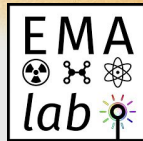




# FRAMING

of the problem:  
A global emulation  
perspective



*Jose M Munoz*  
2026

# The data problem

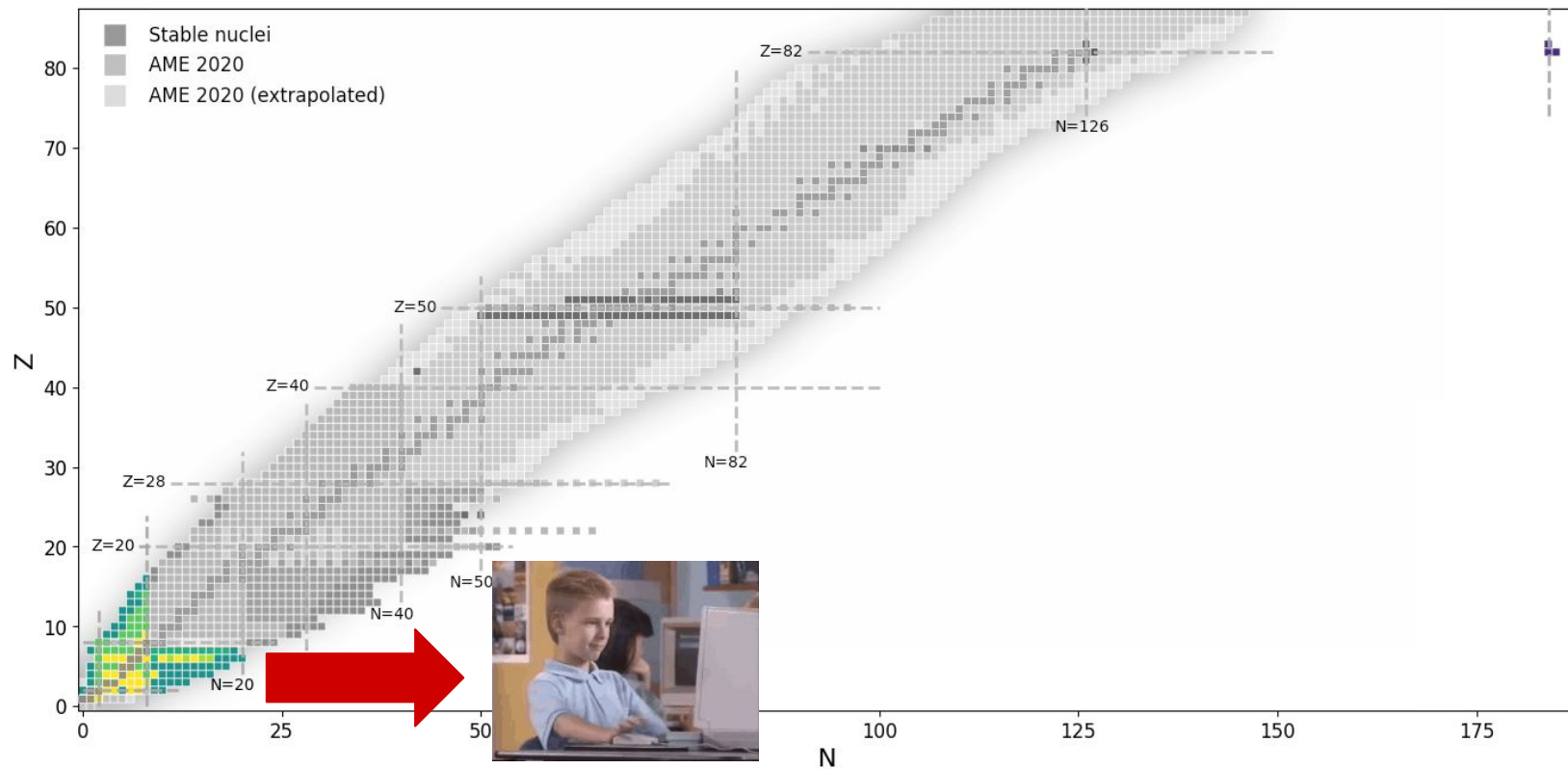


Image Courtesy of Antoine Belley

# The data problem

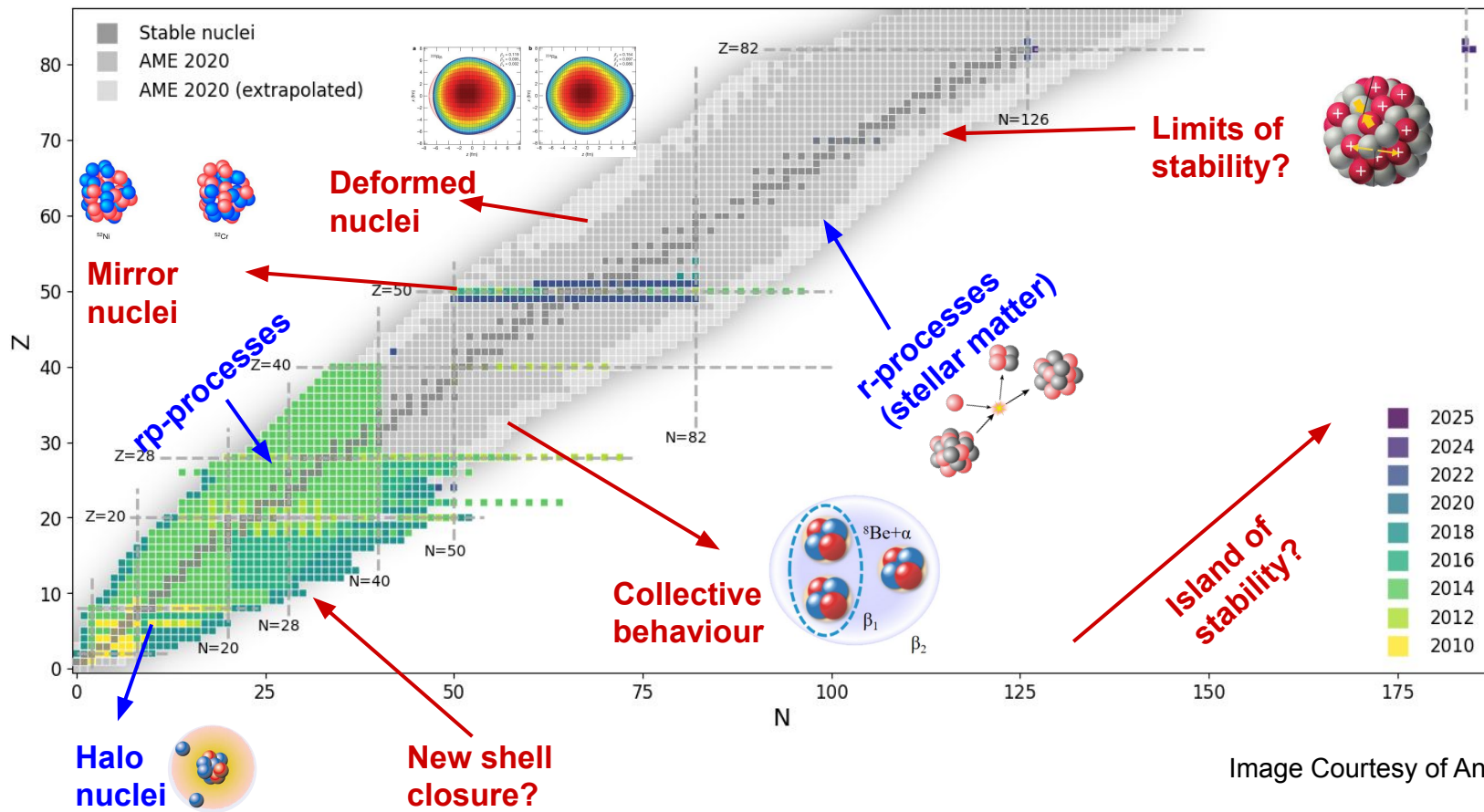
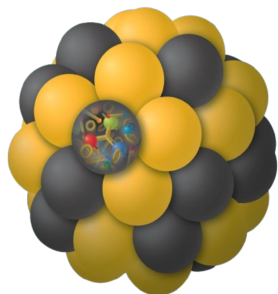


Image Courtesy of Antoine Belley

# From Phenomenology to 'First Principles'

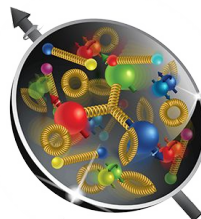
Ab-Initio nuclear physics is a very powerful approach

Interactions

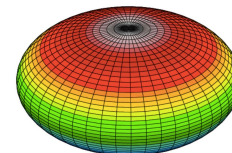


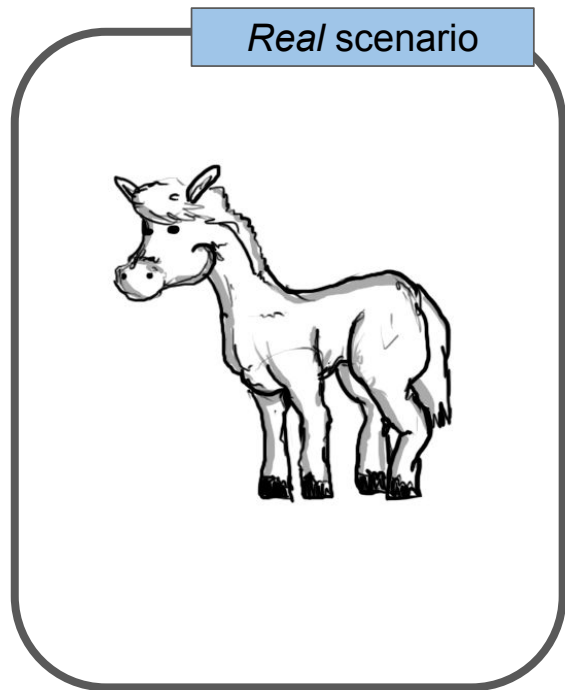
Wavefunctions

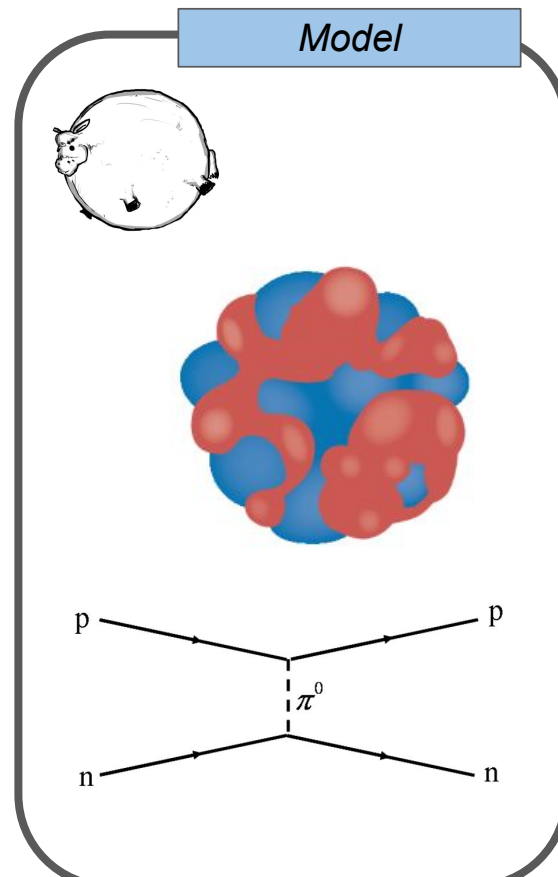
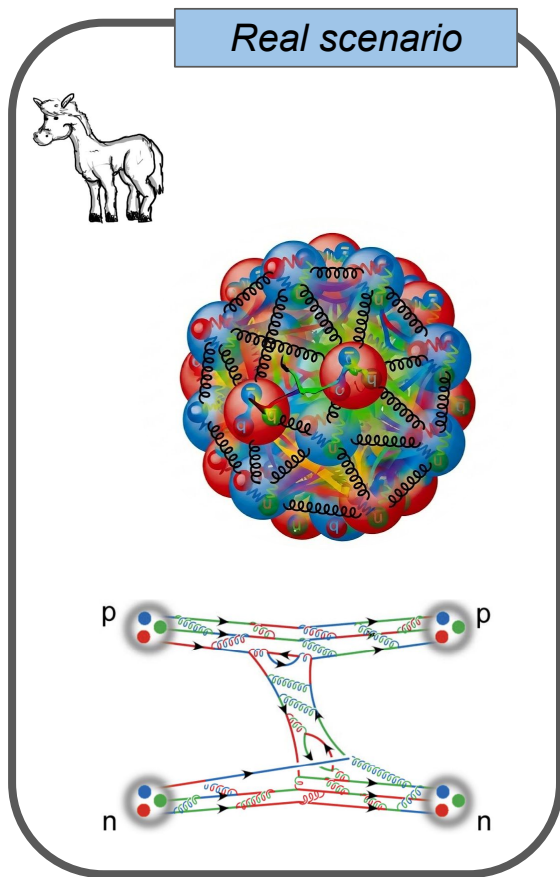
$$(T+V)|\Psi\rangle = E|\Psi\rangle$$



Observables



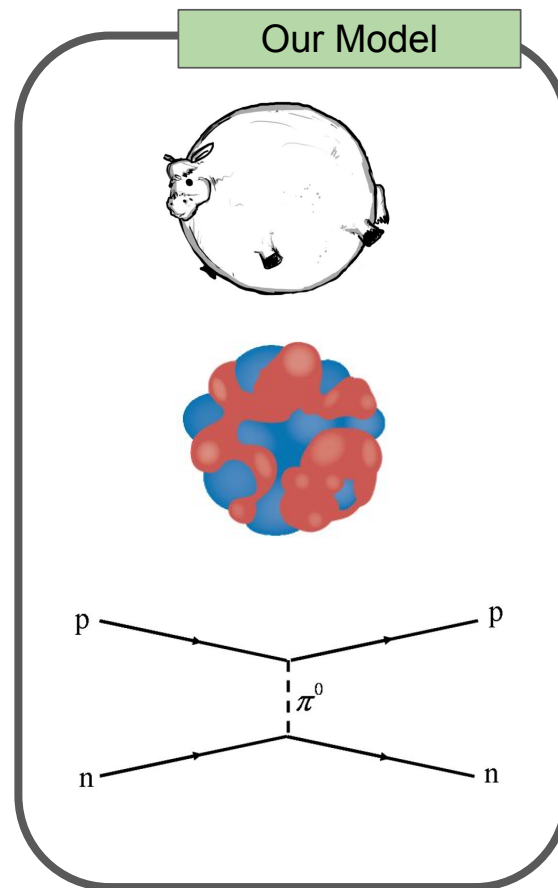


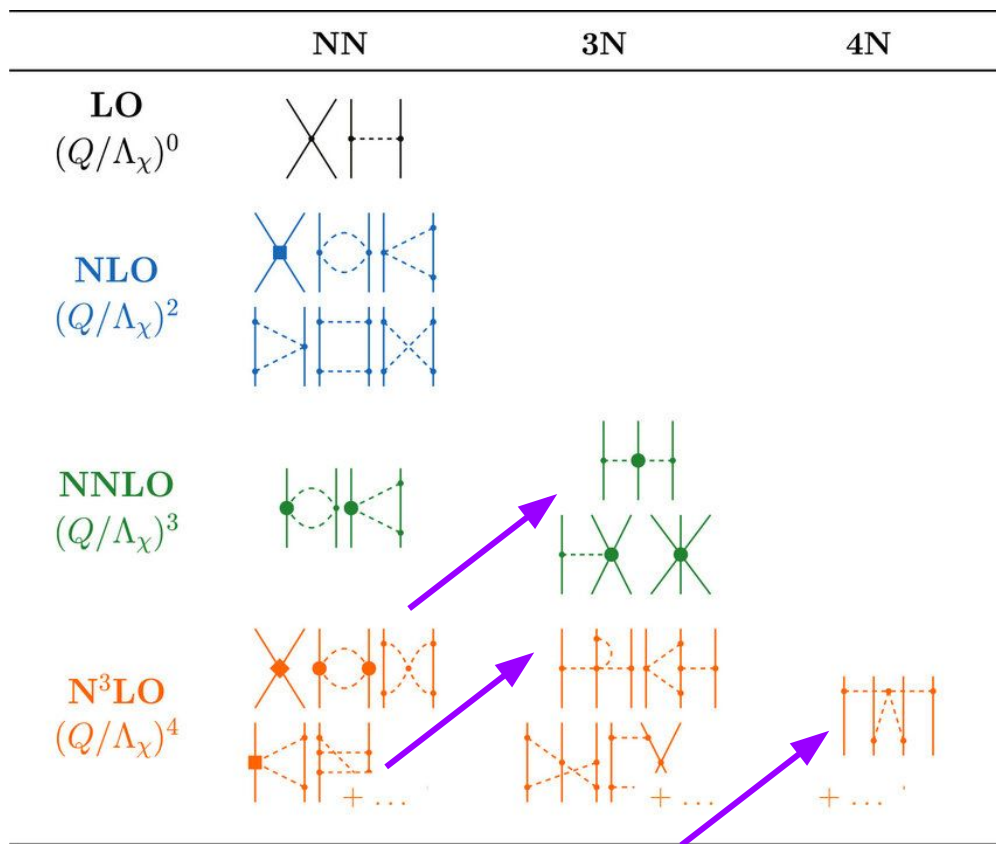


How do we estimate the uncertainties coming from these approximations?


How do we make sure we are not missing important physics?


When and why are these 'simplifications' not valid?





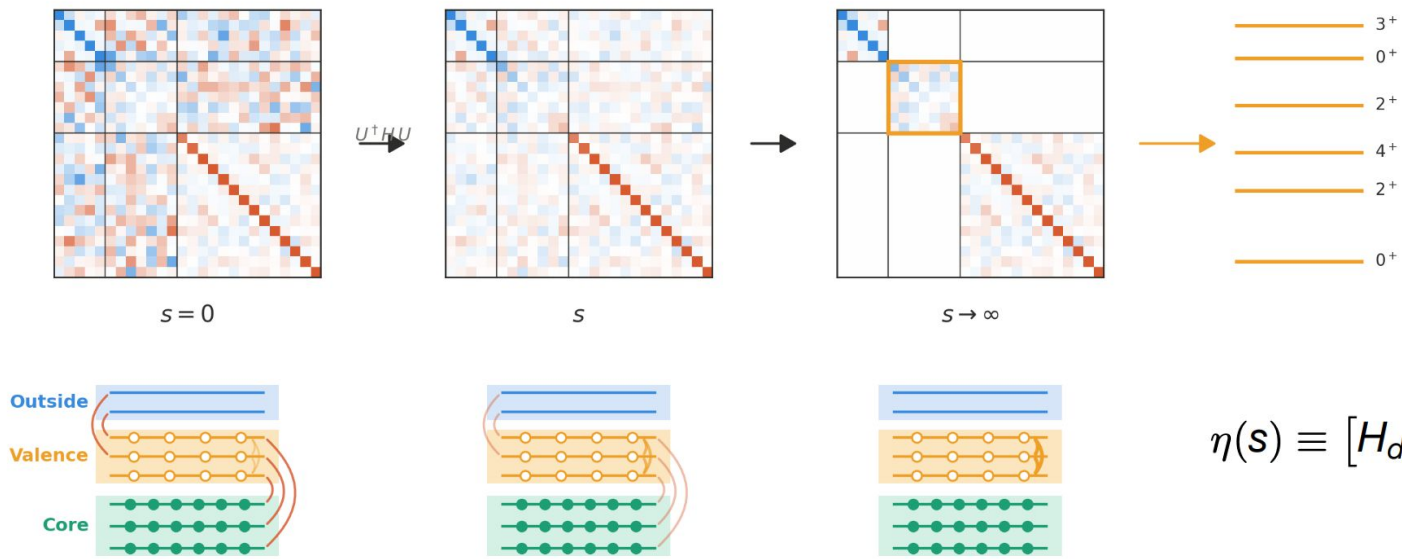
 NN forces  
(fit to scattering data)

