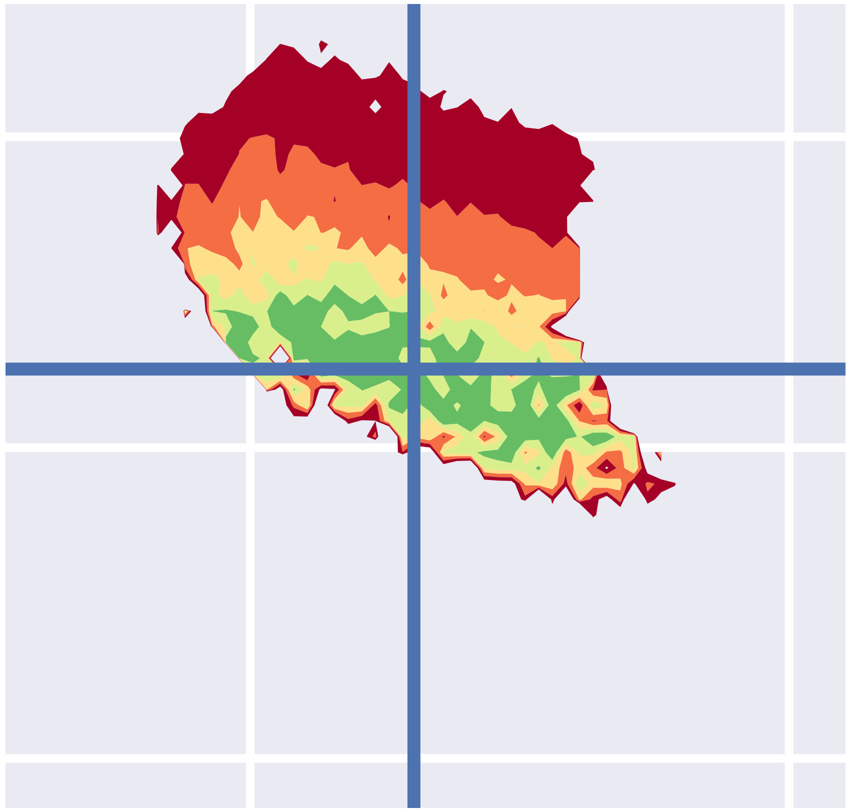
Work in progress



UNCERTAINTY ANALYSIS OF COMPLEX COMPUTER MODELS

ITERATIVE HISTORY MATCHING VIA IMPLAUSIBILITY

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TRIUMF ab initio workshop,
Vancouver, March. 4, 2020

Many thanks to my collaborators

- Andreas Ekström, Weiguang Jiang (Chalmers)
- Gaute Hagen, Gustav Jansen, Thomas Papenbrock, Zhonghao Sun (ORNL/UT)
- Ian Vernon (Durham) and many people in the *ab initio nuclear theory* community for enlightening discussions

Chalmers research funded by:

- Swedish Research Council
- European Research Council

Some numbers

- The analysis presented here relies on an enormous number of *ab initio* computations performed in three waves.
- During the 1st wave we performed ~10^9 scattering phase shift computations (different partial waves, energies and EFT model parametrizations).
- During the 2nd wave we performed ~10^8 few-body computations (A=2-4 observables).
- During the final wave we performed ~10^8 many-body computations (A=16-28).
- As an example, we computed the ^{24}O(gs) energy 10^8 times, which would take ~10^{10} core-h (or 0.7 years of exclusive access to Summit).
- In contrast, with emulators (once constructed) the speedup is on the order of a factor 10^8, meaning that a lower-precision copy of all the ^{24}O(gs) results can be obtained in ~few days on my laptop.

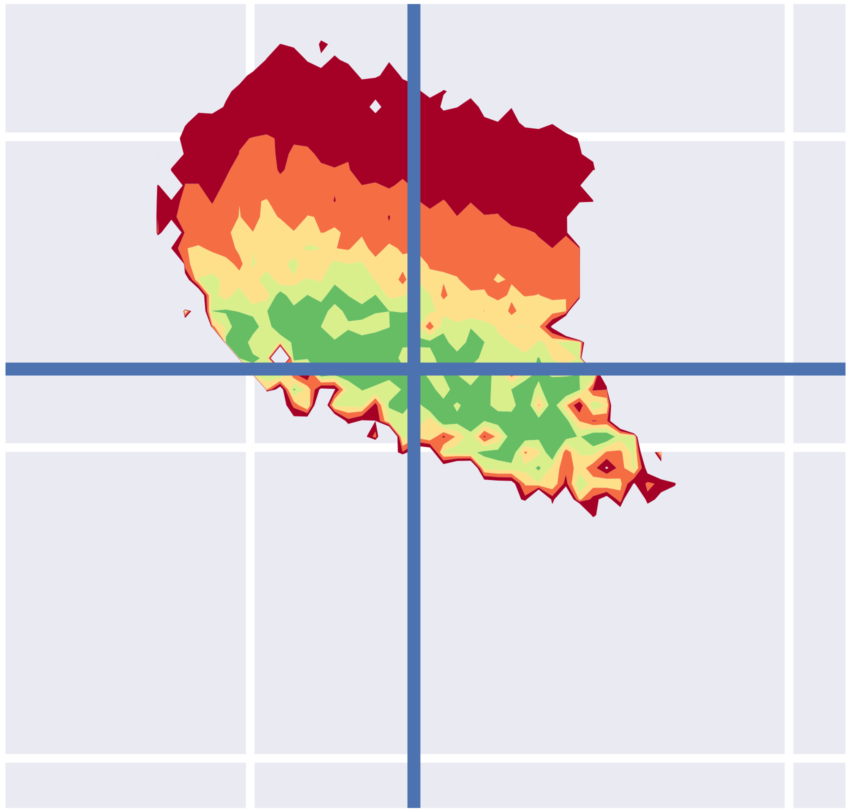
Outline

- **Iterative history matching via implausibility**
  - Global parameter searches
  - Uncertainty analysis of complex computer models
  - Experimental design
- **(Preliminary) results**
  - Implausibility analysis of *ab initio* nuclear many-body computations with the Δ-NNLO interaction.

