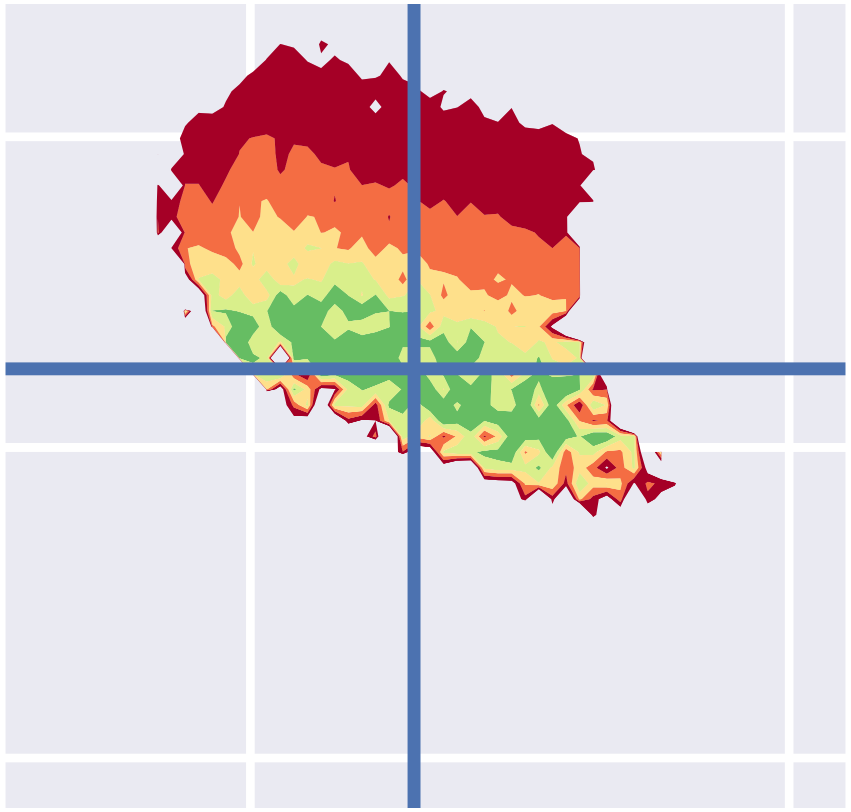
History matching for nuclear *ab initio* calculations

Christian Forssén
Chalmers University of Technology



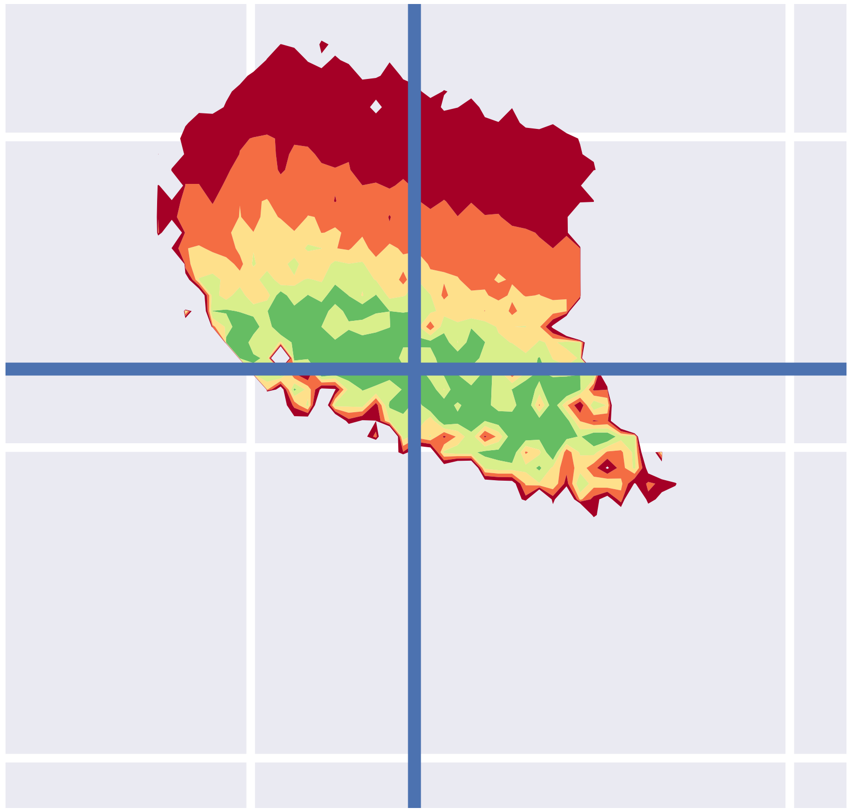
ISNET-9, Washington University in St Louis, May 22-26, 2023

Presenting (mainly) work published in:

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces
by B. Hu, W.G. Jiang, T. Miyagi, Z. Sun, A. Ekström, cf, G. Hagen, J.D. Holt, T. Papenbrock, S.R. Stroberg, I. Vernon, **Nature Phys. 18, 1196 (2022)**

Emergence of nuclear saturation within Δ-full chiral effective field theory
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13203**

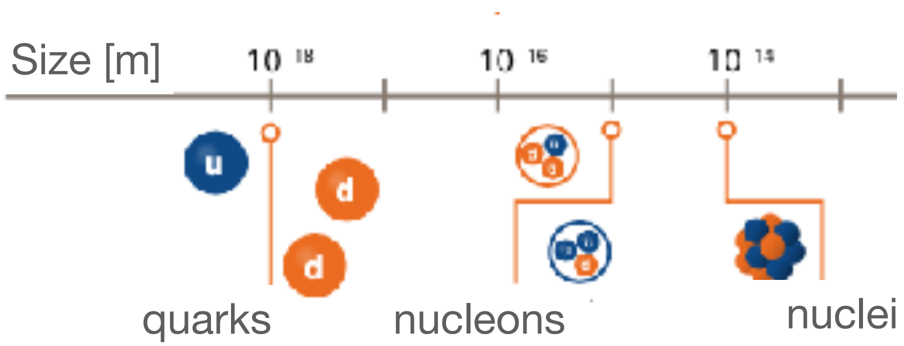
Emulating ab initio computations of infinite nucleonic matter
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13216**



Uncertainty quantification for *ab initio* methods based on effective field theory (EFT)

Scientific goals in *ab initio* nuclear theory

- Model the strong interaction at low-energy
  - At the most fundamental level, the strong interaction is described by Quantum Chromodynamics (QCD);
  - At low energies, quarks condense into hadrons;
  - Atomic nuclei can supposedly be described with relevant low-energy degrees of freedom—nucleons and pions—and residual interactions;
  - Effective field theories (EFTs) offer a systematic description of this physics.



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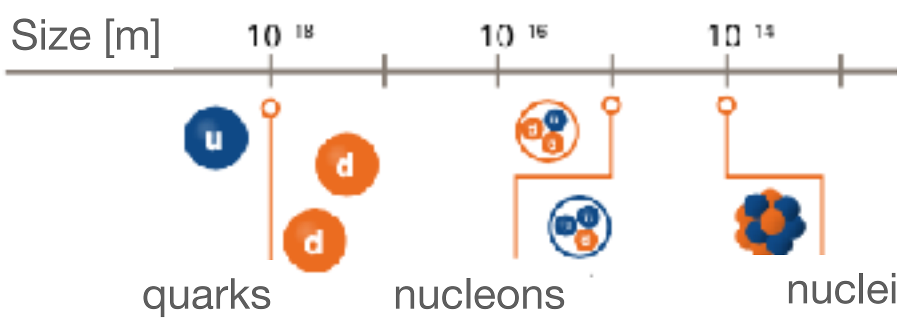
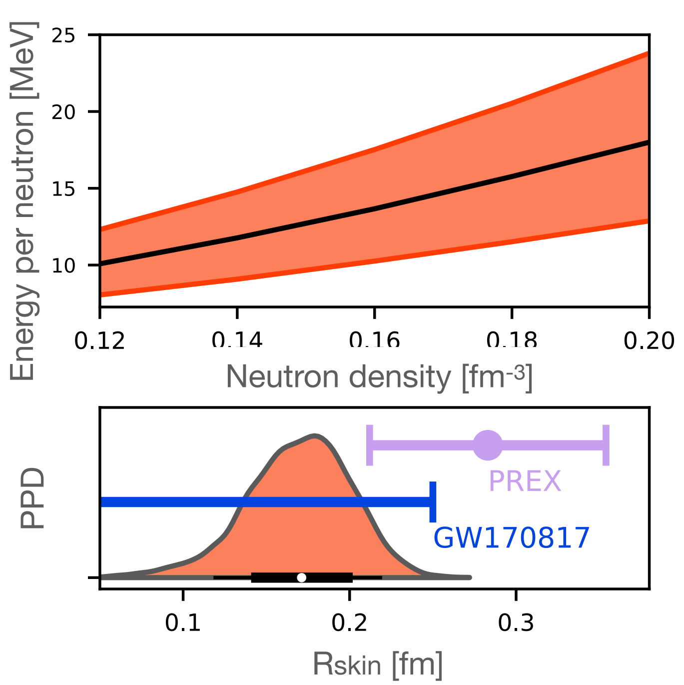


- Parameter estimation and model checking
  - Infer the parameters (low-energy constants = LECs) of chiral EFT from low-energy, nuclear data: E.g. NN scattering observables, few-nucleon or other low-energy observables.
  - Also other parameters might be of interest. E.g.,
    - Can we infer the breakdown scale of the EFT?
    - Can we rigorously test the EFT model assumptions?

- Predictive power
  - Predict scientifically relevant nuclear observables with quantified uncertainties.



Learning from data via Bayes

- Apply **Bayes' theorem**

$$\underbrace{p(\boldsymbol{\alpha}\,|\,\mathscr{D}, I)}_{\text{Posterior}} = \frac{\overbrace{p(\mathscr{D}\,|\,\boldsymbol{\alpha}, I)}^{\text{Likelihood}} \cdot \overbrace{p(\boldsymbol{\alpha}\,|\,I)}^{\text{Prior}}}{\underbrace{p(\mathscr{D}\,|\,I)}_{\text{Marginal likelihood}}}$$

  - The prior encodes our knowledge about parameter values before analyzing the data
  - The likelihood is the probability of observing the data given a set of parameters
  - The marginal likelihood (or model evidence) provides normalization of the posterior.
  - The posterior is the inferred probability density for the parameters.

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- Predictions for "future" data, modeled with y(α), are described by the **posterior predictive distribution** (ppd)

$$\left\{ y(\boldsymbol{\alpha}) : \boldsymbol{\alpha} \sim p(\boldsymbol{\alpha}\,|\,\mathscr{D},I) \right\}$$

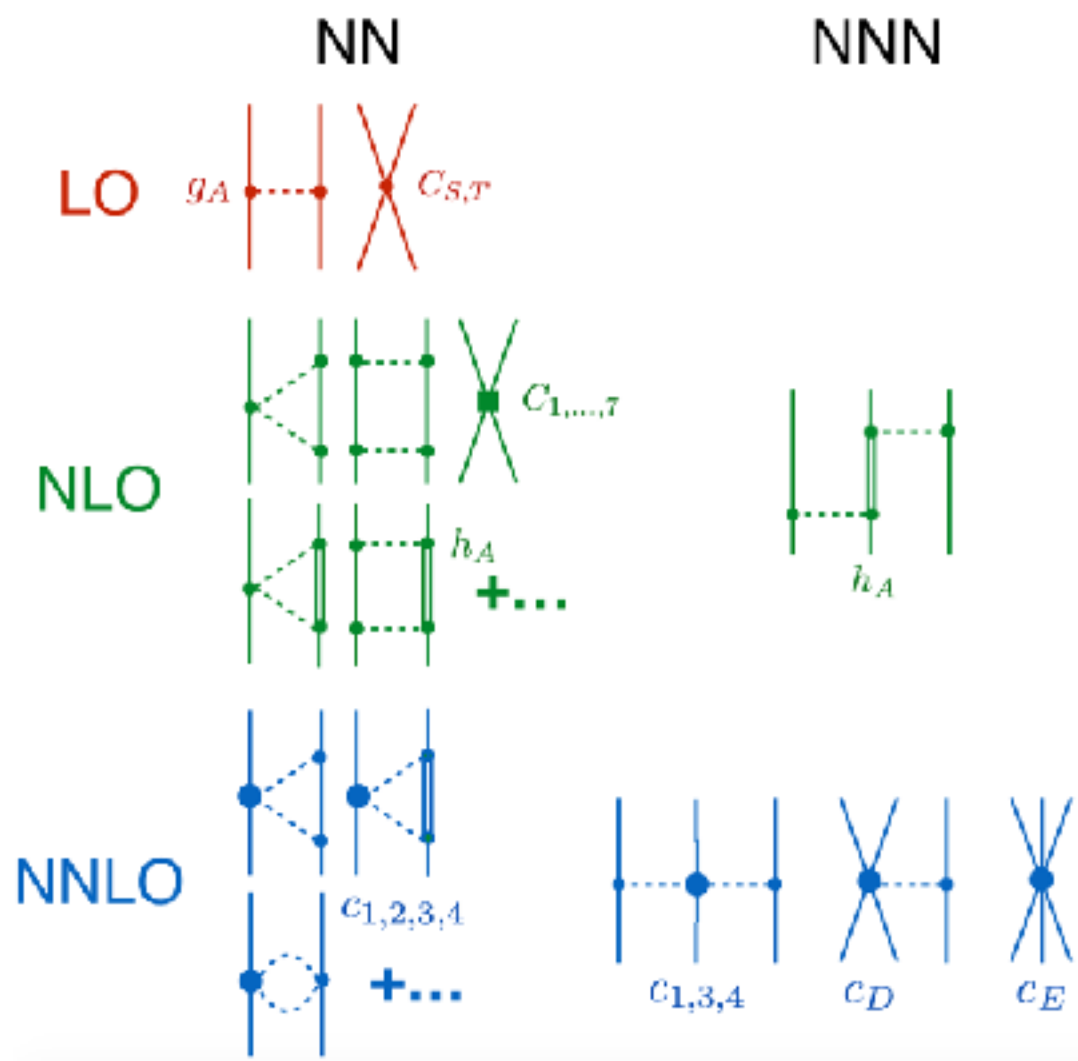
  - We will also introduce **full ppd**:s $\left\{ \boldsymbol{y}(\boldsymbol{\alpha}) + \delta\boldsymbol{y} : \boldsymbol{\alpha} \sim p(\boldsymbol{\alpha}\,|\,\mathscr{D},I),\ \delta\boldsymbol{y} \sim p(\delta\boldsymbol{y}) \right\}$

