Bayesian model calibration for nuclear decays with the Skyrme finite-amplitude method

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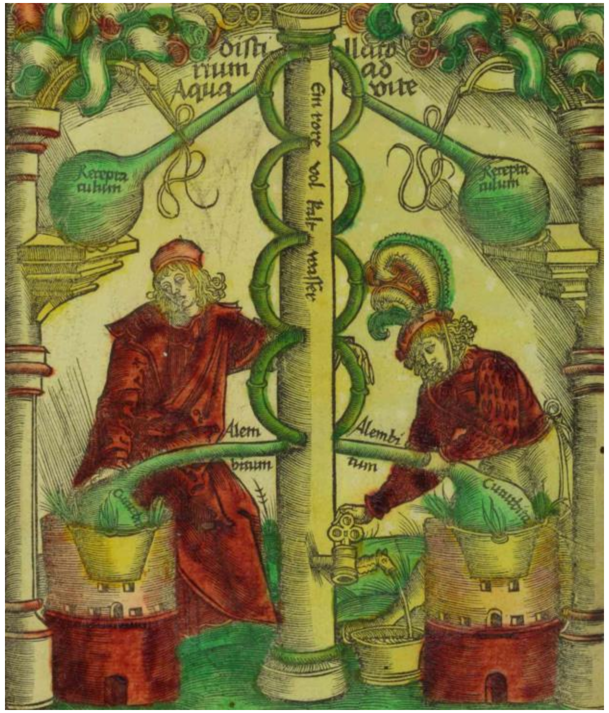
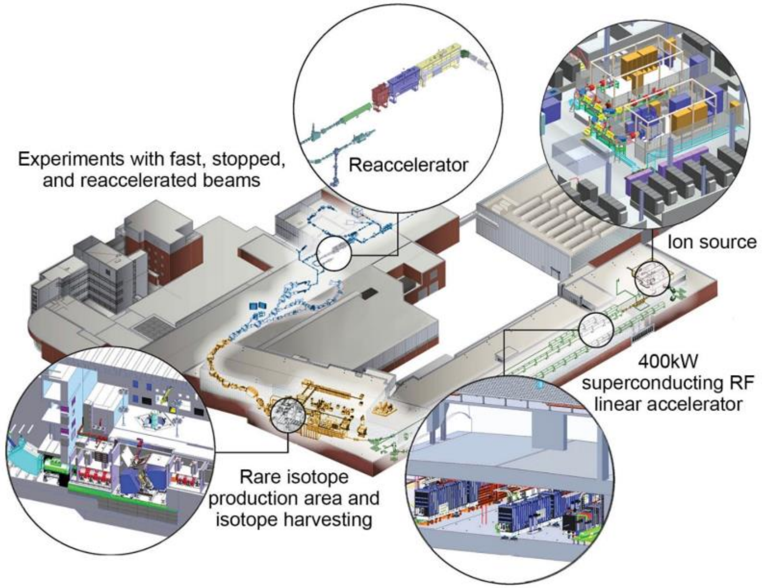
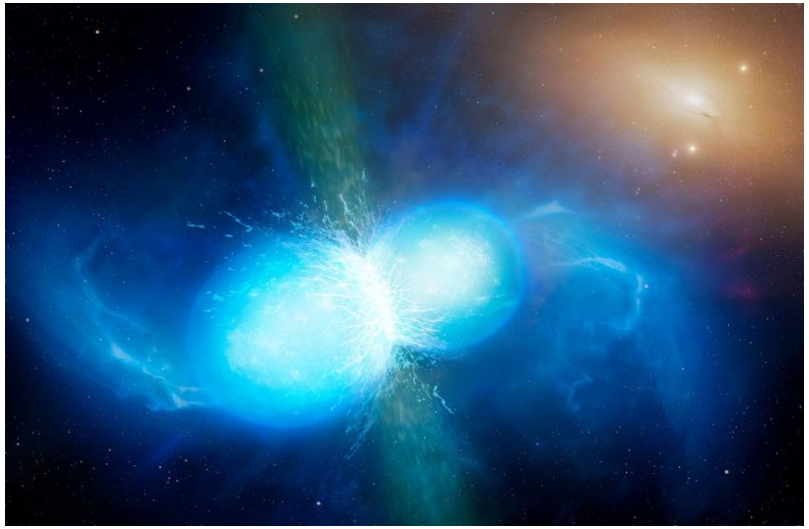
Alchemy on the Earth and in the universe



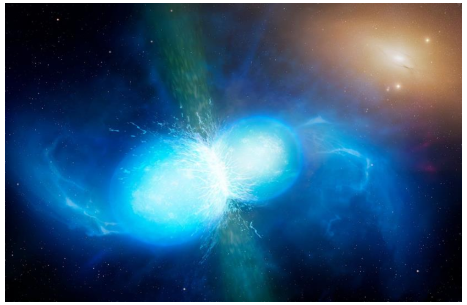




- Medieval alchemists failed to transform one chemical element to another.
- We can now do “modern alchemy” in facilities for nuclear physics!
- Large-scale producers of heavy elements exist in the universe, such as the neutron-star merger.