REFERENCES:

Vernon, I, Goldstein, M, Rowe, J, Liu, J and Lindsey, K, *"Bayesian uncertainty analysis for complex systems biology models: emulation, global parameter searches and evaluation of gene functions."*, arXiv:1607.06358v1 [q-bio.MN].

Vernon, I.; Goldstein, M.; Bower, R. G.; *"Galaxy Formation: Bayesian History Matching for the Observable Universe".* Statistical Science 29 (2014), no. 1, 81–90.



Uncertainty analysis of complex computer models

- In the words of **Ian Vernon** (statistician from Durham) we focus on the following general scenario:
  - We have a **physical model** $f(x)$: a model based on theory, implemented on a computer, that may take a long time to evaluate.
  - The model takes a vector of input parameters x and returns a vector $f(x)$ of outputs.
  - We want to compare the model outputs f, or a subset of them, with **observed data** z.
  - In our case: $f(x)$ is our ab initio model of nuclear few- and many-body systems, x is the vector of interaction parameters (LECs), and z is a vector of nuclear observables.
- This scenario raises several major questions:

Fundamental scientific questions

1. Are there any choices of input parameters x for which theory predictions are consistent with historical observations z? (or at least **non-implausible**)
2. Can we find the region(s) $\mathscr{X}(z)$ of all such input parameters?
3. What design of future experiments will reduce this set $\mathscr{X}(z)$ the most, and hence resolve uncertainty about the input parameters?
4. And what can we predict for yet unmeasured observables using the non-implausible set $\mathscr{X}(z)$.

To answer these questions we need to discuss:

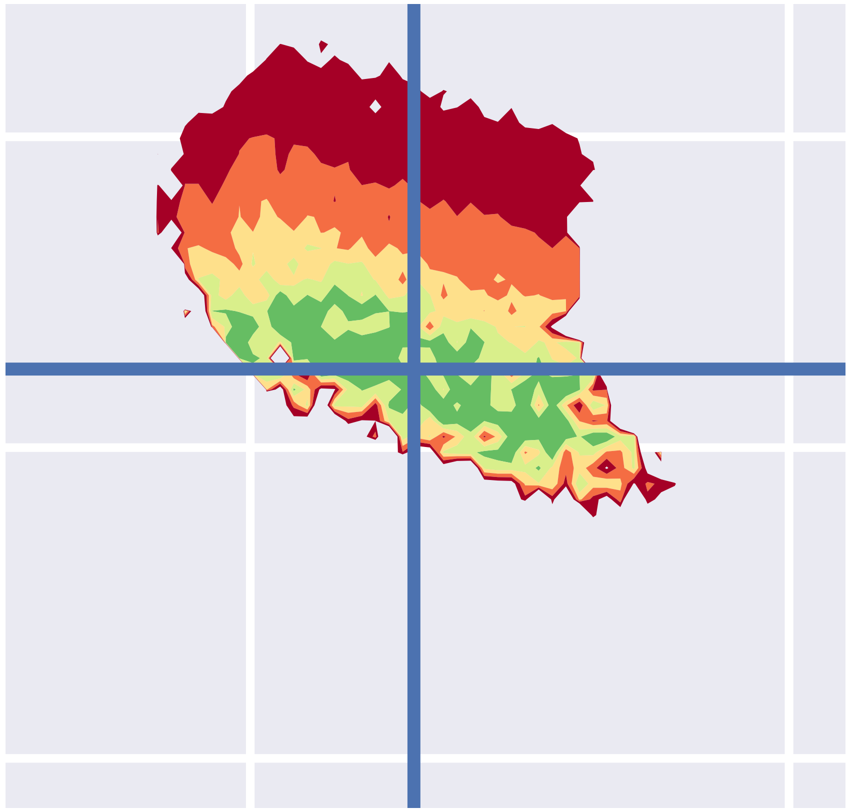
(i) How to **link the model to reality** (incorporating all major uncertainties).

(ii) **Emulation** of the model (to combat speed of $f(x)$ problem)

(iii) A global parameter search strategy known as **iterative history matching**, designed to remove all locations in input parameter space that fail to reproduce the data (according to an **implausibility measure)**.

- I.e. not just searching for a single best match; but instead finding non-implausible parameter regions.