Ab initio modeling of nuclear systems using χEFT

$$\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$$

$$\hat{H}(\boldsymbol{\alpha}) = \hat{T} + \hat{V}(\boldsymbol{\alpha})$$

χEFT promises a connection with QCD



Weinberg, van Kolck, Kaiser, Bernard, Meißner, Epelbaum, Machleidt, Entem, …

A. Ekström, et al. Phys. Rev **C 97**, 024332 (2018)

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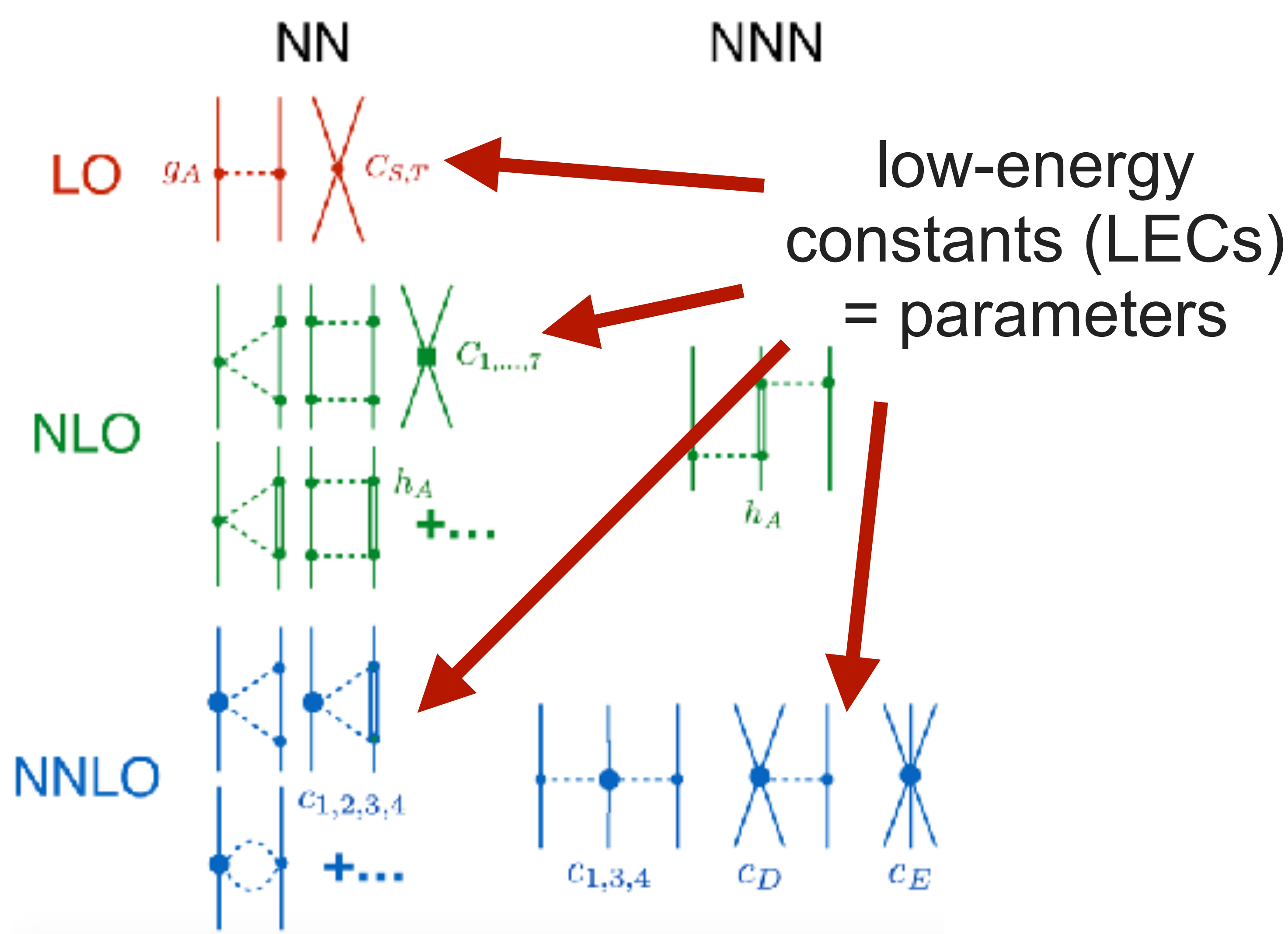

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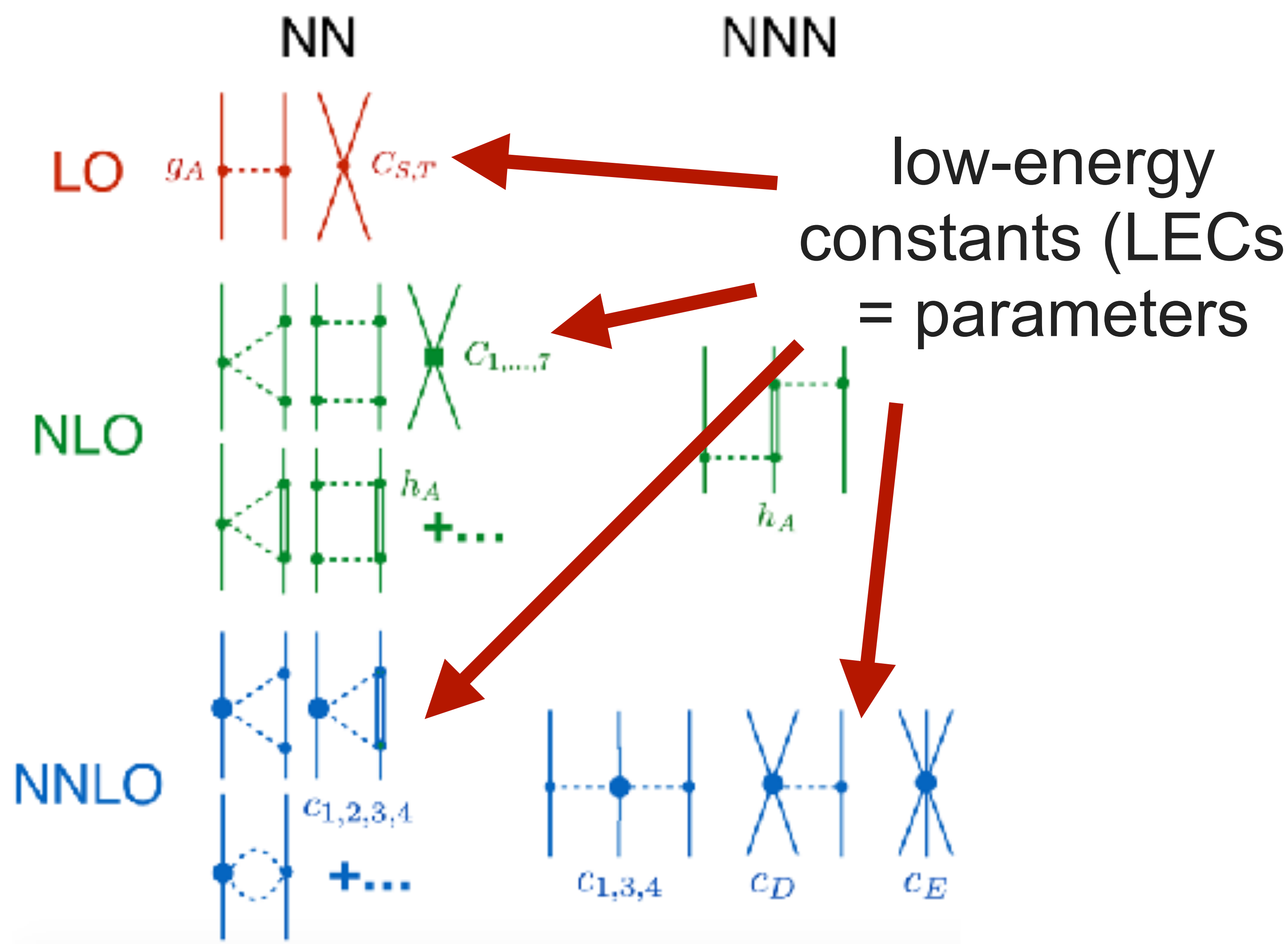
parameters inferred from data.
– **parametric uncertainty**

EFT expansion truncated
– **model/truncation error**

many-body solver relies on approximations:
– **many-body error**

χEFT promises a connection with QCD



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Current UQ frontiers in *ab initio* nuclear theory

- Getting to know your errors
  - Means, variances, and covariances of EFT truncation, many-body method, emulator errors;
  - PDF functional forms;
  - Model calibration and validation
- Sampling PDFs without tears
  - Mimic **costly simulators** with efficient and accurate **emulators**;
  - Hamiltonian MC, sampling / importance resampling, …
- Technologies to be explored
  - Model mixing, experimental design, …

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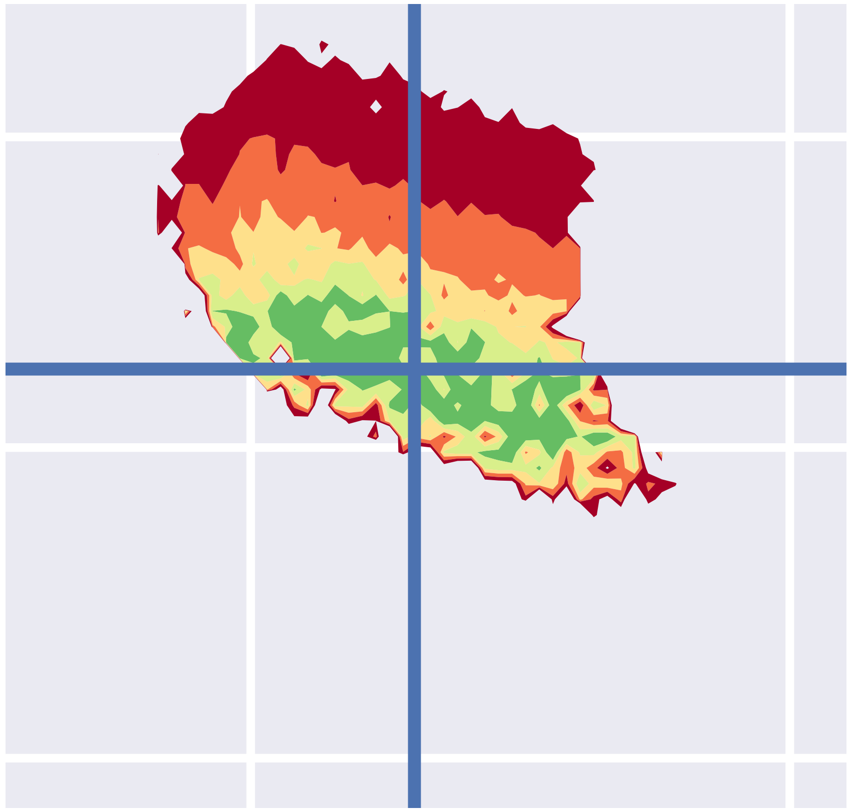
See, e.g., Frontiers in Physics volume on
"*Uncertainty Quantification in Nuclear Physics*"



Emulators

Emulators

- An **emulator** mimics the simulator output at a reduced computational cost:

$$\boldsymbol{y}(\boldsymbol{\alpha}) \approx \tilde{\boldsymbol{y}}(\boldsymbol{\alpha}) + \delta\tilde{\boldsymbol{y}}$$

  - A useful emulator is fast and accurate.
  - Keep track of the emulator uncertainty.

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- Emulators can be non-intrusive (data based)
  - Neural networks, Gaussian processes, etc
- Or intrusive (model based)
  - Translating a high-fidelity model to a low-fidelity one
  - Vast literature on model-order reduction (MOR);
    see, e.g., Melendez et al. (2203.05528) with many refs.

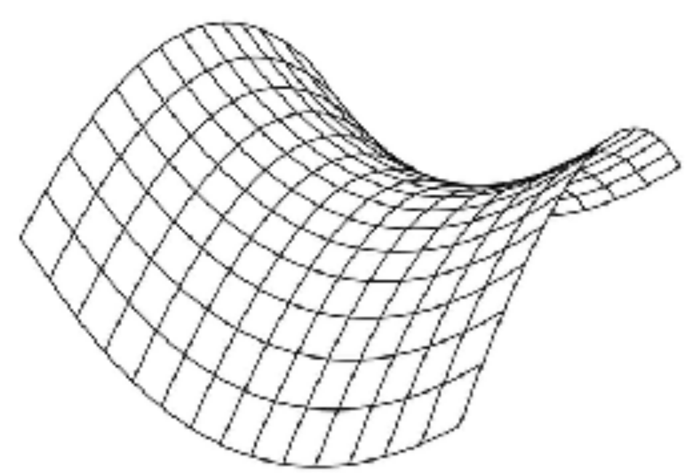
Many talks at this workshop.
E.g., Furnstahl, Ekström, Becker, Odell (model-based)
and several others for data-based emulators

Eigenvector continuation emulators

$$H(\alpha) = H_0 + \alpha H_1$$

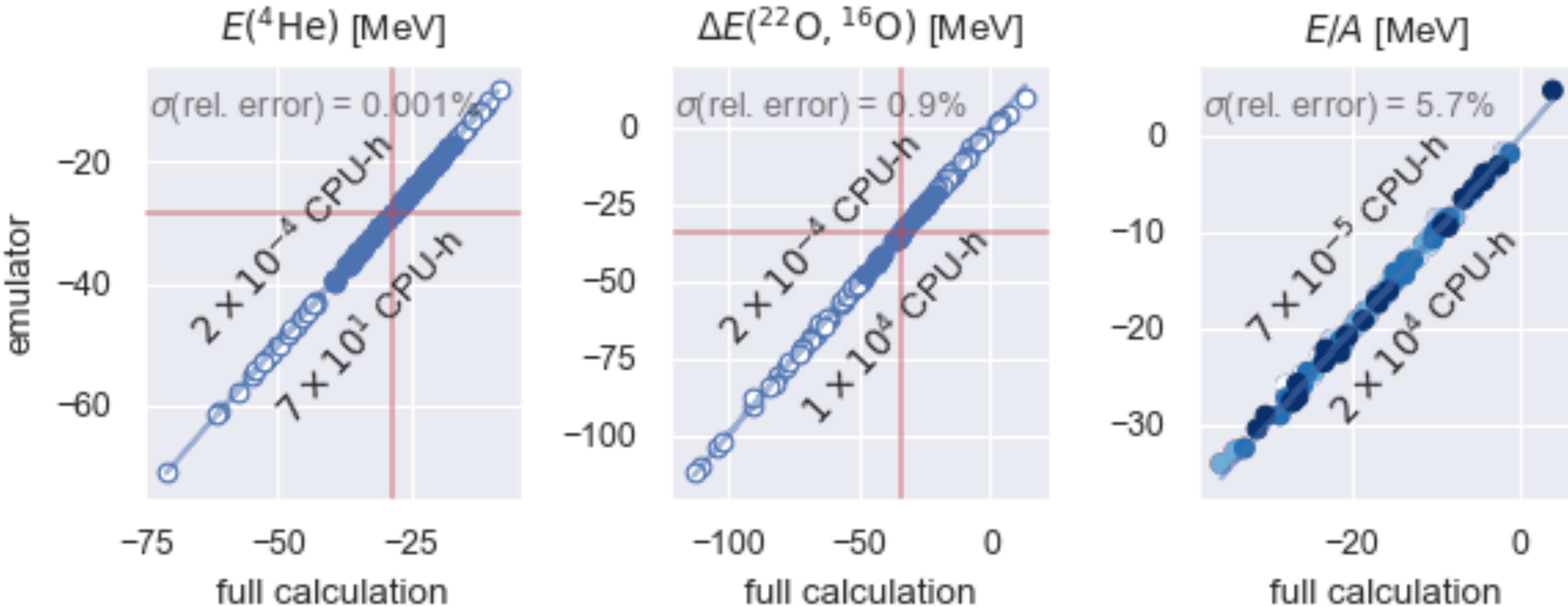
continuous parameter

The key insight is that while an eigenvector resides in a linear space with enormous dimensions, the eigenvector trajectory generated by smooth changes of the Hamiltonian matrix is well approximated by a very low-dimensional manifold.