 3N couplings fit to  
3/4-body systems

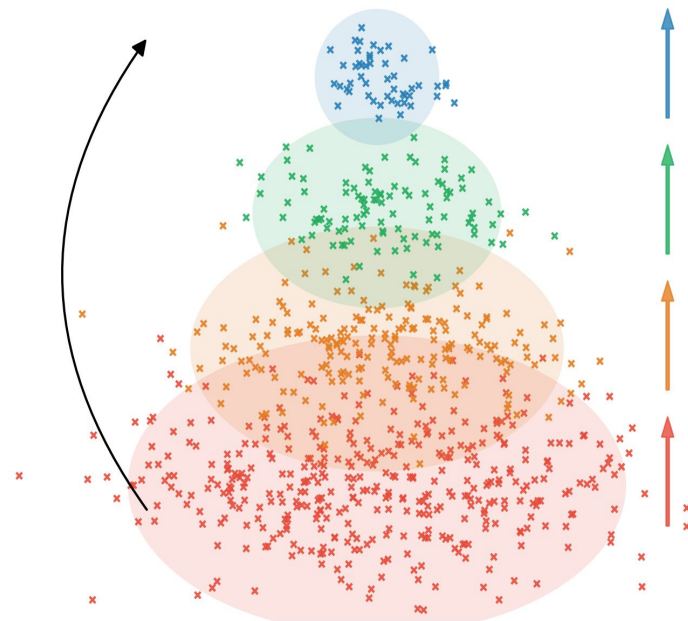
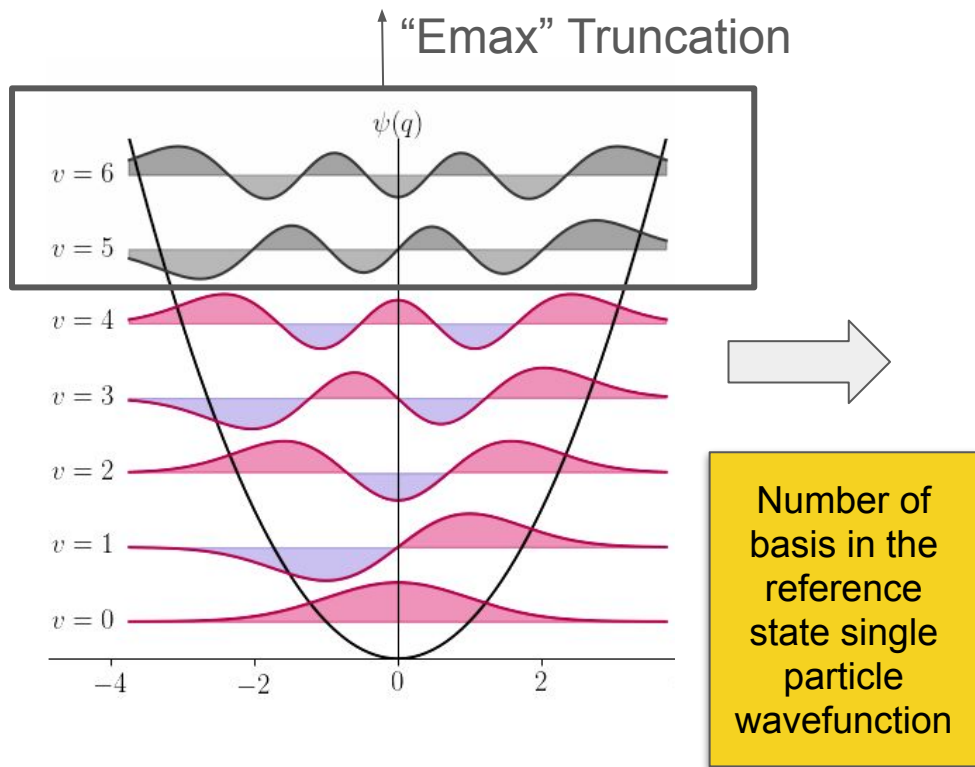
 Higher order terms  
(go) under the rug

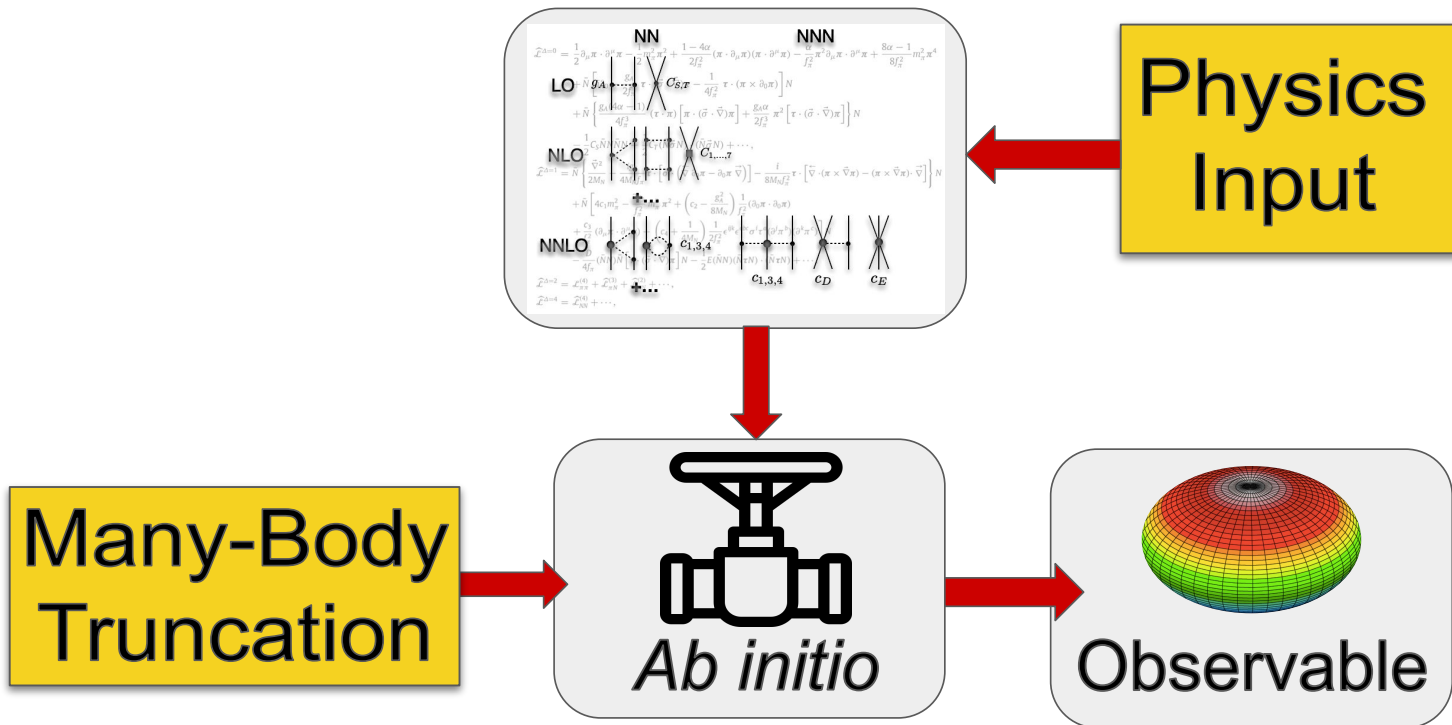


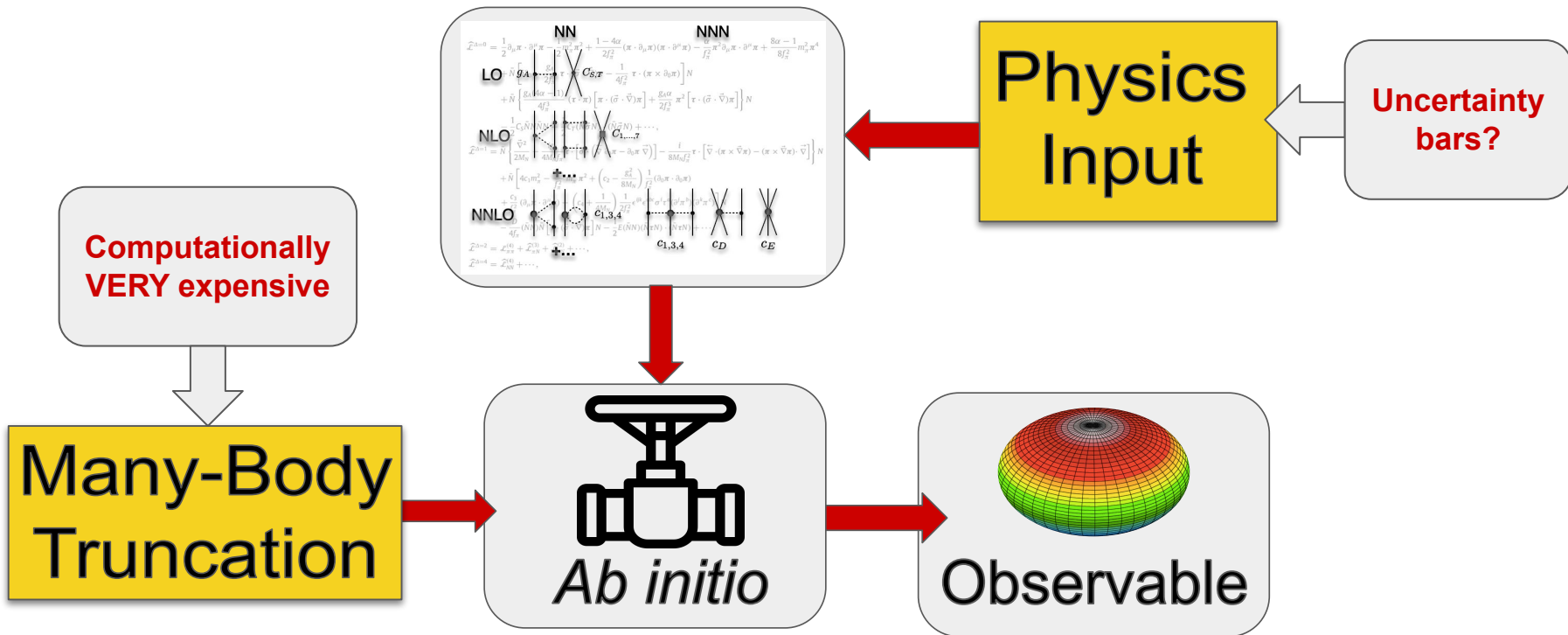
*Diagonalize* a matrix by performing continuous Unitary transformations.  
Then, the reference state is decoupled from excitations

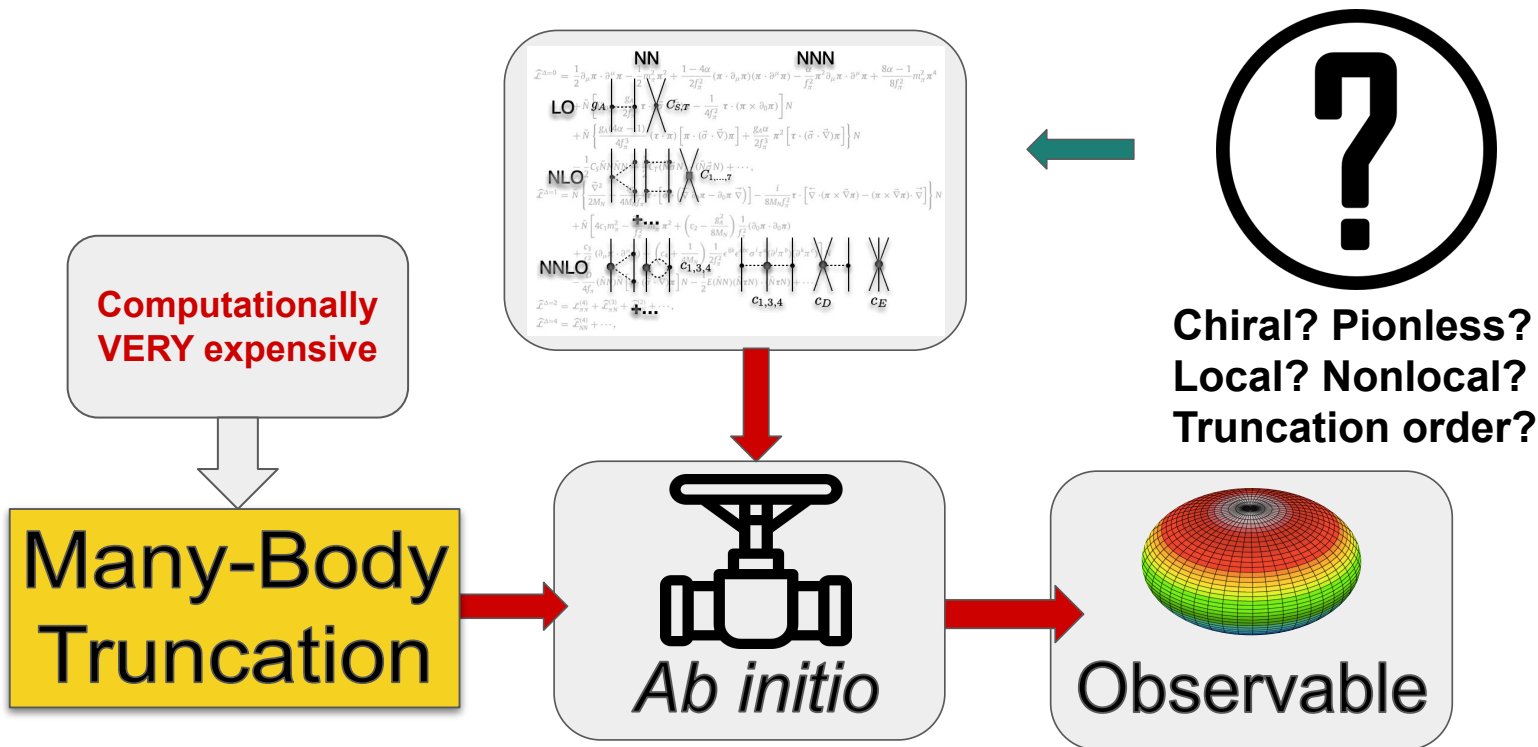


$$\eta(s) \equiv [H_d(s), H_{od}(s)]$$

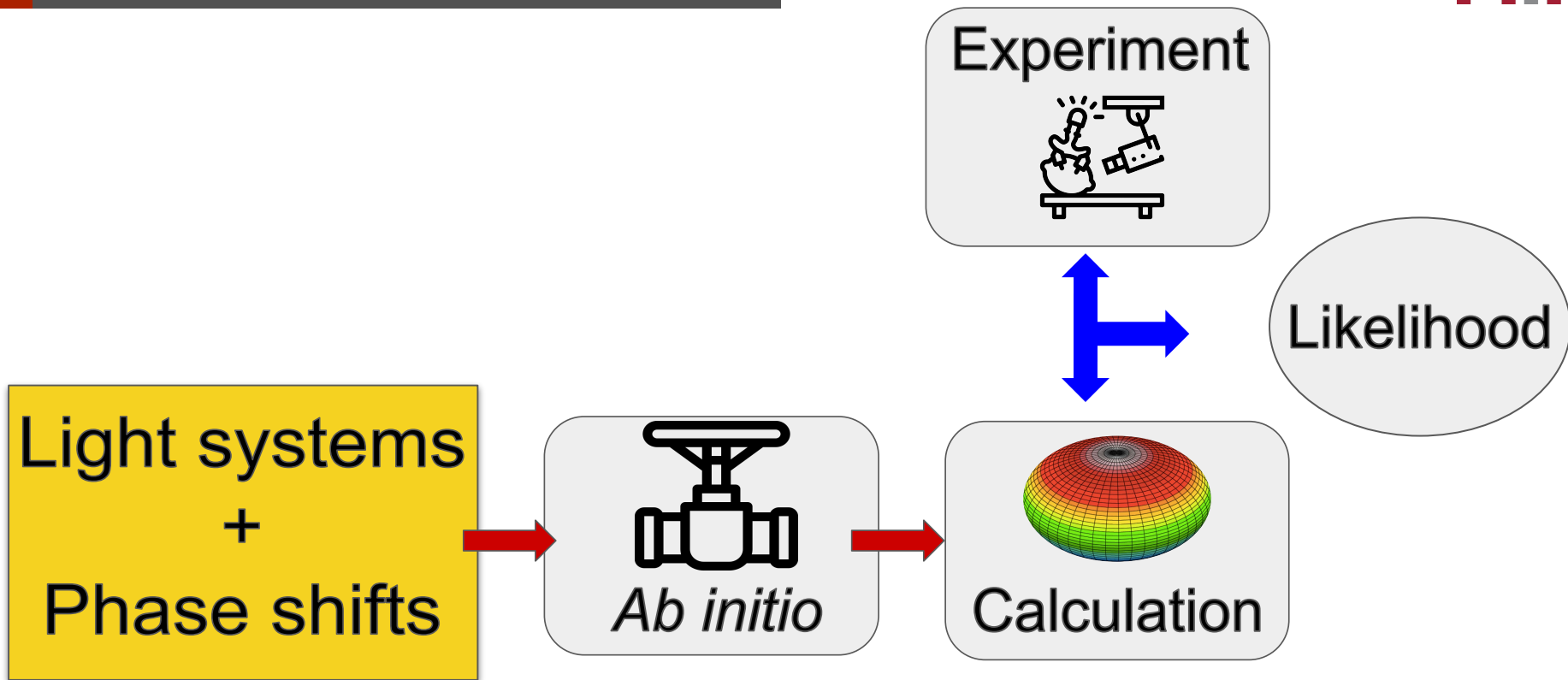








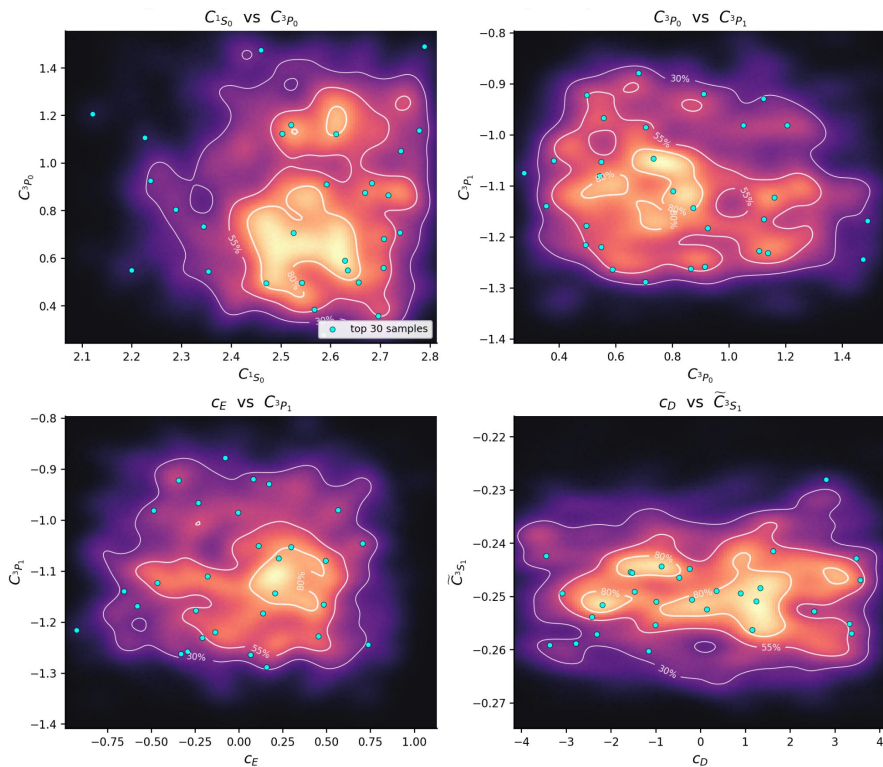
# The problem of Interaction 'calibration'



# A naive problem of optimization



## Likelihood $A=2-4$



→ 17 x 17

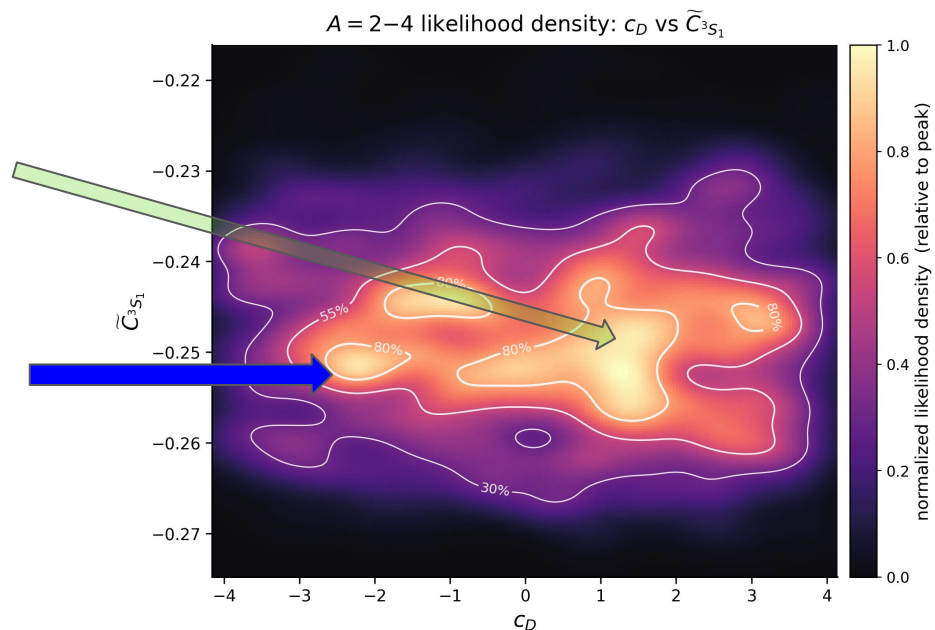
# The infamous $c_D$

Does blue yield better (more physical) results?

Does it 'hide' information about our truncation?

Can we learn more physics from the difference?

Are they artifact of the particular observables we use?

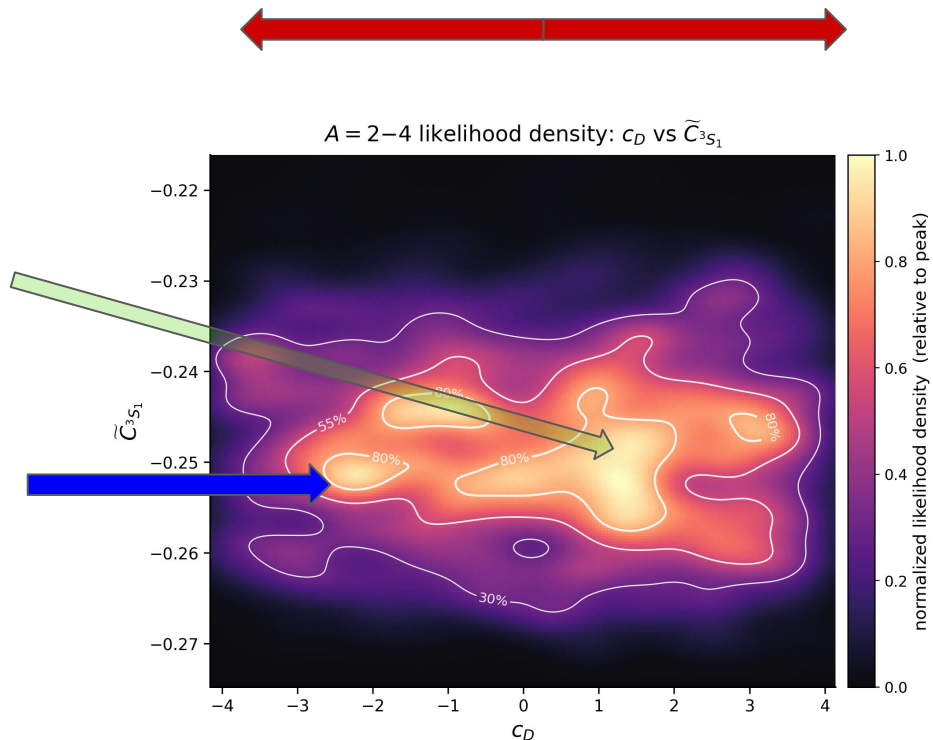


Does blue yield better (more physical) results?