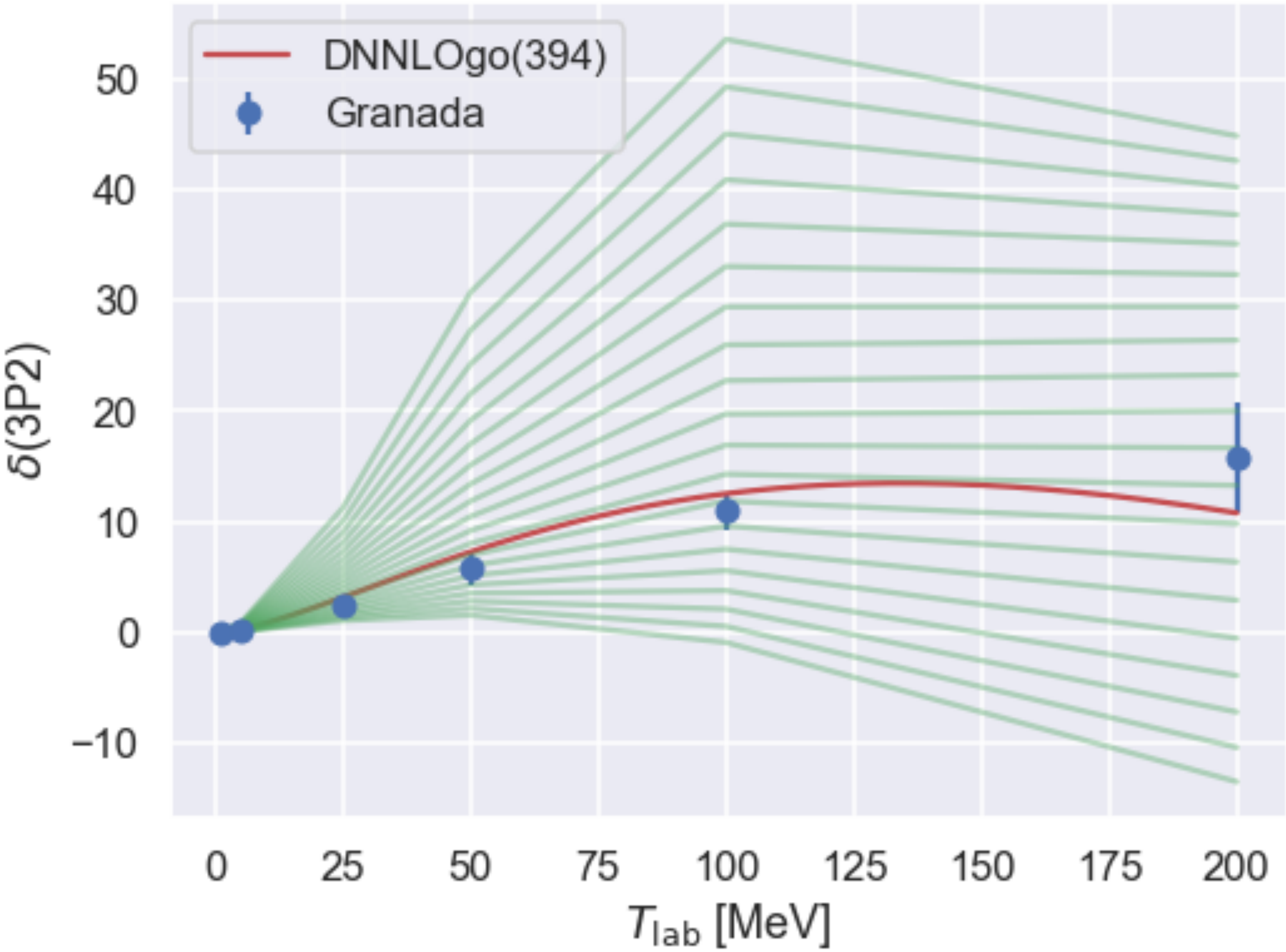
- Somewhat like a Bayesian posterior over x (but not quite...).



One-dimensional example

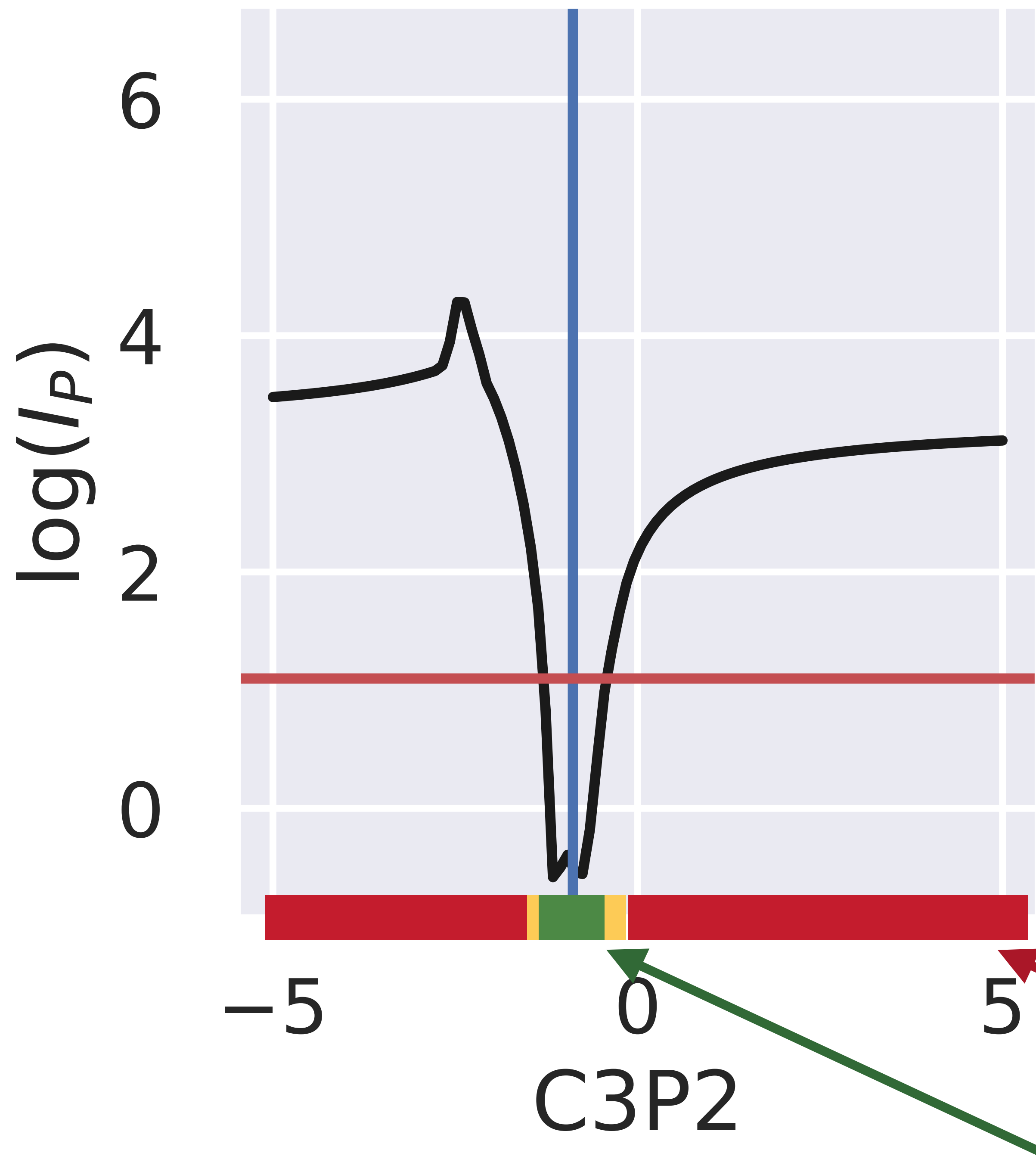
1-parameter example: np scattering (3P2)

- 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.
- We fix c_1, c_2, c_3, c_4 and vary $C_{3P2} \in [-1.5, -0.5]$ (green lines).