D. Frame, et al. Phys. Rev. Lett. **121**, 032501 (2018)

Time(emulation) << Time(simulation)



König et al., PLB 810, 135814 (2020)

Kondo et al., in preparation

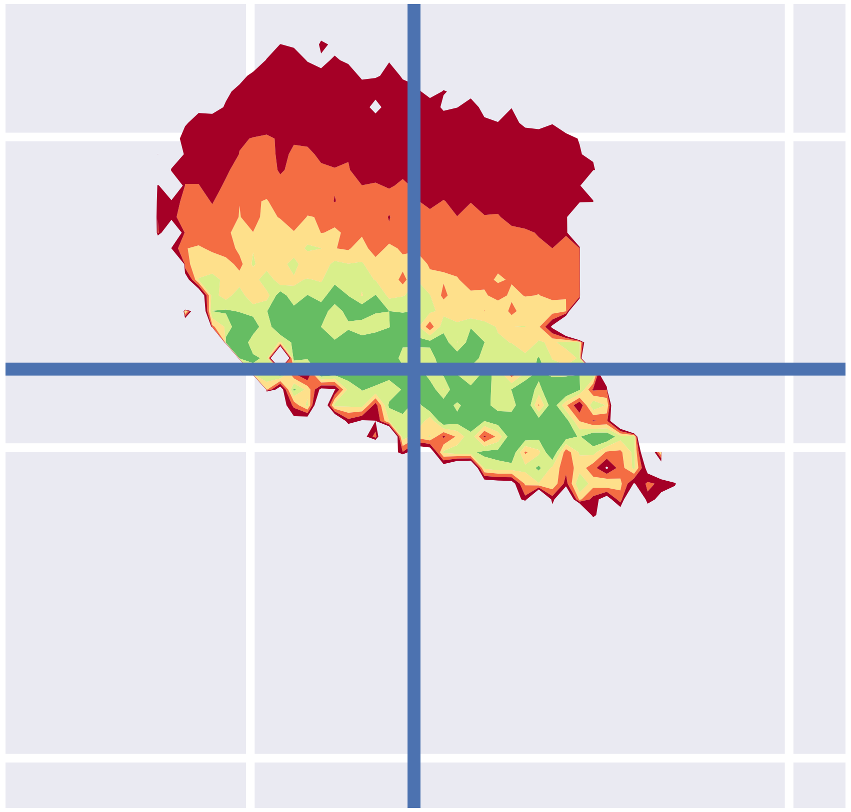
Jiang et al., arXiv 2212.13216 & arXiv 2212.13203

Selected references:

I. Vernon, et al. (Bayesian Anal., 2010)

I. Vernon, et al. (BMC Systems Biology, 2018)

B. Hu et al (Nature Phys. 2022)

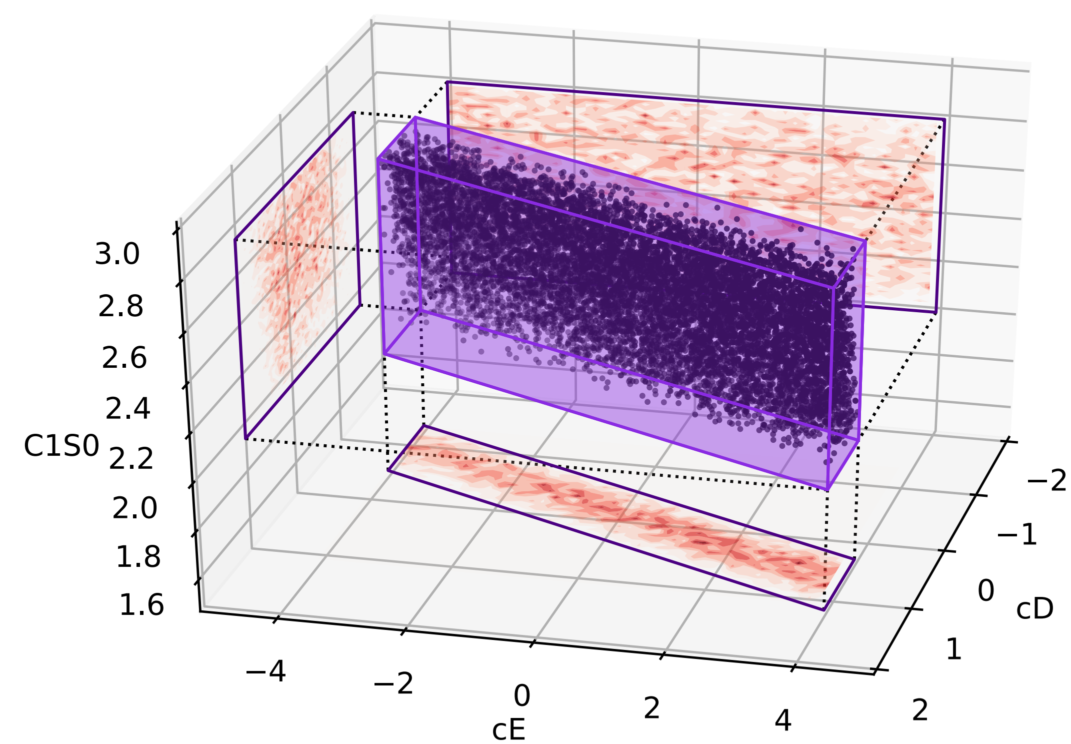


Iterative history matching

Approximate Bayes

- Bayesian linear methods (only means and variances) can be very useful
  - Easier to claim **implausibility** than to quantify likelihood
    $\Theta_{\mathrm{NI}}(\boldsymbol{\alpha})$ versus $p(\mathscr{D}\,|\,\boldsymbol{\alpha}, I) \equiv \mathscr{L}(\boldsymbol{\alpha})$
  - Define **implausibility measure** (using only means and variances)
  - **History matching**: Iteratively remove regions in which $\Theta_{\mathrm{NI}}(\boldsymbol{\alpha}) = 0$

$$\Theta_{\mathrm{NI}}(\boldsymbol{\alpha}) = \begin{cases} 0 & \text{implausible} \\ 1 & \text{non-implausible} \end{cases}$$



Iterative history matching

- Climate modeling
  (Williamson 2013, Edwards 2019)
- Ecosystem ecology
  (Raftery, 1995)
- Epidemiology
  (Andrianakis 2015, 2016, Vernon 2022)
- Galaxy formation
  (Vernon 2010, 2014)
- Oil reservoir modelling
  (Craig 1995, 1996, Cumming 2009)
- Systems biology
  (Vernon 2018)
- Nuclear physics
  (Hu 2022, Jiang 2022, Elhatisari 2022)

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Revisiting Antarctic ice loss due to marine ice-cliff instability

Tamsin L. Edwards, Mark A. Brandon, Gael Durand, Neil R. Edwards, Nicholas R. Golledge, Philip B. Holden, Isabel J. Nias, Antony J. Payne, Catherine Ritz & Andreas Wernecke

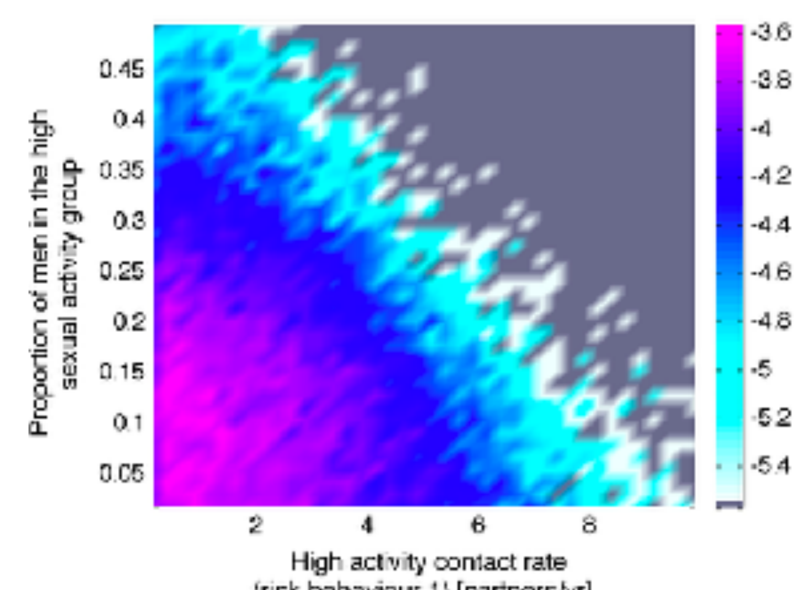
Nature 566, 58–64(2019) Cite this article

ROYAL STATISTICAL SOCIETY
Journal of the Royal Statistical Society
Applied Statistics
Series C

Original Article | Open Access

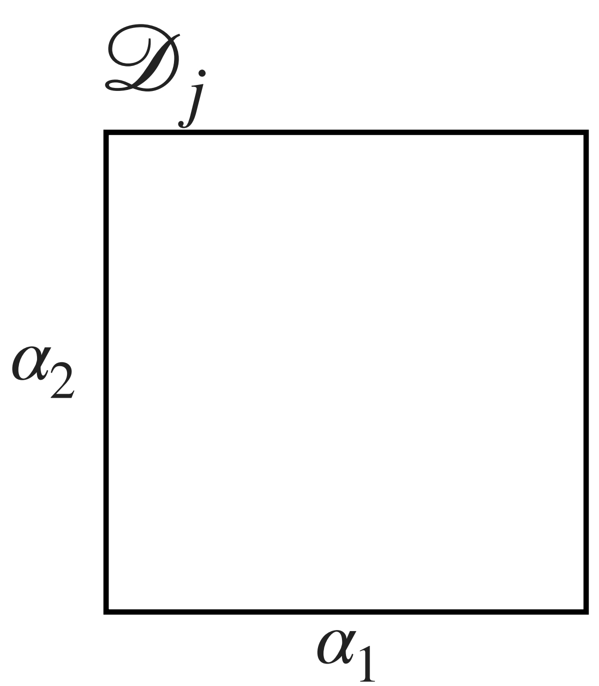
History matching of a complex epidemiological model of human immunodeficiency virus transmission by using variance emulation

I. Andrianakis, I. Vernon, N. McCreesh, T. J. McKinley, J. E. Oakley, R. N. Nsubuga, M. Goldstein, R. G. White



Iterative history matching strategy

1. At iteration j: Construct or **refine emulator(s)** for the model predictions across the current non-implausible volume $\mathscr{D}_j$.
   Choose a **rejection strategy based on implausibility measures** for the chosen set $\mathscr{Z}_j$ of informative observables.



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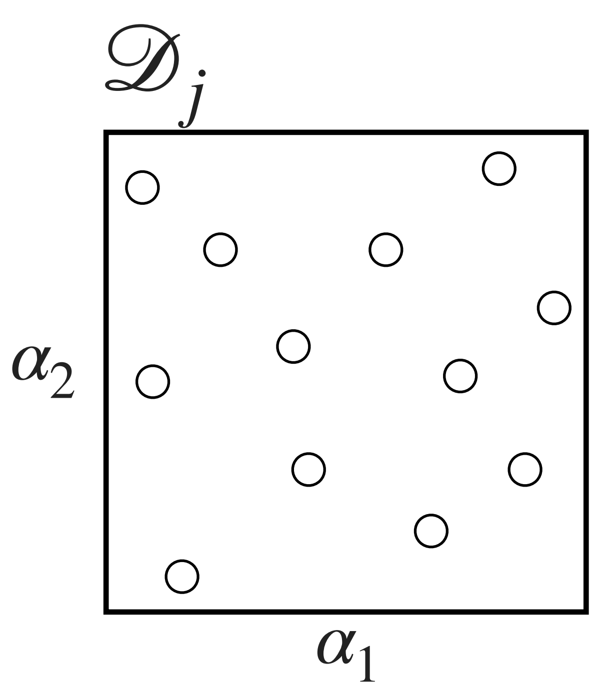

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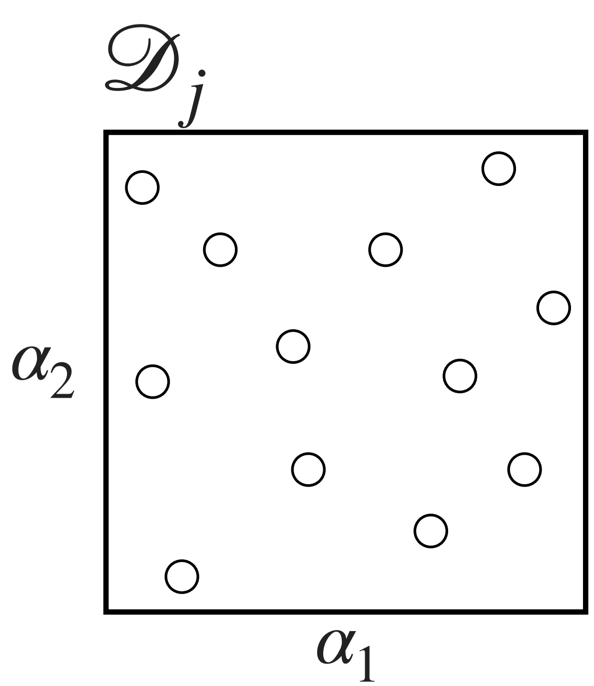
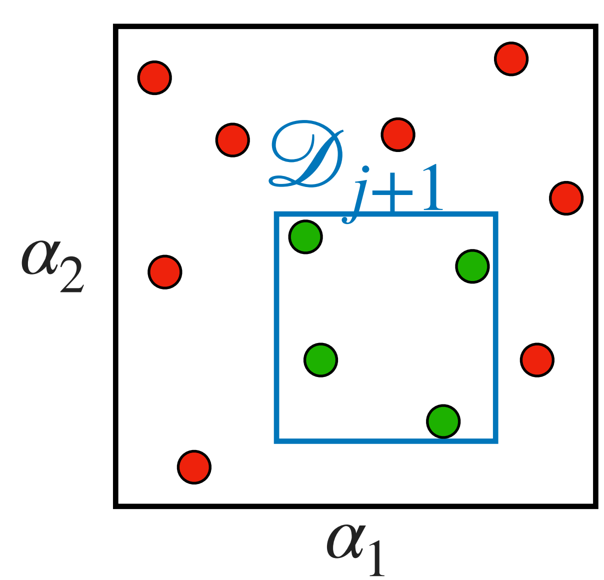
3. The implausibility measures are then calculated over $\mathscr{D}_j$, using the emulators, and implausibility cutoffs are imposed. Define a **new (smaller) non-implausible volume** $\mathscr{D}_{j+1}$ which should satisfy $\mathscr{D}_{j+1} \subset \mathscr{D}_j$.





