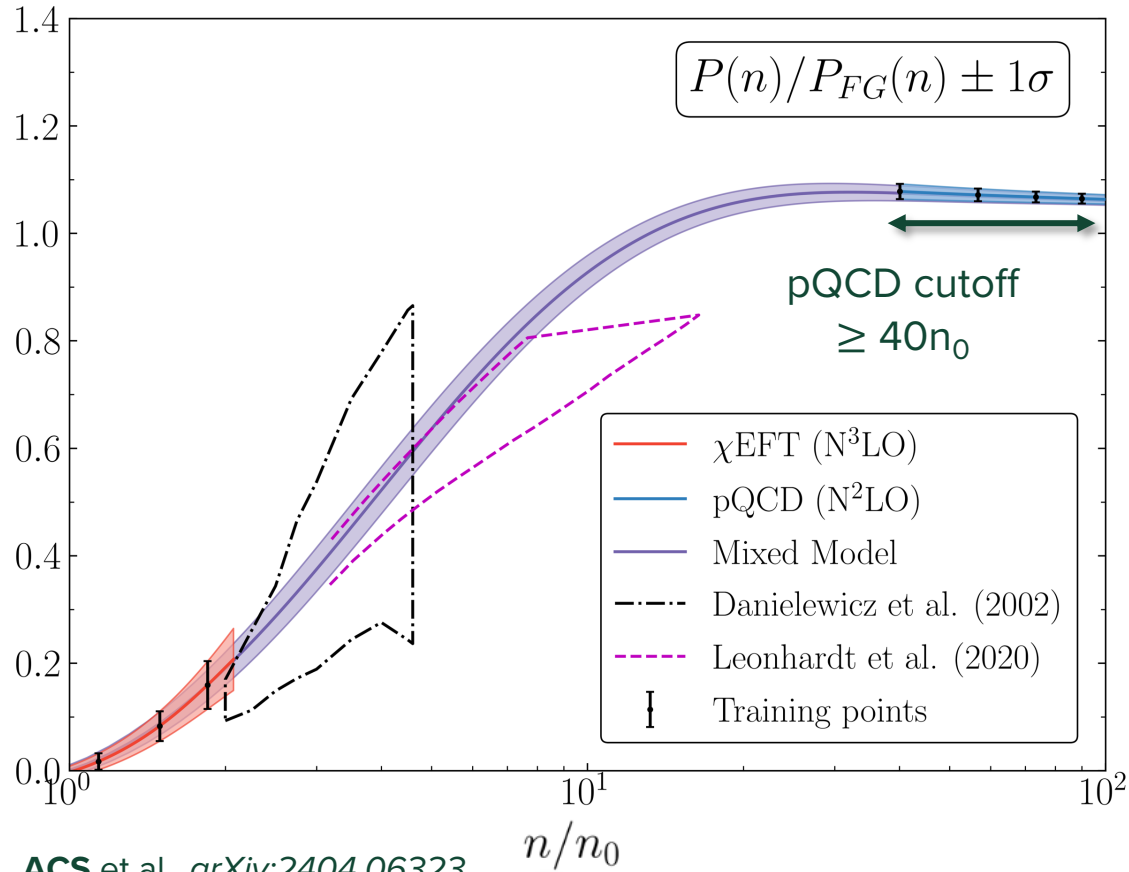
## Constrained prior on lengthscale

Reduction of the correlation length between the two EOSs  $\Rightarrow$  wider uncertainty bands



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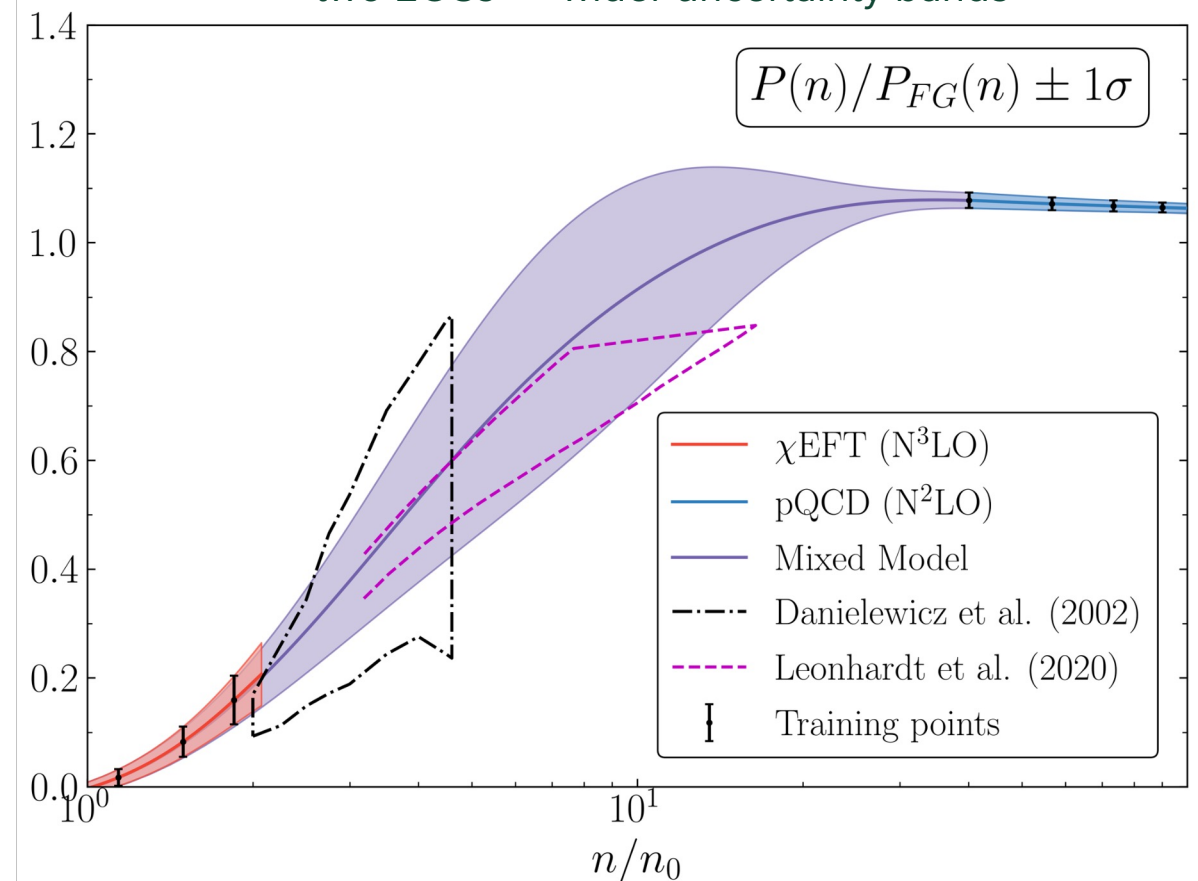
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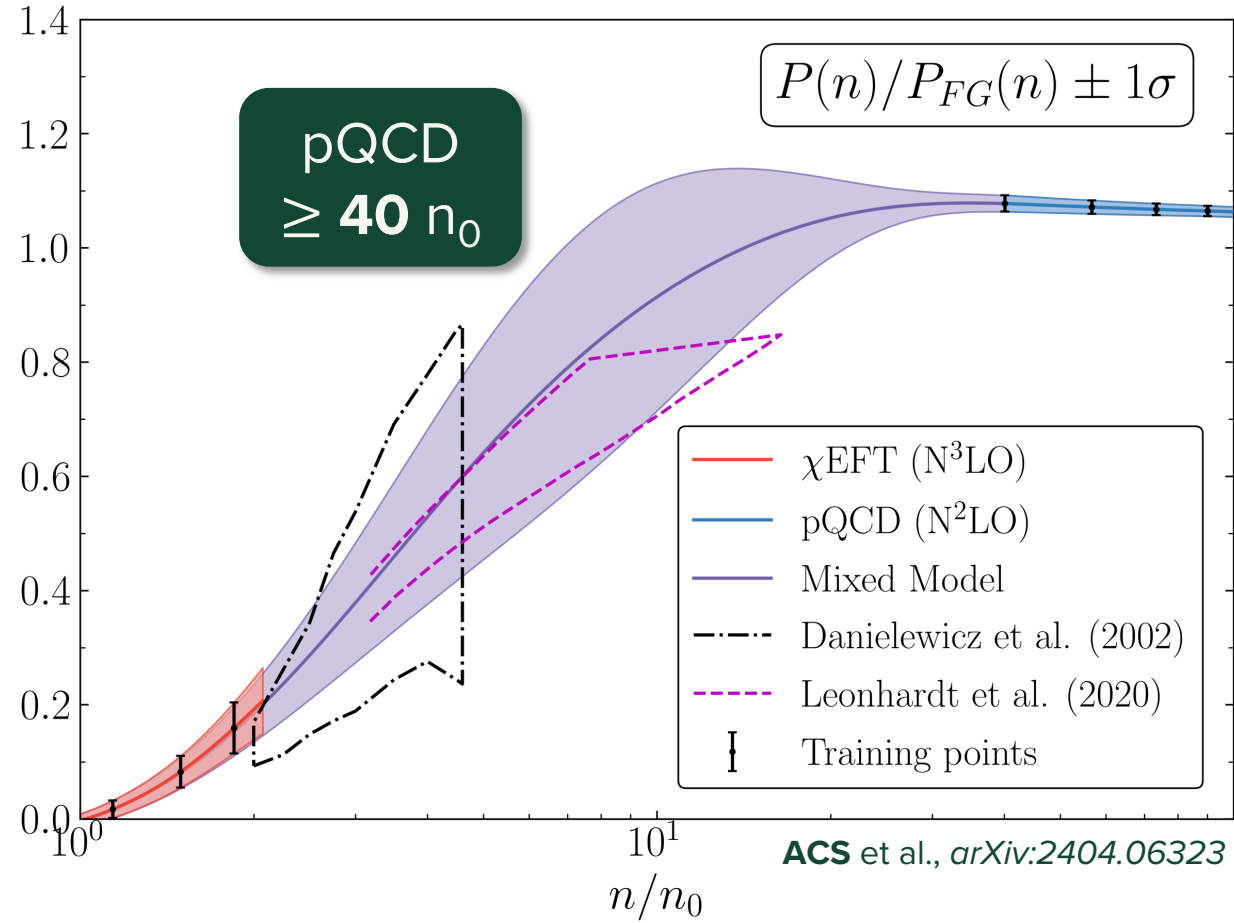
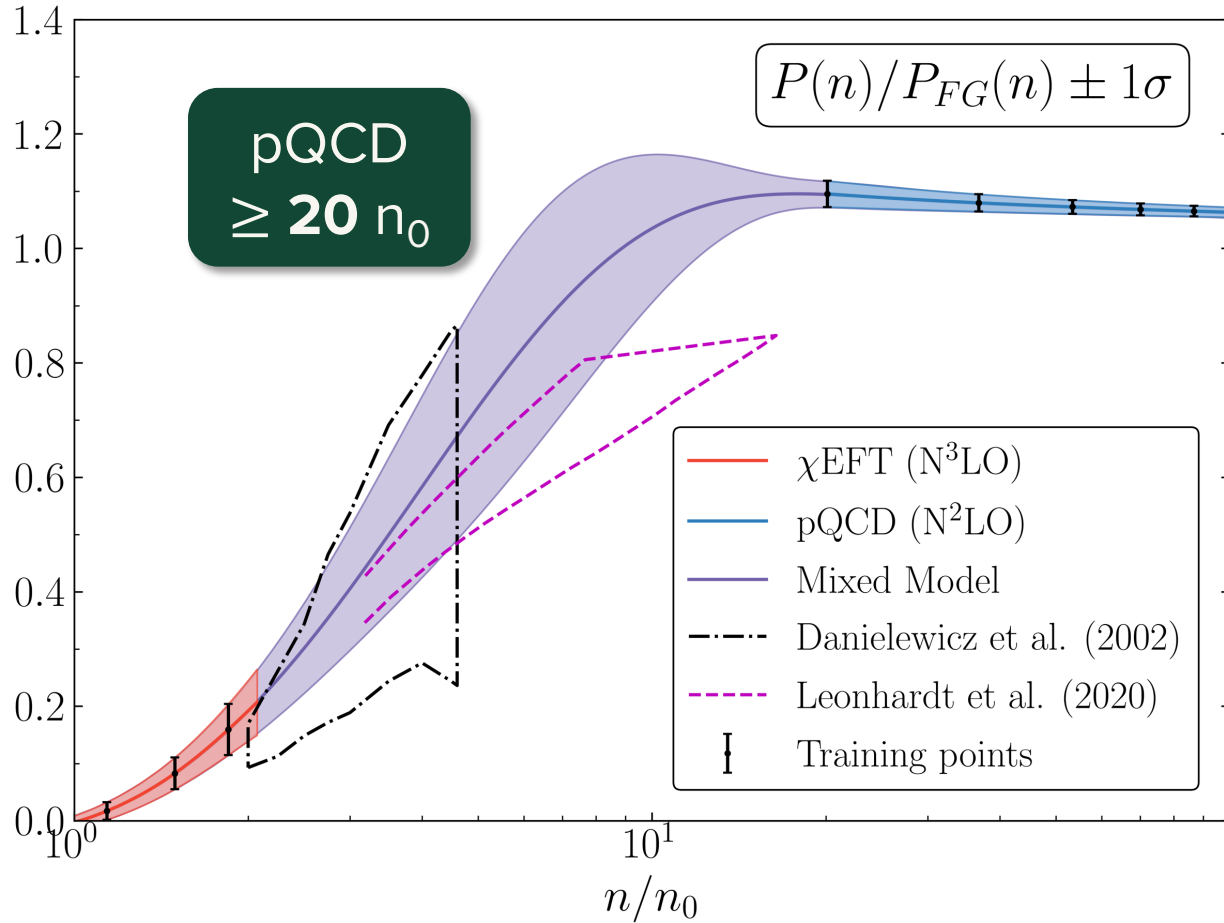
Reduction of the correlation length between the two EOSs  $\Rightarrow$  wider uncertainty bands