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

Implausibility measure

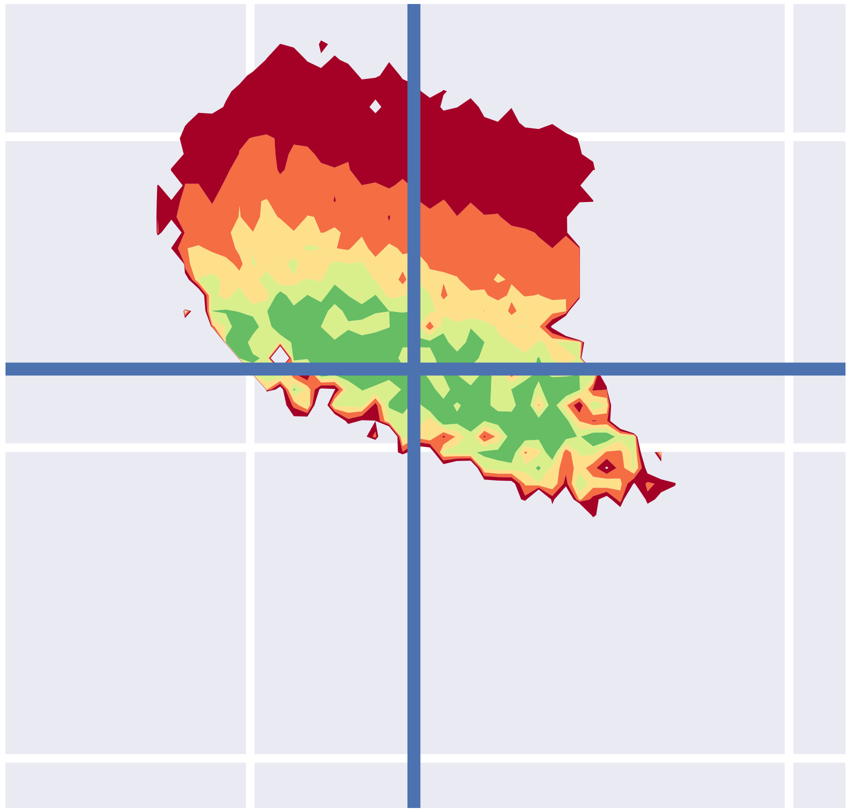


$$I_P(x_0) = \min_{x_{1,\ldots} \in X} I_M(x_0, x_{1,\ldots})$$

$$I_M^2(x) = \max_{i \in Z} \frac{|f_i(x) - z_i|^2}{\mathrm{Var}_i(x)}$$

Implausible!

Non-implausible!



Iterative history matching for the Δ-NNLO interaction model

- Here we consider the *Δ*-NNLO(394) interaction with 17 parameters. See e.g. Ekström et al (1707.09028)
- A benchmark parametrisation is the optimized *Δ*-NNLO$_{GO}$(394) interaction (W. Jiang et al; Gaute's talk yesterday).
- The outputs z_i are scattering and bound-state observables, and we use **emulators** based on ***eigenvector continuation*** (König et al. 2019) and ***subspace-projected coupled cluster*** (Ekström and Hagen, 2019).
- E.g., the ^{16}O binding energy and radius is obtained in ~ms.

- The **implausibility measure** is
$$I_M^2(x) = \max_{i \in Z} I_i^2(x) \equiv \max_{i \in Z} \frac{|\,\mathbb{E}\left(f_i(x)\right) - z_i\,|^2}{\mathrm{Var}_i(x)}.$$
where Z is the collection of outputs that are being considered and $\mathrm{Var}_i(x)$ is the combined variances of **observational, model, and emulator uncertainties**.

- Large values of $I_M(x)$ imply that we are highly unlikely to obtain acceptable matches between model output and observed data at input x. We consider a particular input x as **implausible** if
$$I_M(x) > c_M,$$
where we may choose $c_M = 3$, appealing to Pukelheim's three-sigma rule.

- Small values of $I_M(x)$ do not necessarily imply that x is very good; just **non-implausible**!

Linking the model to reality

We represent the model as a function, which maps the vector of 17 inputs x (LECs) to the vector of outputs $f(x)$ (nuclear observables).