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4. Unless (a) computational resources are exhausted, or (b) all considered points in the parameter space are deemed implausible, we:
   i. include any additional informative observables in the considered set $\mathscr{Z}_{j+1}$, and return to step 1.

5. If 4(a) is true we generate a large number of acceptable runs from the final NI volume $\mathscr{D}_{\text{final}}$, sampled according to scientific need.

Implausibility measure

- The **implausibility measure** does not use the full likelihood, but just means and variances

$$I_M^2(\boldsymbol{\alpha}) \equiv \max_{z_i \in \mathcal{Z}} \frac{\left| \mathbb{E}\left[\tilde{f}_i(\boldsymbol{\alpha})\right] - z_i \right|^2}{\mathrm{Var}\left[\tilde{f}_i(\boldsymbol{\alpha}) - z_i\right]}.$$

where $\mathcal{Z}$ is the collection of outputs that are being considered and $\mathrm{Var}[\ldots]$ is the combined variance of **observational, model, method, and emulator uncertainties**.

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- Large values of $I_M(\boldsymbol{\alpha})$ imply that we are highly unlikely to obtain acceptable matches between model output and observed data at input α. We consider a particular input $\boldsymbol{\alpha}$ as **implausible** if

$$I_M(\boldsymbol{\alpha}) > c_M,$$

where we may choose $c_M = 3$, appealing to Pukelheim's three-sigma rule, or a ladder of cutoffs for the first, second, etc., maximum.

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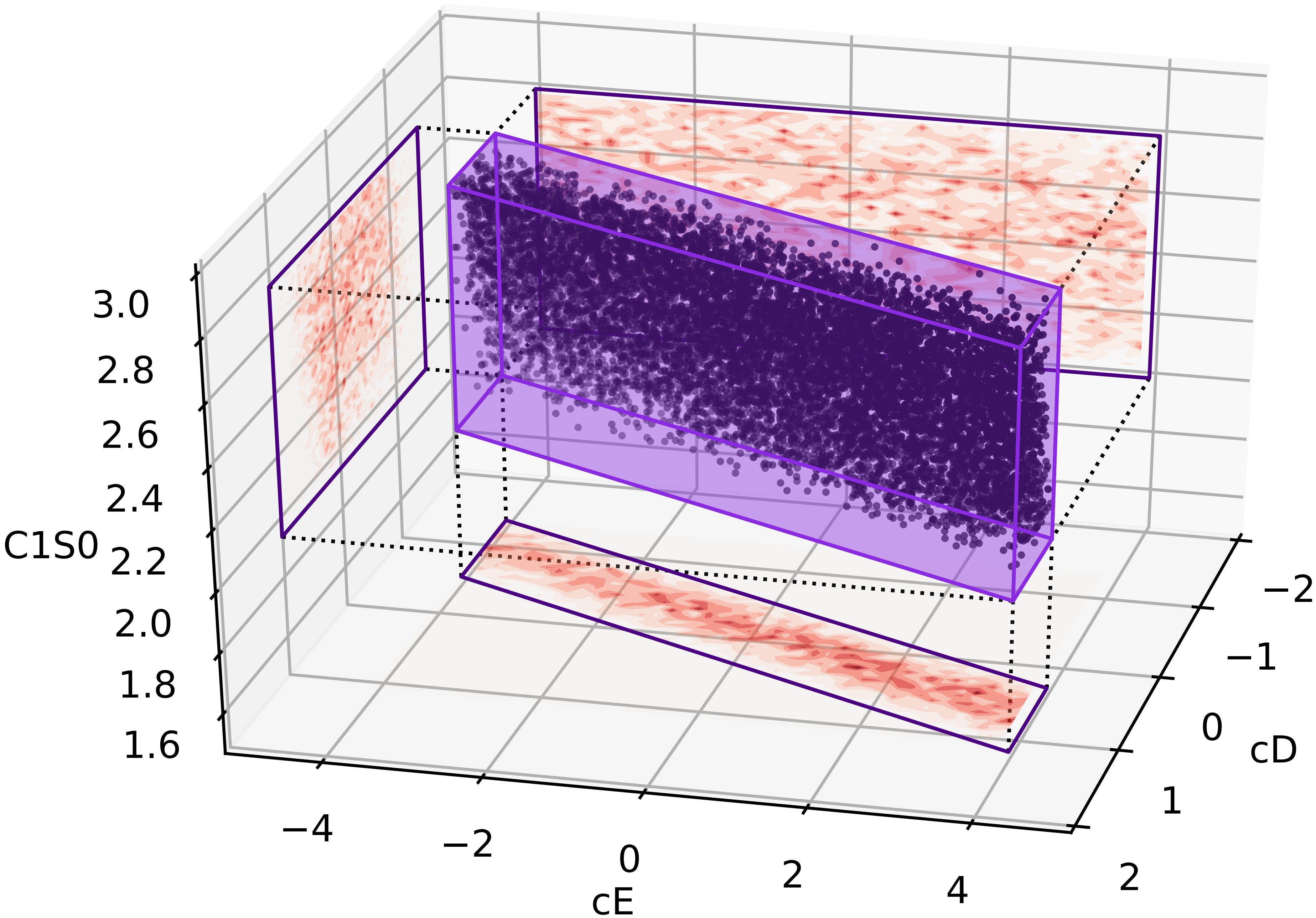
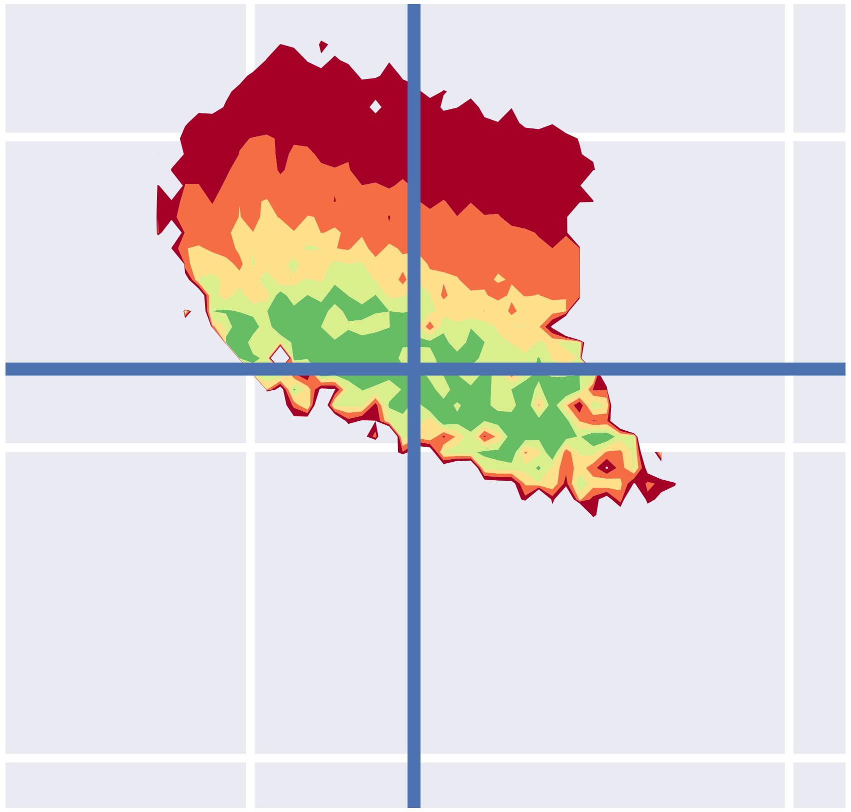
where we may choose $c_M = 3$, appealing to Pukelheim's three-sigma rule, or a ladder of cutoffs for the first, second, etc., maximum.

- Surviving the implausibility cutoff does not necessarily imply that $\boldsymbol{\alpha}$ is very good; just **non-implausible**!

Non-implausible domain



The parameter region emerging from history matching is where we expect the posterior distribution to reside.



Emergence of nuclear saturation

Emergence of nuclear saturation within Δ-full chiral effective field theory
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13203**

Emulating ab initio computations of infinite nucleonic matter
by W.G. Jiang, cf, T. Djärv, G. Hagen, **arXiv:2212.13216**

Emergence of nuclear saturation within $\Delta - \chi\mathrm{EFT}$

- $\chi\mathrm{EFT}$ **with explicit Δ isobar**.
- Extensive **error model**
  (EFT truncation, method convergence, finite-size errors).
- **Iterative history-matching** for global parameter search. Study *ab initio* model performance, and provide a large (>10^6) number of non-implausible samples.
  - Implausibility criterion involves only $A \leq 4$ observables.
- Bayesian **posterior predictive** distributions for nuclear matter properties.
  - Importance resampling with two different data sets:
    $\mathscr{D}_{A=2,3,4}$ and $\mathscr{D}_{A=2,3,4,16}$ (see the talk by Weiguang).
- Relies on sub-space projected coupled cluster (SP-CCD) **emulators** for infinite nuclear matter systems at different densities.

History matching waves

- np S- and P-wave phase shifts at T_{lab}=1, 5, 25, 50, 100, 200 MeV

[wave 1] & [wave 2] & final

History matching waves

- np S- and P-wave phase shifts at T_{lab}=1, 5, 25, 50, 100, 200 MeV

  [wave 1] & [wave 2] & final

- ^{2}H (E, R_p^2, Q),

  [wave 3] & [wave 4] & final

History matching waves

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- ^{2}H (E, R_p^2, Q), — [wave 3] & [wave 4] & final
- ^{3}H (E), ^{4}He (E, R_p^2) — [wave 4] & final
- Prior for c_1, c_2, c_3, c_4 from a Roy-Steiner analysis of πN data (Siemens 2017)