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

# Results: pressure

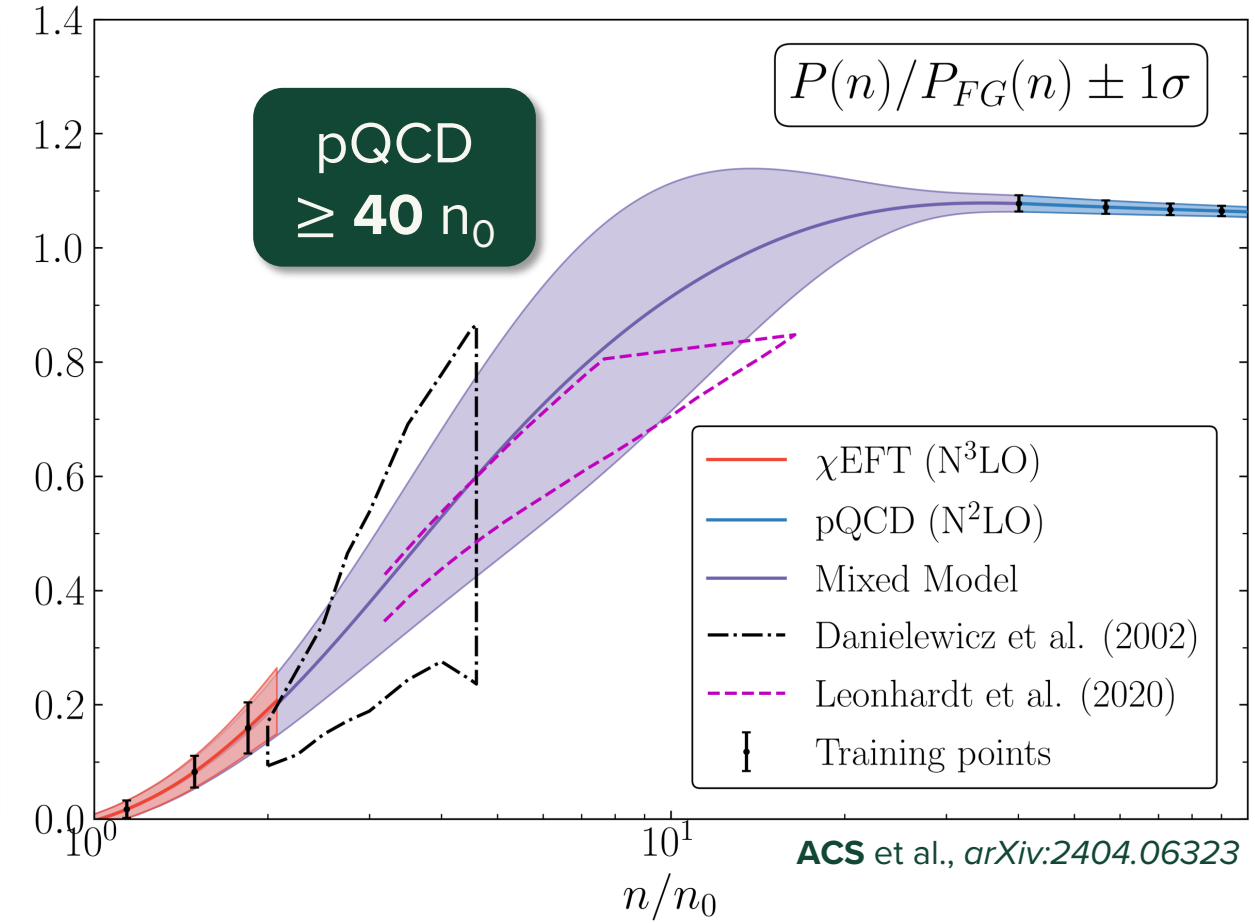
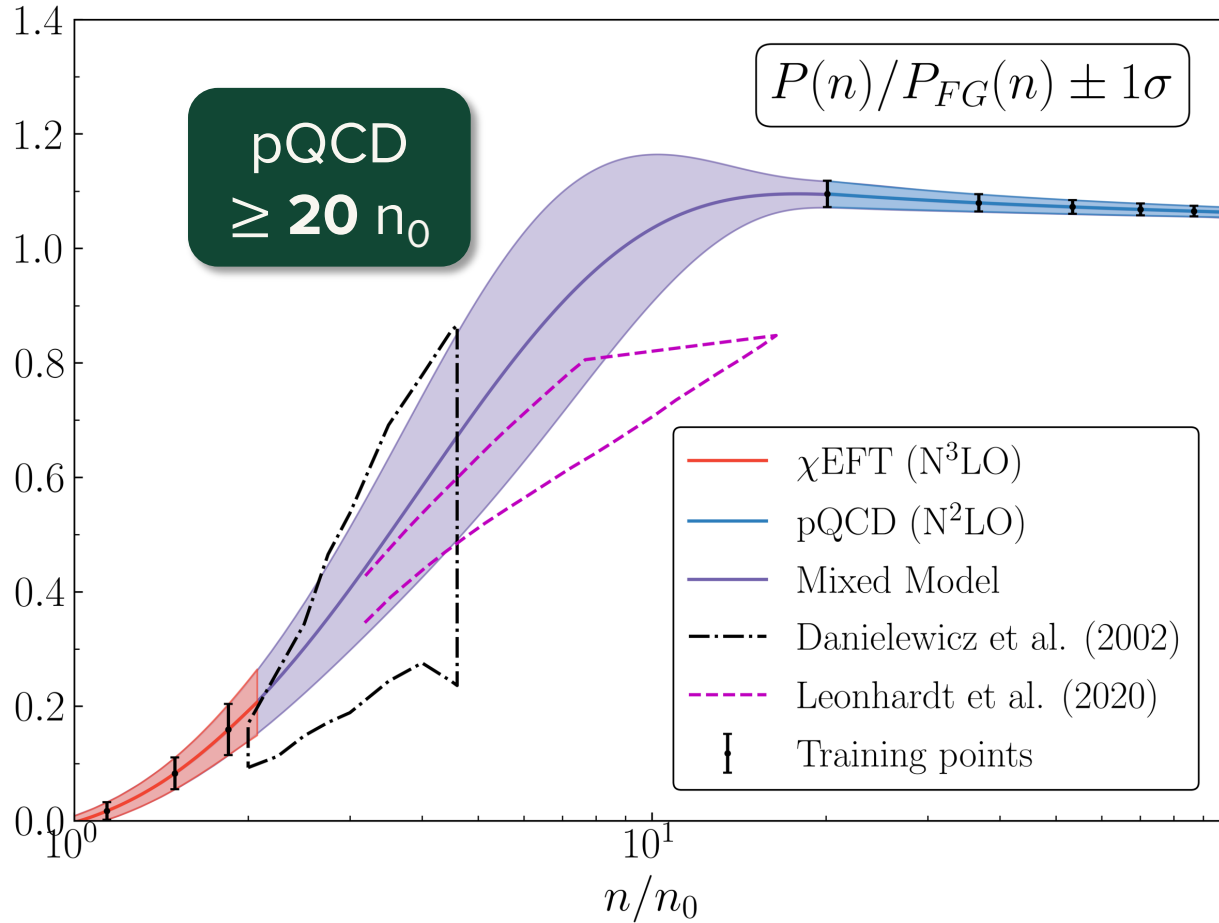
Unknown cutoff of pQCD validity = testing with **two cases**:  
 pQCD cutoffs for  $\geq 20 n_0$  and  $\geq 40 n_0$