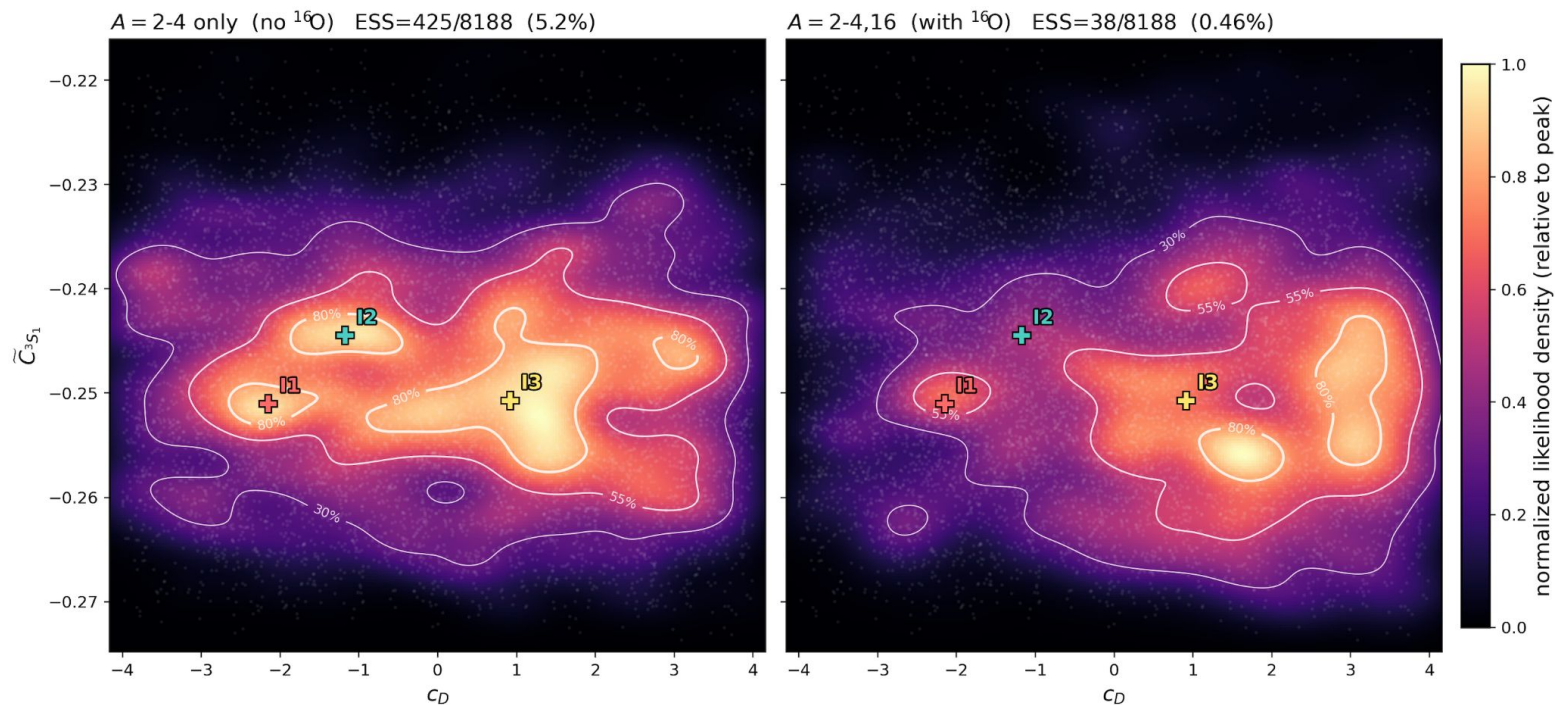
Does it 'hide' information about our truncation?

Can we learn more physics from the difference?

Are they artifact of the particular observables we use?



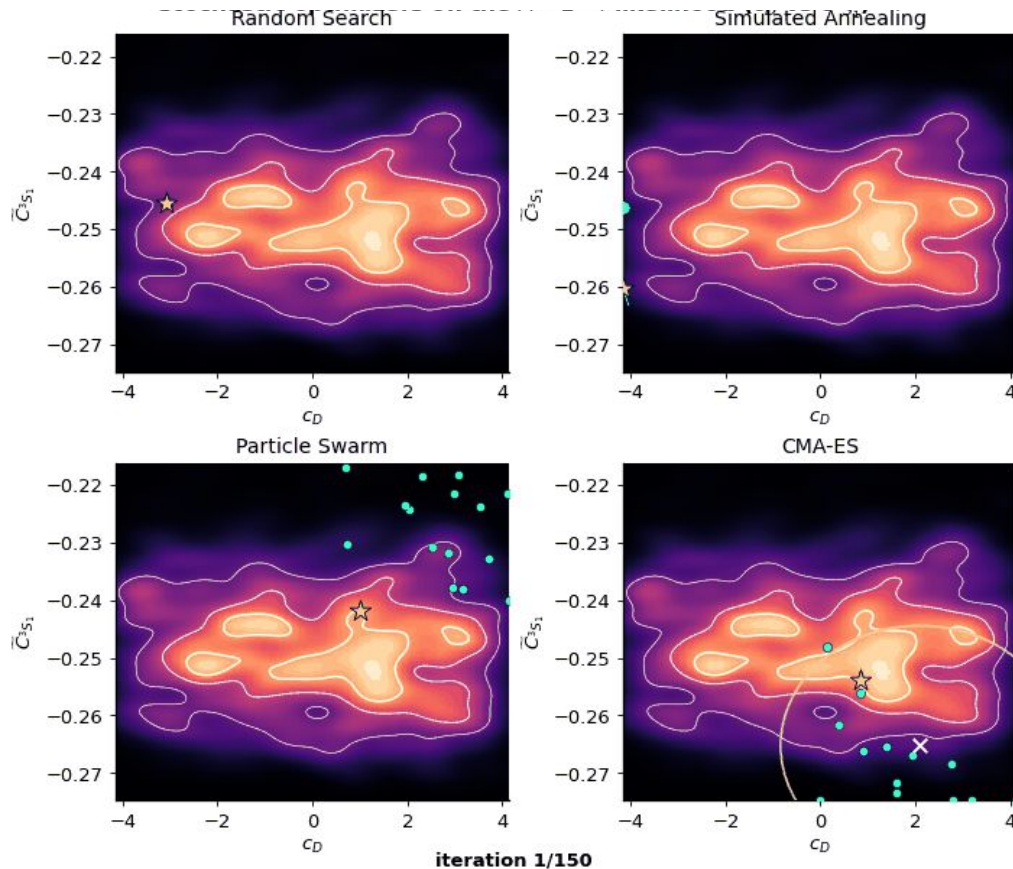
Or including O16.



Of course... optimizing the interaction with the same observables will only get you so far...

And no, better optimization is not the answer!

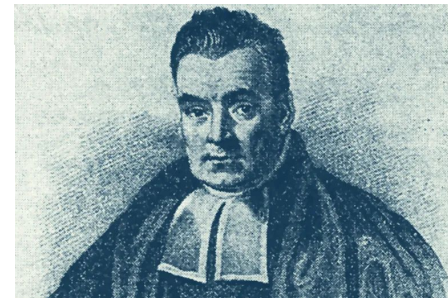
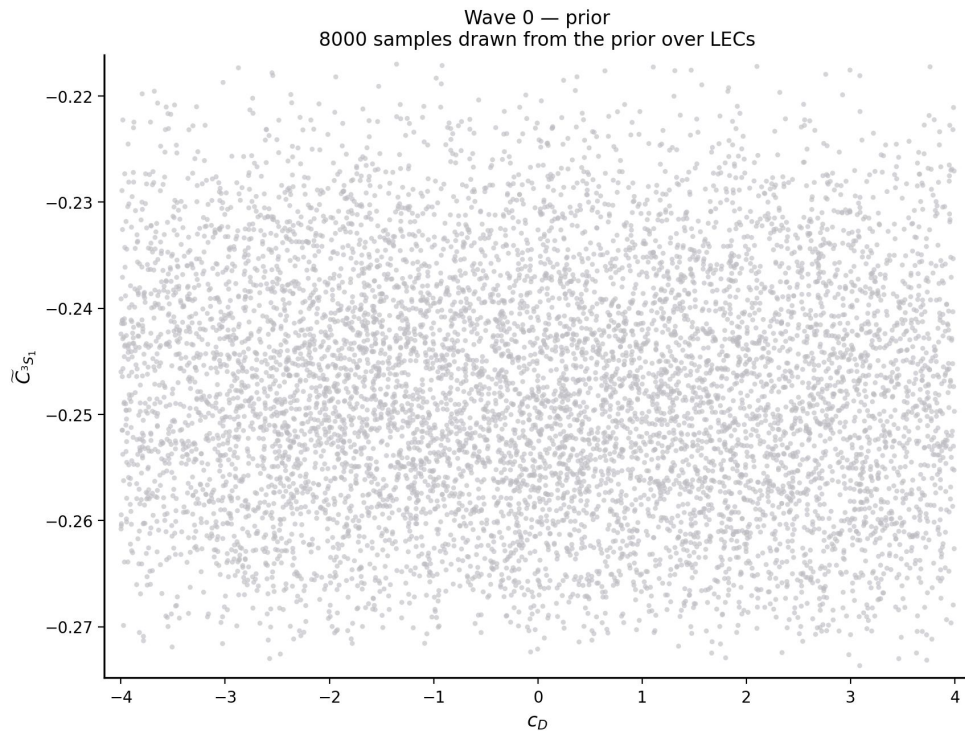
Don't estimate uncertainty by just using different optimizers!



So... which one is right?



None!  
You need to consider them  
all...

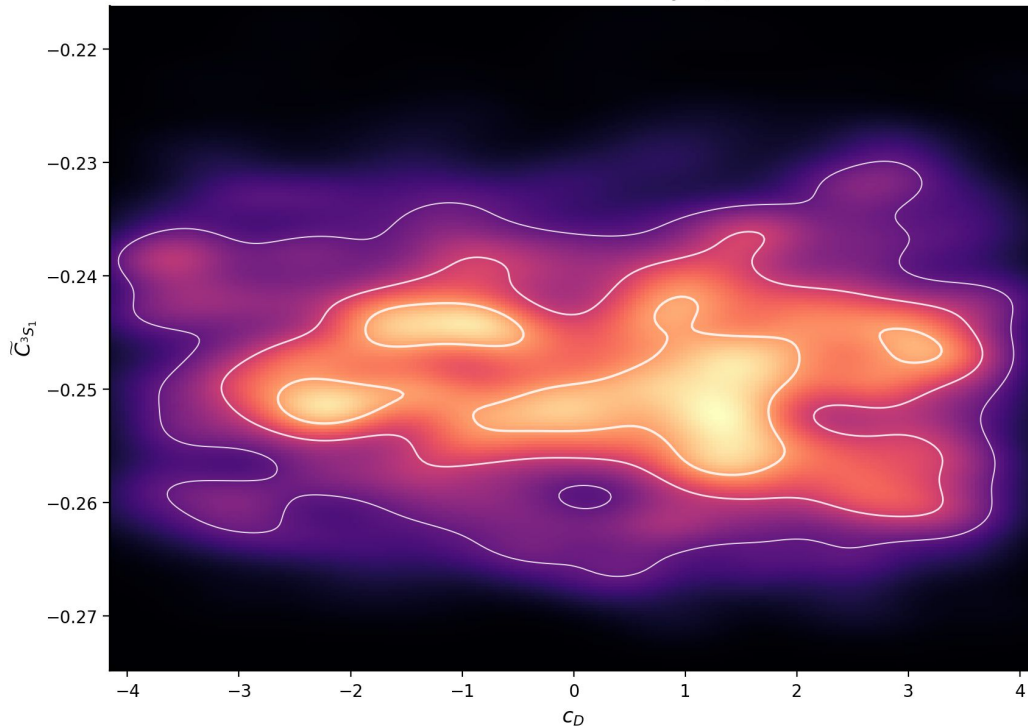


So... which one is right?



None!  
You need to consider them  
all...

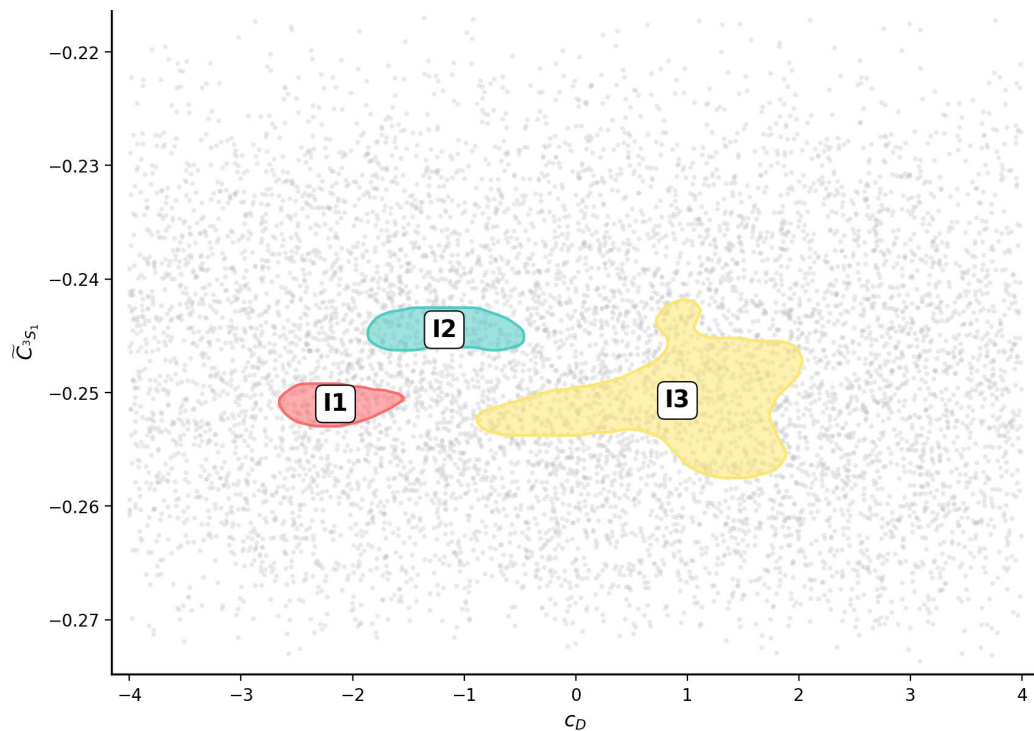
Evaluate likelihood  
 $A = 2-4$  likelihood density  $\mathcal{L}(\theta)$



So... which one is right?



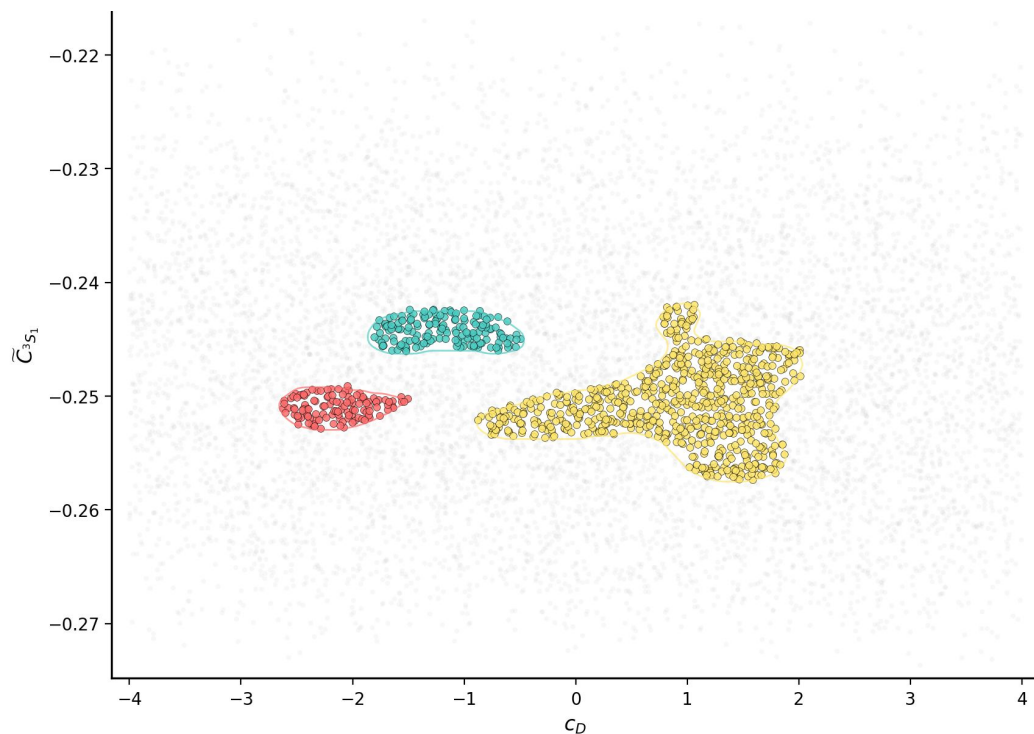
None!  
You need to consider them  
all...



So... which one is right?



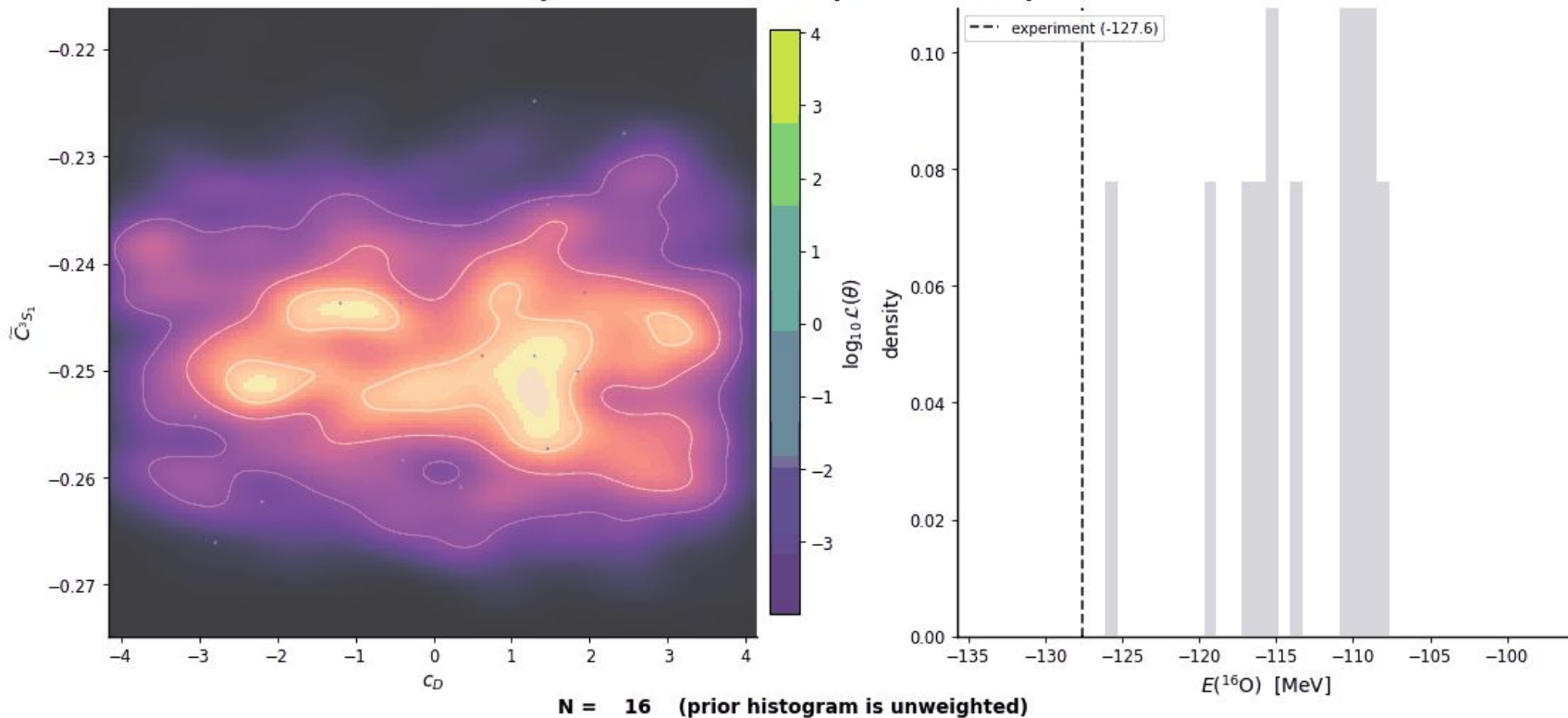
None!  
You need to consider them  
all...



# So... which one is right?



## Step 1 / 3 — draw samples from the prior



This leaves order 10k samples left 'non-implausible'...