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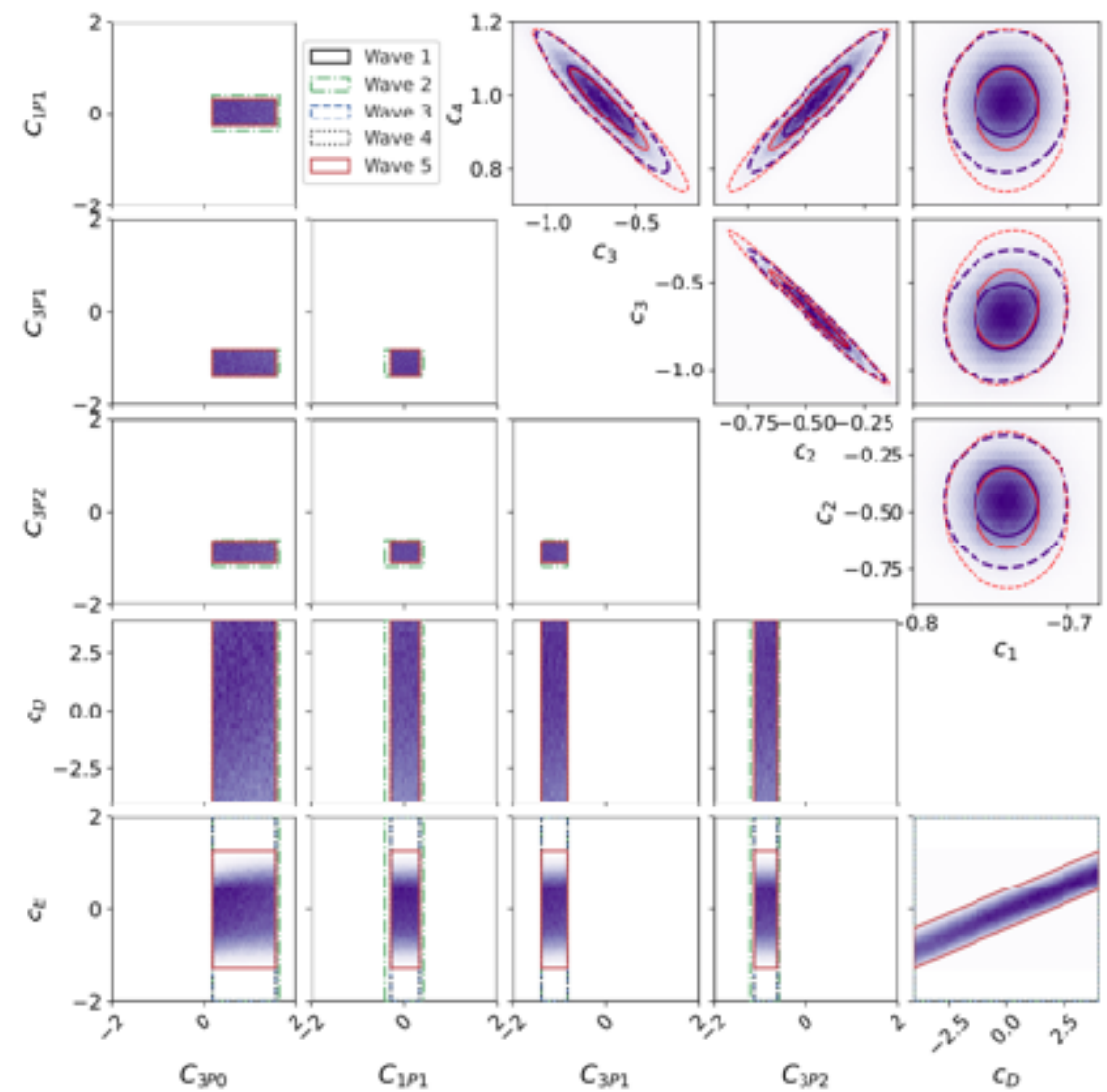
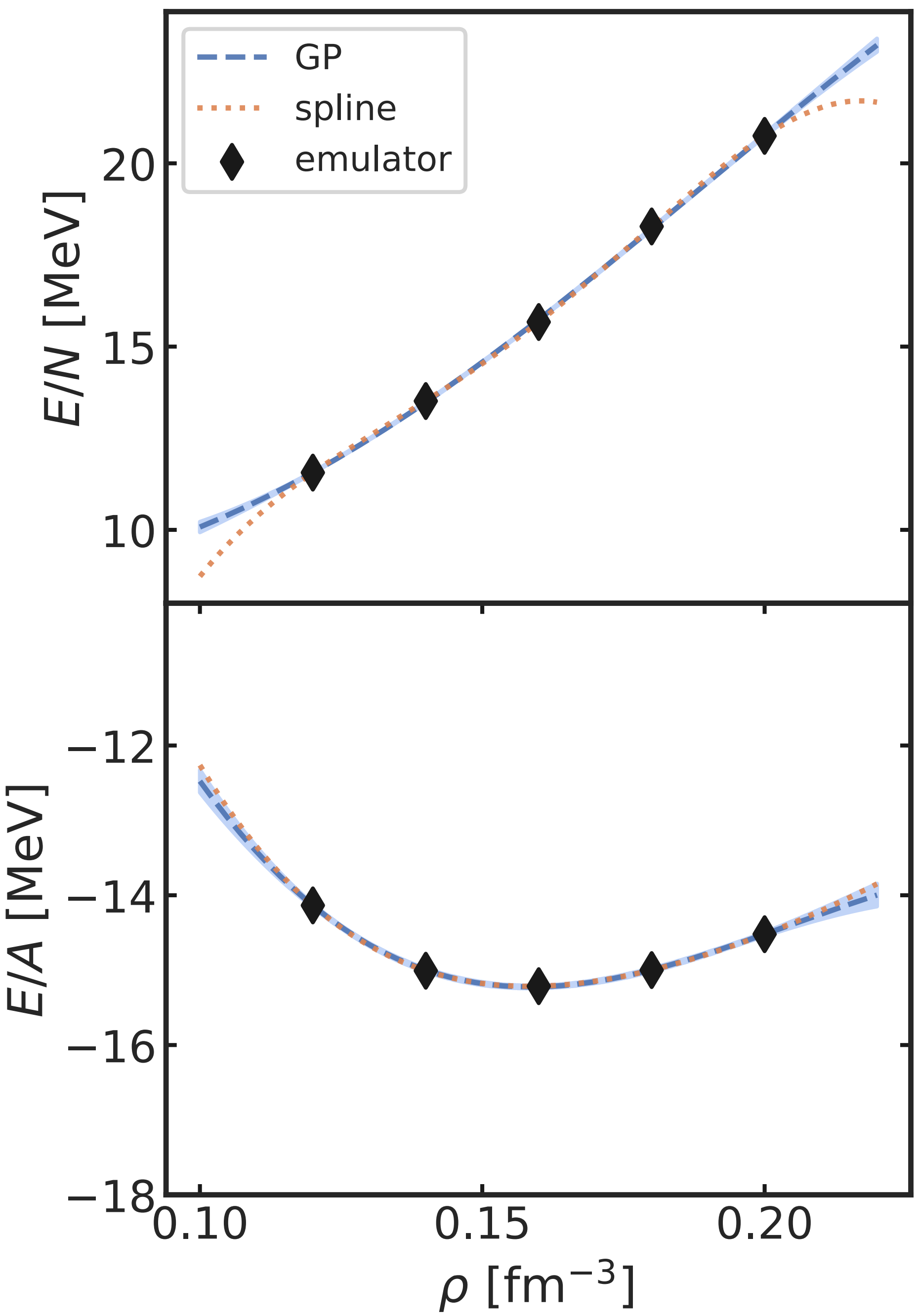
Observable	z	$\varepsilon_{\rm exp}$	$\varepsilon_{\rm model}$	$\varepsilon_{\rm method}$	$\varepsilon_{\rm em}$
$E(^2\mathrm{H})$	-2.2298	0.0	0.05	0.0005	0.001%
$r_p(^2\mathrm{H})$	1.976	0.0	0.005	0.0002	0.0005%
$Q(^2\mathrm{H})$	0.27	0.01	0.003	0.0005	0.001%
$E(^3\mathrm{H})$	-8.4818	0.0	0.17	0.0005	0.01%
$E(^4\mathrm{He})$	-28.2956	0.0	0.55	0.0005	0.01%
$r_p(^4\mathrm{He})$	1.455	0.0	0.016	0.0002	0.003%



Model output for EOS parameters



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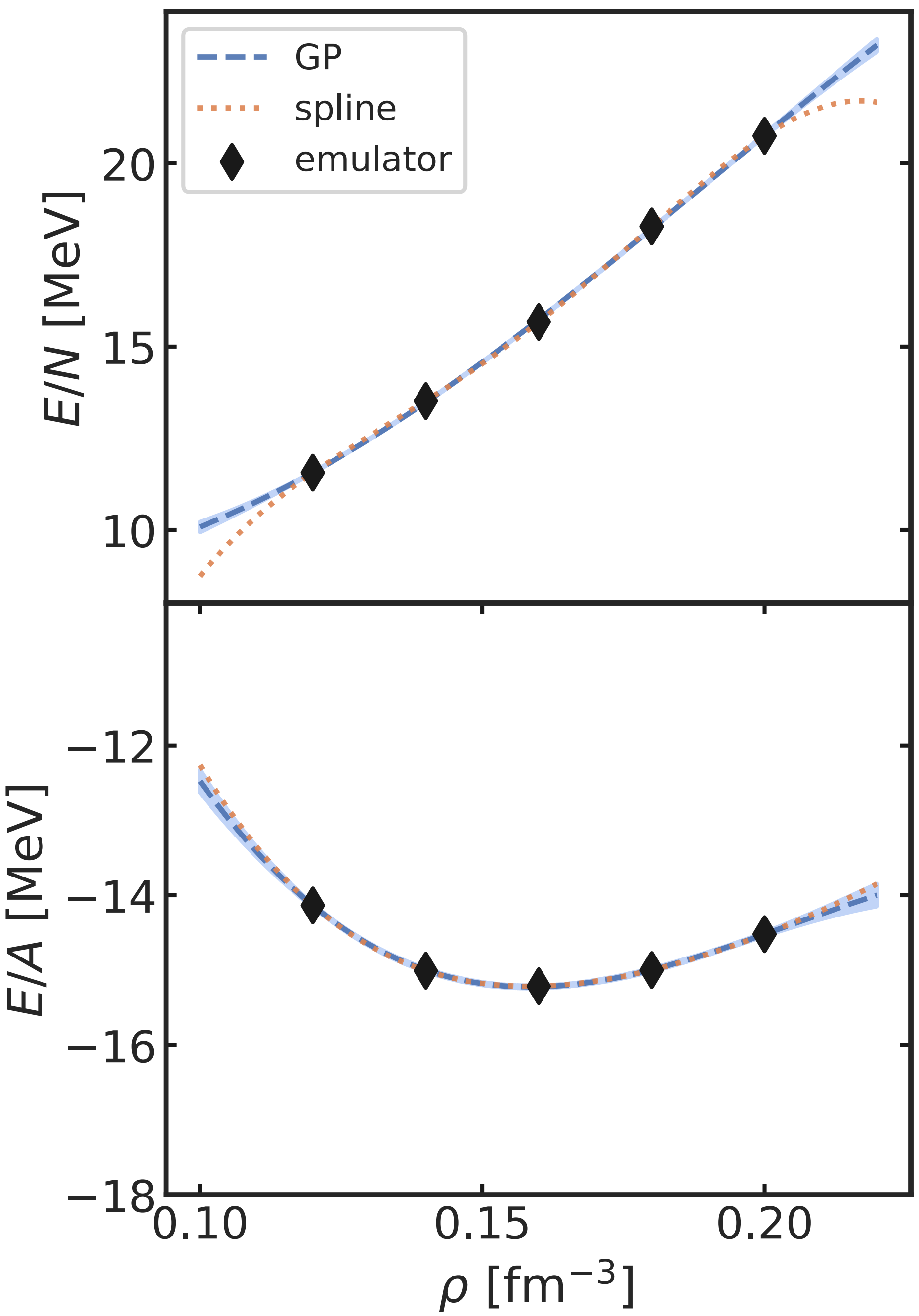
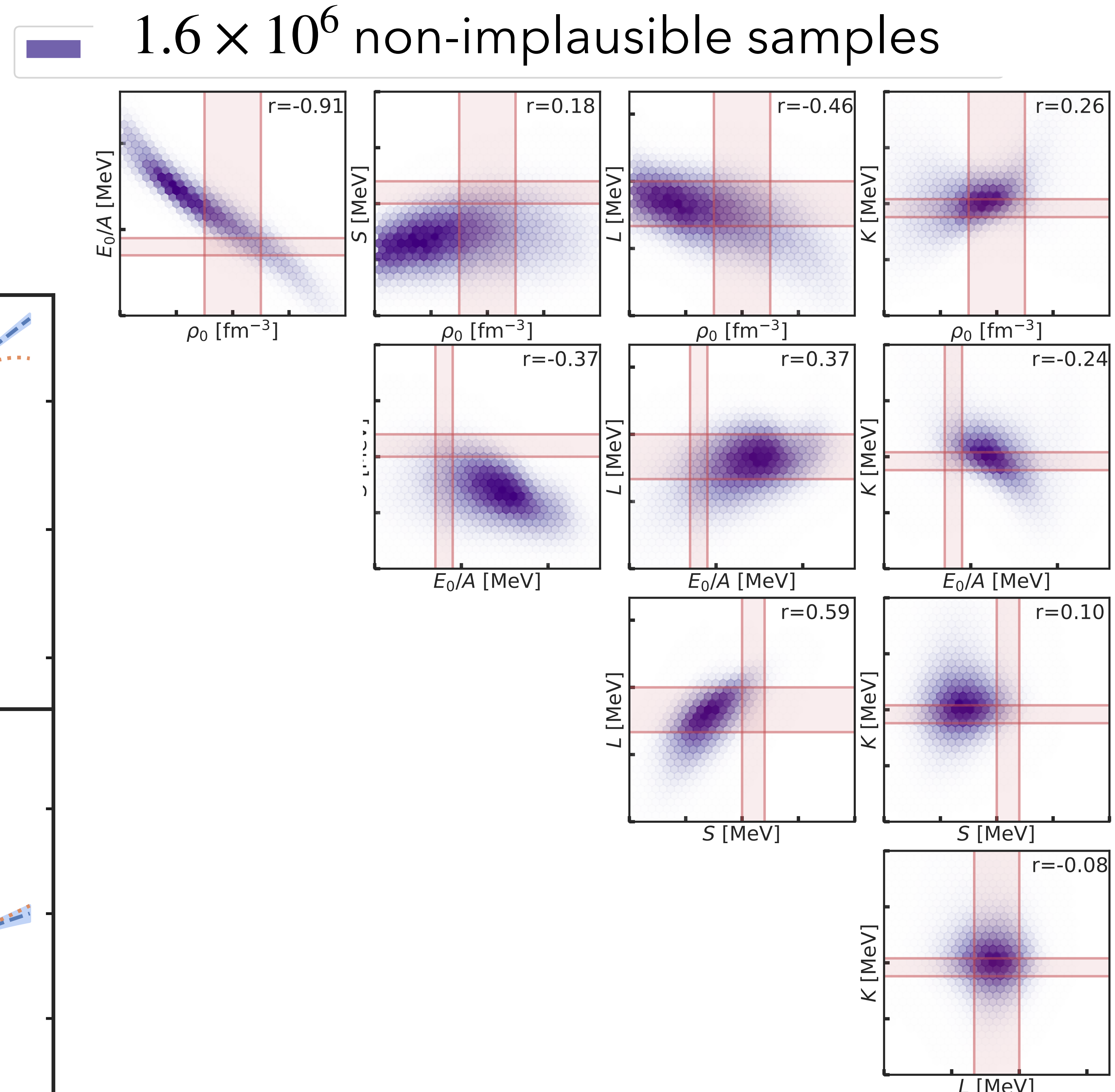




See the talk by Weiguang for step 2:
History matching + Importance Resampling = Bayesian posterior

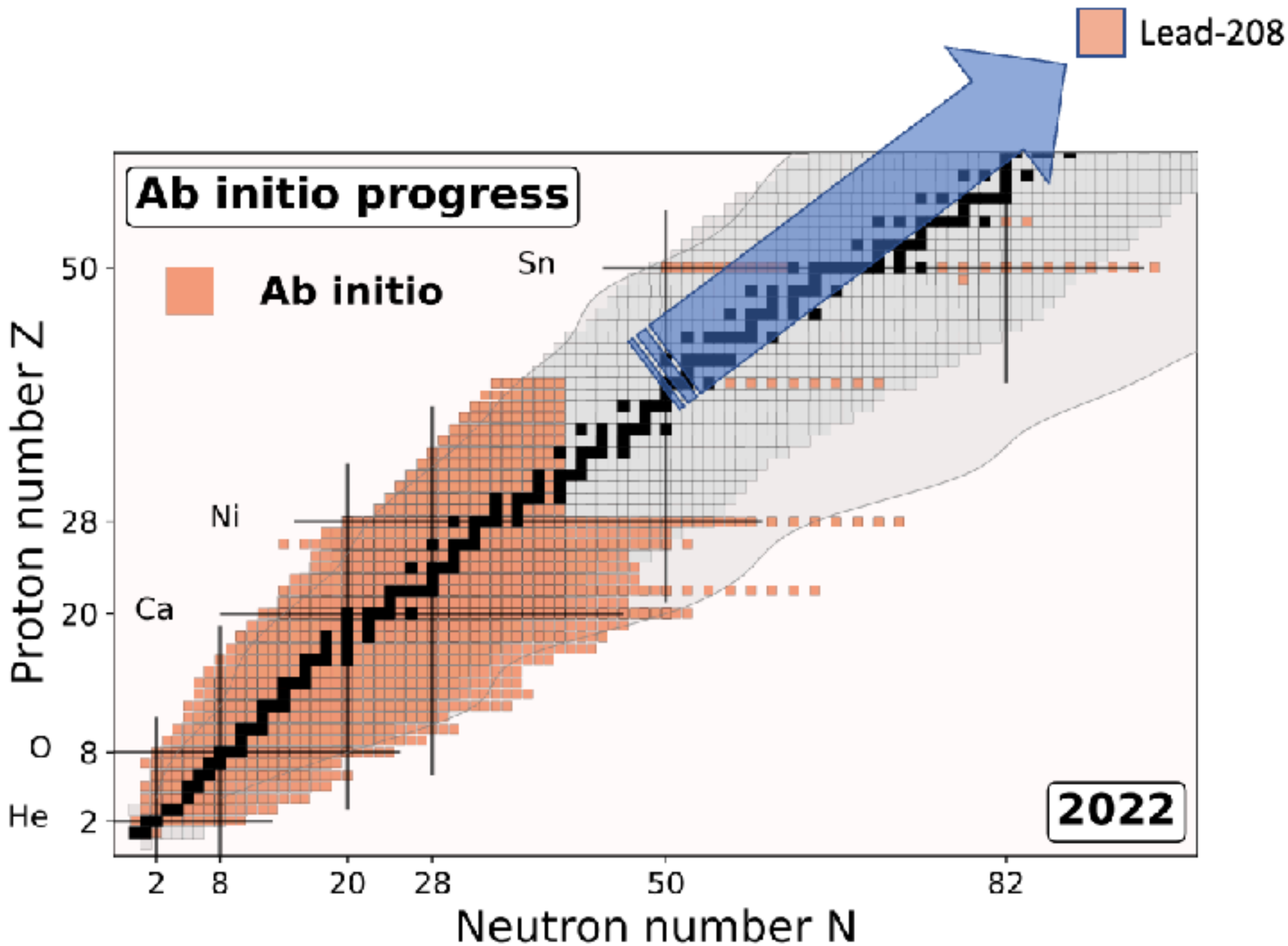
Summary and outlook

- *The concept of **tension in science** relies on statements of uncertainties*
- It is natural to strive for **accuracy** in theoretical modeling; but actual predictive power is more associated with quantified **precision**.
- Ab initio methods + χEFT + Bayesian statistical methods in combination with fast & accurate emulators is enabling **precision nuclear theory**.
- We have developed a unified ***ab initio* framework** to link the physics of NN scattering, few-nucleon systems, medium- and heavy-mass nuclei up to ^{208}Pb, and the nuclear-matter equation of state near saturation density.
- **Challenges**:
  - Getting to know our uncertainties;
  - How to define implausibility when conditioning on many outputs;
  - Have identified a need to revisit the leading (and subleading) orders of χEFT (from explorations of the model discrepancy).