Rapid neutron-capture process and nuclear inputs for simulation

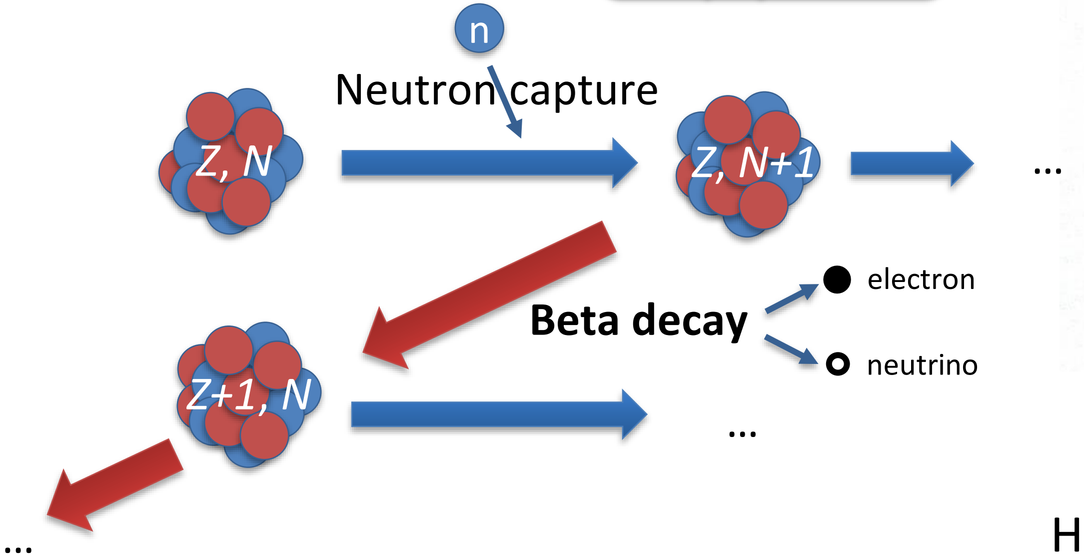
- The rapid neutron-capture process (*r* process) plays a key role in the synthesis of heavy nuclei.