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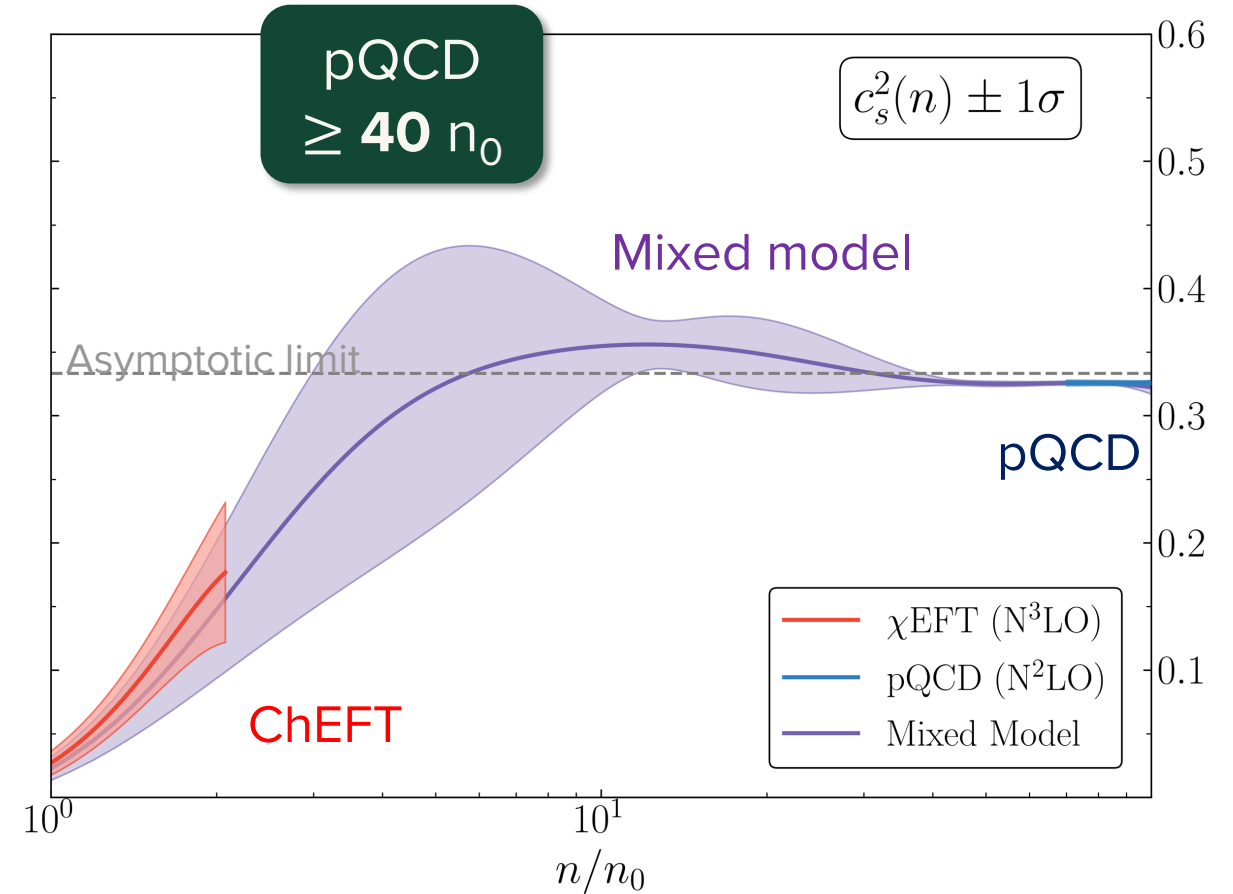
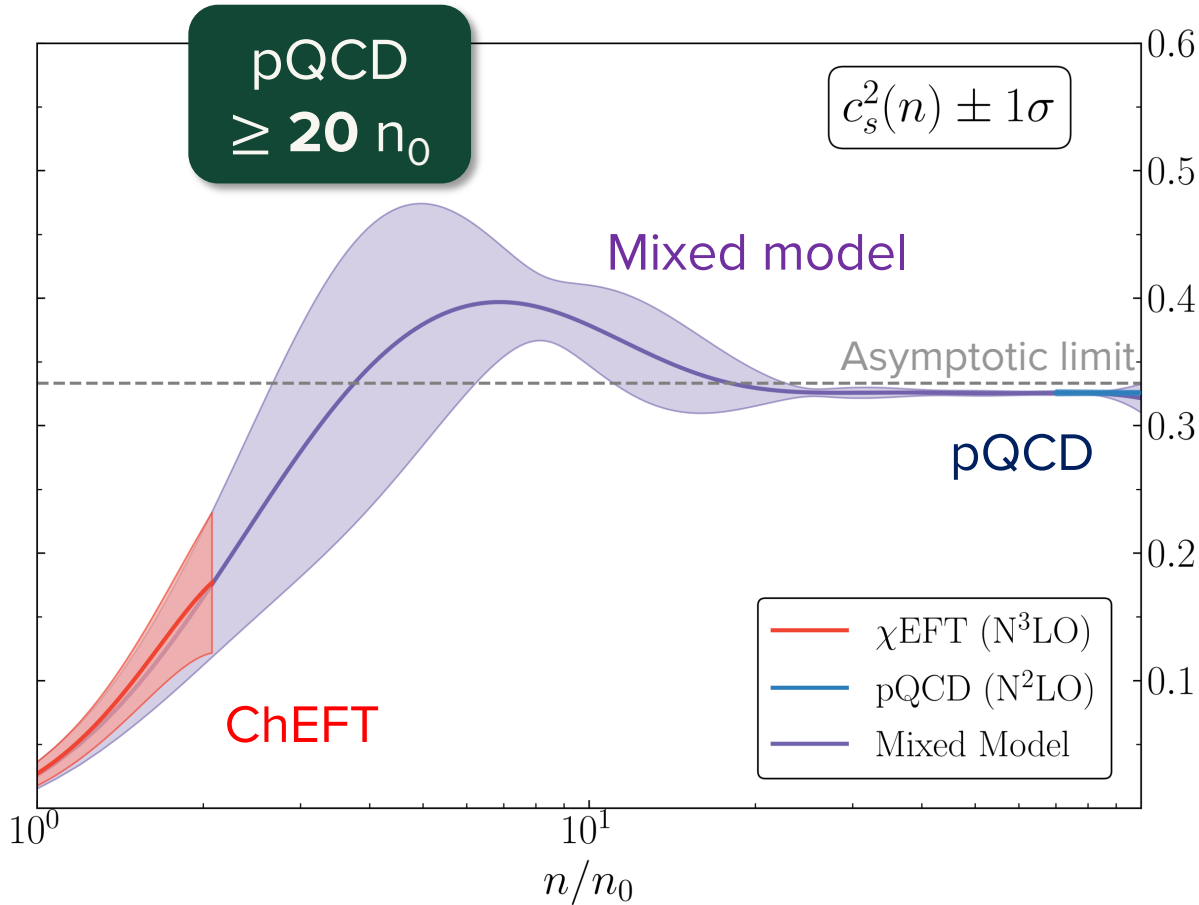