Appendix

Recent UQ progress in χEFT modeling

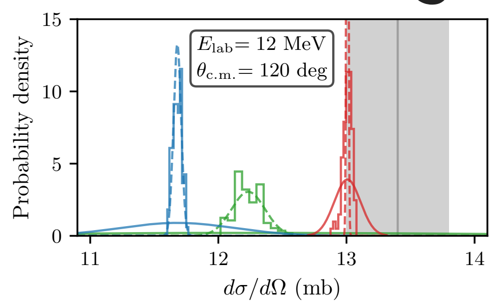
From light…



Recent UQ progress in χEFT modeling

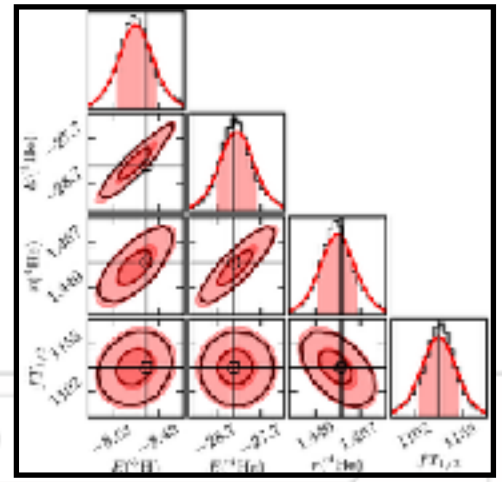
From light…

nd-scattering



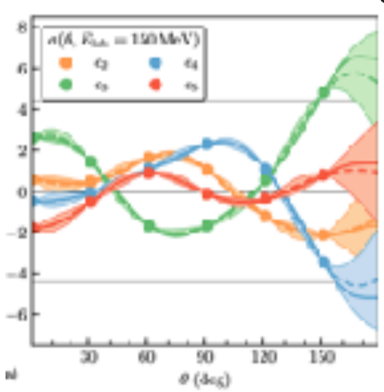
S. B. S. Miller et al. PRC (2023)

Few-nucleon systems

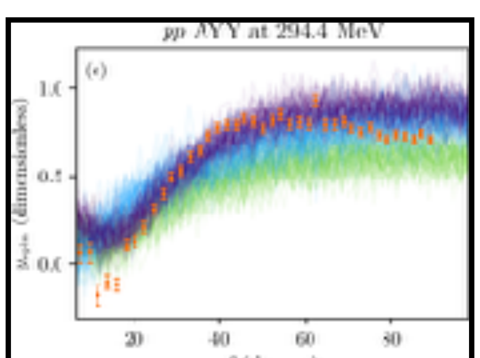


S. Wesolowski et al PRC (2021)

NN-scattering

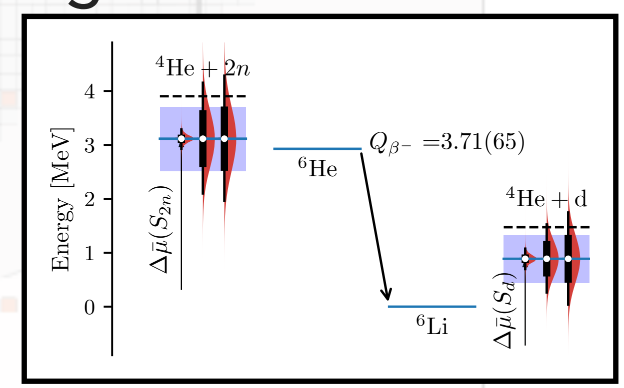


J. Melendez et al PRC (2019)



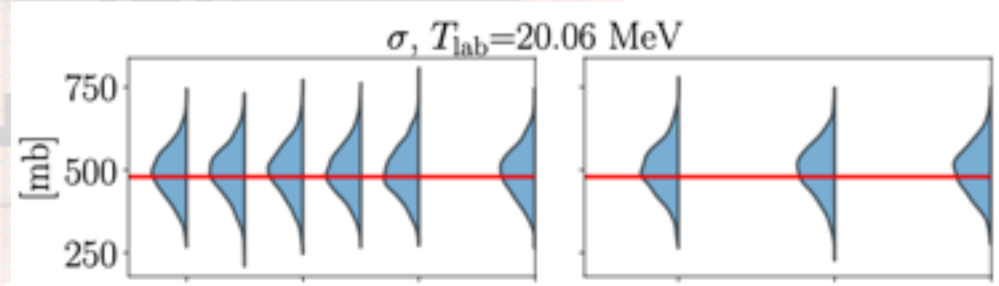
I. Svensson et al PRC (2022)

Light nuclei



T. Djärv et al PRC (2022)

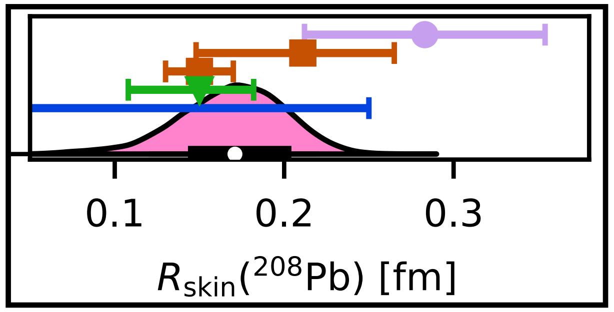
Modified LO



O. Thim et al. arXiv (2023)

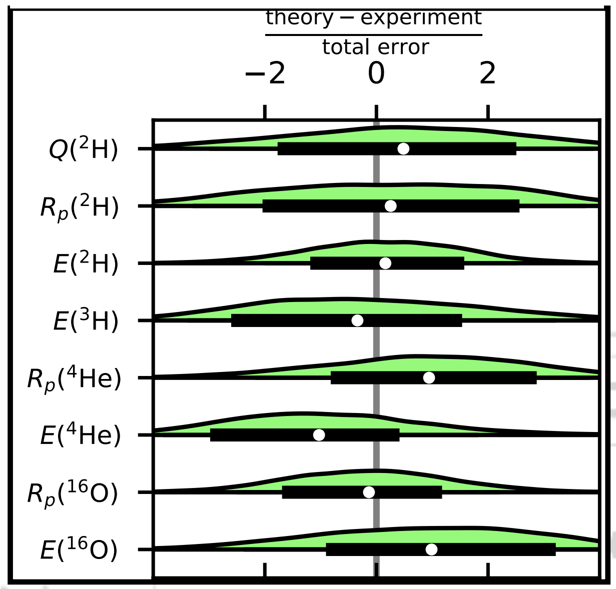
Recent UQ progress in χEFT modeling

… to heavy



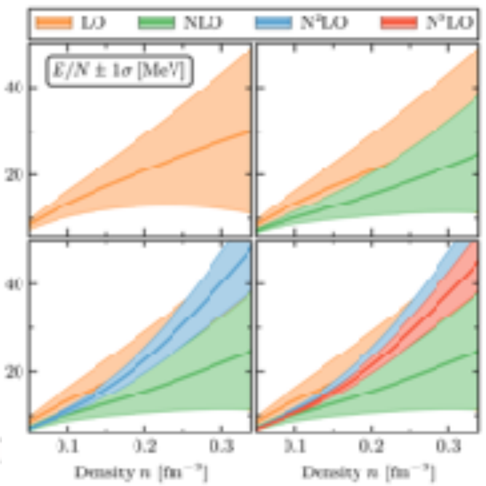
B. Hu et al
Nature Phys. (2022)

History matching



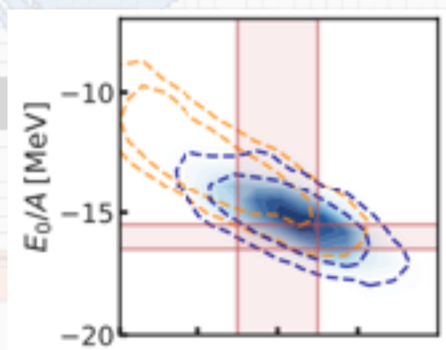
B. Hu et al Nature Phys. (2022)

Nuclear matter EoS (correlated errors)



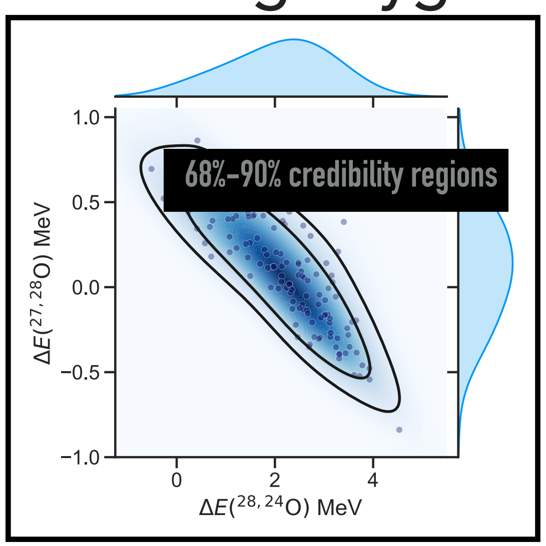
C. Drischler et al PRL,PRC (2020)

(importance resampling)



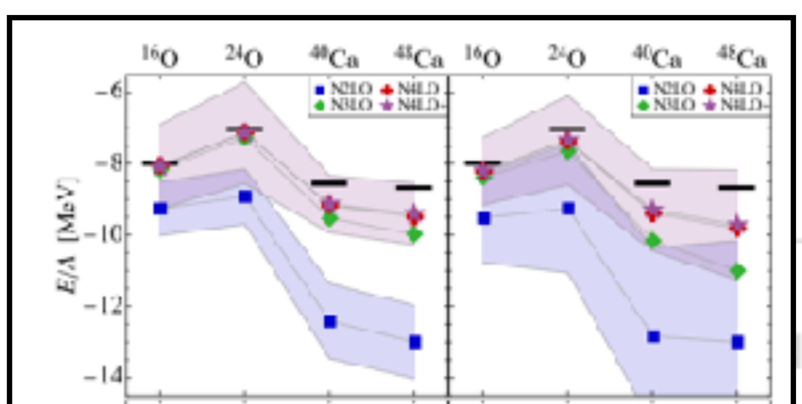
W.G. Jiang et al
Frontiers Phys.,
+ arXiv (2022)

Predicting oxygens



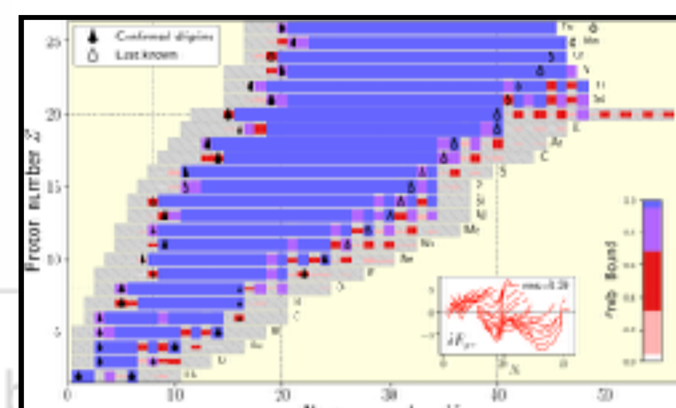
in preparation

Truncation errors/Model checking



P. Maris et al PRC (2022)

Bayesian linear regression



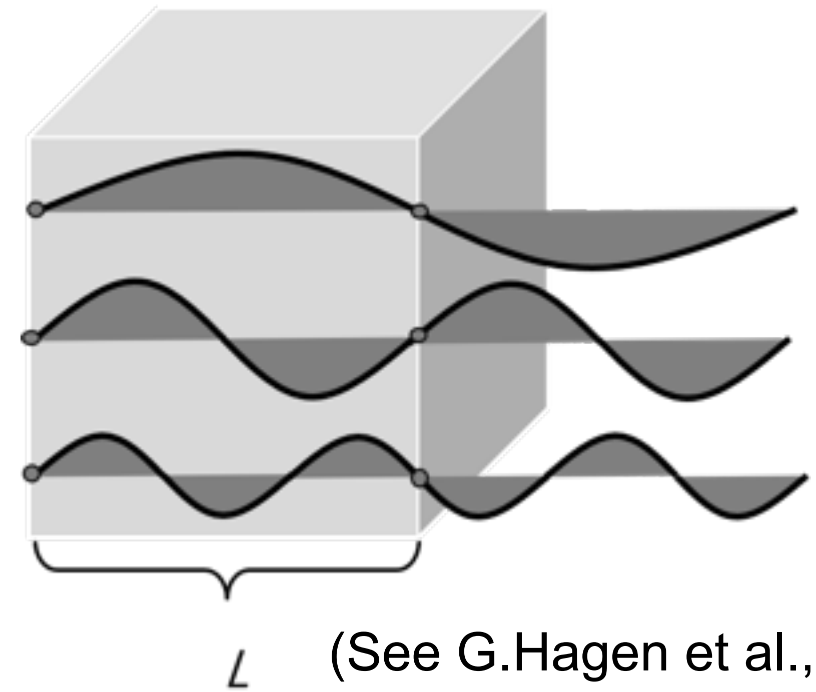
S. R. Stroberg et al PRL (2021)