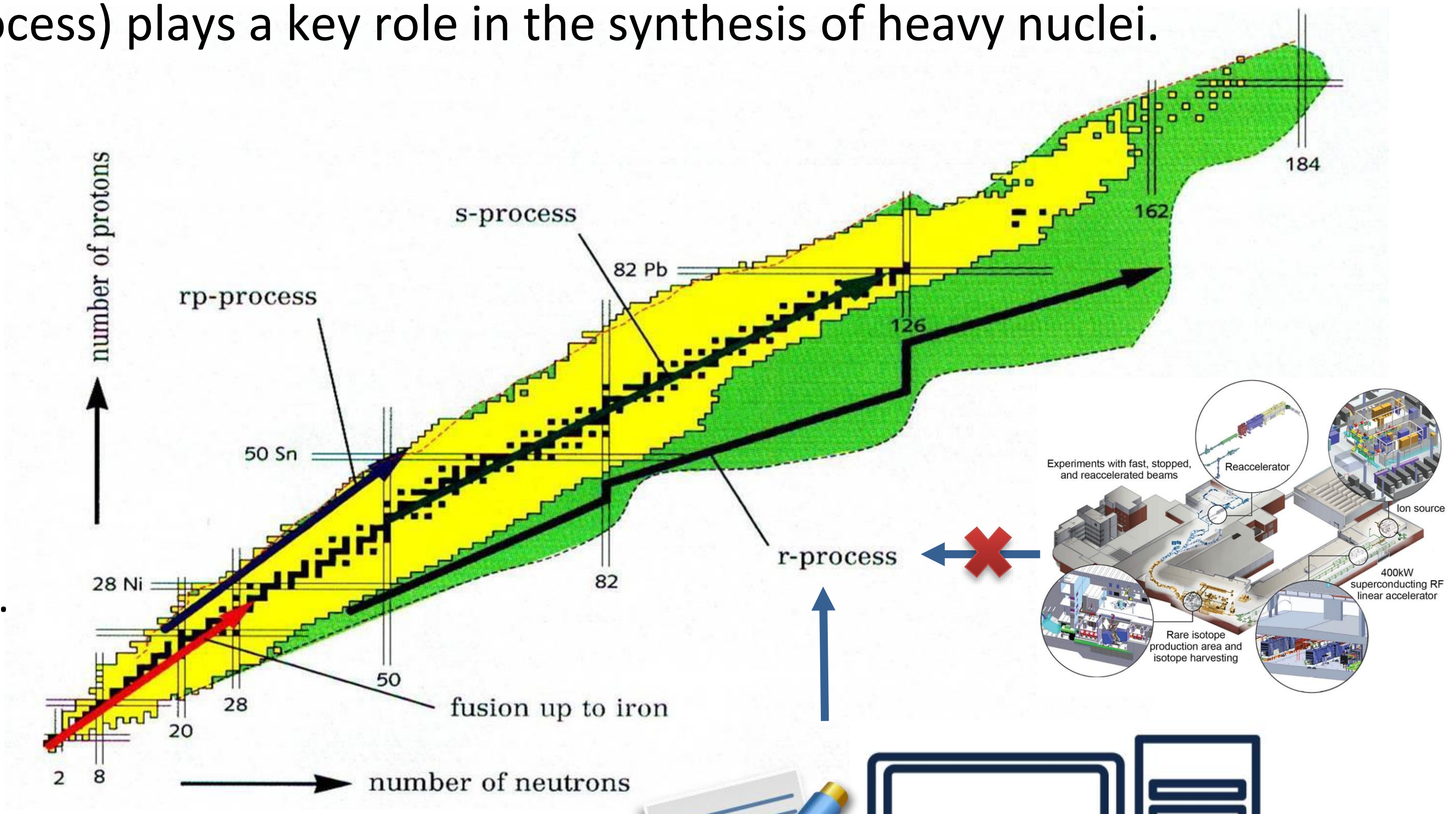


Astrophysical environment

+

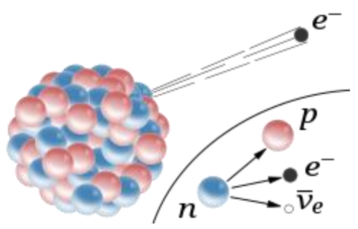
Nuclear physics



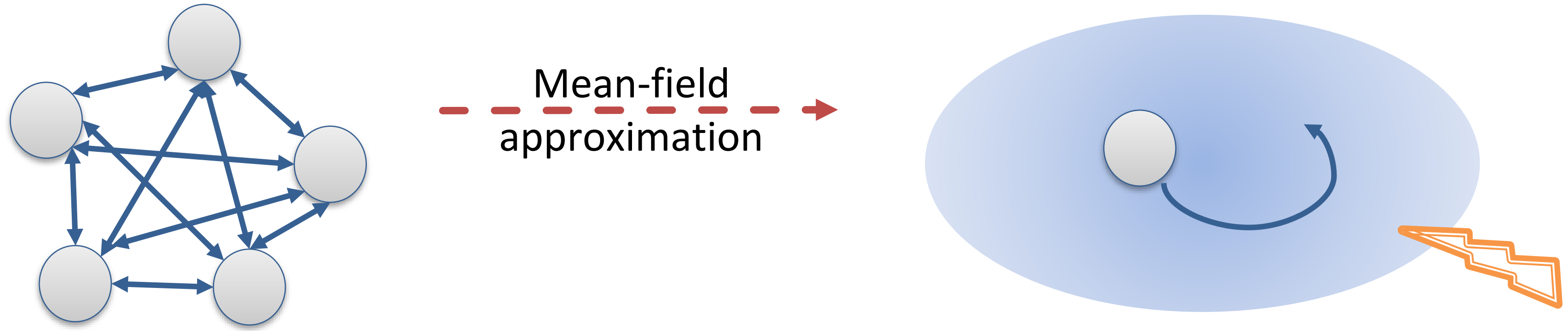


How uncertain is our model?

Finite amplitude method enables large-scale studies



- New algorithms in the framework of nuclear density functional theory make it feasible to perform self-consistent microscopic calculations of beta decays through the nuclear landscape.



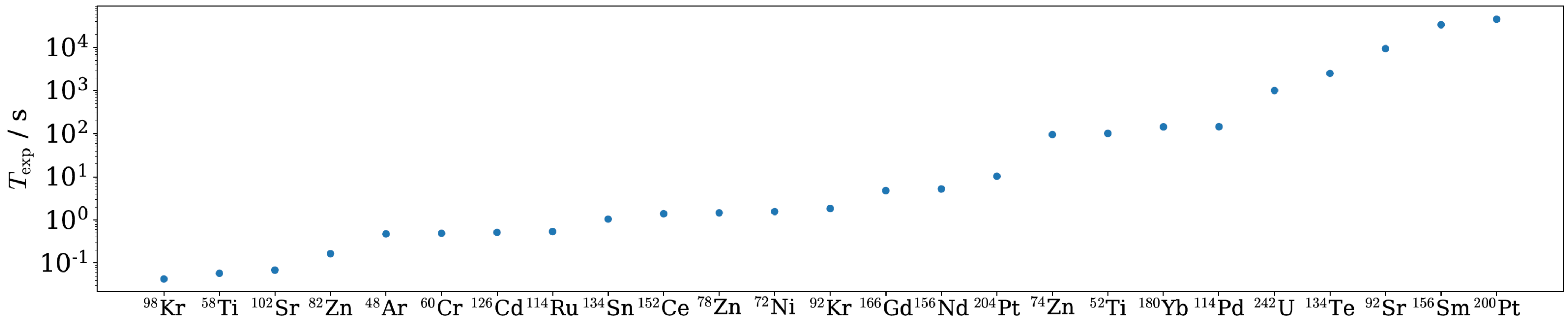
- Each nucleon moves in the **mean field** generated by other nucleons.
  The mean field is specified by the Skyrme energy density functional (EDF).
- The ground state is described by the Hartree-Fock-Bogoliubov (HFB) approach.
- The beta-decay transition is calculated through the finite-amplitude method (FAM), where an external charge-changing field is applied as perturbation to trigger the transition.

- Some EDF parameters need to be constrained by experimental data on the beta decay.