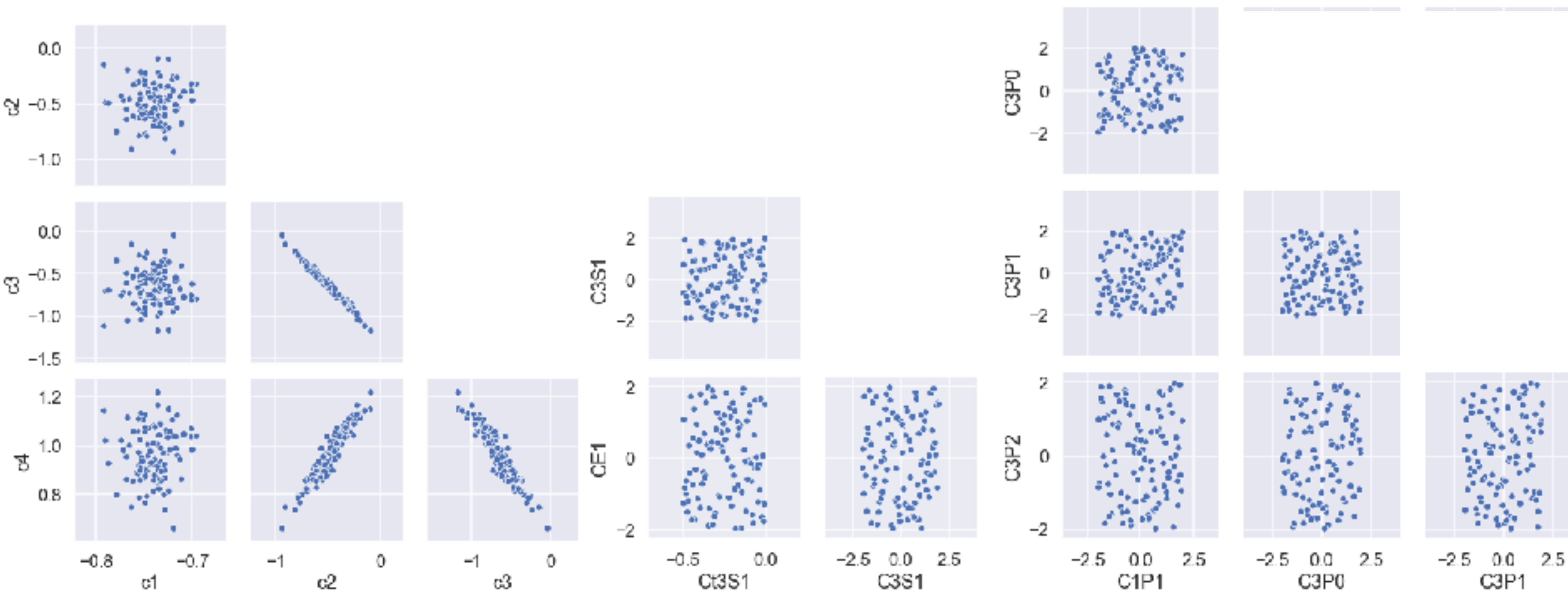
- We relate the true data y to the observational data z by,
  $$z = y + e$$
  where e represents the observational errors specified via $\mathbb{E}[e] = 0$ and $\mathrm{Var}[e]$.

- We link the model $f(x)$ to the real system y (observables of the nuclear system) via:
  $$y = f(x) + \varepsilon$$
  where ε is the model discrepancy and we assume that it is independent of x . We specify $\mathbb{E}[\varepsilon] = 0$ and $\mathrm{Var}[\varepsilon]$ via order-by-order estimates and expert assessment.

- Emulators of model output $f_i(x)$ are assumed to give an expectation $\mathbb{E}[f_i(x)]$ and a variance $\mathrm{Var}[f_i(x)] = \left(\alpha_i \mathbb{E}[f_i(x)]\right)^2$ at point x with a relative error α_i estimated via cross-validation.

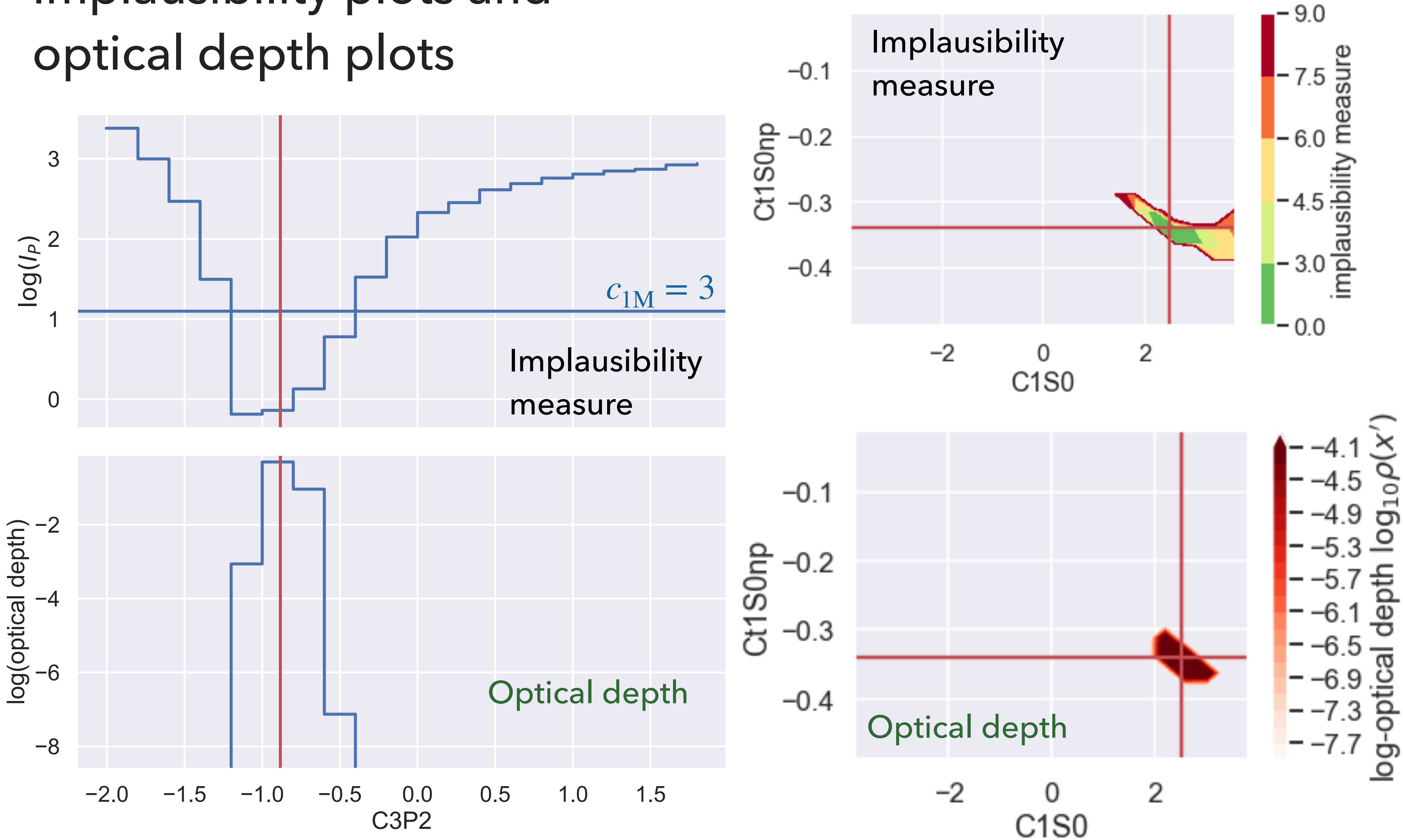
Wave 1: np scattering

- Start with huge ranges for the LECs.
- Use space-filling lhs sampling.
- ci: uncertainty defined by covariance matrix from Roy-Steiner analysis (Siemens et al, 2017).