Infinite nuclear matter: computational approach

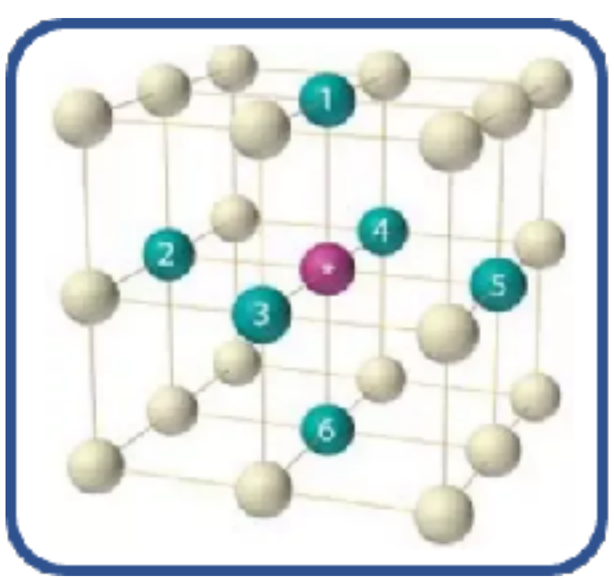
See the talk by Weiguang

- Discrete momentum basis states $\psi_k(x) \propto e^{ikx}$
- Cubic lattice in momentum space, (k_x, k_y, k_z)
- $k_n = \dfrac{2\pi n}{L}$, with $n = 0, \pm 1, \pm 2, \ldots \pm n_{\max}$
- Results should converge with increasing $n_{\max}$

- Periodic boundary conditions $\psi_k(x + L) = \psi_k(x)$



(See G.Hagen et al., 2014)

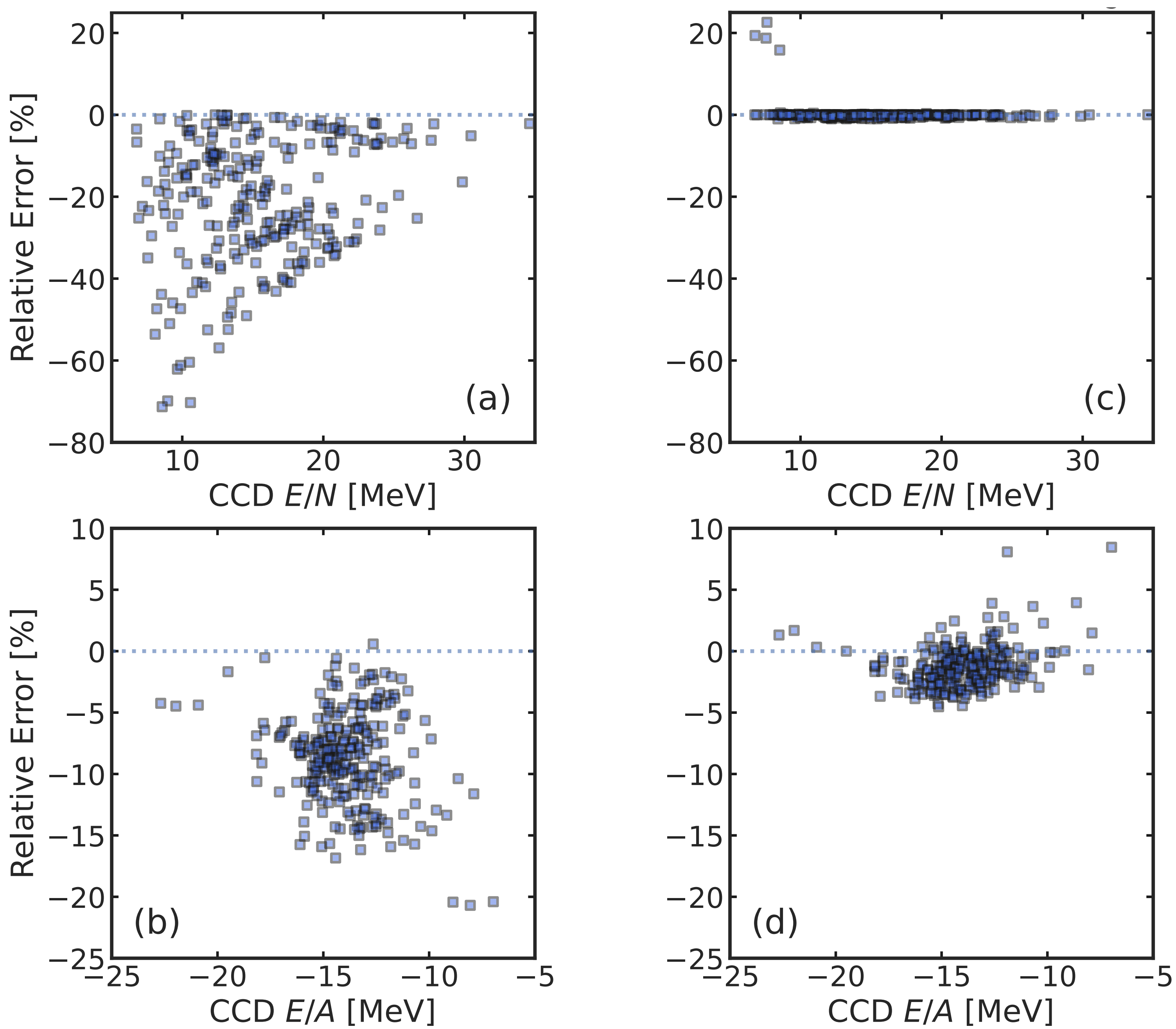


- The box size (L) and the nucleon number (N) controls the density (ρ)
- Computational challenge ($n_{\max} = 4$):
  - PNM: 1458 orbits with 66 neutrons
  - SNM: 2916 orbits with 132 nucleons

SPCC with small-batch voting

See the talk by Weiguang

SPCC SPCC w. small-batch voting

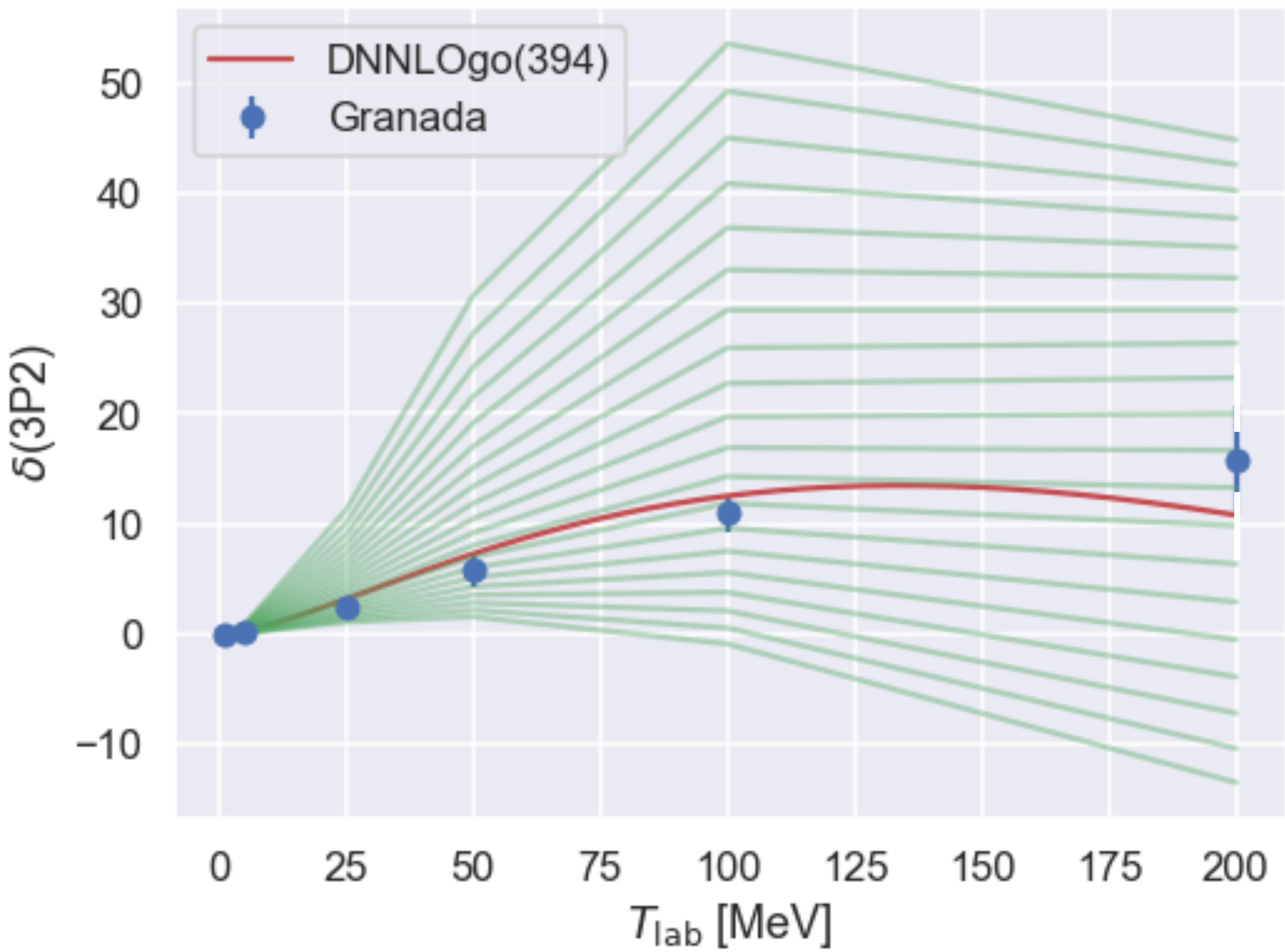


Physical states are stable w.r.t. subspace variations

$$|\Psi(\boldsymbol{\alpha}_{\odot})\rangle = e^{T(\boldsymbol{\alpha}_{\odot})}|\Phi_0\rangle \approx \sum_{i=1}^{N_{\text{sub}}} c_i^{\star}|\Psi_i\rangle$$

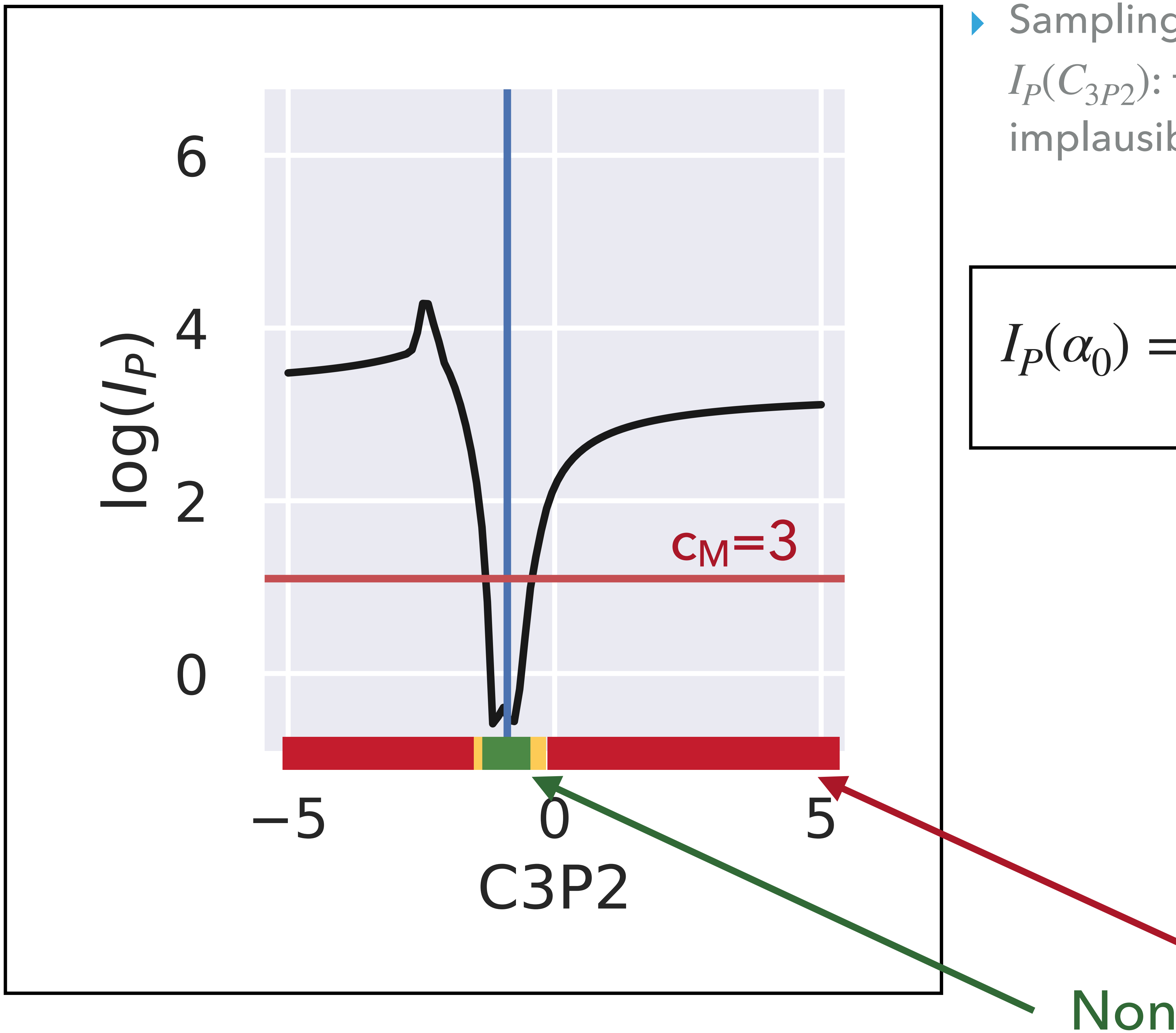
1-parameter example: np scattering (3P2)

- The "observations" are the 3P2 phase shift at 6 different energies.
- Our theoretical model is the solution of the L-S equation for the np system.
- Below, we fix c_i:s and vary $C_{3P2} \in [-1.5, -0.5]$ (green lines).