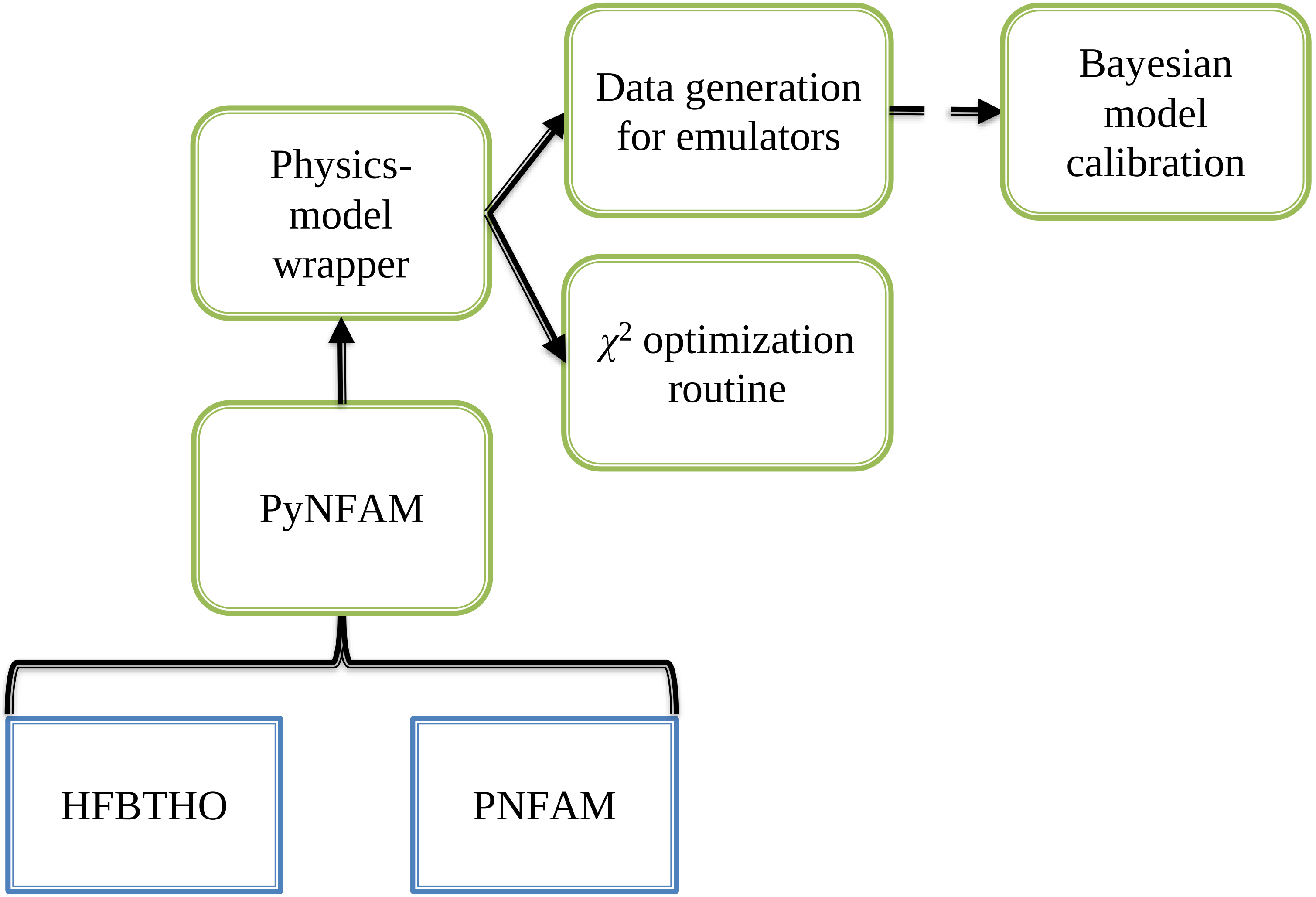
Parameters to calibrate and fit targets

- Skyrme parameterization UNDEF1-HFB is employed.
- Parameters to calibrate include:
  - Landau-Migdal parameter g_0',
  - Normalized isoscalar pairing strength v_0,
  - Axial-vector coupling g_A (quenching effect).

- Fit targets include two types of data:
  - Gamow-Teller-resonance energies of 4 selected doubly and semi-magic systems,
  - β^--decay half lives of 25 even-even nuclei.
- The data selection is based on Phys. Rev. C **93**, 014304 (2016).



Numerical Framework



χ^2 optimization is the first step for model calibration

- We minimize the weighted sum of squared errors (residuals) with POUNDERS:

$$\chi^2(\boldsymbol{x}) = \frac{1}{n_d - n_x} \sum_{i=1}^{n_d} \left(\frac{s_i(\boldsymbol{x}) - d_i}{w_i} \right)^2 .$$

- Parameter values obtained from the χ^2 optimization are shown in the table below. These parameters are weakly correlated.

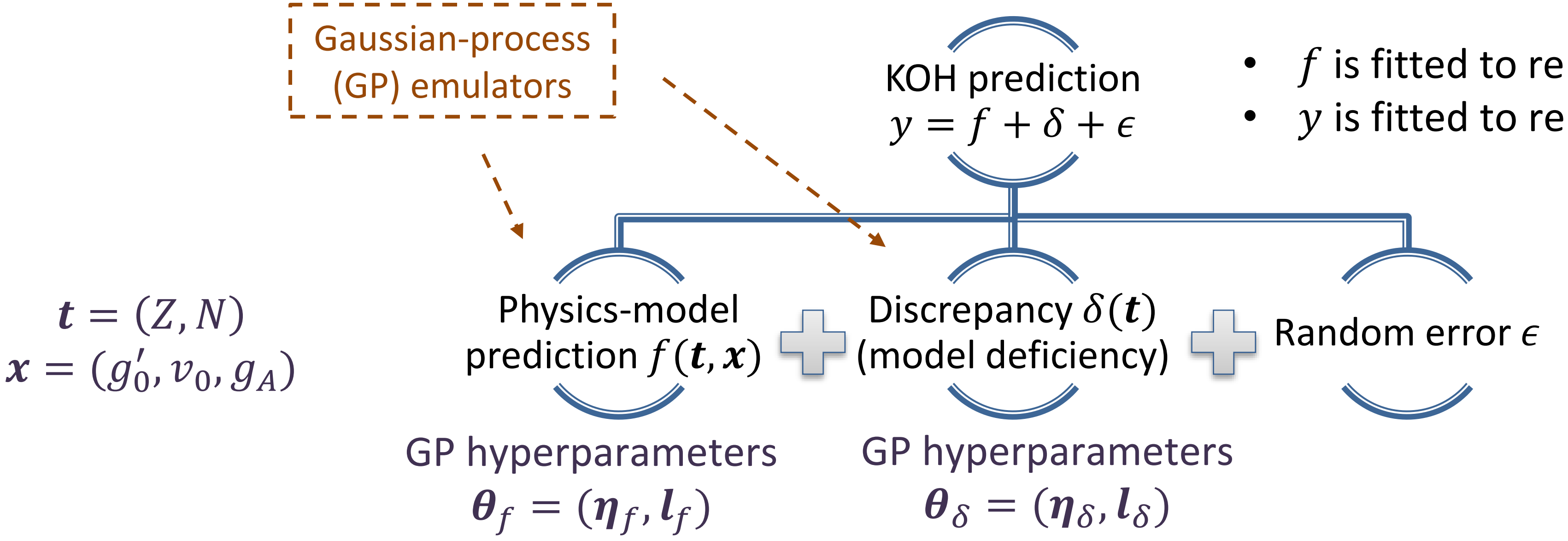
Fit	g_0'	g_1'	v_0	g_A
A	1.59560 (0.039)	0 (fixed)	−0.99993 (0.178)	1 (fixed)
B	1.59184 (0.034)	0 (fixed)	−1.19745 (0.179)	0.50345 (0.143)