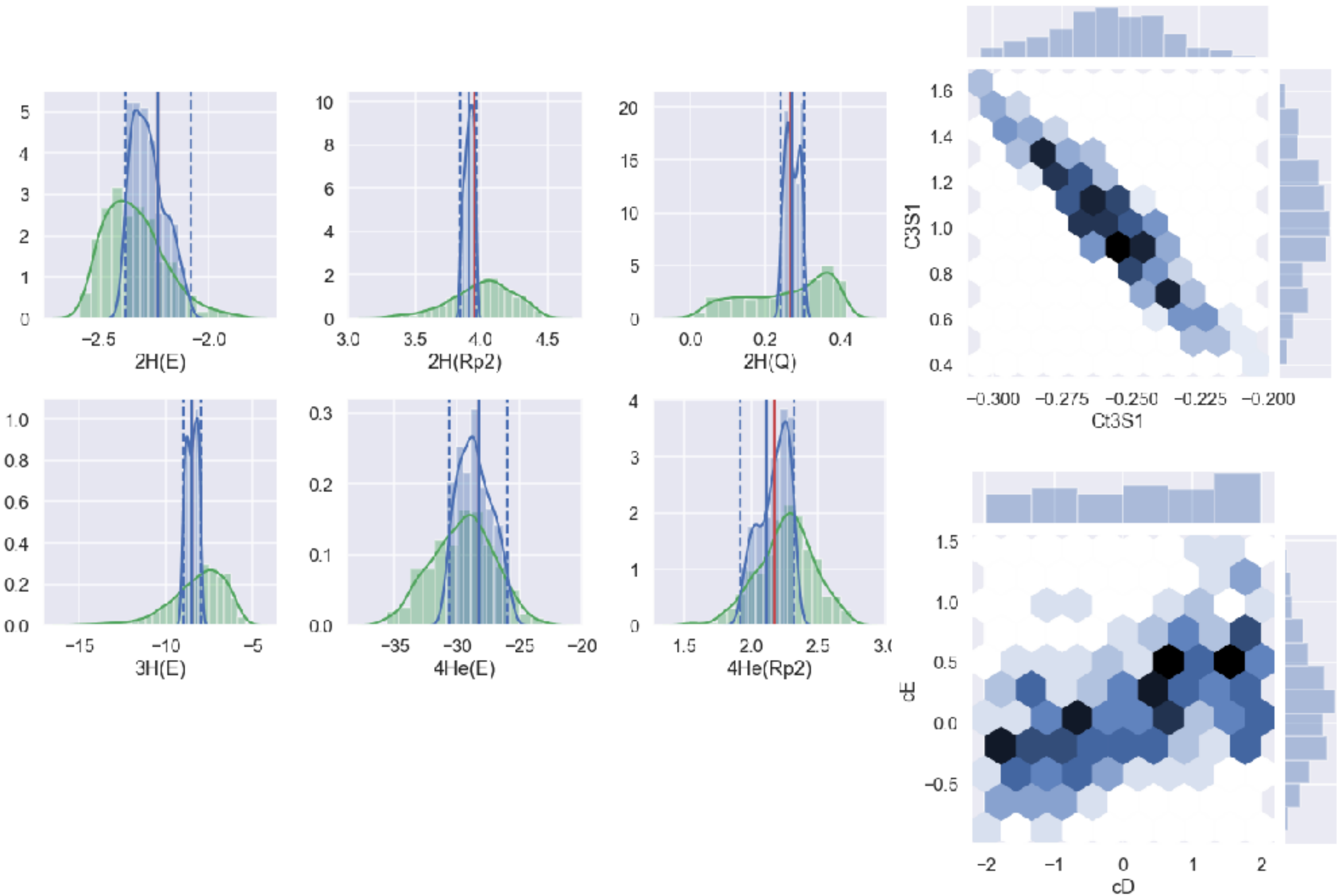
Wave 1: np scattering

Implausibility plots and optical depth plots



- The implausibility measure and optical depth gives the non-implausible volume used as input for wave 2.
- 8 parameters are noticeably constrained; for those the non-implausible volume is now a factor 10^{-6} smaller
- Now we include isospin breaking effects: Ct_{1S0np} +/- 2%.
- And also introduce c_D, c_E.
- However, P-wave contacts are fixed during this wave; The effect is modelled with an emulator nugget (white noise).