ACS et al., arXiv:2404.06323

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

# Results: speed of sound

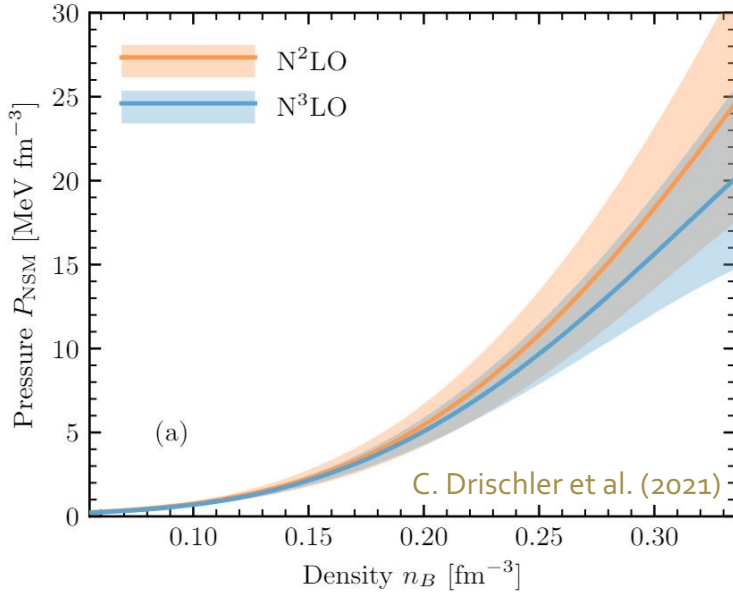
Mixed models both approaching 0.33 asymptotically (from below)



ACS et al., *arXiv:2404.06323*

**Causal, stable EOS**

## Next steps: neutron-rich matter



Extending **BMM** calculations to  
neutron-rich matter

Goal: global, microscopic, QCD-based  
EOSs for merger simulations

Inclusion of important **astrophysical  
observations** (NICER, ...) and  
**experimental constraints** (FRIB400, ...)

## Opportunities for discussion...

**UQ of the pQCD expansion**

Scale variation techniques vs.  
missing higher orders UQ =>  
possibly double-counting  
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**Exploring kernel design**

EOS as a case study:  
constraints from astro./exp.  
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## ... and some challenges

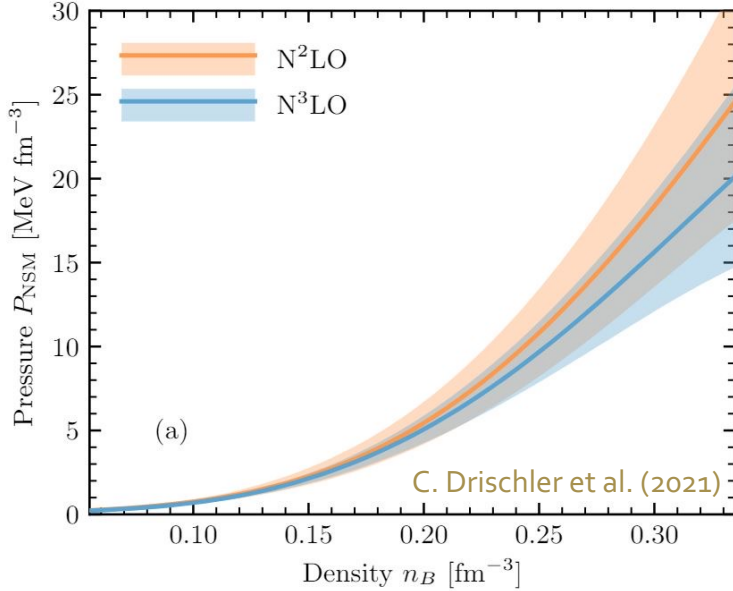
**Extending this version of  
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Crucial for performing UQ in any  
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**Prior choices**

How to best incorporate known  
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Extending **BMM** calculations to neutron-rich matter

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Scale variation techniques vs. missing higher orders UQ => possibly double-counting information if using both

### Exploring kernel design

EOS as a case study: constraints from astro./exp. could inform choices via type of phase transition allowed

**This BMM framework is *not* restricted to the EOS!**

**So, you might ask...**

## ... and some challenges

**Extending this version of BMM to multiple dimensions**

Crucial for performing UQ in any multi-dimensional nuclear physics problem

### Prior choices

How to best incorporate known physics => priors other than GPs



**How do I use this BMM framework for *my* particular problem?**



# Taweret: BMM software

Open-source repository:

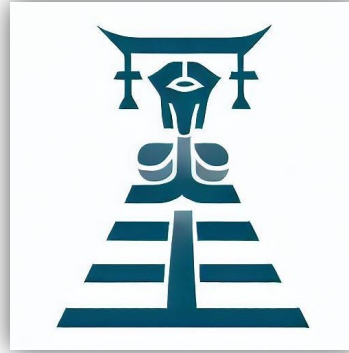
<https://github.com/bandframework/Taweret>

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



John Yannotty

Kevin Ingles

Dan Liyanage

Picture credit: Dick Furnstahl

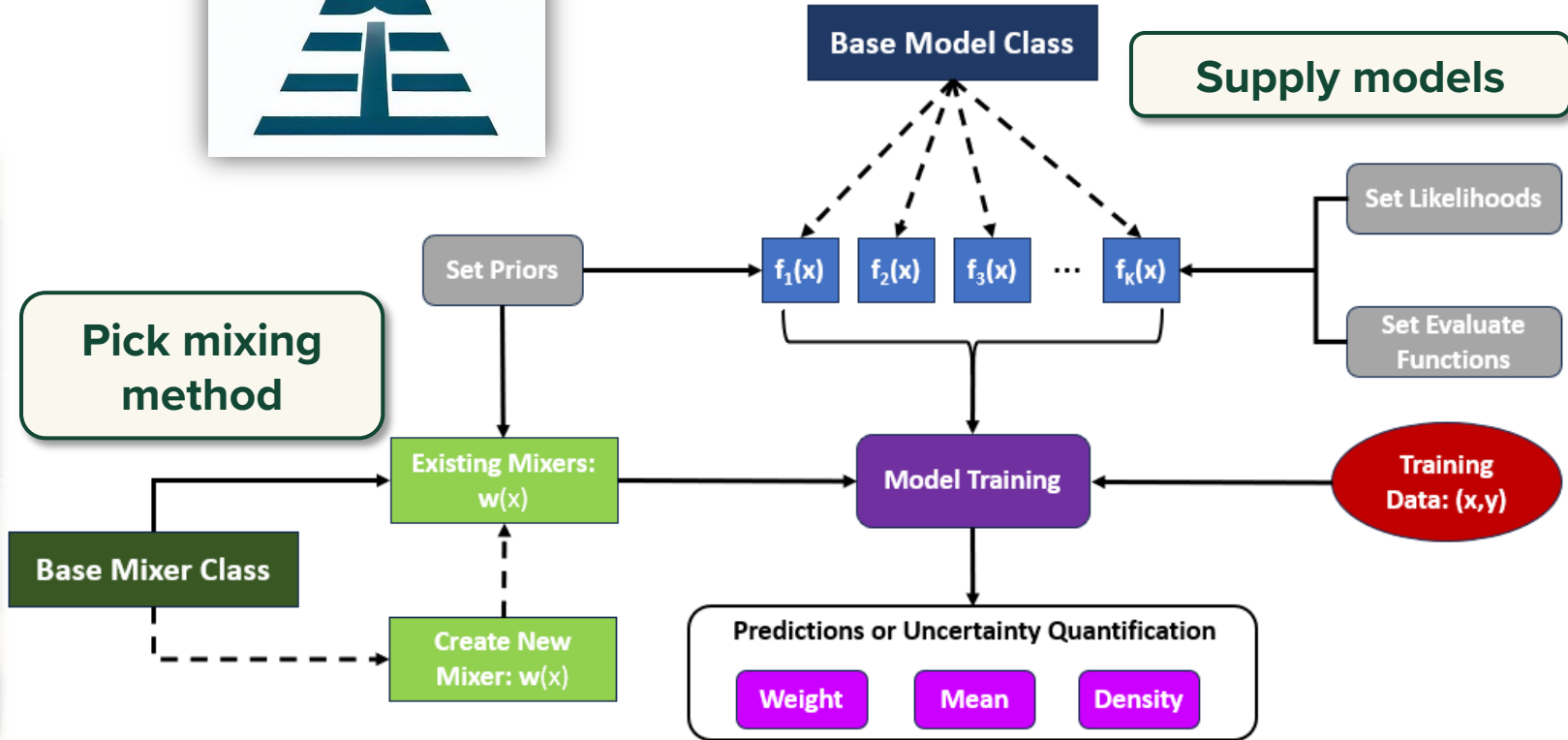


Figure credit: John Yannotty



Daniel Phillips (OU)



Dick Furnstahl (OSU)



Christian  
Drischler (OU)