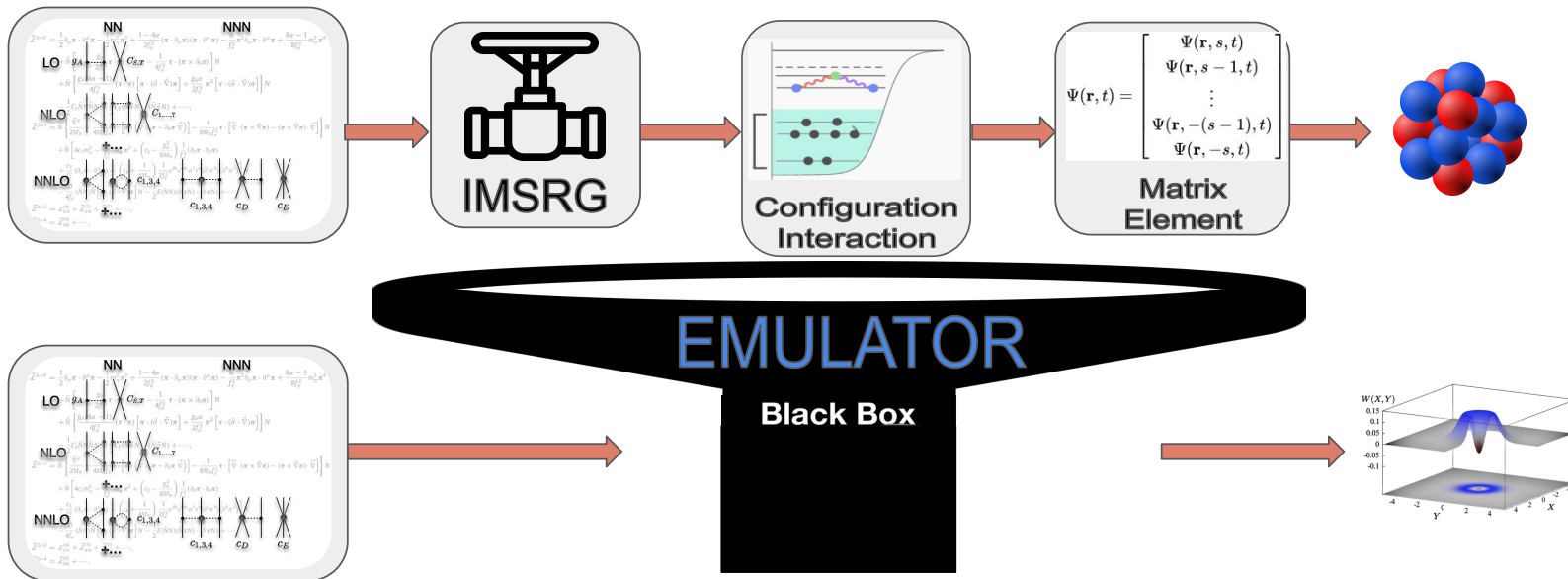
So if we want to have our uncertainty bar... we need to compute the converged calculations for all of them.

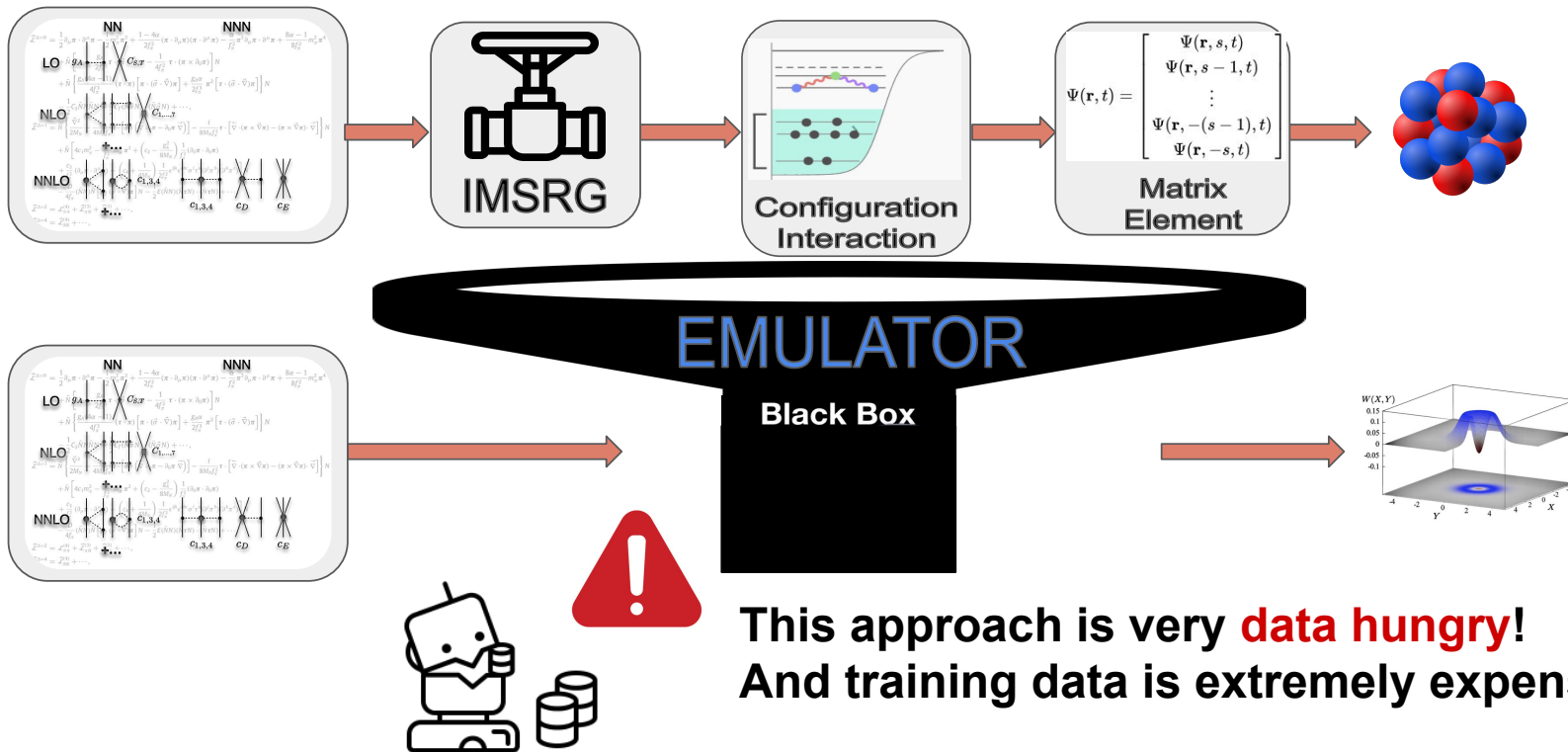
This is O(years) on MIT compute cluster (not too small)...  
+ This has to be done per nuclei...



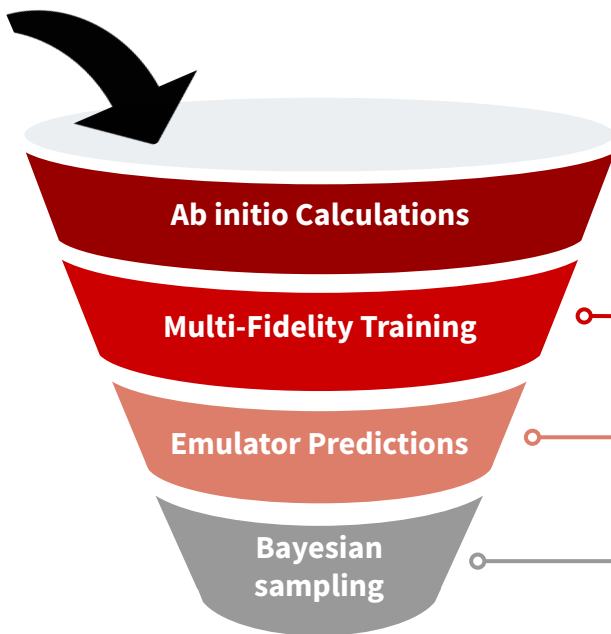
+ This is only one of the possible uncertainty sources!

# Emulating the nucleus





Physical  
Parameters  
Samples  
(with  
likelihoods)



Constrain LEC values using history-matching techniques.

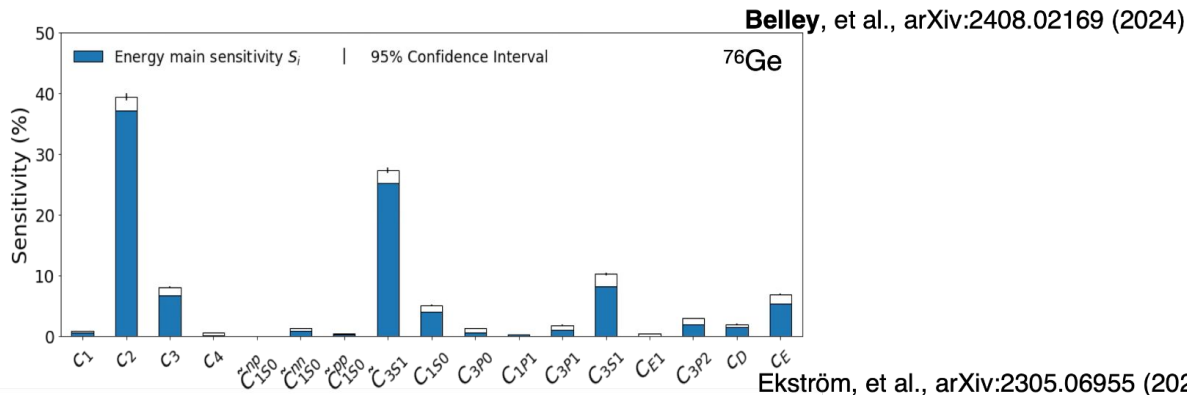
Train a BNN emulator to approximate ab initio calculations.

Predict the emulator posterior Using the generated samples.

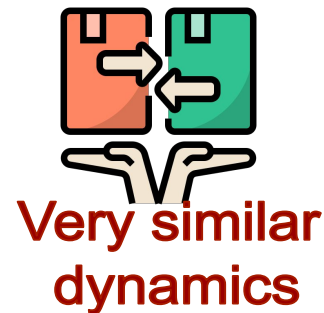
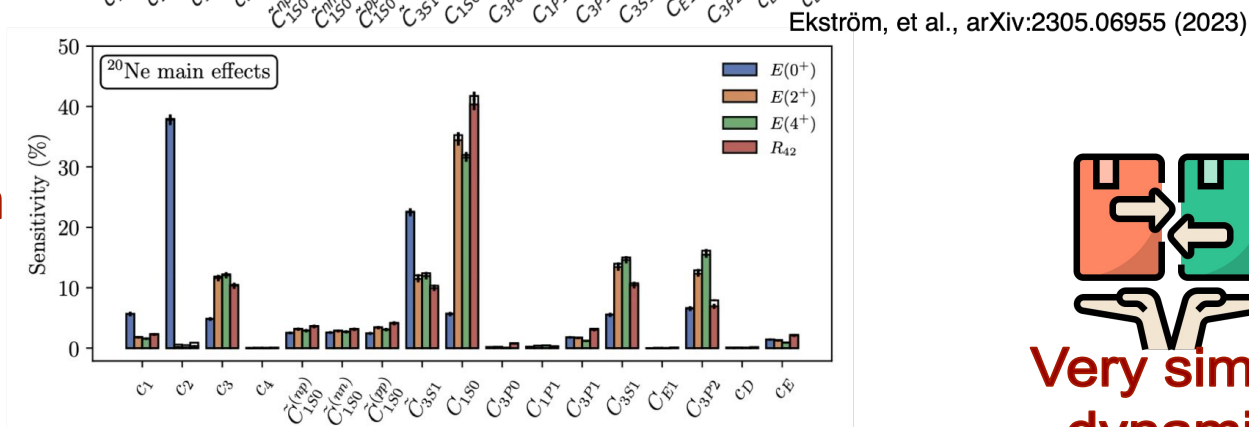
Likelihood based resampling of the estimated observables.

Uncertainty  
Estimation

Data-Driven emulators



Physics-driven reduction

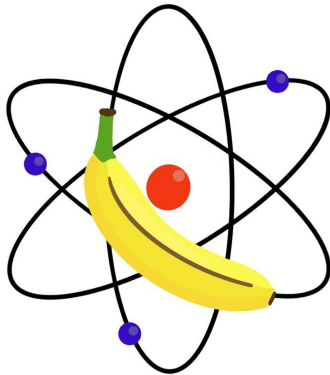




# Global Framework for Emulation of Nuclear Calculations

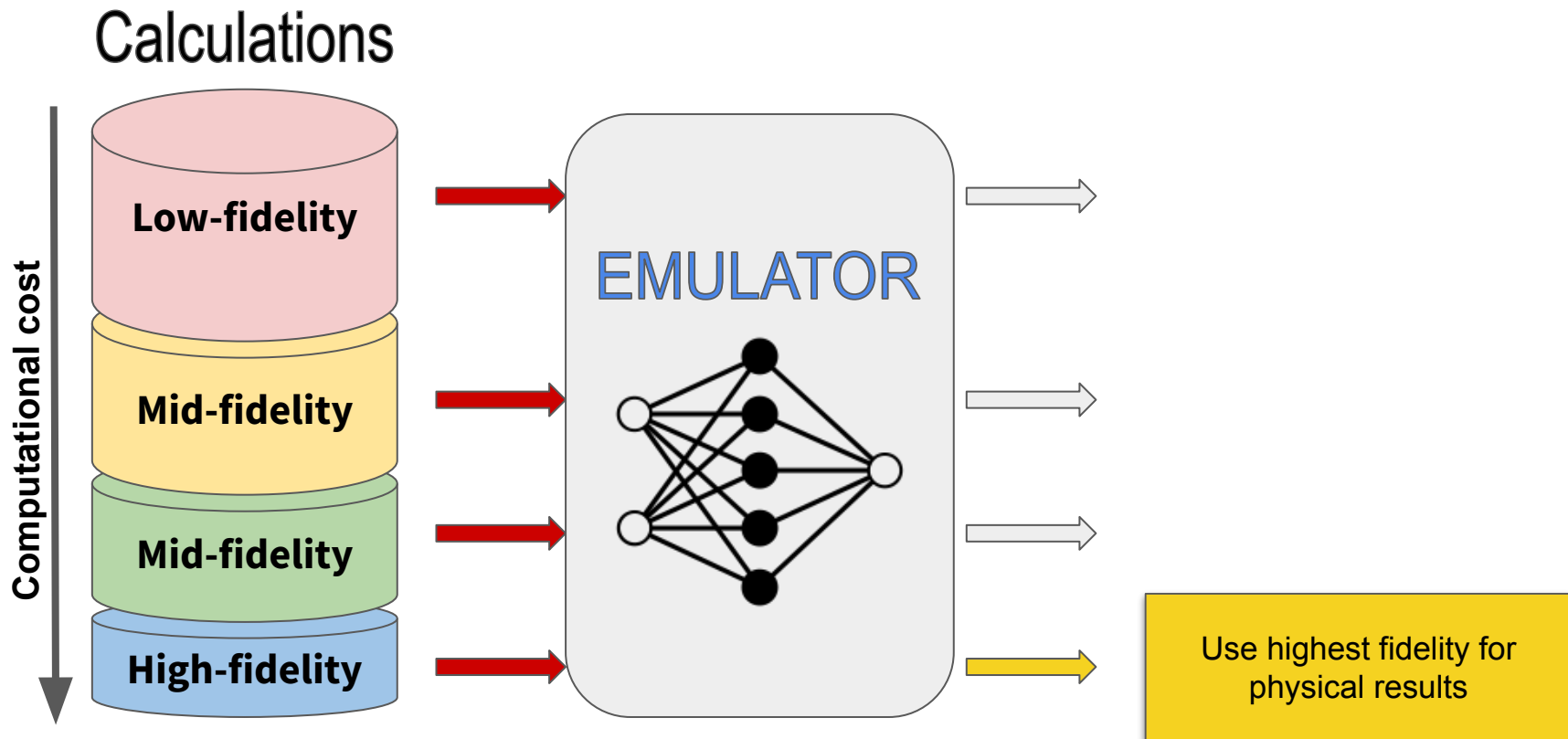
Antoine Belley<sup>†,\*</sup> Jose M. Munoz<sup>†,†</sup> and Ronald F. Garcia Ruiz<sup>‡</sup>

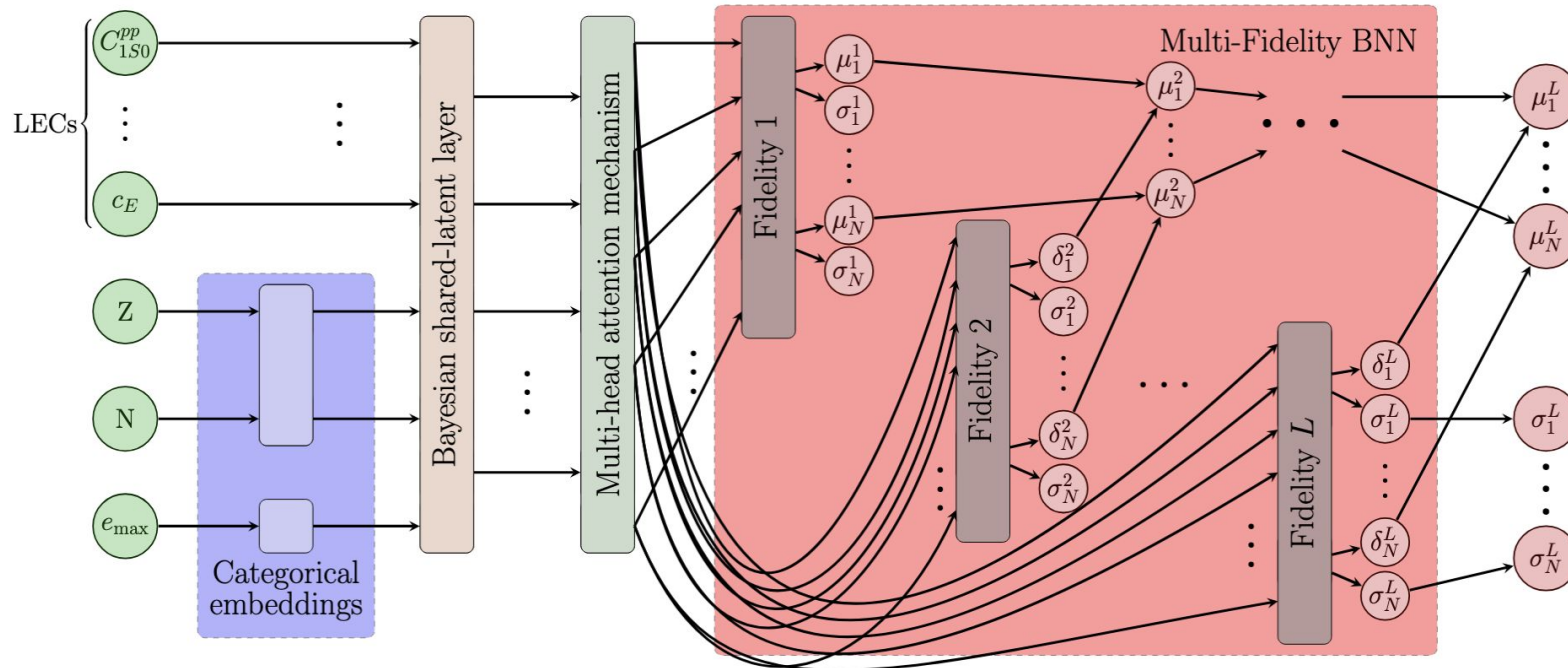
*Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*



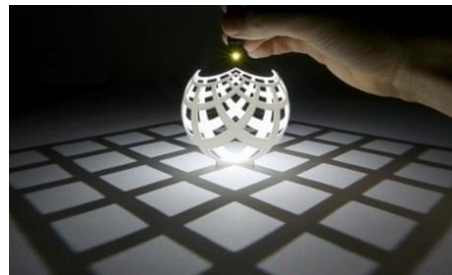
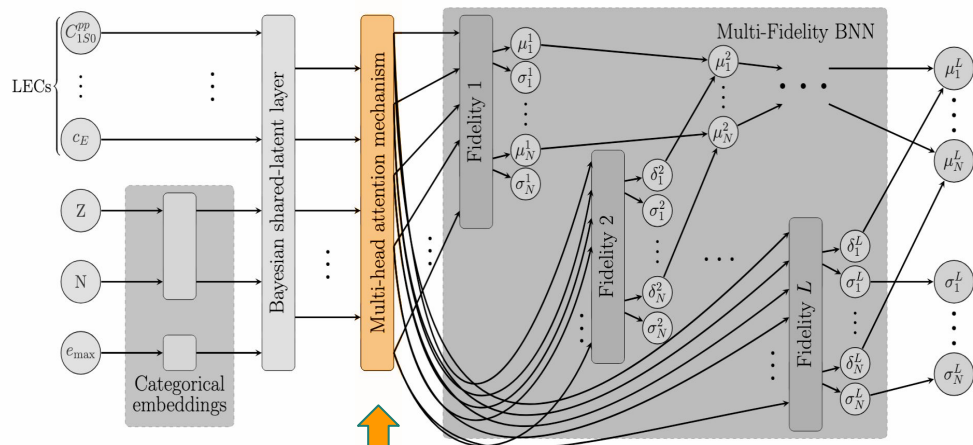
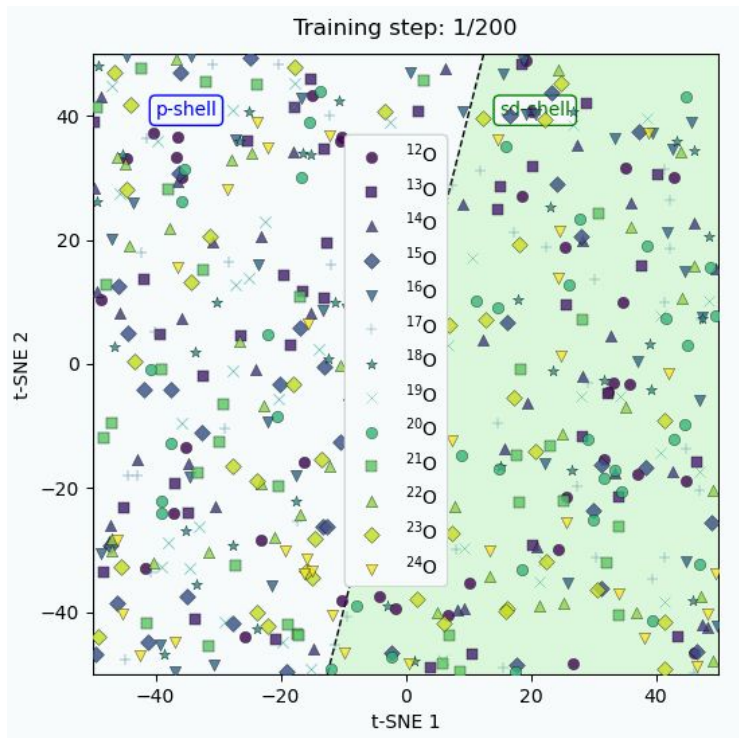
Phys. Rev. Lett. **136**, 082501 – Published 23 February, 2026