Bayesian model calibration with model deficiency

- Compared with the χ^2 optimization, Bayesian inference provides a reliable approach to obtain the distributions of parameter values, which is useful for uncertainty quantification and propagation.
- The foundation of the Bayesian model calibration is Bayes' theorem:

$$P(\text{ params } \mid \text{ obs }) \propto P(\text{ obs } \mid \text{ params })P(\text{ params }).$$

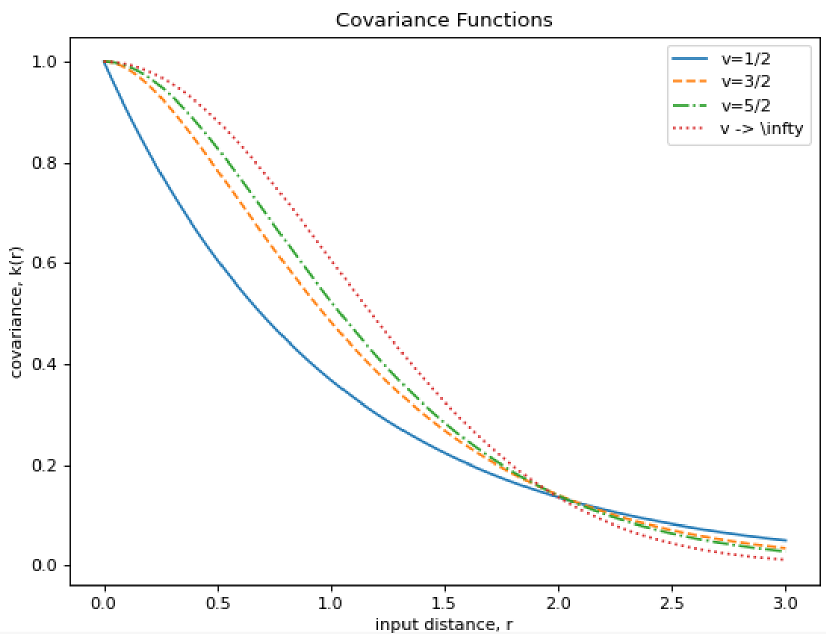
- The likelihood is specified by the Kennedy-O'Hagan (KOH) model.

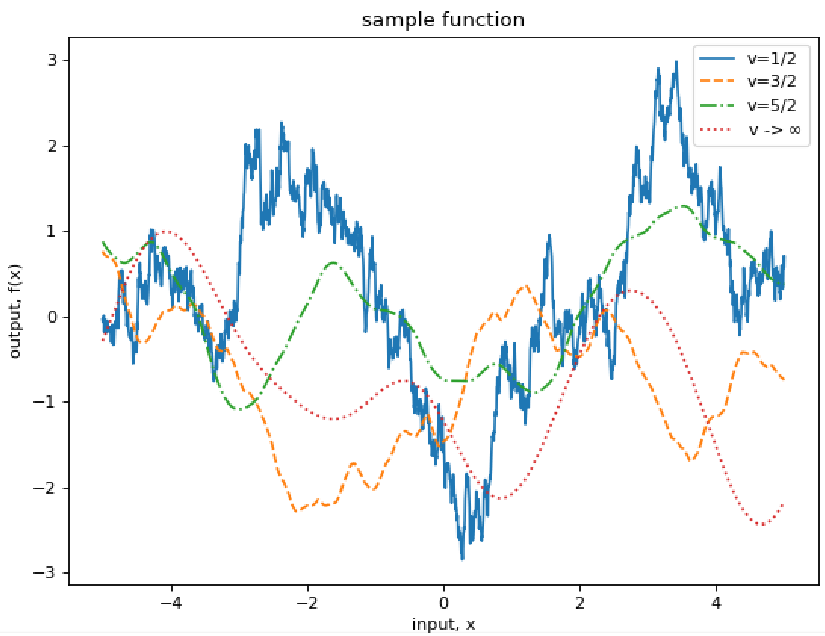


- f is fitted to reproduce physics-model outputs.
- y is fitted to reproduce experimental data.

Unsmooth covariance function is better for GP emulators

- We use the Matérn kernel as the covariance function: $k(\boldsymbol{x}, \boldsymbol{x}') = \eta \frac{2^{1-v}}{\Gamma(v)} \left(\frac{\sqrt{2v}|\boldsymbol{x}-\boldsymbol{x}'|}{l} \right)^{v} K_v \left(\frac{\sqrt{2v}|\boldsymbol{x}-\boldsymbol{x}'|}{l} \right)$, where K_v is the modified Bessel function.
- Compared with the radial basis function, samples generated by the GP with a Matérn covariance function are **not smooth**, making it easier to emulate unsmooth outputs of the physics model.





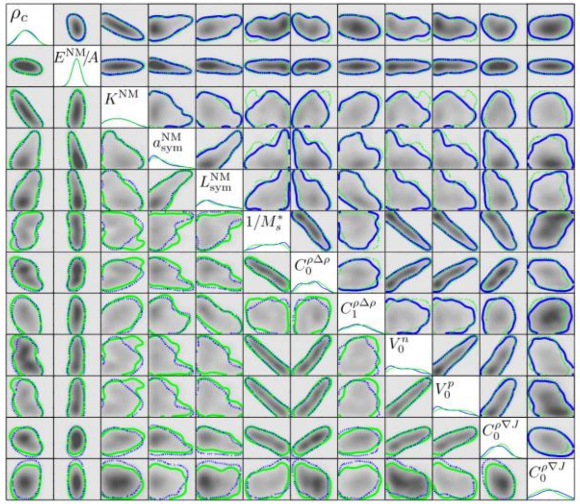
Can the KOH model kill two birds with one stone?

- Fitting the KOH model does not only calibrate parameters $\boldsymbol{x}$ used in the physics model, but also build a statistical model δ that can correct the physics model.