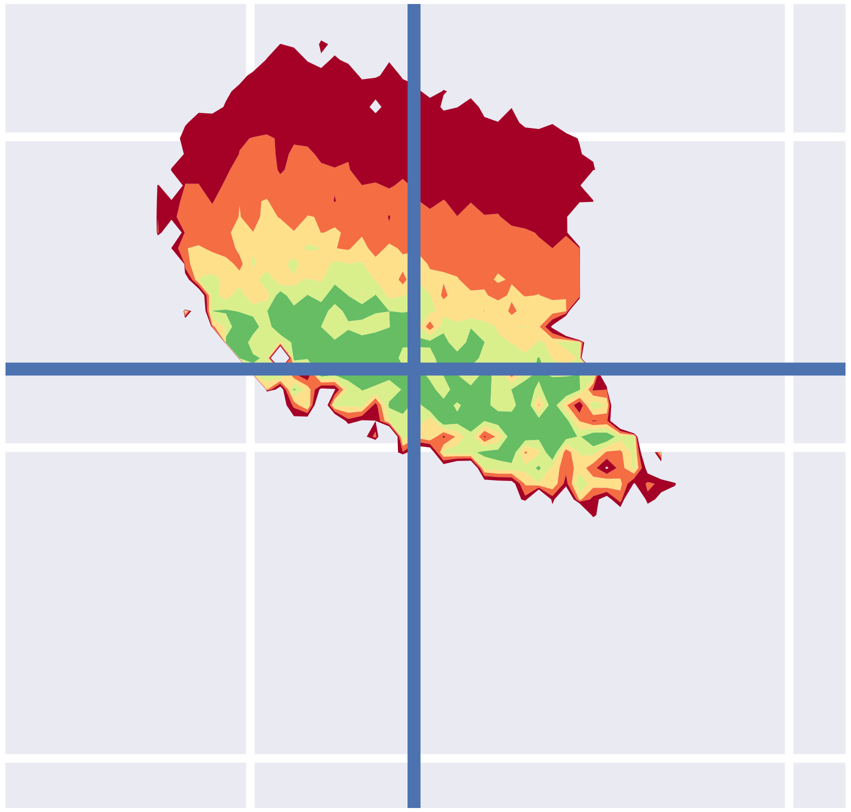
Most choices for C_{3P2} are deemed **implausible** when confronted with data.

Projected implausibility measure



- Sampling the c_i:s we study $I_P(C_{3P2})$: the projected implausibility measure

$$I_P(\alpha_0) = \min_{\alpha_{1,\ldots} \in \mathscr{D}_\alpha} I_M(\alpha_0, \alpha_{1,\ldots})$$



Ab initio computations of ^{208}Pb

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces
by B. Hu, W.G. Jiang, T. Miyagi, Z. Sun, A. Ekström, cf, G. Hagen, J.D. Holt, T. Papenbrock, S.R. Stroberg, I. Vernon, **Nature Phys. 18, 1196 (2022)**

Ab initio computations of ^{208}Pb

We start from a ΔNNLO(394) chiral Hamiltonian. Order by order results provide estimates of the model errors. Pion-nucleon couplings are from a Roy-Steiner analysis.

W. Jiang, et al. Phys Rev **C 102,** 054301 (2020)
M. Hoferichter et al, Phys. Rev. Lett. **115**, 192301 (2015)

Approximately solve the Schrödinger equation in HF basis using Coupled-Cluster, IMSRG, and MBPT methods. Comparisons and domain knowledge provide estimates of the method errors.

G. Hagen, et al. Rep. Prog. Phys. **77**, 096302 (2014)
H. Hergert, et al. Phys Rep. **621** 165 (2016)

3NFs are captured using the NO2B approx. Large emax (=14) and E3max (=28) spaces. For ^{208}Pb, IR extrapolation adds only ~2% to the skin thickness and ~6% to the energy.

T. Miyagai, et al. Phys. Rev. **C 105**, 014302 (2022)

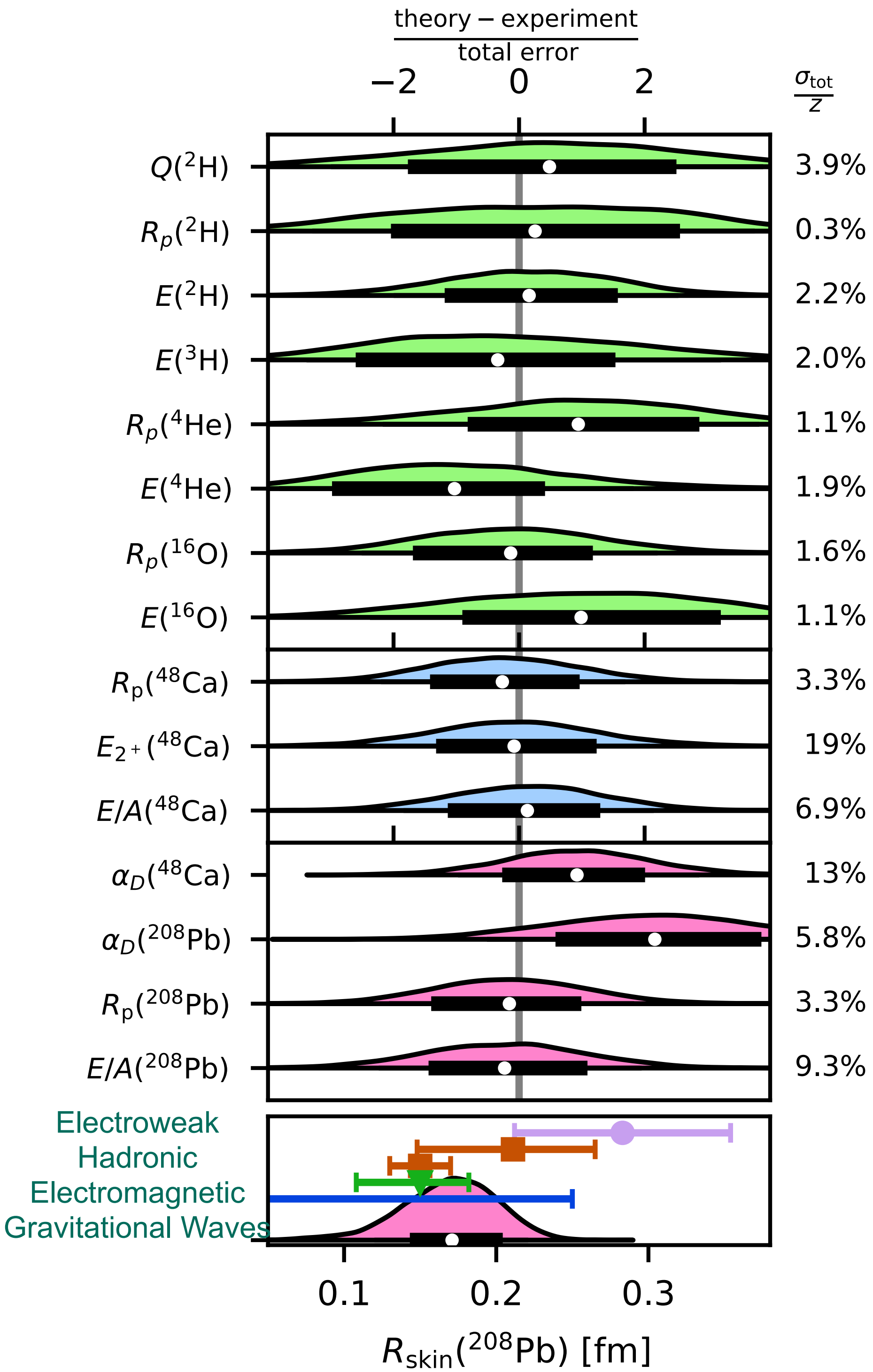
EC-emulators for observables with $A \leq 16$. Validated and trusted to within 0.5%

S. König, et al. Phys. Lett. **B 810**, 135814 (2020)
A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

Nuclear matter computed using CCD(T) with estimates of the method error from systematics. Conflated with estimates for the model error using a multitask Gaussian Process.

C. Drischler, et. al. Phys. Rev. Lett. **125**, 202702 (2020)

Ab initio predictions link the skin of ^{208}Pb to nuclear forces



History Matching

We explore 10^9 different interaction parameterizations

Confronted with A=2-16 data + NN scattering information

Find 34 non-implausible interactions

Calibration

Importance resampling

Validation

Inspect ab initio model and error estimates

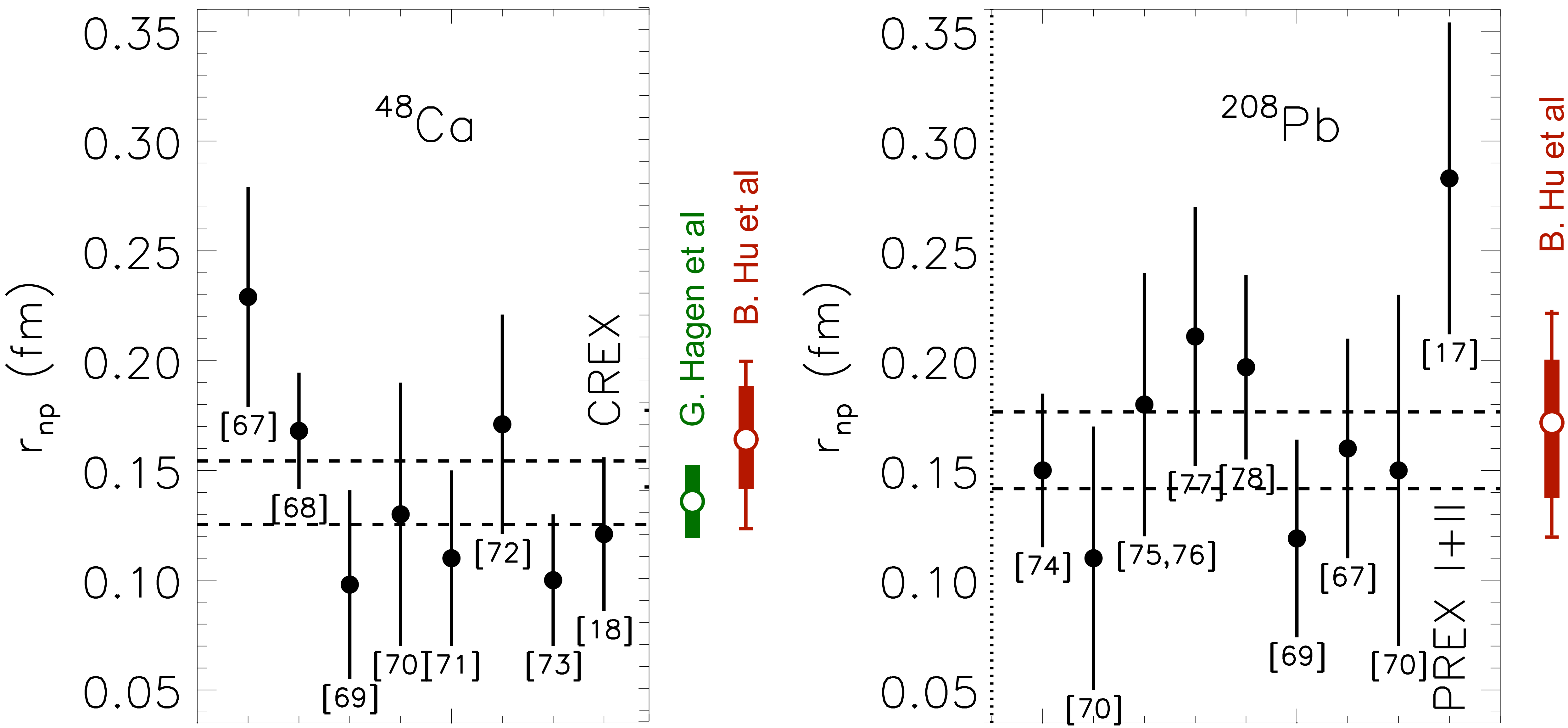
Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
History-matching observables						
$E(^2\mathrm{H})$	-2.2246	0.0	0.05	0.0005	0.001%	$-2.22^{+0.07}_{-0.07}$
$R_p(^2\mathrm{H})$	1.976	0.0	0.005	0.0002	0.0005%	$1.98^{+0.01}_{-0.01}$
$Q(^2\mathrm{H})$	0.27	0.01	0.003	0.0005	0.001%	$0.28^{+0.02}_{-0.02}$
$E(^3\mathrm{H})$	-8.4821	0.0	0.17	0.0005	0.01%	$-8.54^{+0.34}_{-0.37}$
$E(^4\mathrm{He})$	-28.2957	0.0	0.55	0.0005	0.01%	$-28.86^{+0.86}_{-1.01}$
$R_p(^4\mathrm{He})$	1.455	0.0	0.016	0.0002	0.003%	$1.47^{+0.03}_{-0.03}$
$E(^{16}\mathrm{O})$	127.62	0.0	1.0	0.75	0.5%	$-126.2^{+3.0}_{-2.8}$
$R_p(^{16}\mathrm{O})$	2.58	0.0	0.03	0.01	0.5%	$2.57^{+0.06}_{-0.06}$
Calibration observables						
Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{48}\mathrm{Ca})$	-8.667	0.0	0.54	0.25	—	$-8.58^{+0.72}_{-0.72}$
$E_{2^+}(^{48}\mathrm{Ca})$	3.83	0.0	0.5	0.5	—	$3.79^{+0.86}_{-0.96}$
$R_p(^{48}\mathrm{Ca})$	3.39	0.0	0.11	0.03	—	$3.36^{+0.14}_{-0.13}$
Validation observables						
Observable	z	ε_{exp}	ε_{model}	ε_{method}	ε_{em}	PPD
$E/A(^{208}\mathrm{Pb})$	-7.867	0.0	0.54	0.5	—	$-8.06^{+0.99}_{-0.88}$
$R_p(^{208}\mathrm{Pb})$	5.45	0.0	0.17	0.05	—	$5.43^{+0.21}_{-0.23}$
$\alpha_D(^{48}\mathrm{Ca})$	2.07	0.22	0.06	0.1	—	$2.30^{+0.31}_{-0.26}$
$\alpha_D(^{208}\mathrm{Pb})$	20.1	0.6	0.59	0.8	—	$22.6^{+2.1}_{-1.8}$

B. Hu et al (Nature Phys. 2022)

<u>Prediction</u>: small skin thickness 0.14-0.20 fm in mild (1.5 sigma) tension with PREX.

Neutron skin thickness

Constraints on Nuclear Symmetry Energy Parameters
J. Lattimer (2023)



Observable	median	68% CR	90% CR
$R_{\mathrm{skin}}(^{48}\mathrm{Ca})$	0.164	[0.141, 0.187]	[0.123, 0.199]
$R_{\mathrm{skin}}(^{208}\mathrm{Pb})$	0.171	[0.139, 0.200]	[0.120, 0.221]

B. Hu et al (Nature Phys. 2022)

Why does ab initio predict thin skins?

- Tune C1S0 while adjusting cE to maintain saturation
- Study the effect on various observables. Note *L* & $\delta_{1S0}(50)$