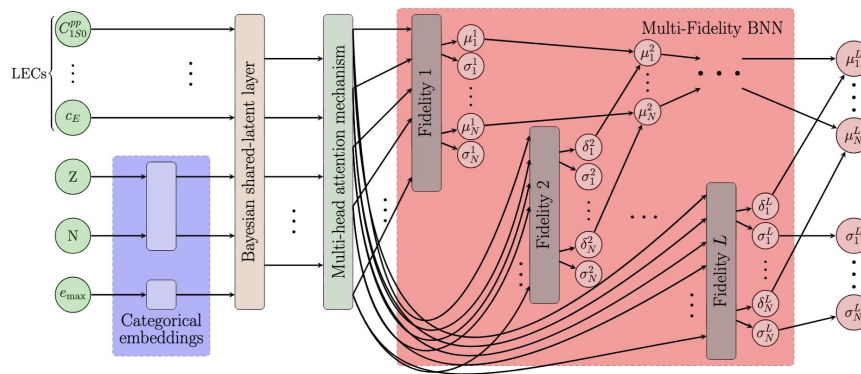
DOI: <https://doi.org/10.1103/mvc3-qdtc>





# From months to seconds!

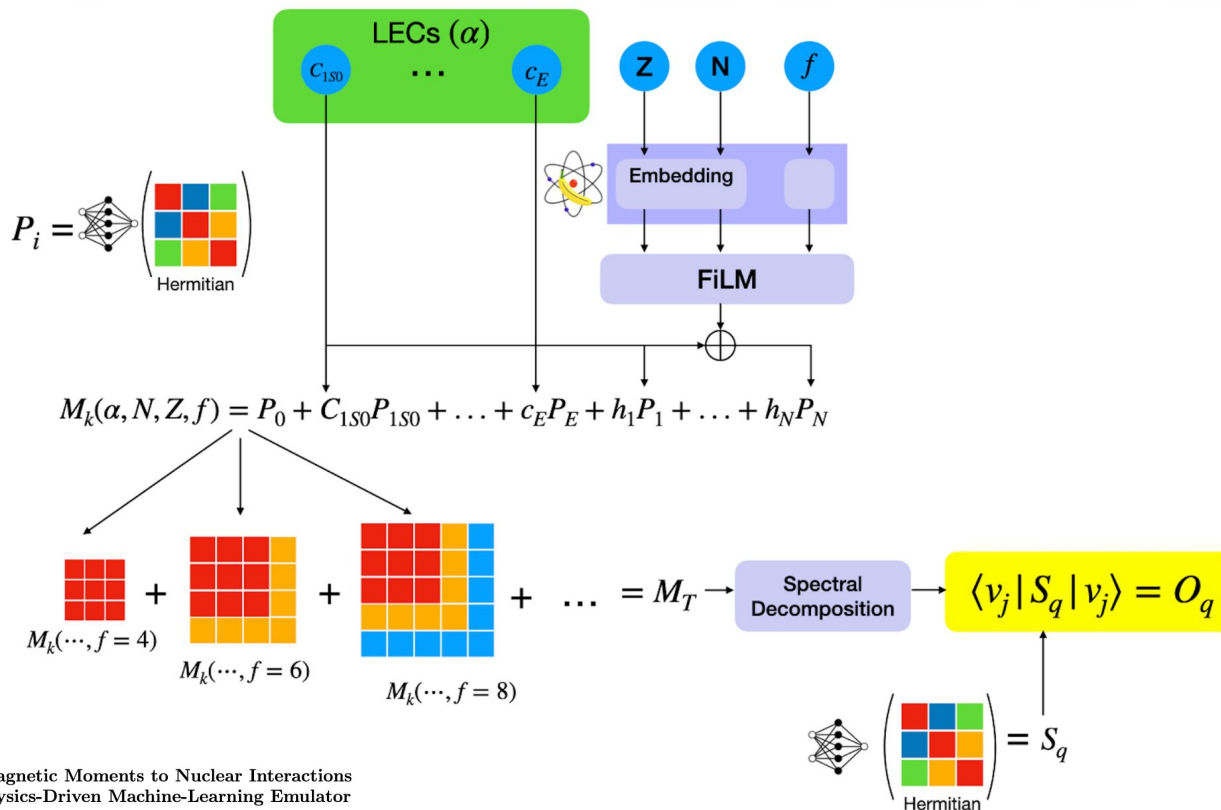




Can we really trust an AI model  
(no)  
to extrapolate nicely?

# The need to inject more physics

# A physics first approach!



Linking Electromagnetic Moments to Nuclear Interactions with a Global Physics-Driven Machine-Learning Emulator

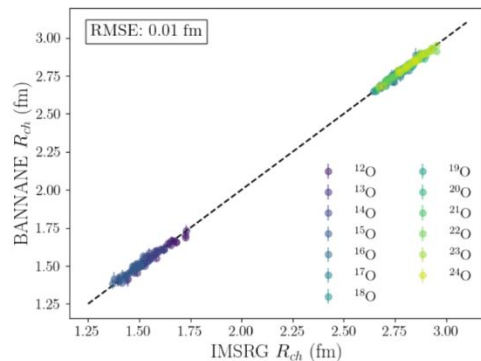
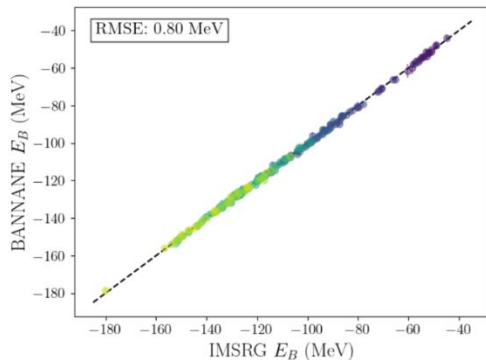
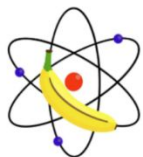
$$M^{(k)}(z, n, \ell) = a_0 I_{m_k} + \lambda_1 \begin{matrix} \color{red}{\square} & \color{red}{\square} & \color{red}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} \end{matrix} + \lambda_2 \begin{matrix} \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} \end{matrix} + \lambda_3 \begin{matrix} \color{green}{\square} & \color{green}{\square} & \color{green}{\square} & \color{green}{\square} & \color{green}{\square} \\ \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} & \color{green}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} \end{matrix} + \lambda_3 \begin{matrix} \color{blue}{\square} & \color{blue}{\square} & \color{blue}{\square} & \color{blue}{\square} & \color{blue}{\square} & \color{blue}{\square} \\ \color{green}{\square} & \color{green}{\square} & \color{green}{\square} & \color{green}{\square} & \color{green}{\square} & \color{blue}{\square} \\ \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} & \color{yellow}{\square} & \color{green}{\square} & \color{blue}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} & \color{blue}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} & \color{blue}{\square} \\ \color{red}{\square} & \color{red}{\square} & \color{red}{\square} & \color{yellow}{\square} & \color{green}{\square} & \color{blue}{\square} \end{matrix} + \dots$$

Fitted with  $\longrightarrow$  emax-4      emax-6      emax-8      emax-10

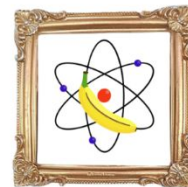
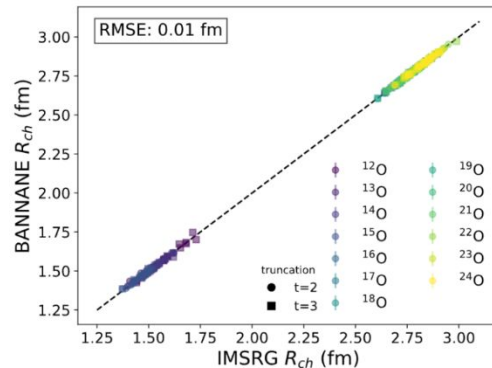
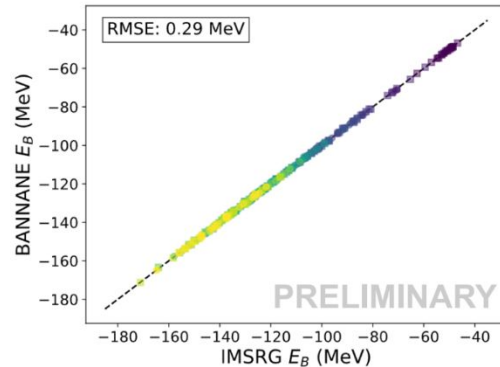
See it in action:

<https://frame-architecture-explorer-553167399436.us-west1.run.app>

# A physics first approach!



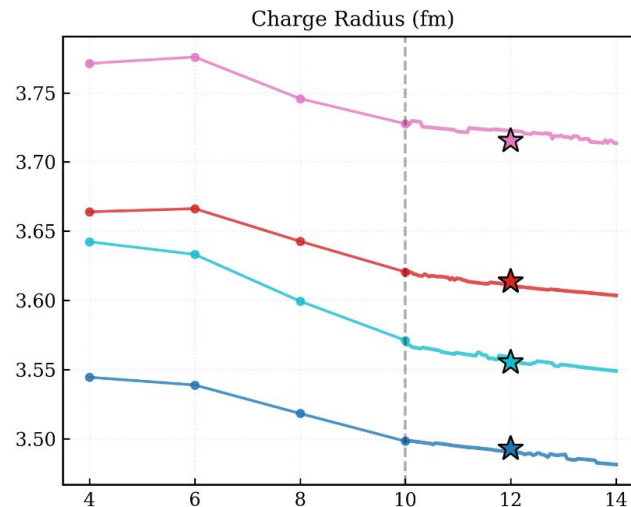
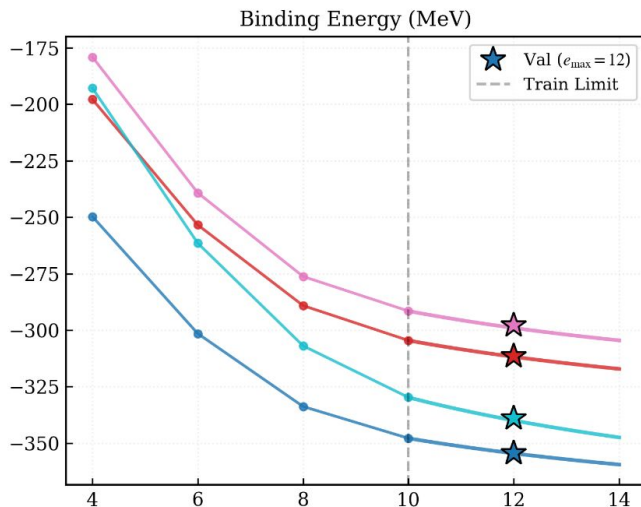
Training cost  
was reduced by  
a factor of 5!



$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^J \xi(f; N, Z, \alpha) \Delta M_p]$$

Anchor: Matrix at the lowest fidelity

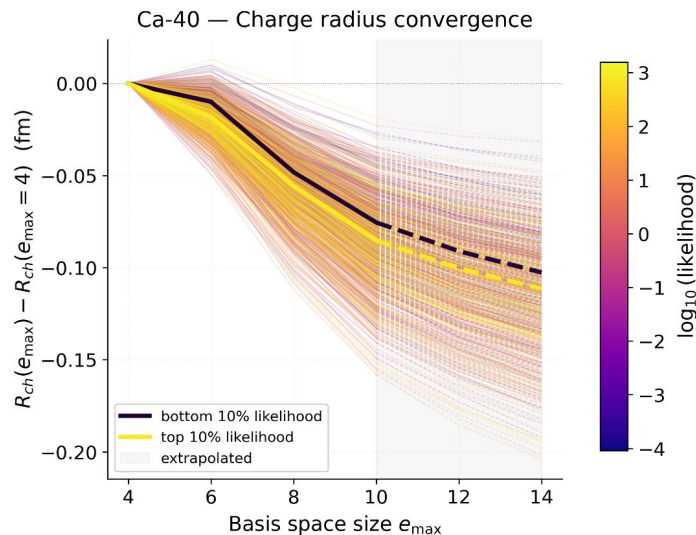
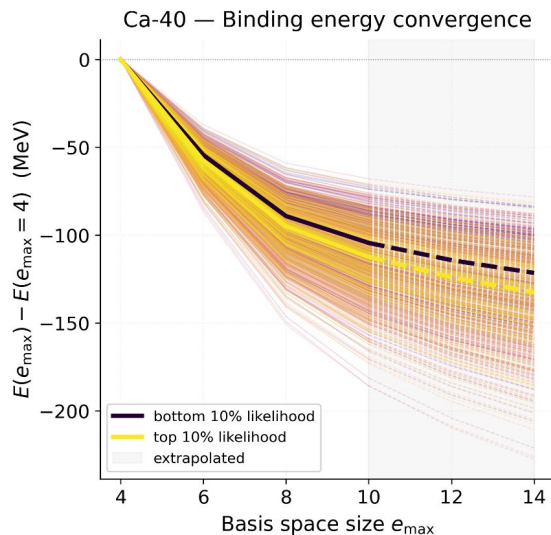
Refinement: Corrections from higher fidelities

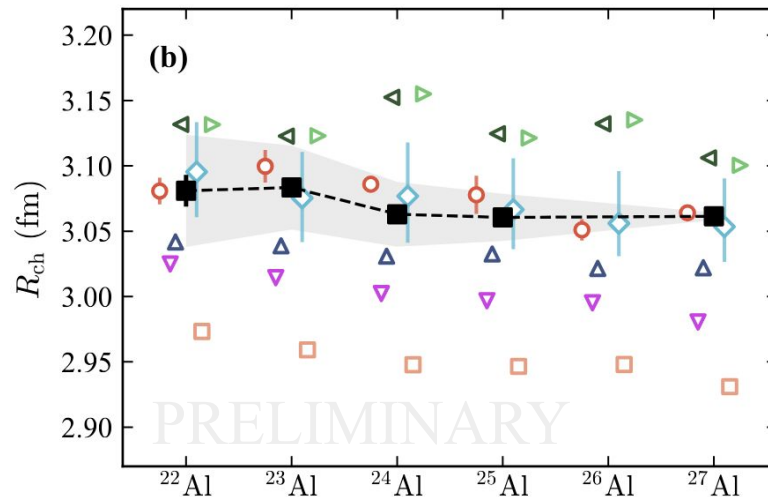
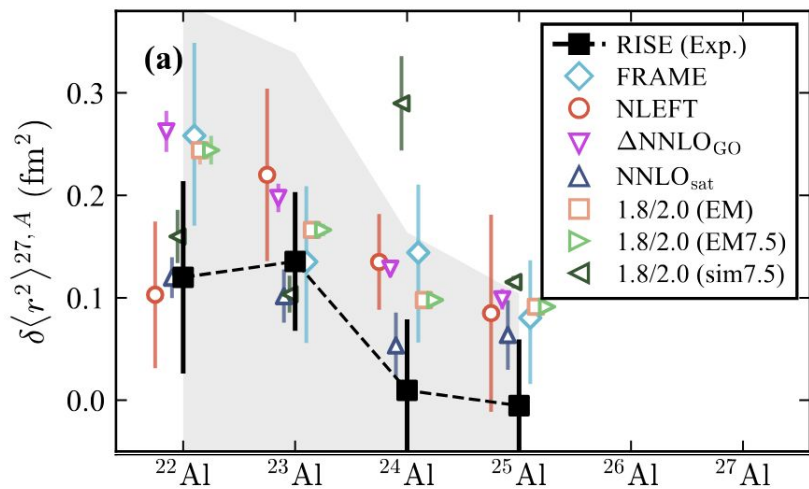


$$M(N, Z, f, \alpha) = [M_{f_{min}} + \sum_{p=1}^J \xi(f; N, Z, \alpha) \Delta M_p]$$