PRL **114,** 122501 (2015) PHYSICAL REVIEW LETTERS week ending 27 MARCH 2015

Uncertainty Quantification for Nuclear Density Functional Theory and Information Content of New Measurements

J. D. McDonnell,[1,2] N. Schunck,[2] D. Higdon,[3] J. Sarich,[4] S. M. Wild,[4] and W. Nazarewicz[5,6,7]



We limit the number of experimental data points to reduce computational cost and avoid overfitting.

The more data points we provide, the better the discrepancy model performs.

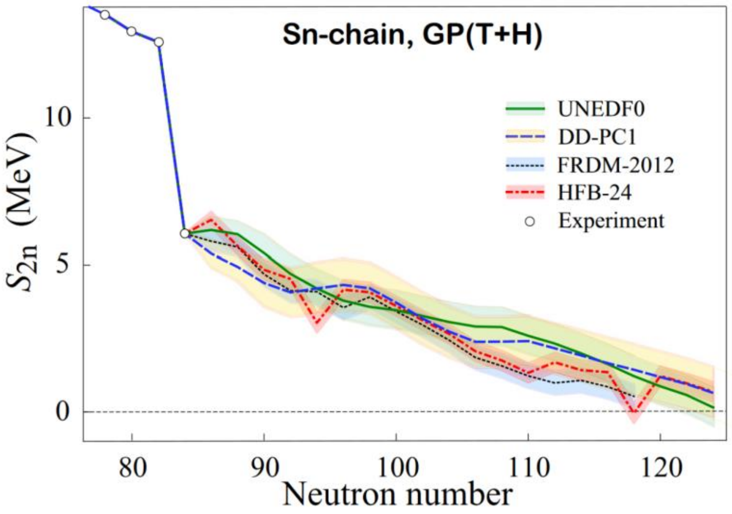
Possible solution:
Iterative model calibration?
Fit different parts against different data?

PHYSICAL REVIEW C **98**, 034318 (2018)

Editors' Suggestion

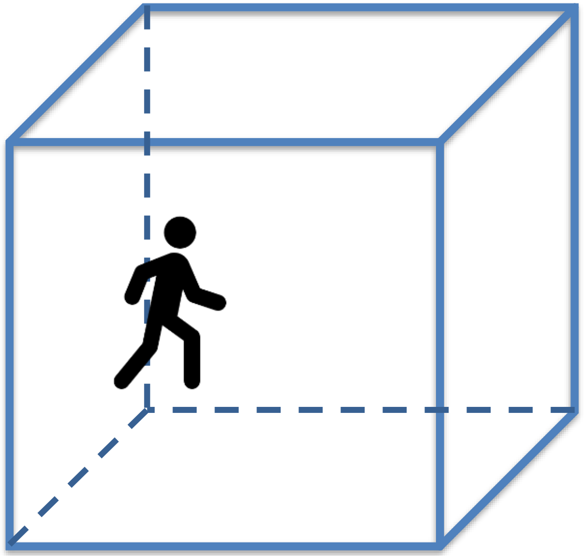
Bayesian approach to model-based extrapolation of nuclear observables

Léo Neufcourt,[1,2] Yuchen Cao (曹宇晨),[3] Witold Nazarewicz,[4] and Frederi Viens[1]



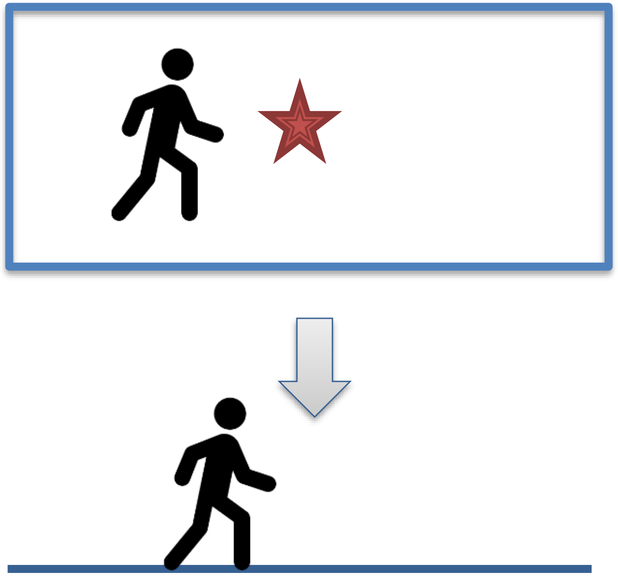
Integrated vs. modular approaches

- With all the priors of parameters (including GP hyperparameters) and the likelihood specified, we can directly perform MCMC sampling in full parameter space.
- A faster but more approximate method is to sample different sets of parameters step-by-step.



Integrated method:
Sample in full parameter space

vs.



Module method: Sample step-by-step

1. Build the physics-model emulator f: Sample $\boldsymbol{\theta}_f$ to fit physics-model outputs.
2. Fix $\boldsymbol{\theta}_f$ at its mean value.
3. Sample other parameters to fit experimental data.

Hierarchical priors ensure that we calibrate the physics model

- If priors of GP hyperparameters are not chosen carefully, f can perform badly (far from experimental data) but δ can well reproduce experimental observations.