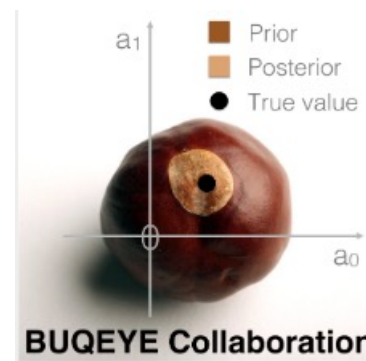


Jordan  
Melendez

# Thank you!



U.S. DEPARTMENT OF  
**ENERGY**



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



# Backup slides

# Crash course: Gaussian Processes (GPs)

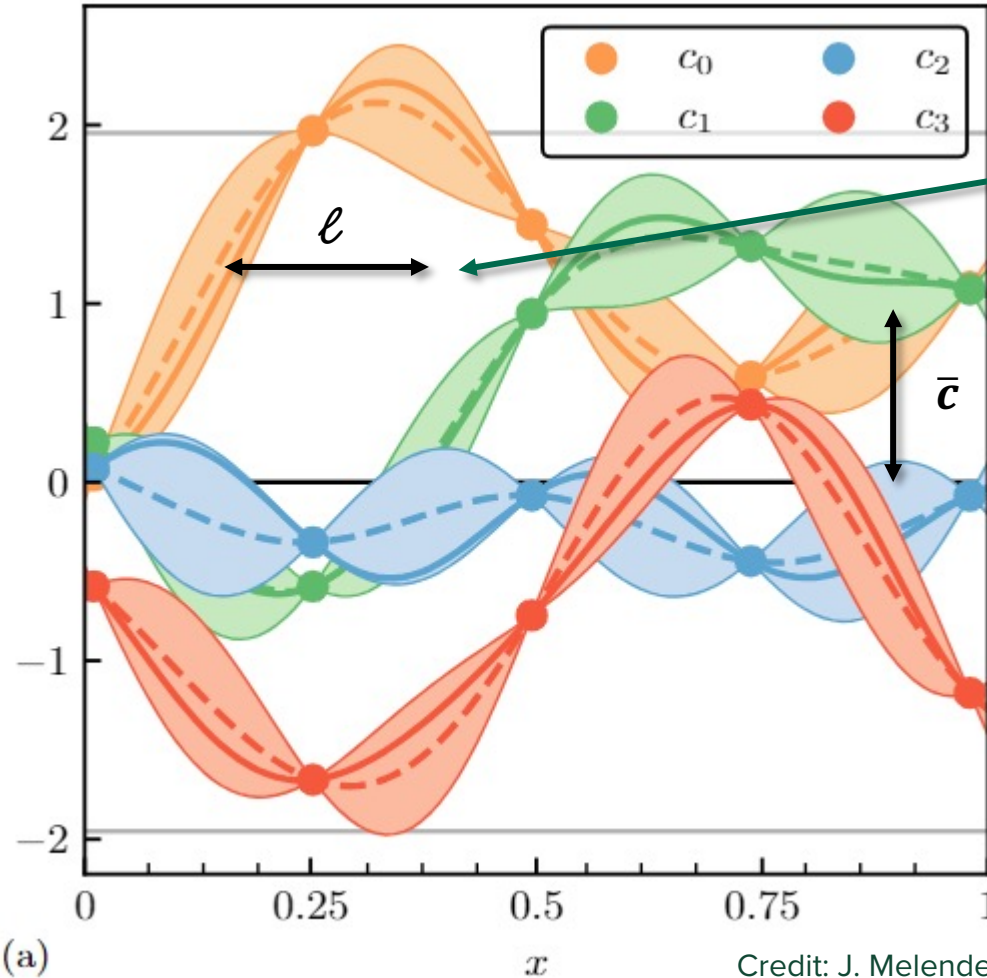
“Set of random variables, any subset of which possesses a Gaussian distribution”

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.)



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

Credit: J. Melendez et al. (2019)

# 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  $\Rightarrow n(\mu) = \frac{\partial P(\mu)}{\partial \mu} \rightarrow n(\mu_{FG}) \equiv n(\mu_{FG} + \mu_1 + \mu_2) \equiv \bar{n}$  Input number density

**3** Equate terms by counting powers of  $\alpha_s$   $\bar{n}(\mu) = c_0(\mu) \frac{\partial P_{FG}(\mu)}{\partial \mu} \Big|_{\mu=\mu_{FG}}$ ,  $\mu_1 = - \frac{c_1 Q(\bar{\Lambda}) \frac{\partial P_{FG}(\mu)}{\partial \mu}}{c_0 \frac{\partial^2 P_{FG}(\mu)}{\partial \mu^2}} \Big|_{\mu=\mu_{FG}} + \mu_2$  expression

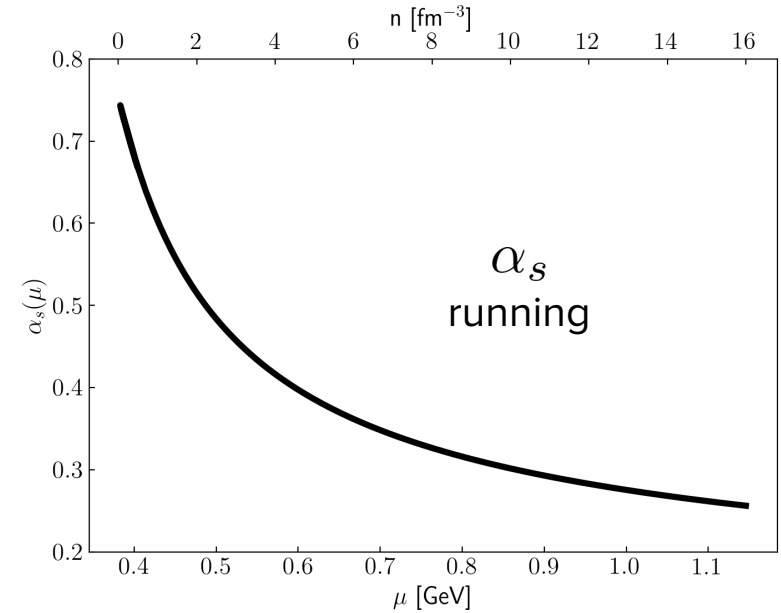
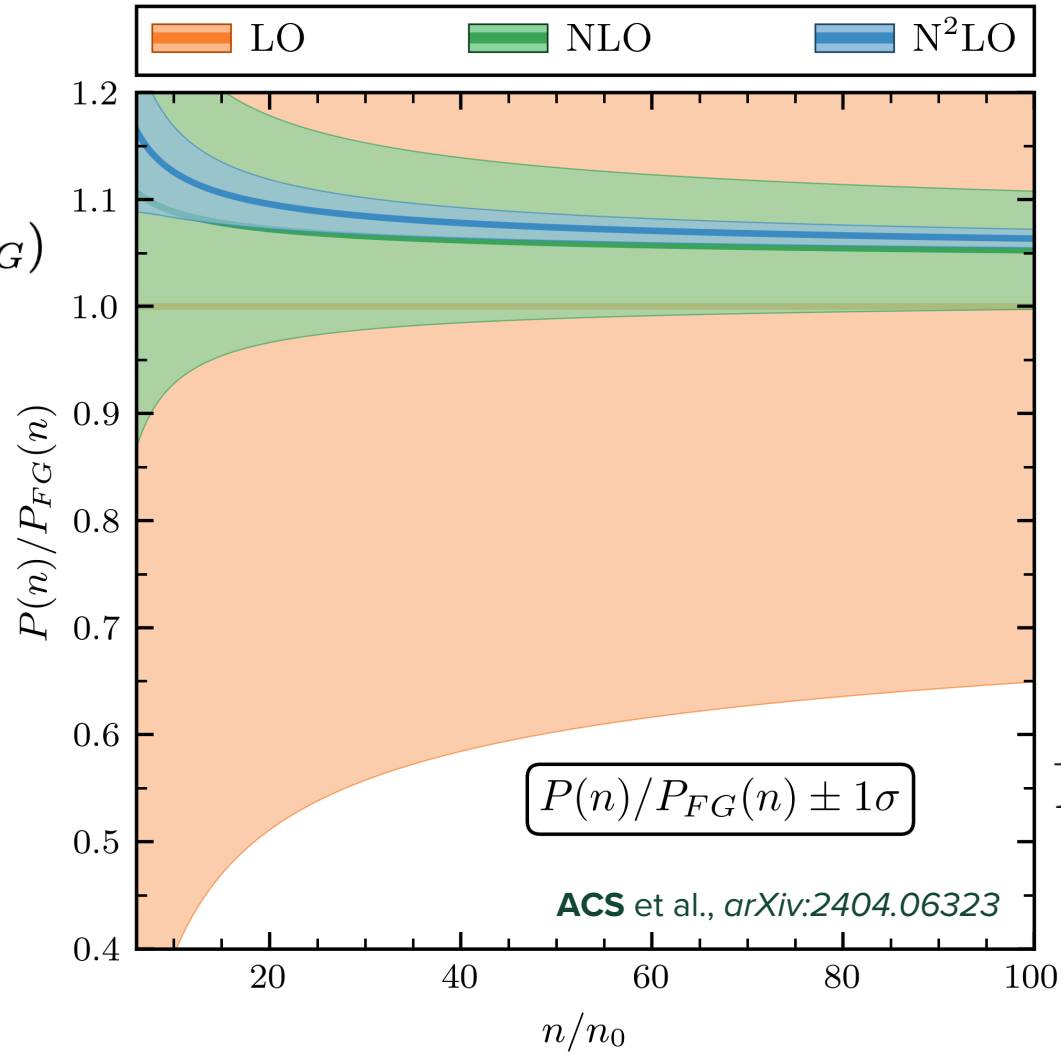
**4** Expand  $P(\mu)$ , insert terms, keep up to second order in  $\alpha_s$

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

# High densities: pQCD EOS

Invoke the Kohn-Luttinger-Ward inversion theorem

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



$P(n)$  scaled by FG pressure:

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

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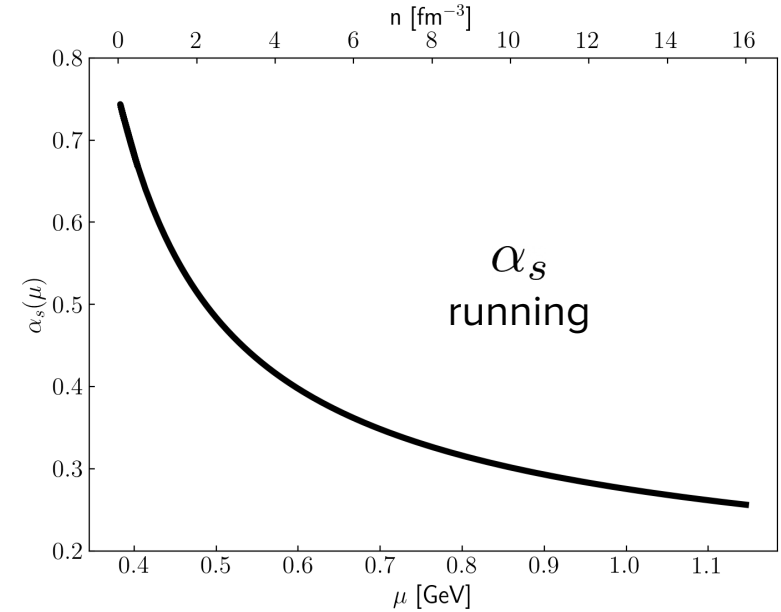
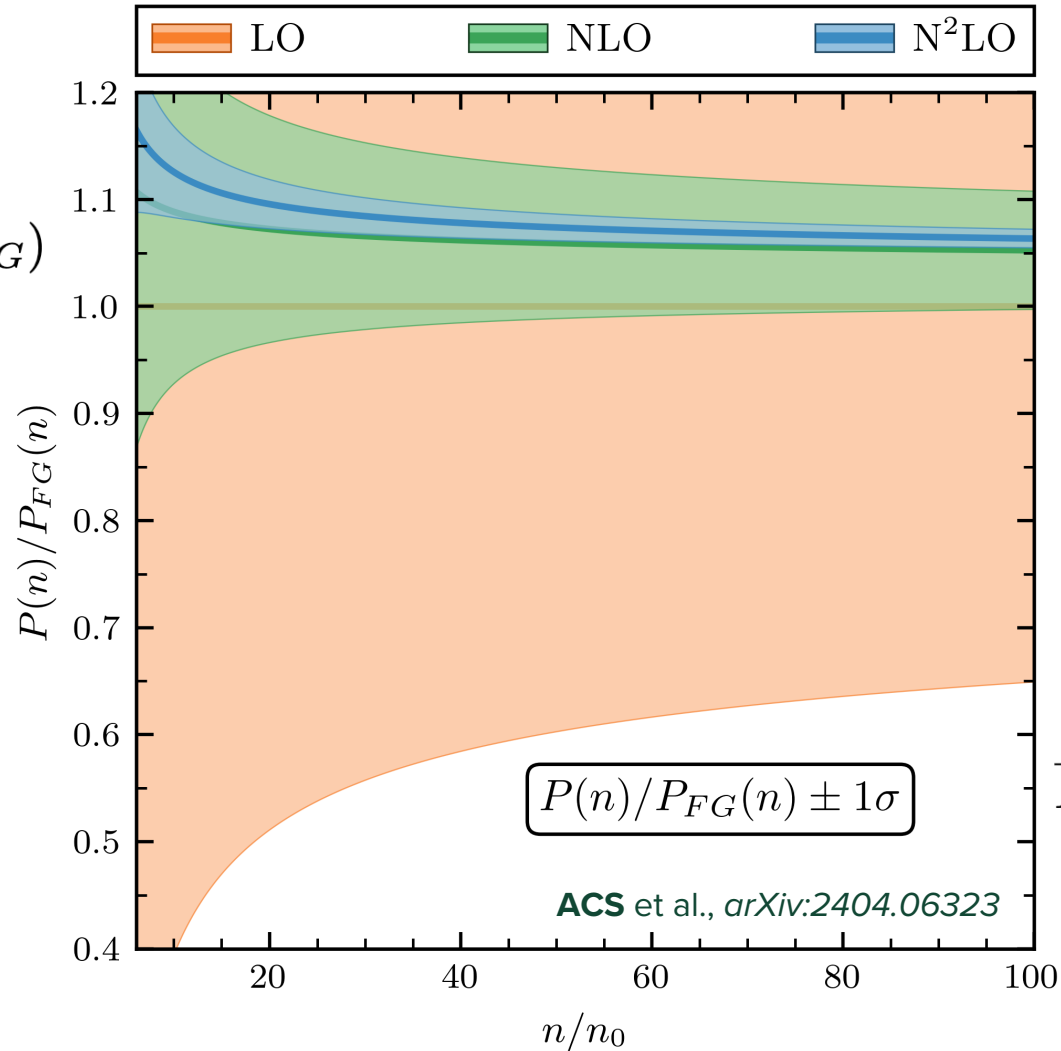
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Apply **gsum** to **P(n)**

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

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



**P(n) scaled by FG pressure:**

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

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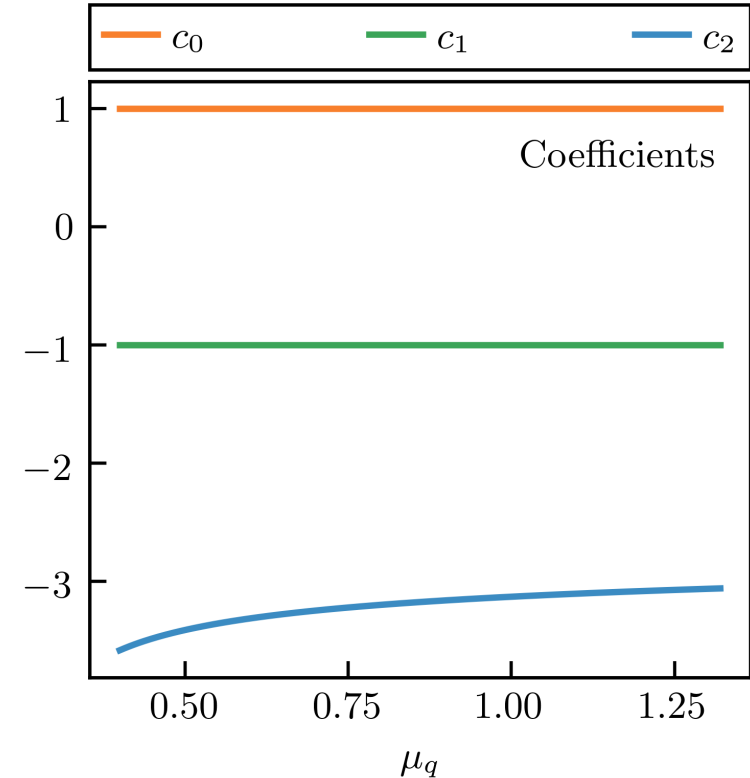
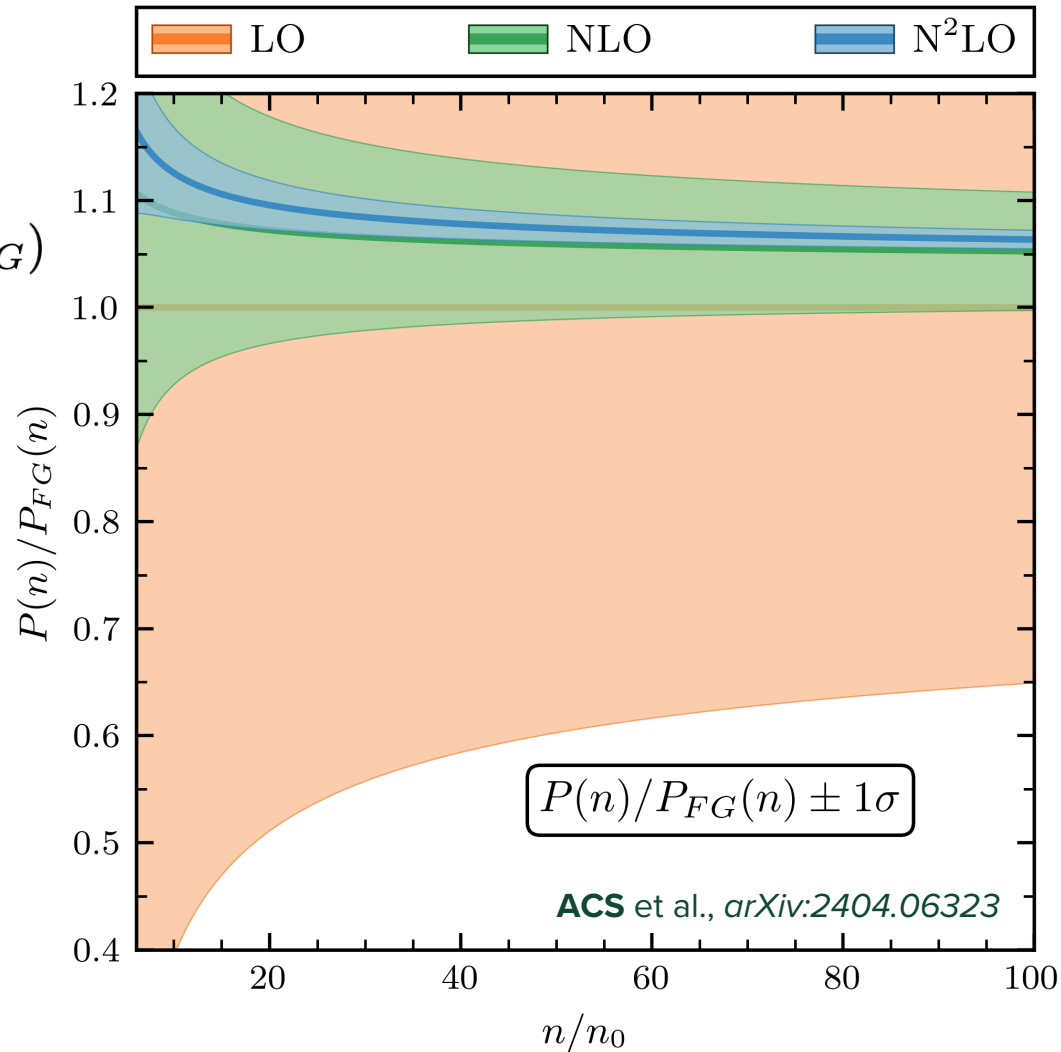
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**Truncation error** historically not assessed in a Bayesian way\* -> vary renormalization scale to obtain band