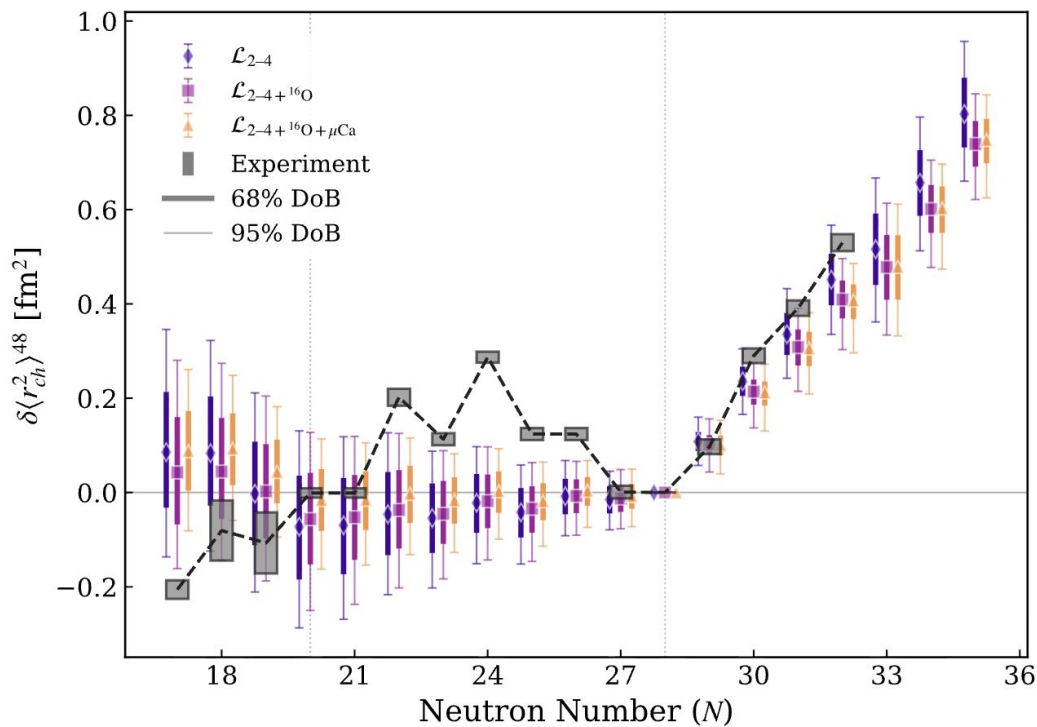
Anchor: Matrix at the lowest fidelity

Refinement: Corrections from higher fidelities

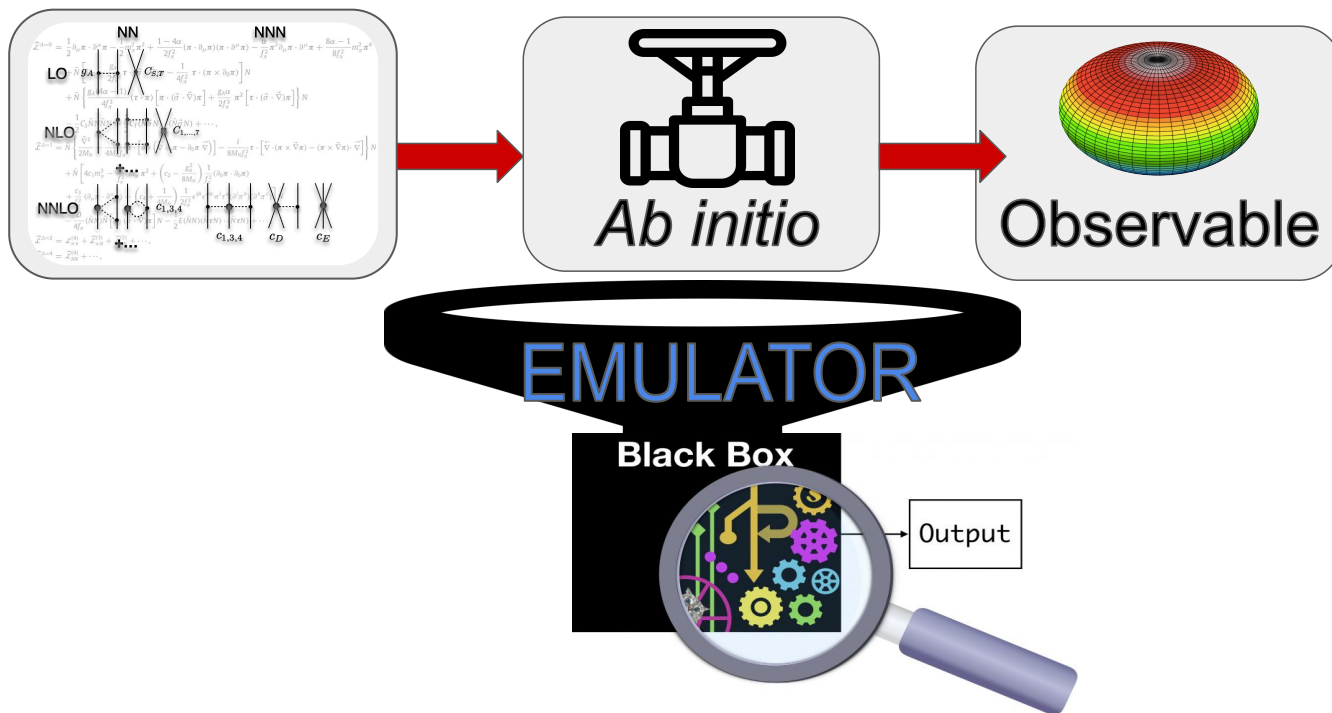


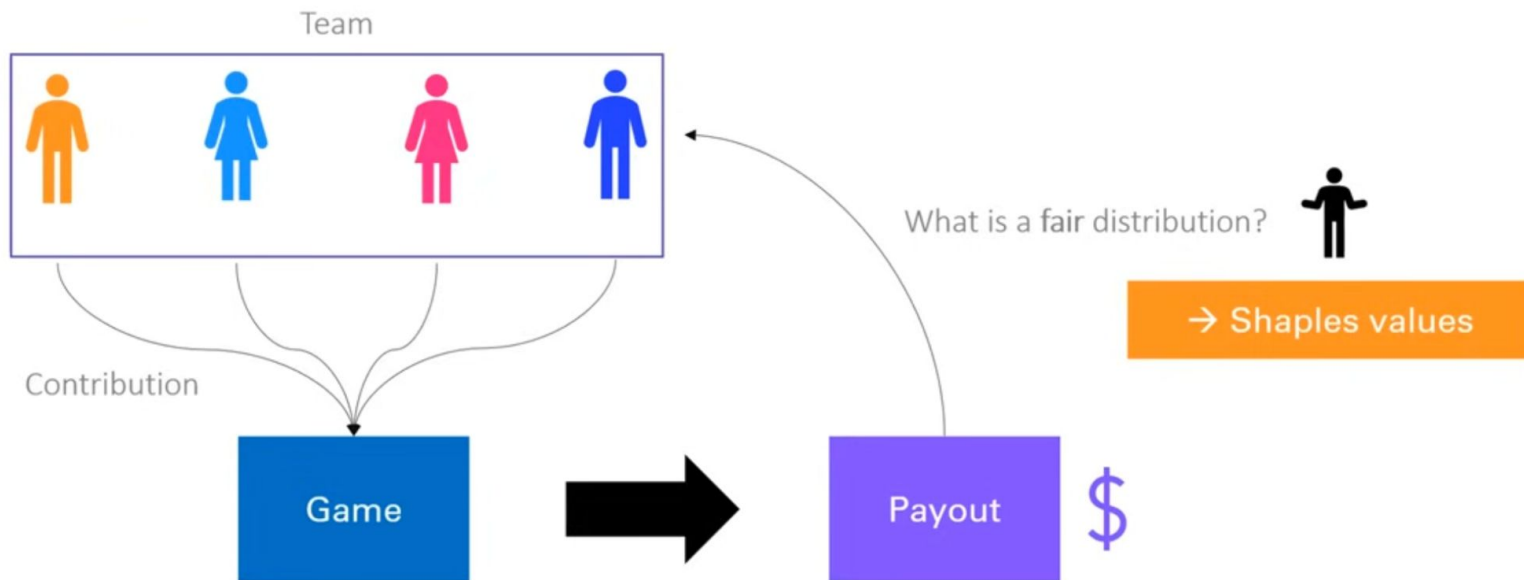


# A physics first approach!

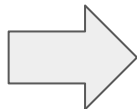
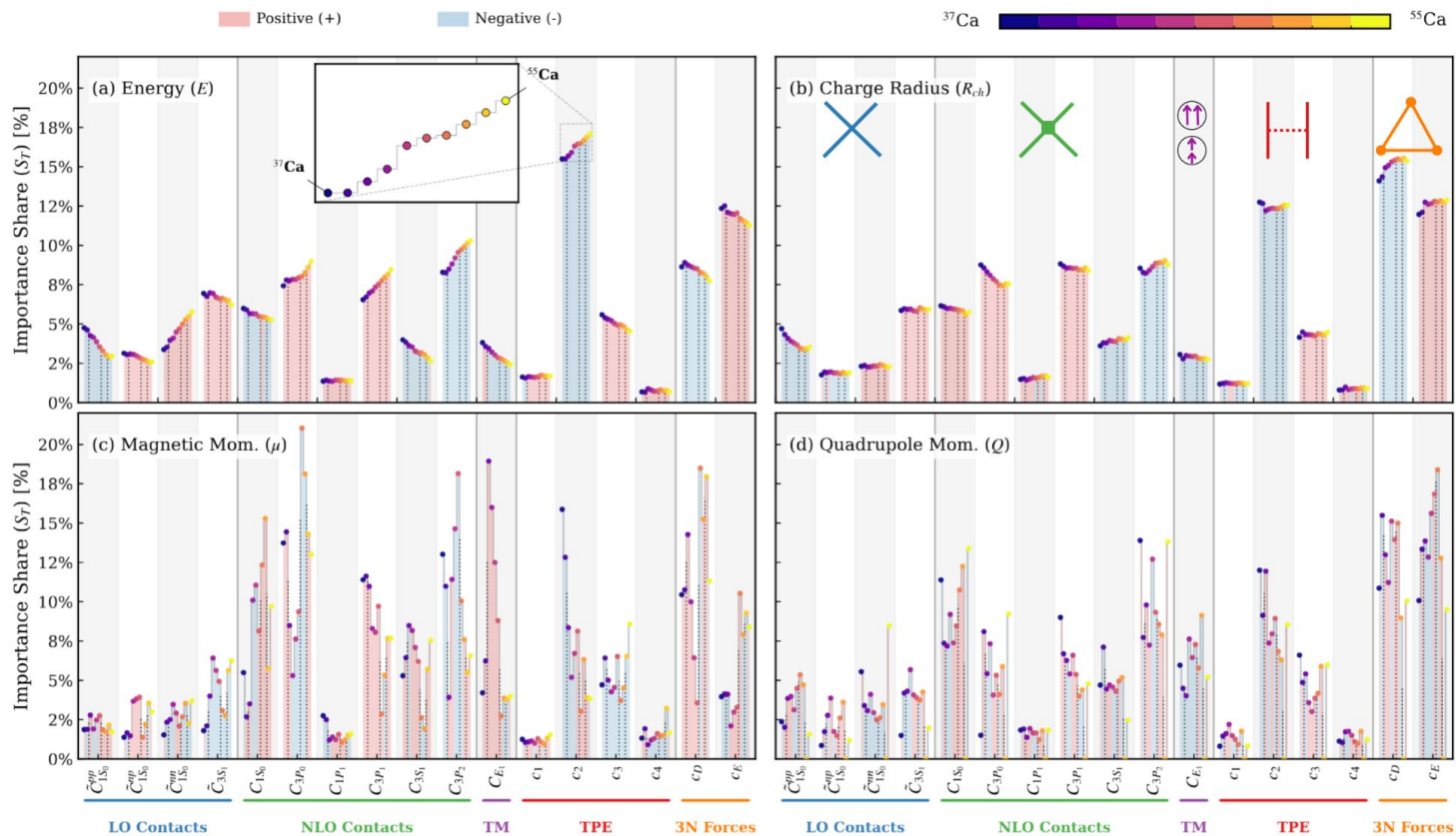


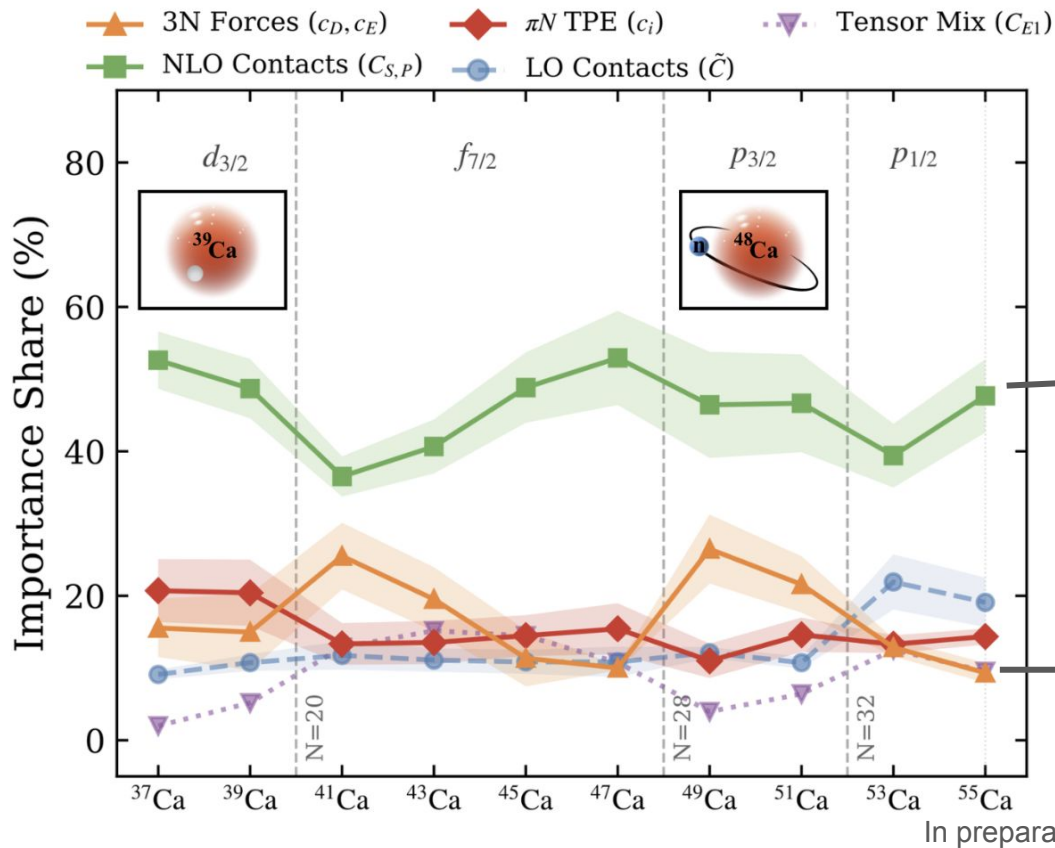
# A physics first approach!



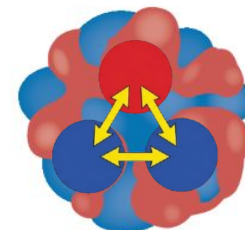
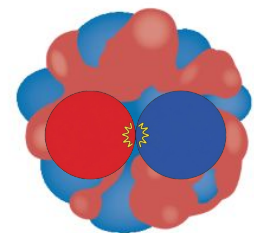


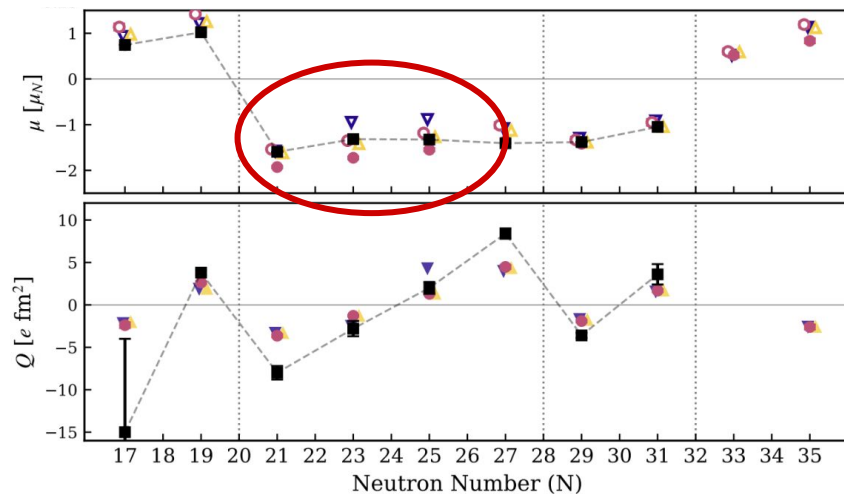
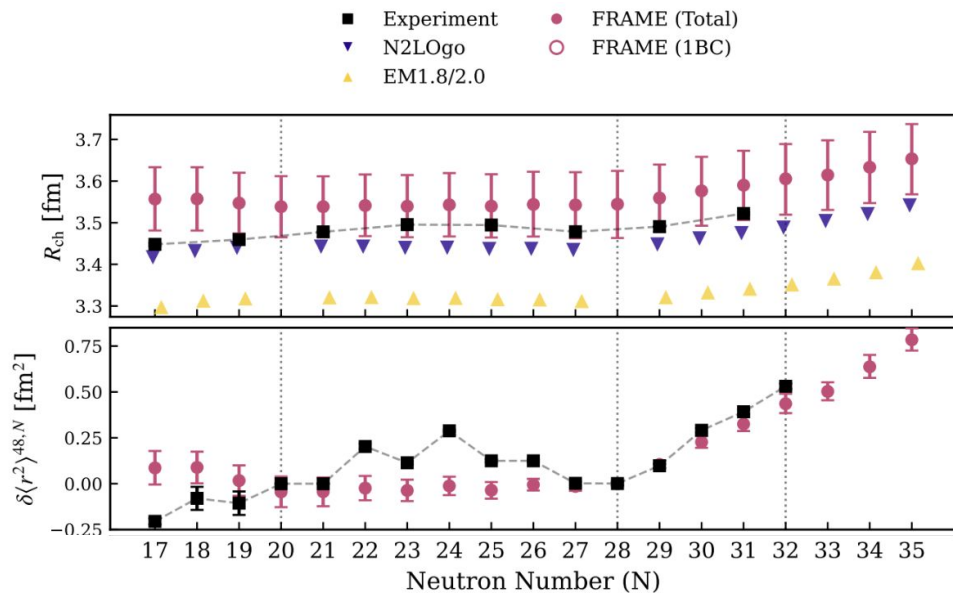
# Understanding importances

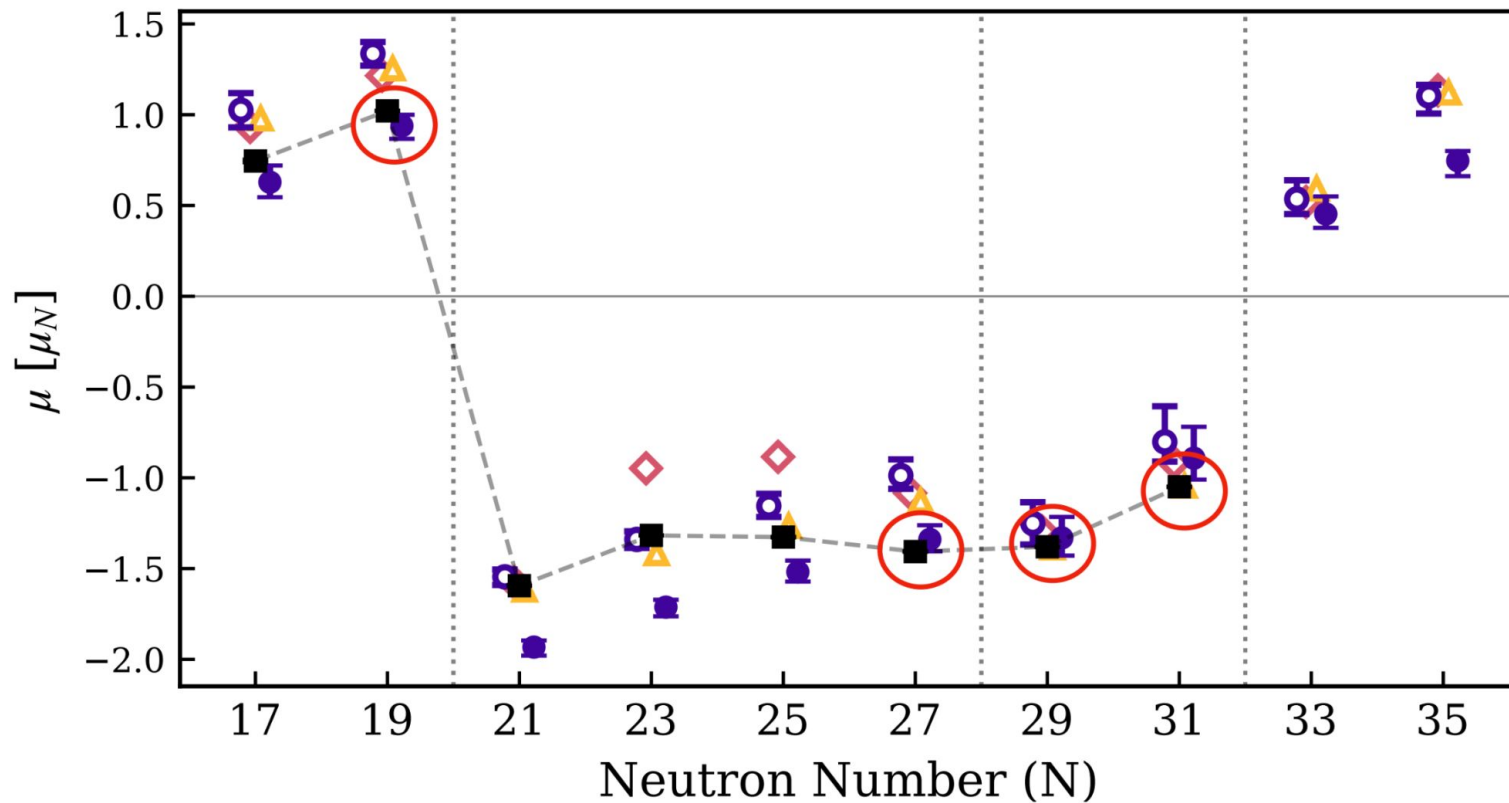




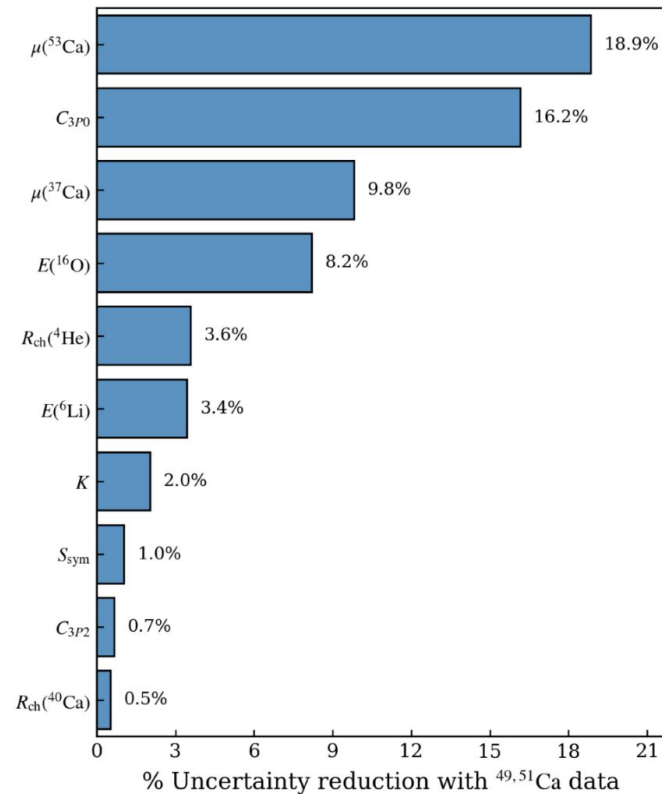
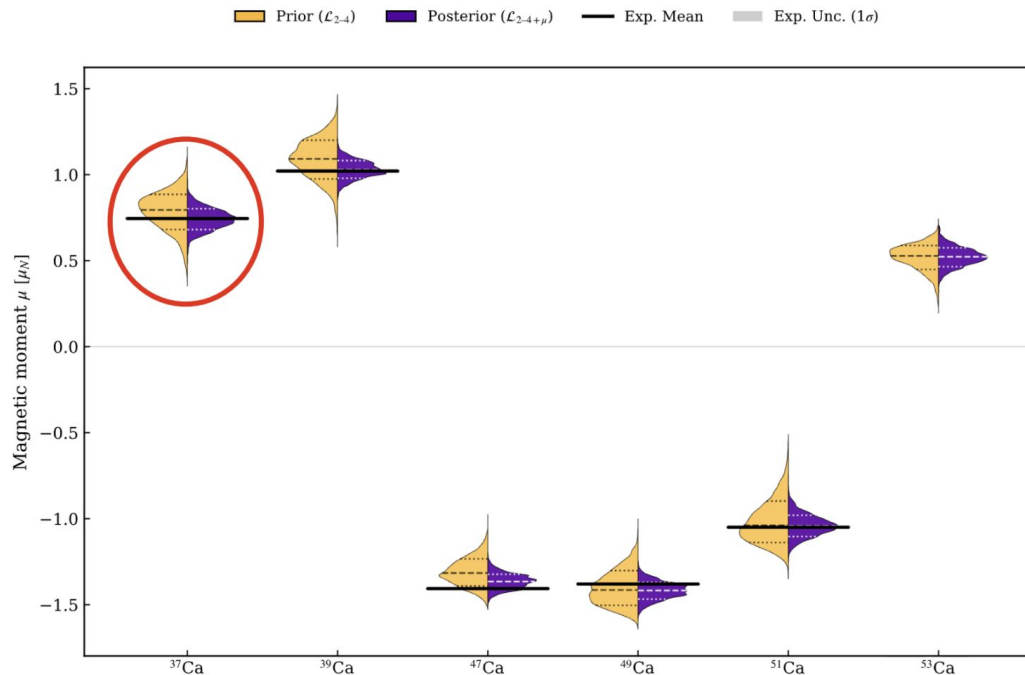
Now it's possible to 'connect' elements of the nuclear force with physical observables!