- A hierarchical prior structure for the magnitudes of variances ($\sigma_\epsilon^2 < \sigma_\delta^2 < \sigma_f^2$) is thus adopted:

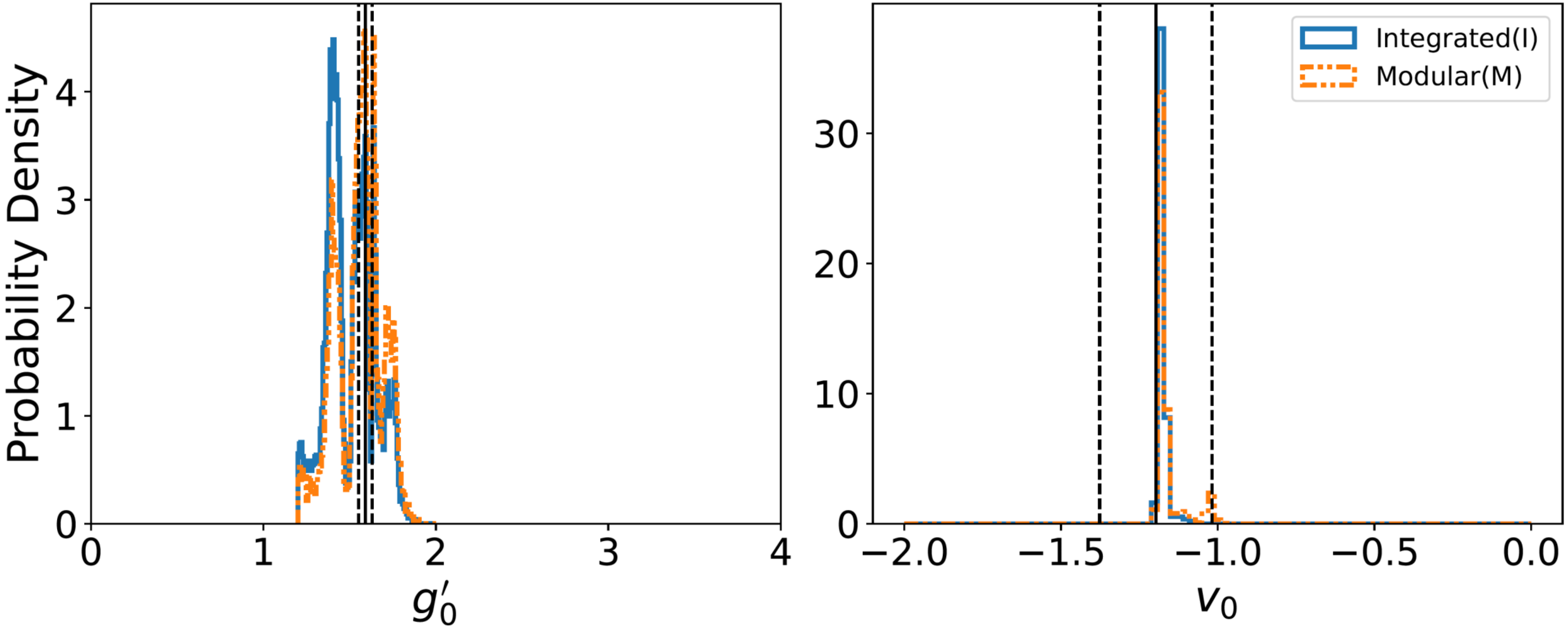
$$1/\eta_f \sim \Gamma(a = 10, b = 10),$$
$$1/\eta_\delta \sim \Gamma(a = 10, b = 0.3),$$
$$1/\sigma_\epsilon^2 \sim \Gamma(a = 10, b = 0.012).$$

  — The mean value of the Gamma distribution is a/b.

- This prior structure ensures that the variance in experimental data is most explained by f, less by δ, and least by ϵ.

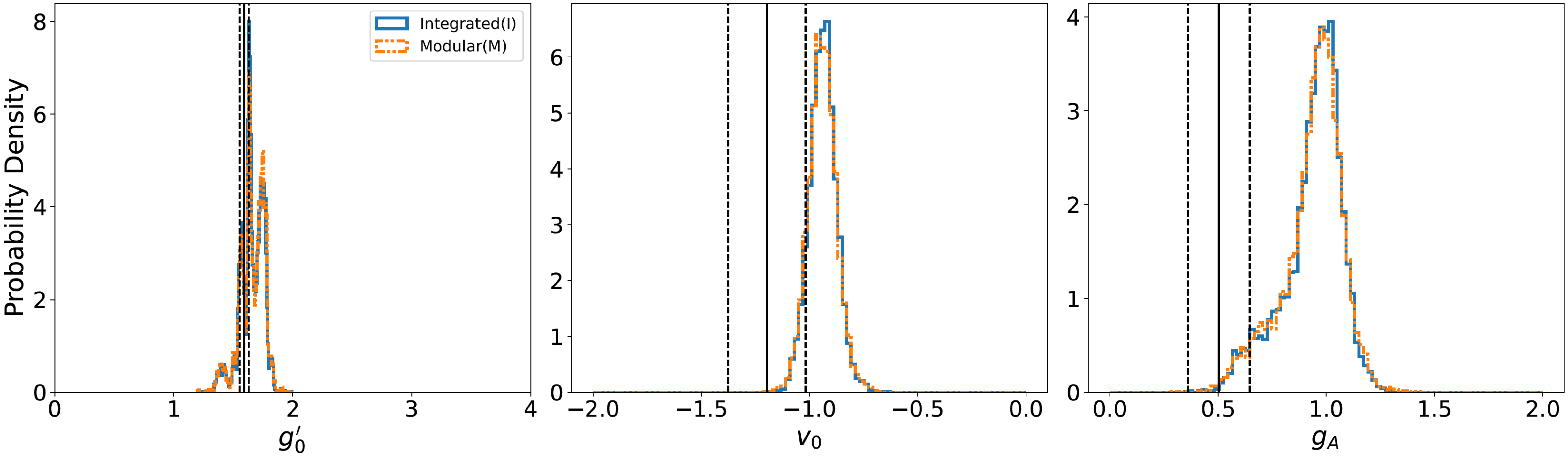
- Is the choice of η_δ for different data types equivalent to the choice of weights in the χ^2 optimization?