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





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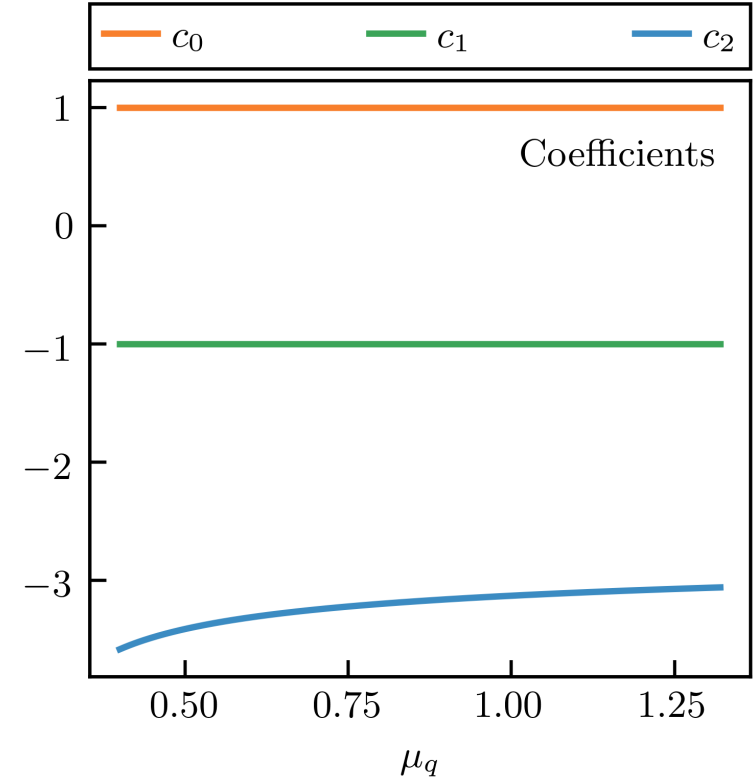
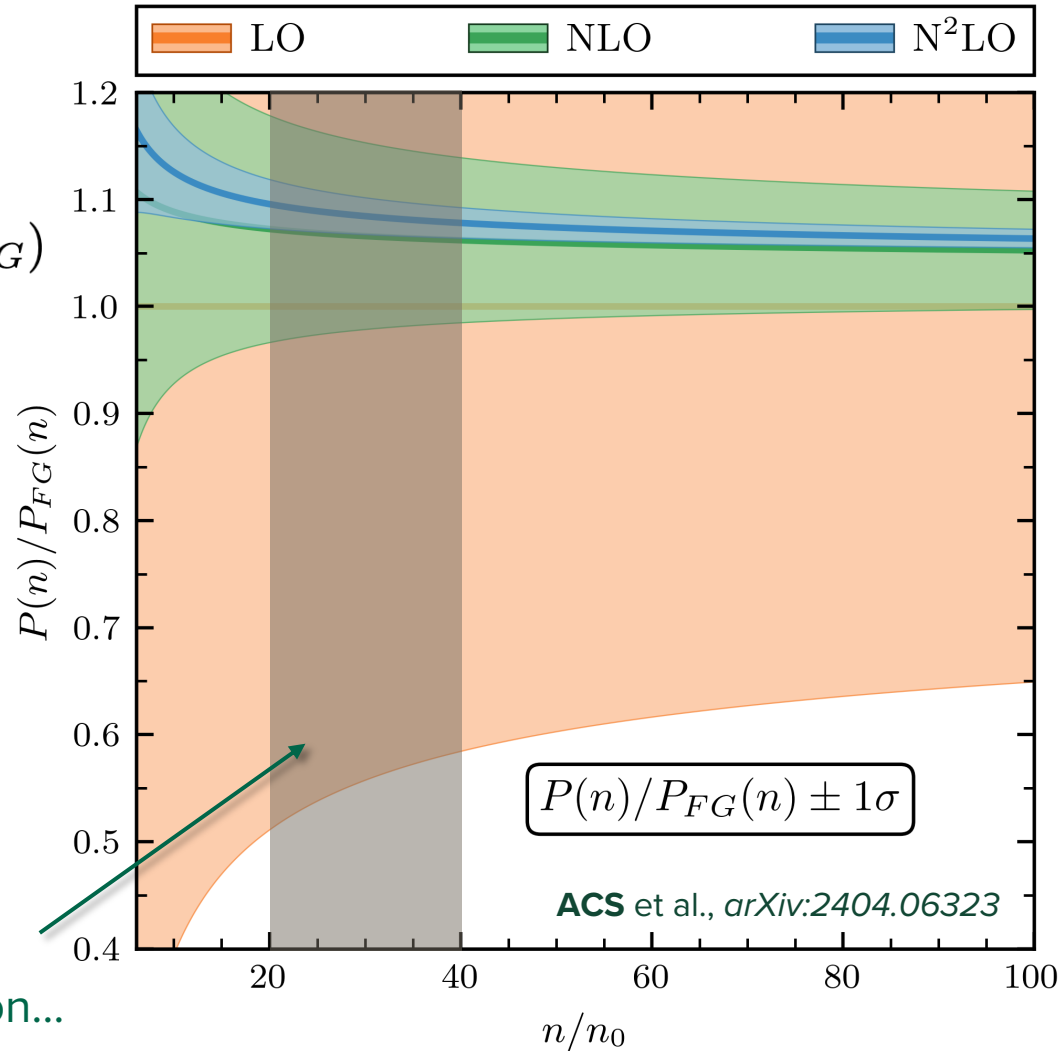
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Nonperturbative effects under (20-40)  $n_0$ : pairing, hadronization...



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# High densities: pQCD EOS

Calculate speed of sound squared using KLV expansion:

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

[**Equal** at N<sup>2</sup>LO to the calculation of  $c_s^2(\mu)$  using the pressure directly]