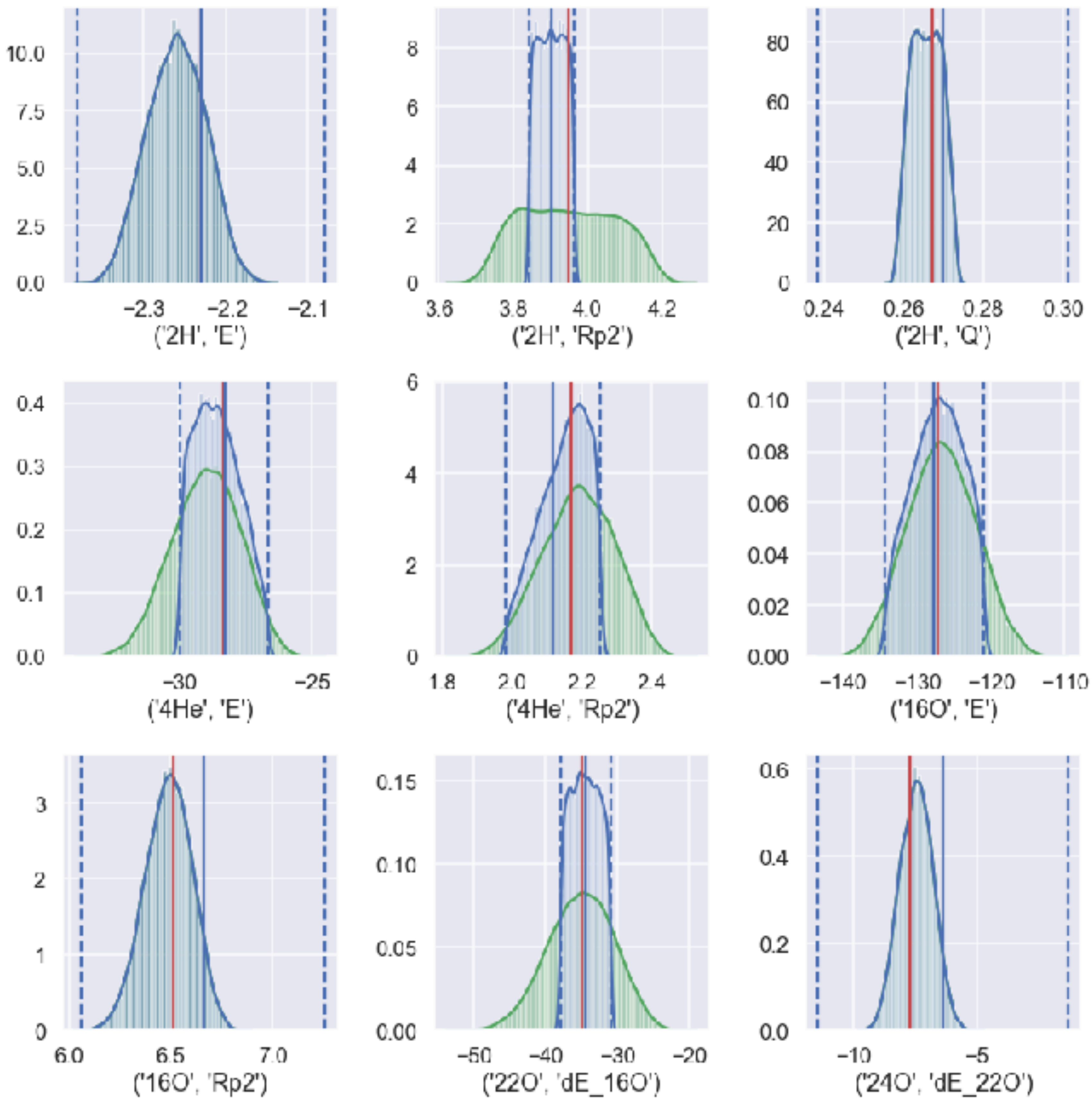
Wave 2: Few-body



Wave 3: DNNLOgo10

- The preceding waves and experience from the Δ-NNLO$_{GO}$ optimisation give the wave 3 non-implausible volume.
- We select 10^8 samples (lhs) of the 17 parameters and evaluate nine observables (in ^{2}H, ^{4}He, ^{16,22,24}O) at each point.
- These ~10^9 many-body computations take in total 25 k-cpu-h.