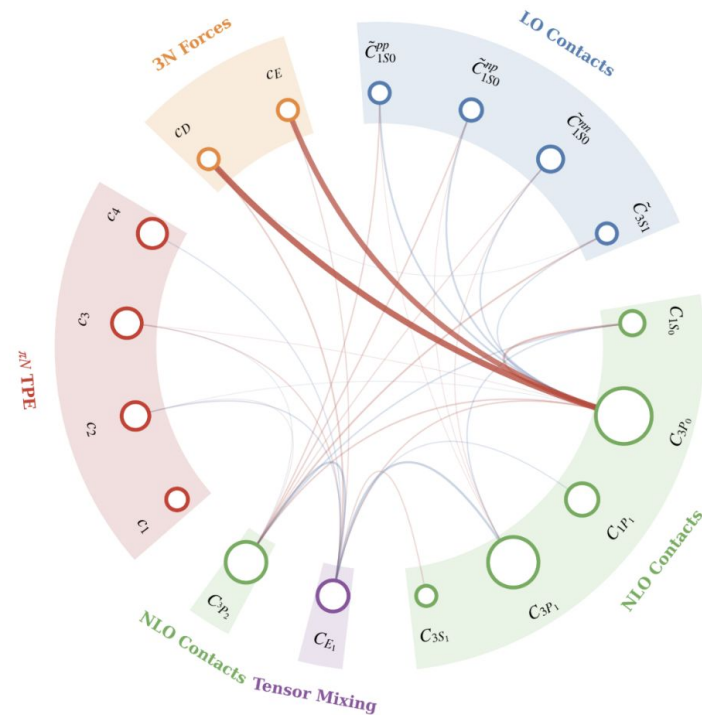
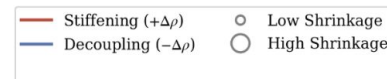
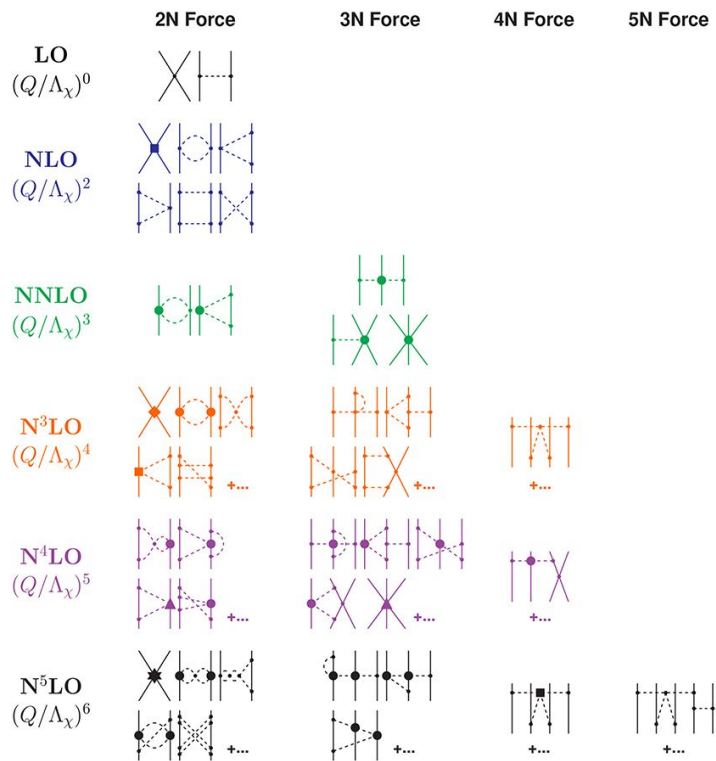




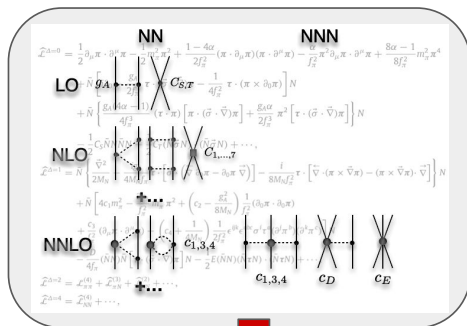
# Updating our likelihood



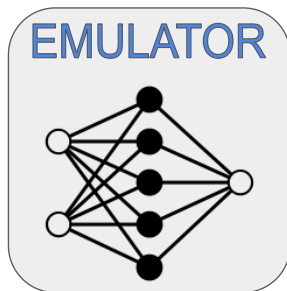
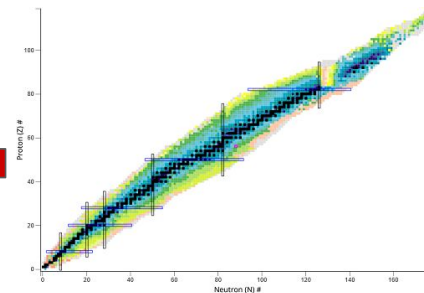
# Updating our knowledge



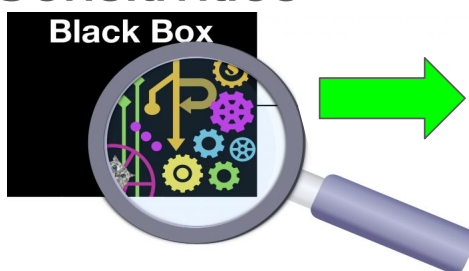
# A bridge between experiment and theory



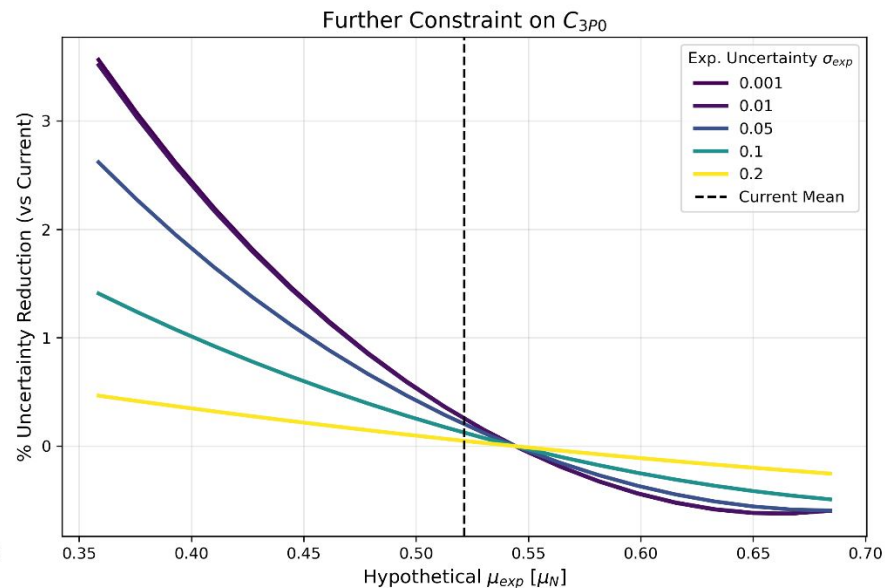
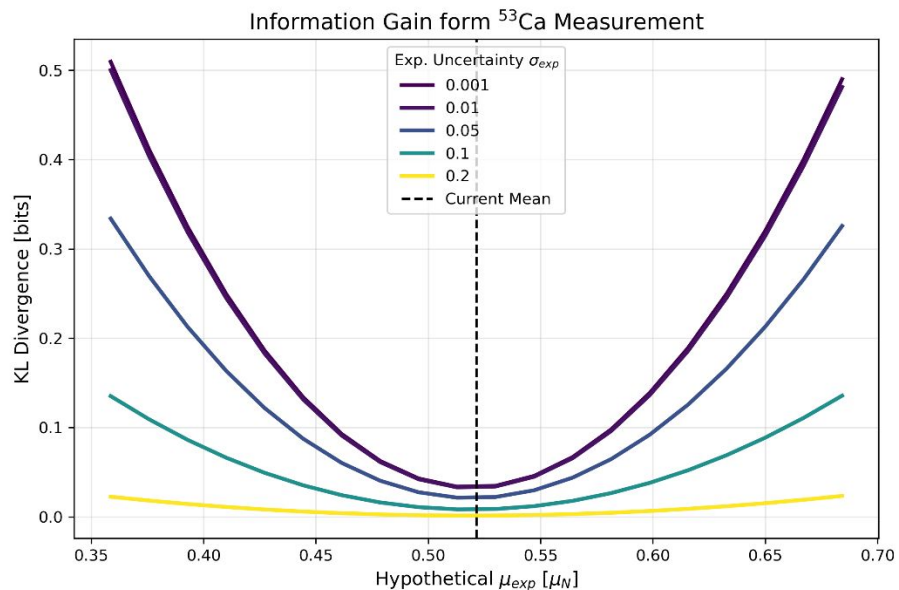
Physics Input



Sensitivities

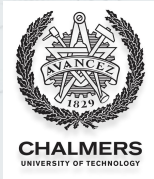


## Blind Simulation: Impact of a Future $^{53}\text{Ca}$ Measurement



- Proper treatment of uncertainties is necessary to assess model quality, and make proper inference of failure modes.
- Rigorous correlation across sources of uncertainty
- Emulators as a tool! (never a replacement).
- Can we emulate your lattice?

# Acknowledgements



**Andreas Ekström**



**Gaute Hagen**



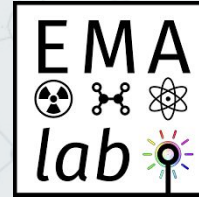
**Jason Holt**

# Acknowledgements

Prof.  
Ronald García



Antoine  
Belley



G. Mondel



A. Brinson



H. Kakiota



S. Moroch



F. Pastrana



D. Gonzales



J.  
Hacias



M Fulghieri



F. Shungo



A. Jadbabaie

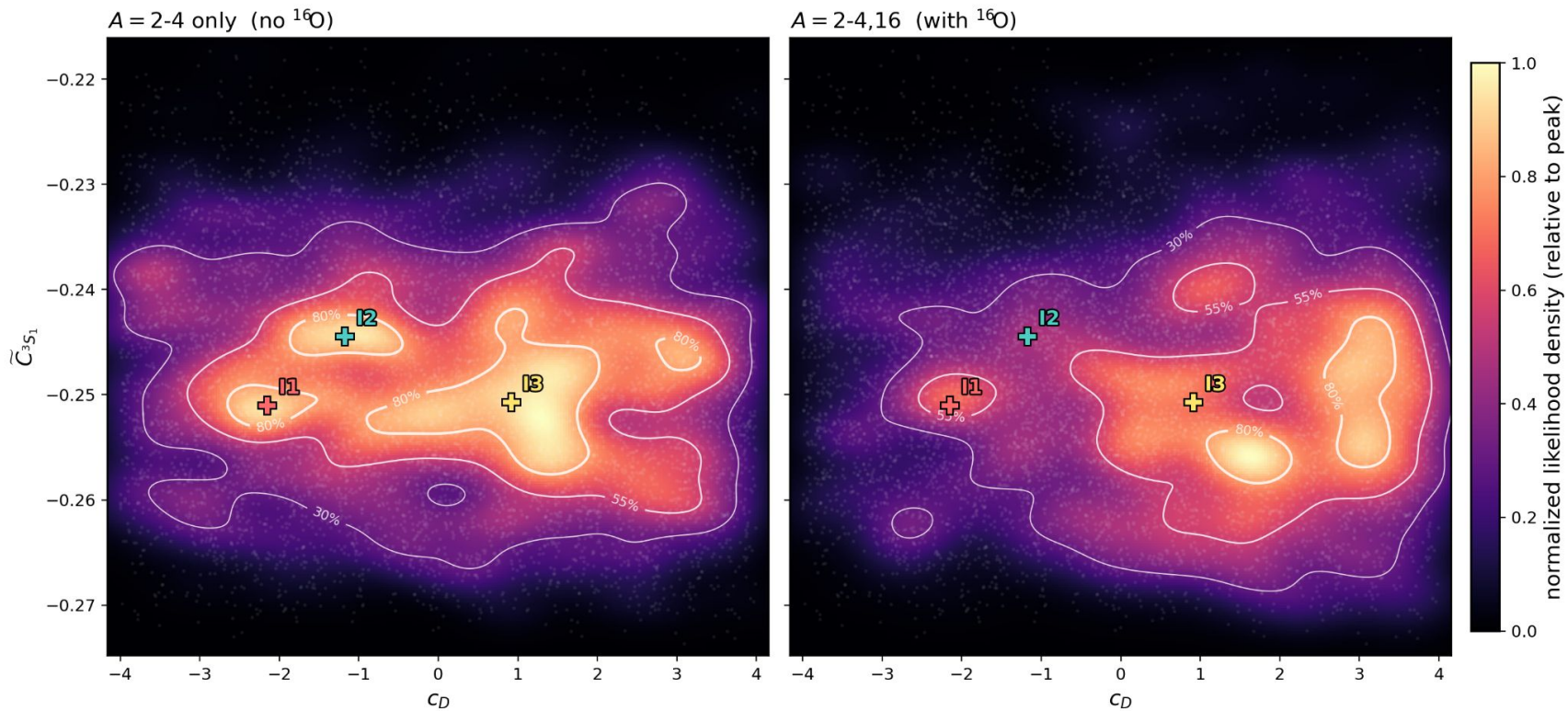


C. Konig

**Thanks!**

# Backup

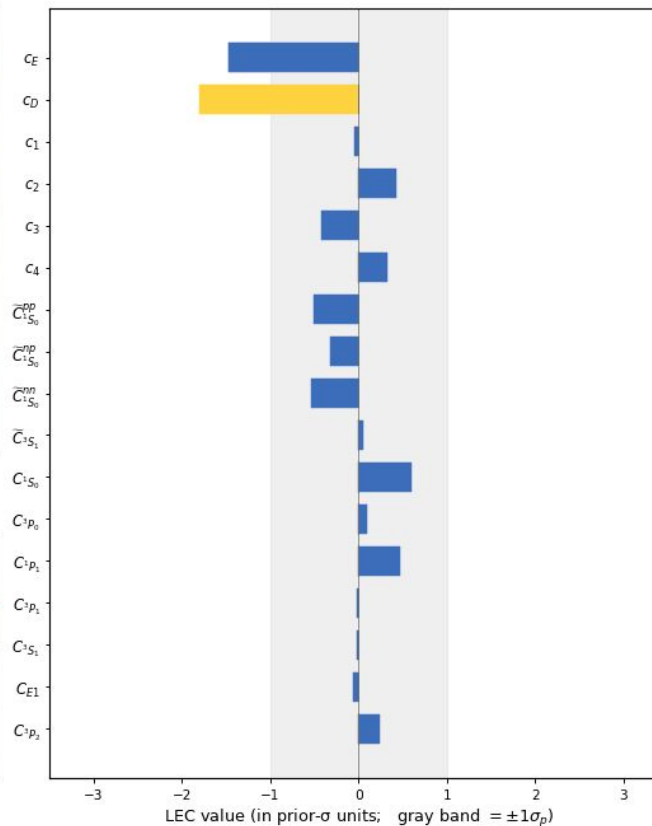
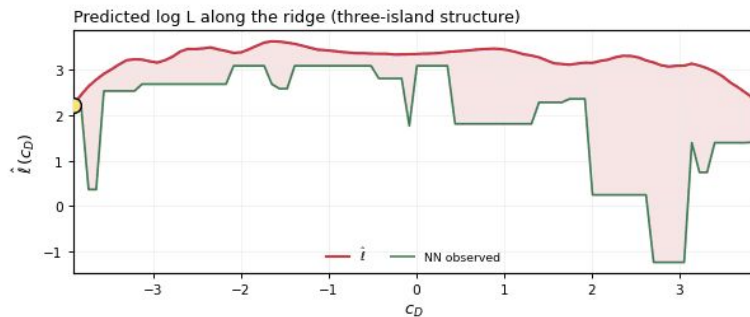
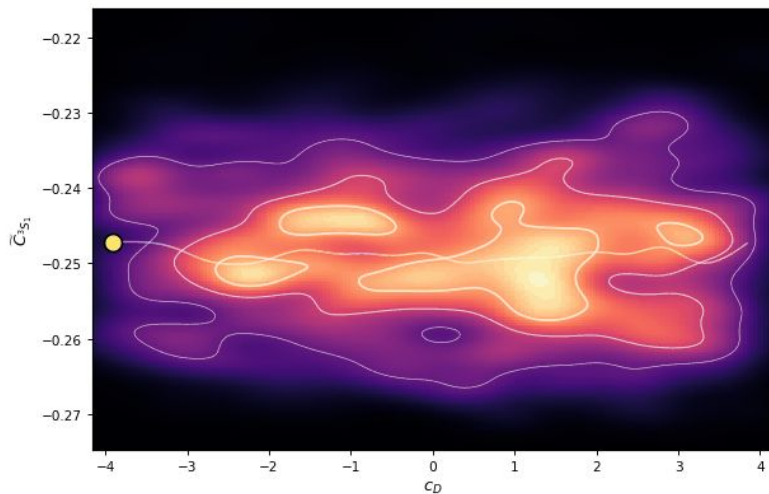
# Phase shifts