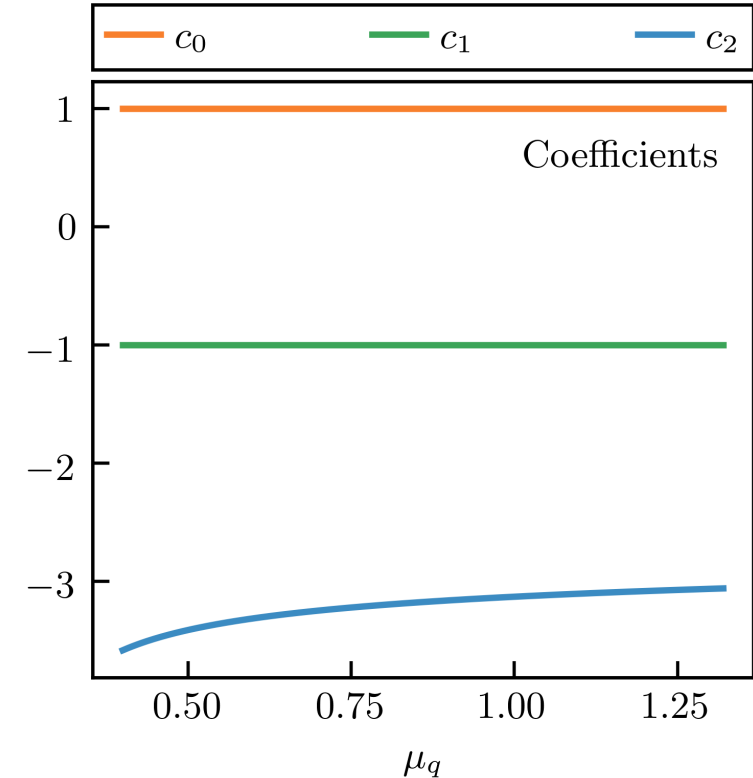
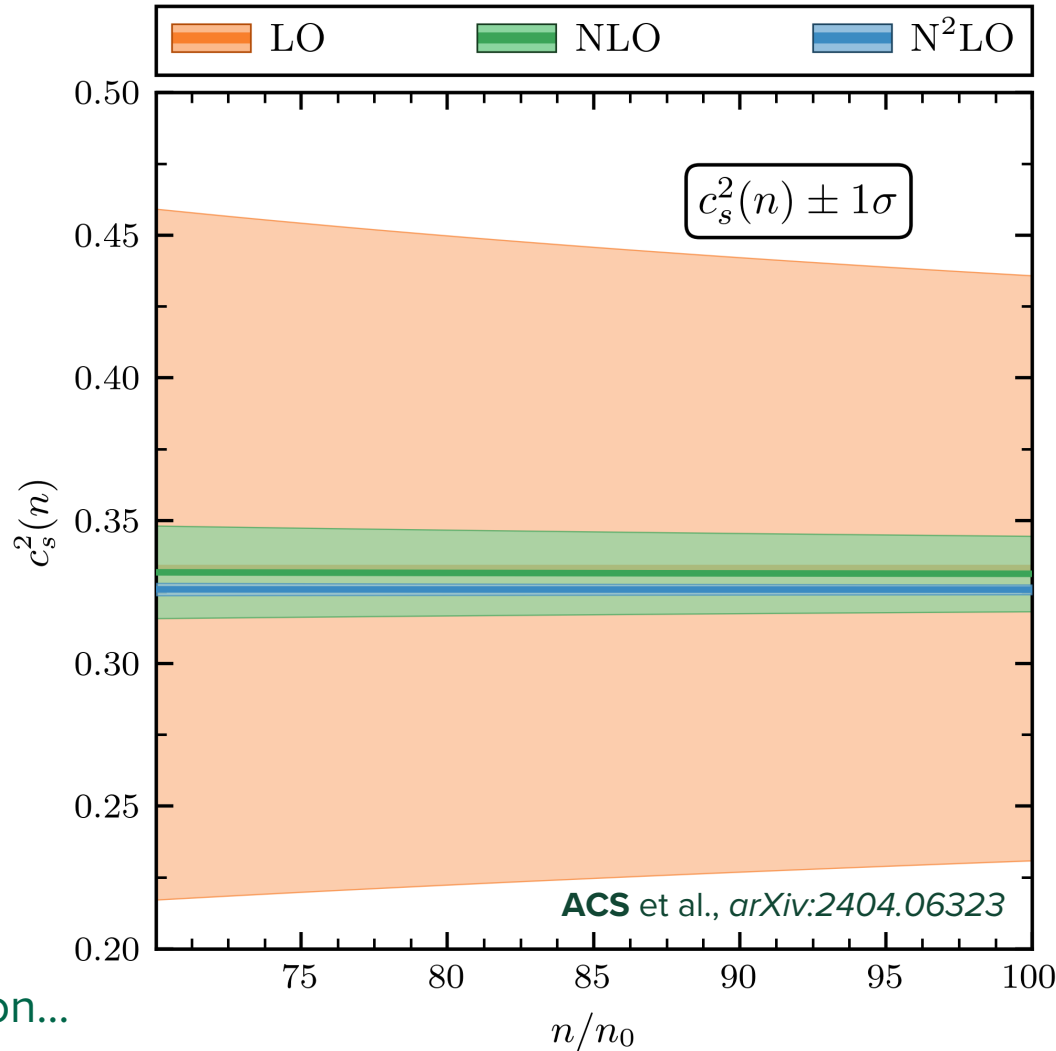
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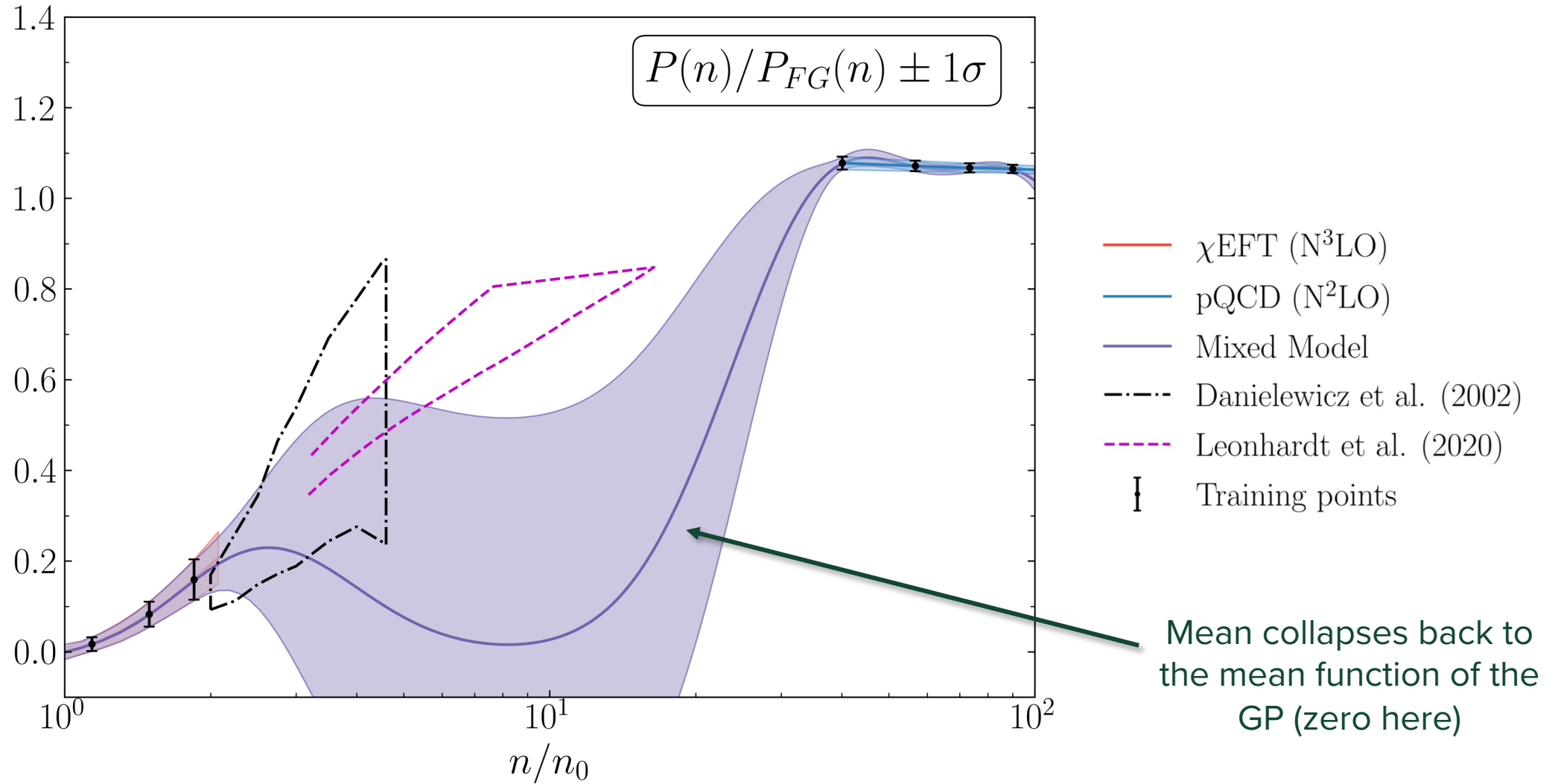


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# Extreme case: very short lengthscale





# collaboration: efforts

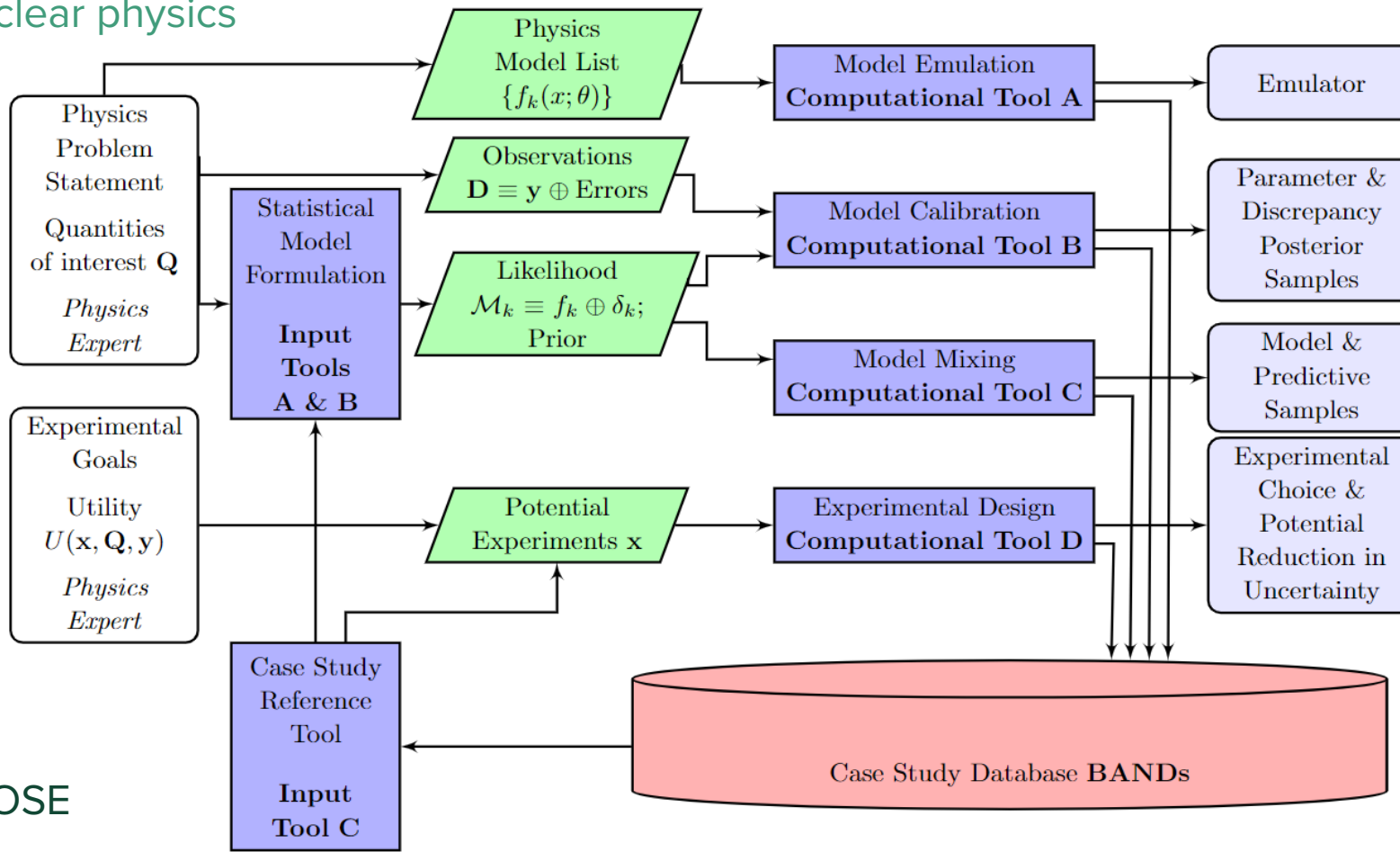
v0.3 of the BAND framework is out!



<https://github.com/bandframework/bandframework>

## Cyber-infrastructure

Develop tools for nuclear physics community  
Test on toy models and real-world applications



Our model mixing software!

SAMBA



Taweret