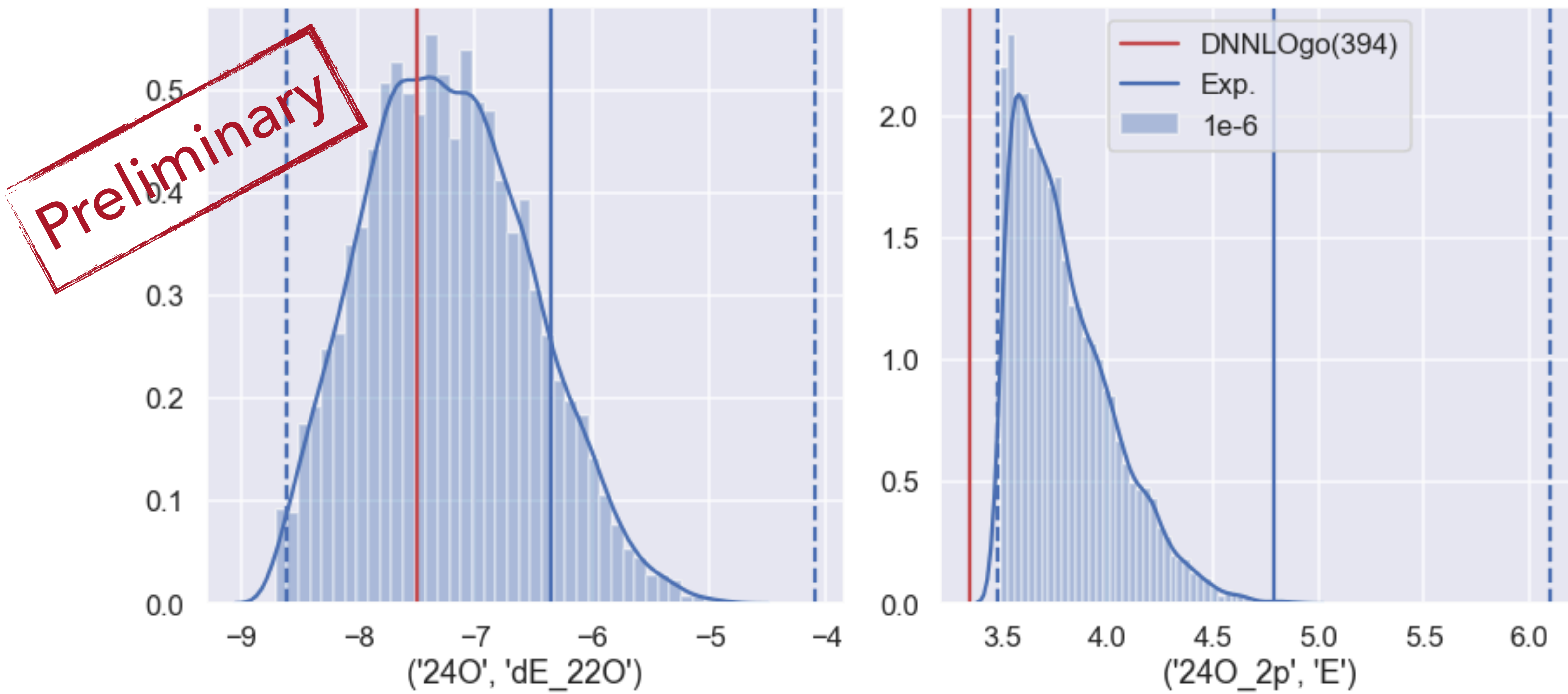
Wave 3: DNNLOgo10



- 22,000 non-implausible samples (blue histograms) [out of 10^8]
- Exp. (blue line)
  3-sigma (dashed blue)
  DNNLOgo (red line)
- Green histograms are predictions.

Final wave

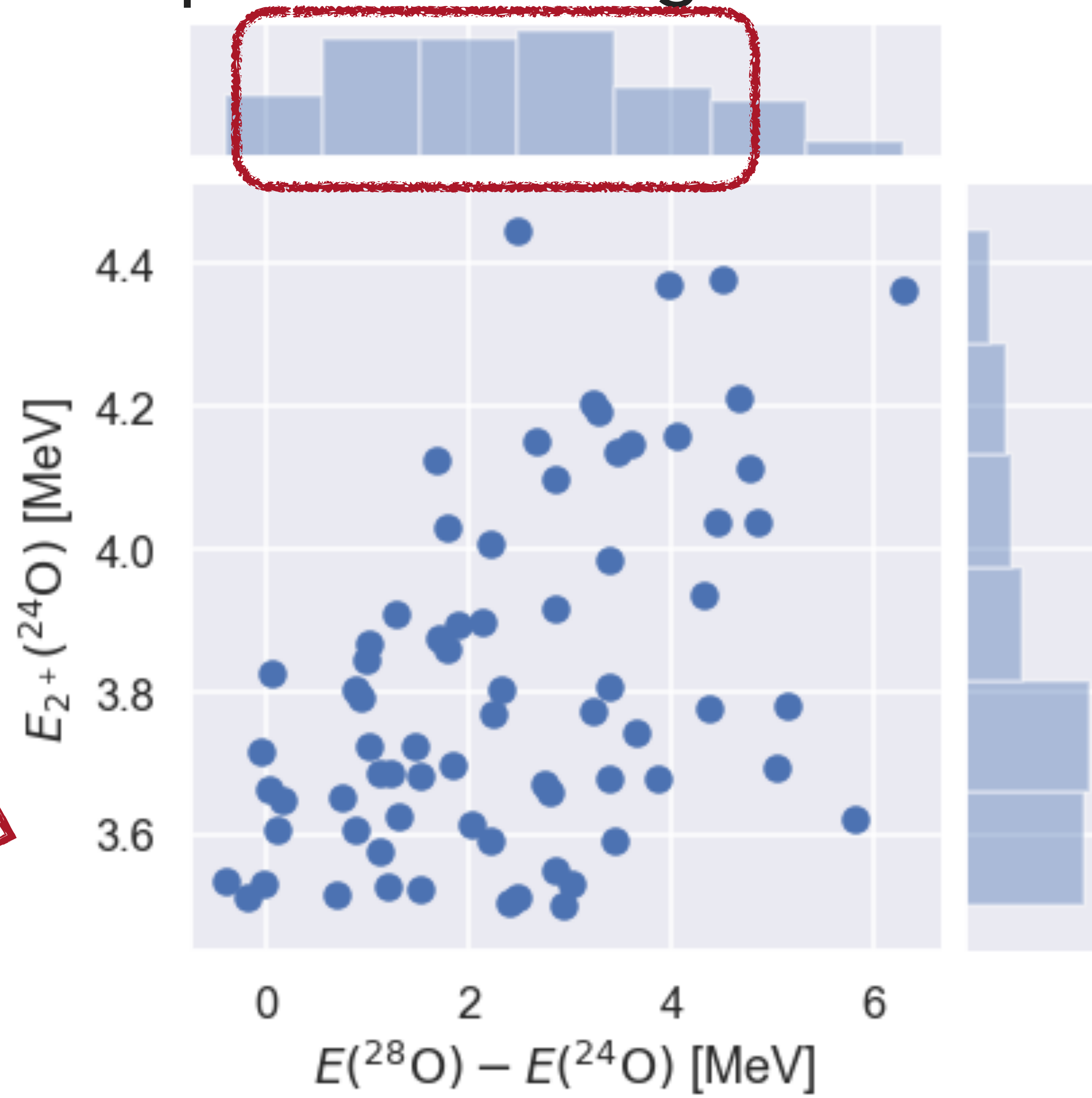
- For the final wave we created a high-precision ^{24}O(gs) emulator [going from 20% to 4% precision]
- And developed an $E_{2+}(^{24}O)$ emulator [~50 keV precision!]
- A set of 8,343 non-implausible samples survive.



Oxygen dripline

- Performing a history match of ab initio methods with the Δ-NNLO interaction model produces a huge volume reduction and a set of non-implausible samples.
- Does this set predict bound or unbound ^{28}O?
- First tests indicate a slightly unbound ^{28}O.

Very preliminary



Outlook

- Additional explorative computations for ^{28}O (continuum? deformation? create and test emulators);
- Further exploration of iterative history matching;
- Additional emulators (nuclear matter, transition strengths, …);
- Statistics interpretations: from the non-implausible region to Bayesian posteriors;
- Experimental design;
- …