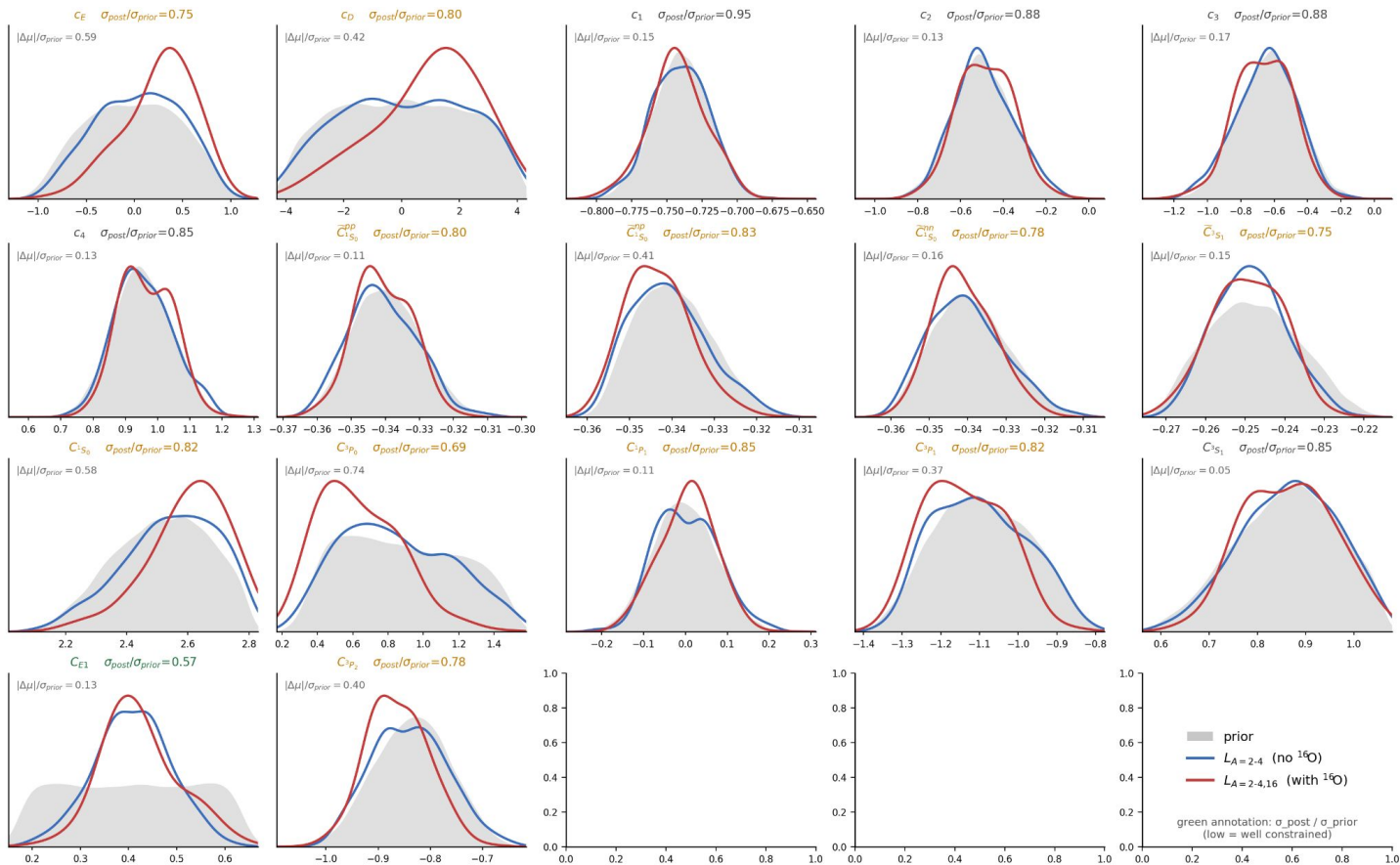
# Phase shifts



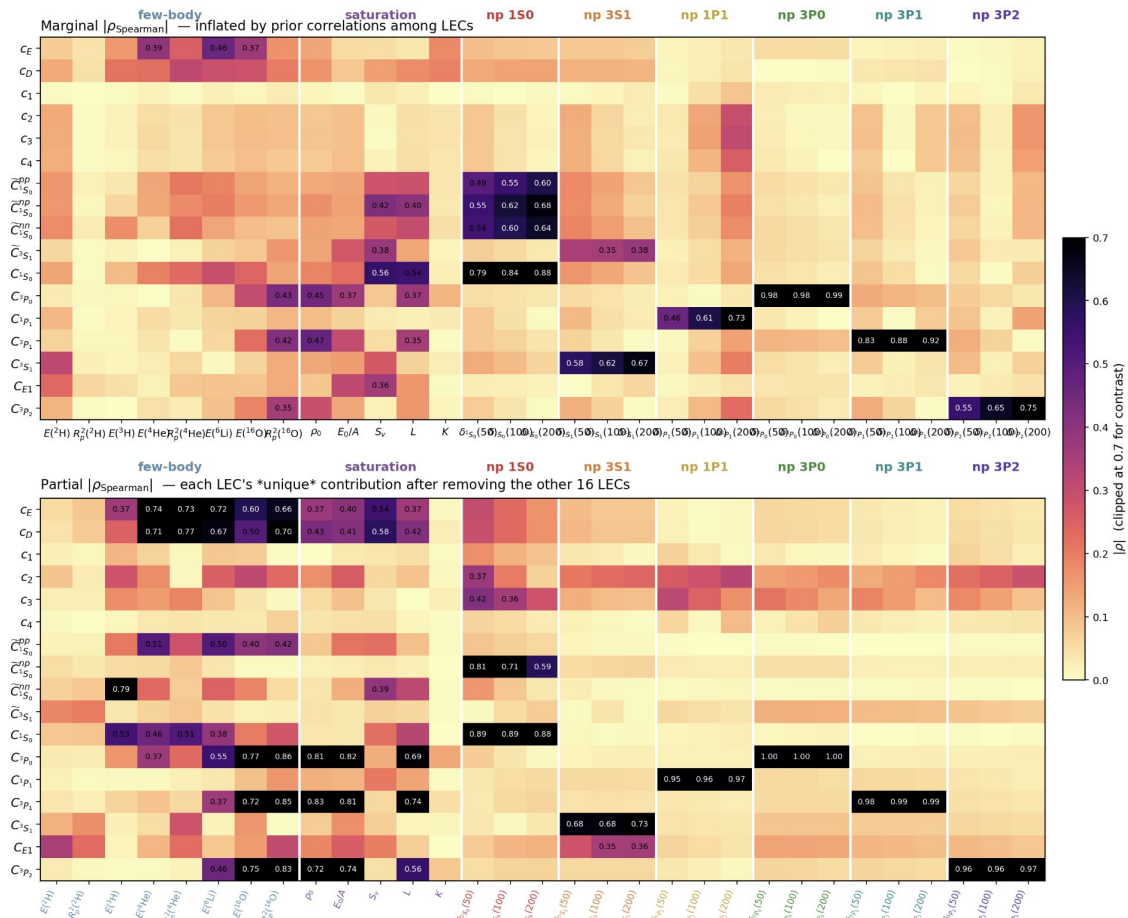
$c_D = -3.91$     $\hat{l}(c_D) = +2.23$    (other 16 LECs adjust)



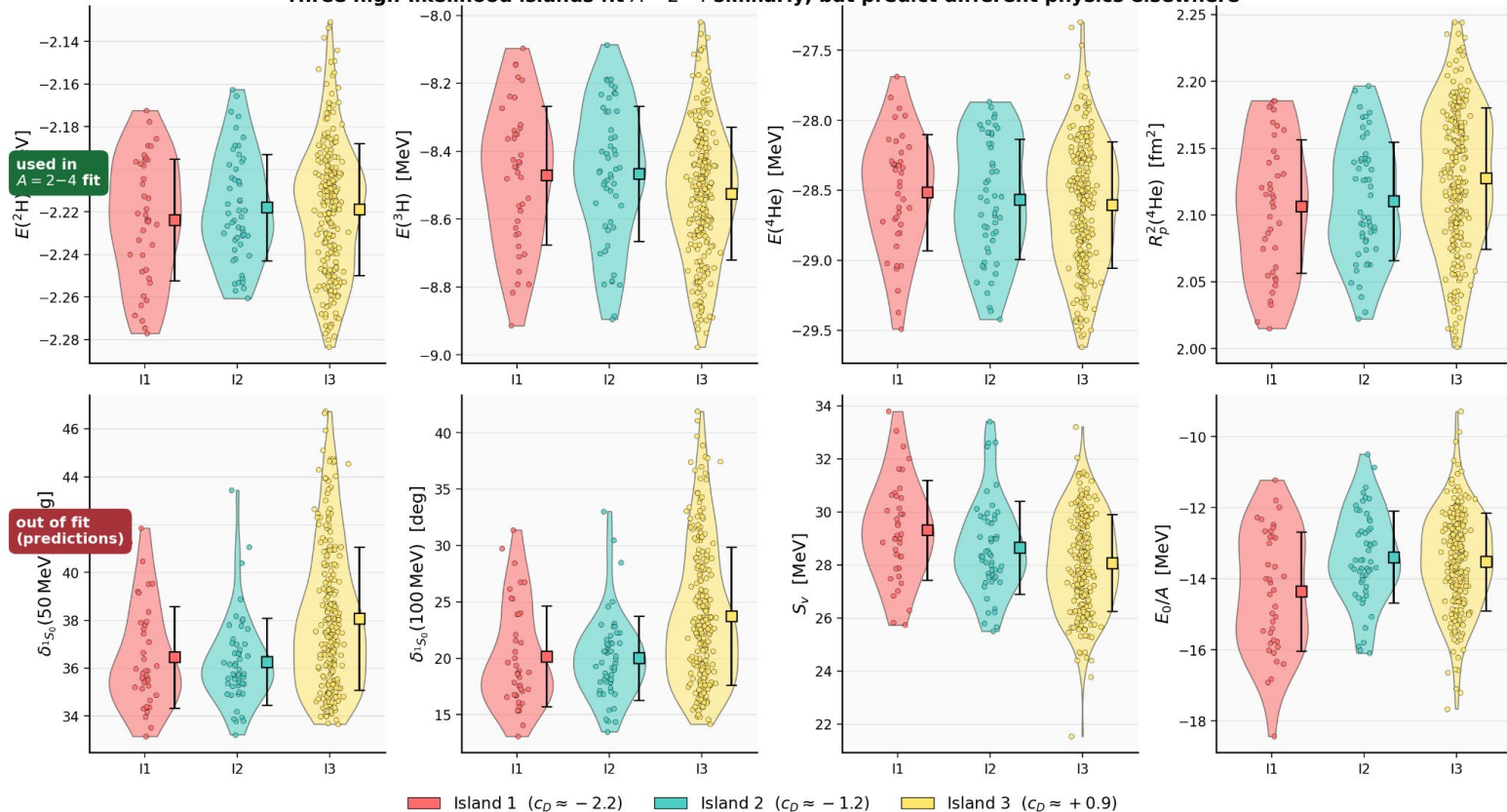
# Phase shifts



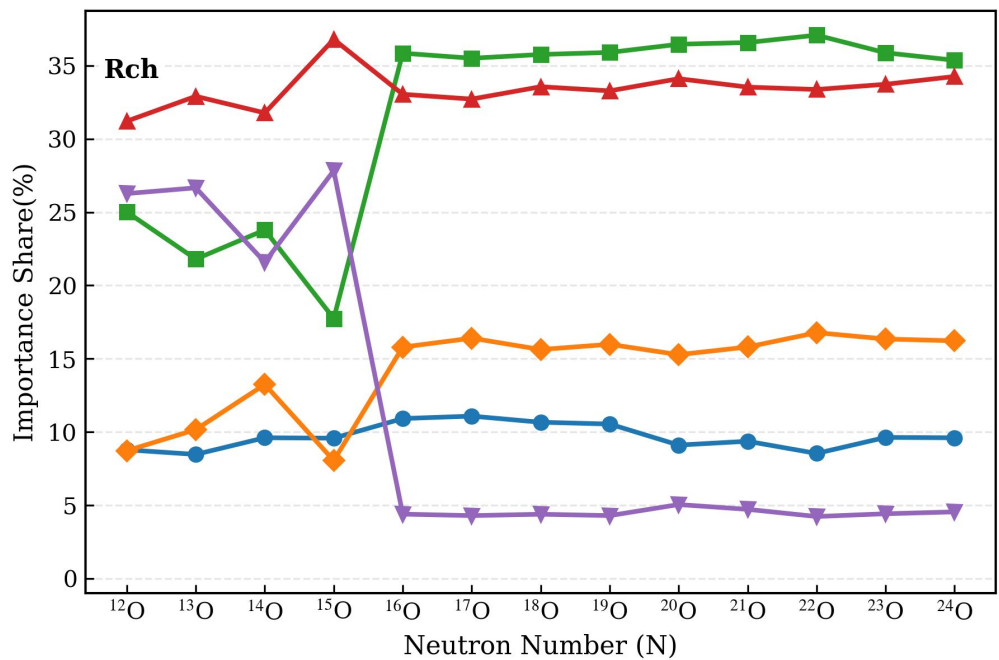
# Phase shifts



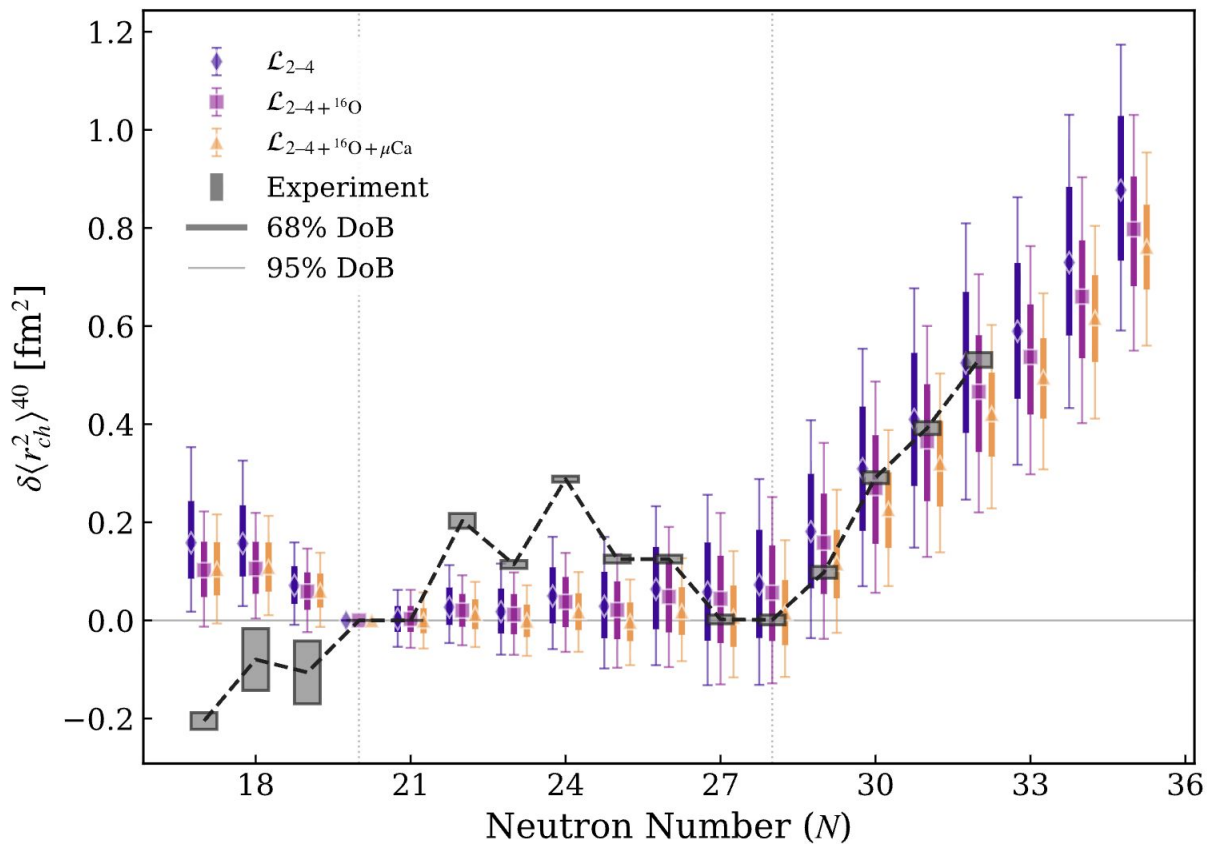
Three high-likelihood islands fit  $A = 2-4$  similarly, but predict different physics elsewhere

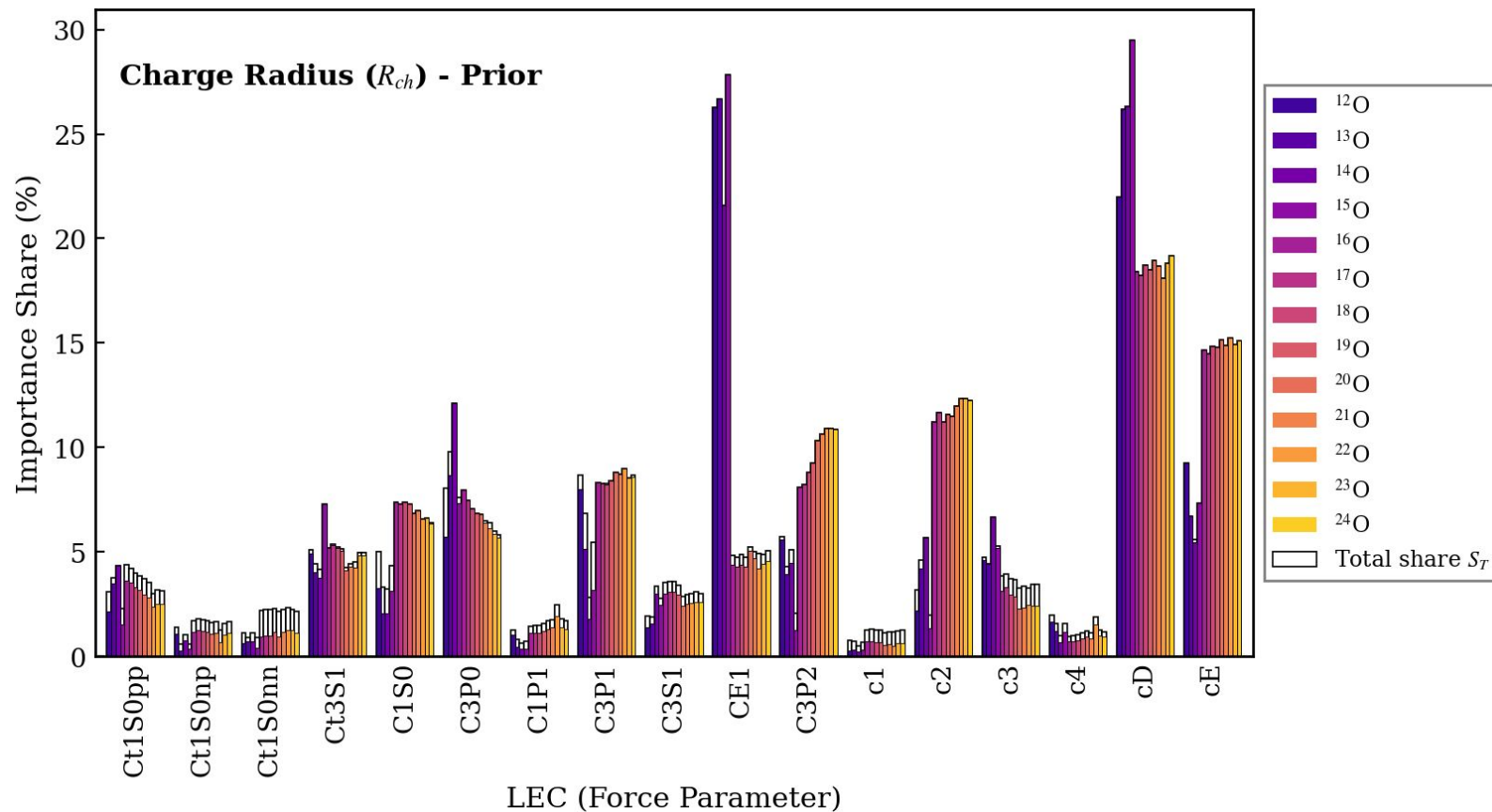


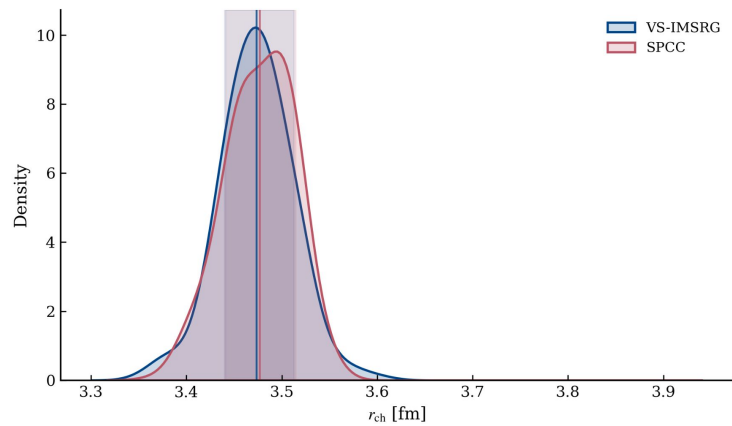
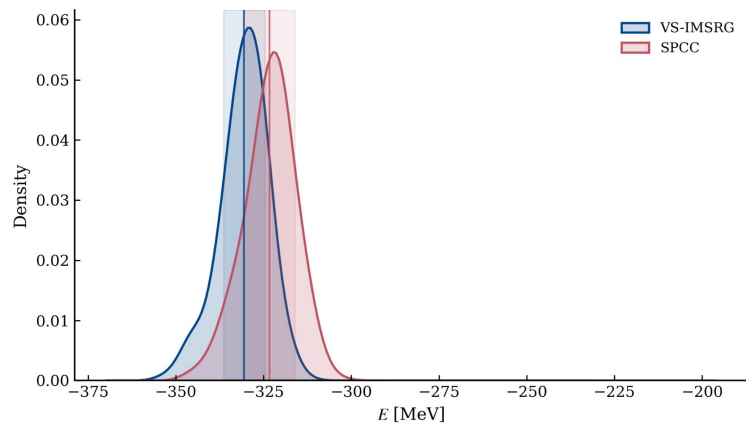
- LO Contacts ( $\tilde{C}$ )
- N2LO Contacts ( $C_{S,P}$ )
- ◆  $\pi N$  TPE ( $c_i$ )
- ▲ 3N Forces ( $c_D, c_E$ )
- ▼ Tensor Mixing ( $C_{E1}$ )

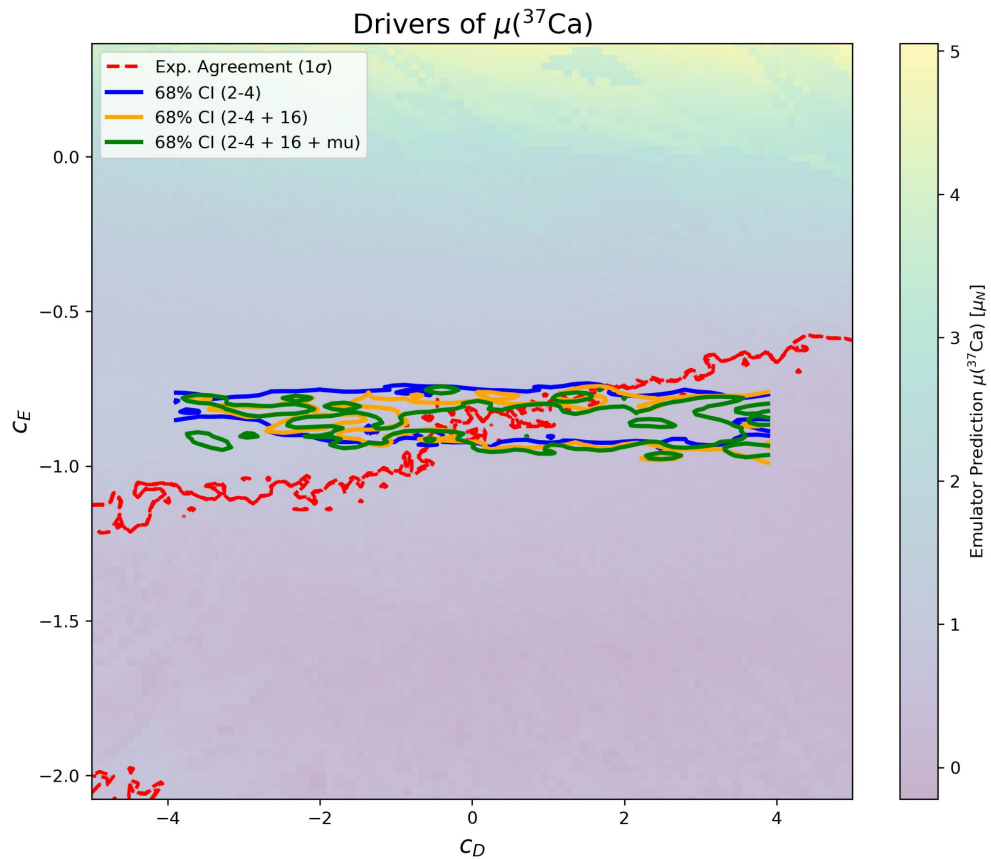












# Distributions