Preliminary results: Posterior distributions



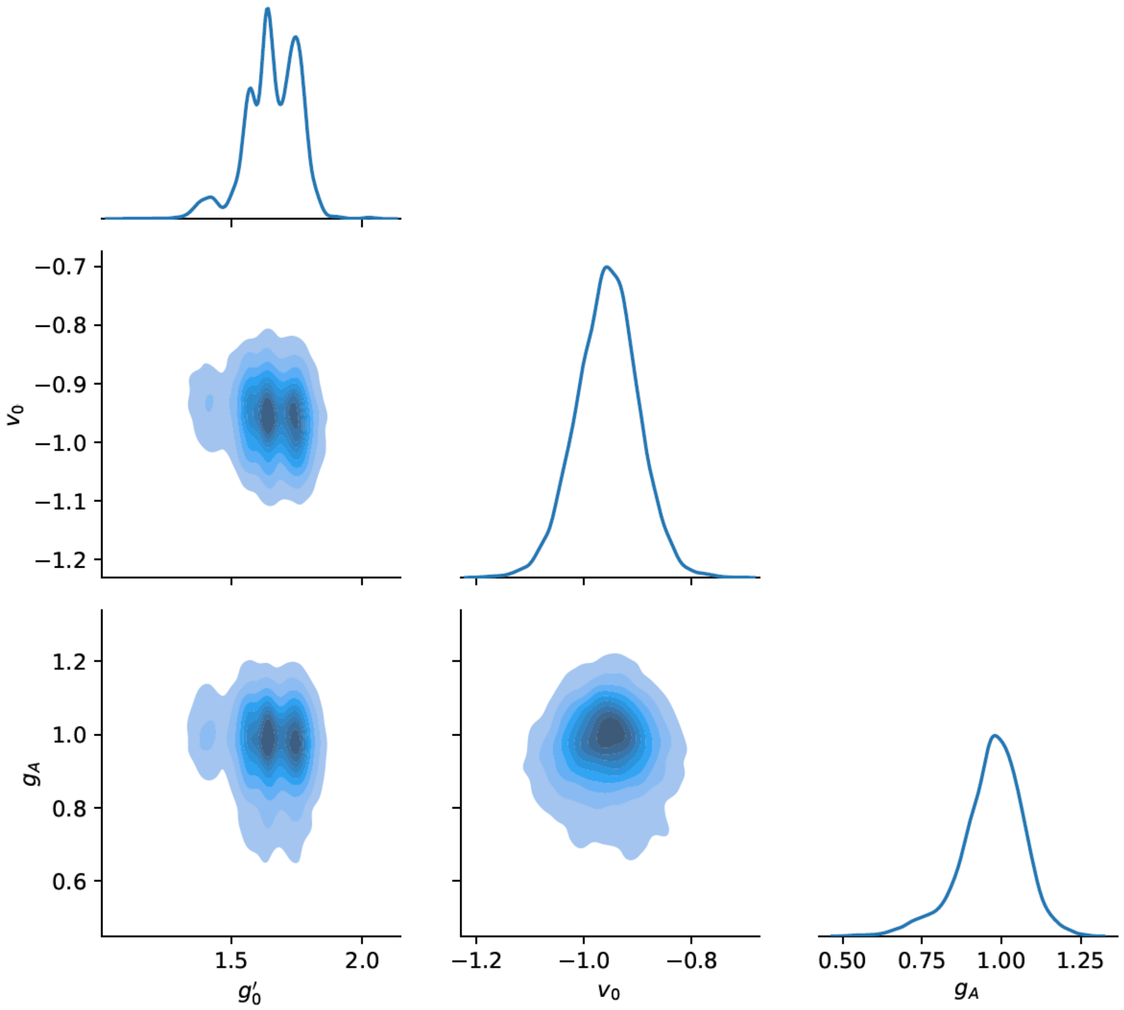
$g_A = 1$

Preliminary results: Posterior distributions

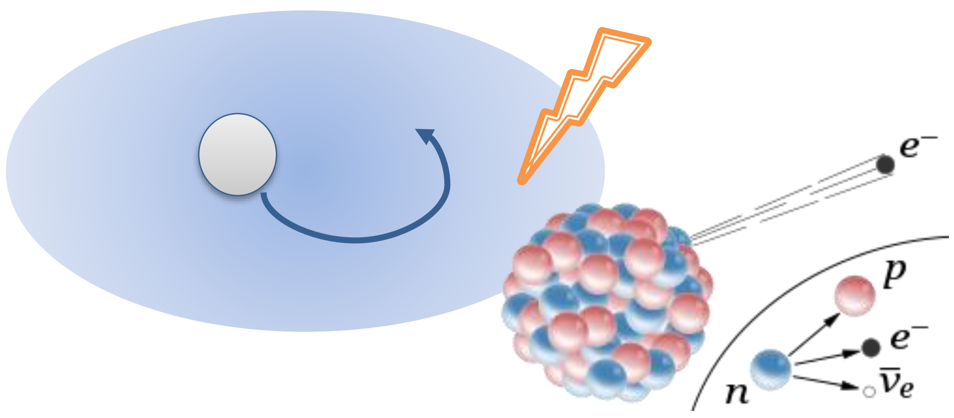


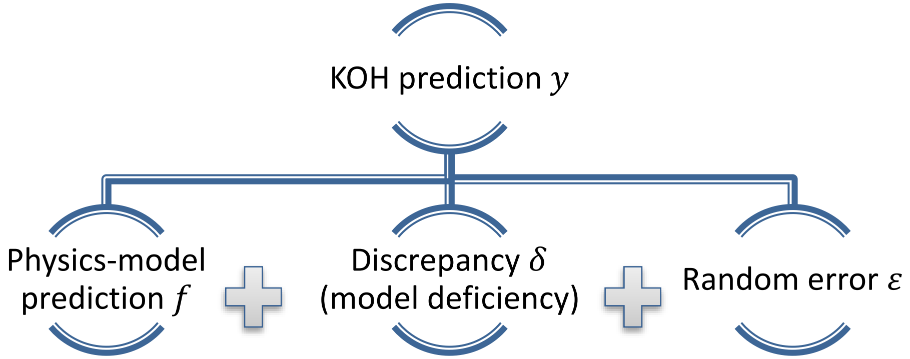
Preliminary results: Correlation

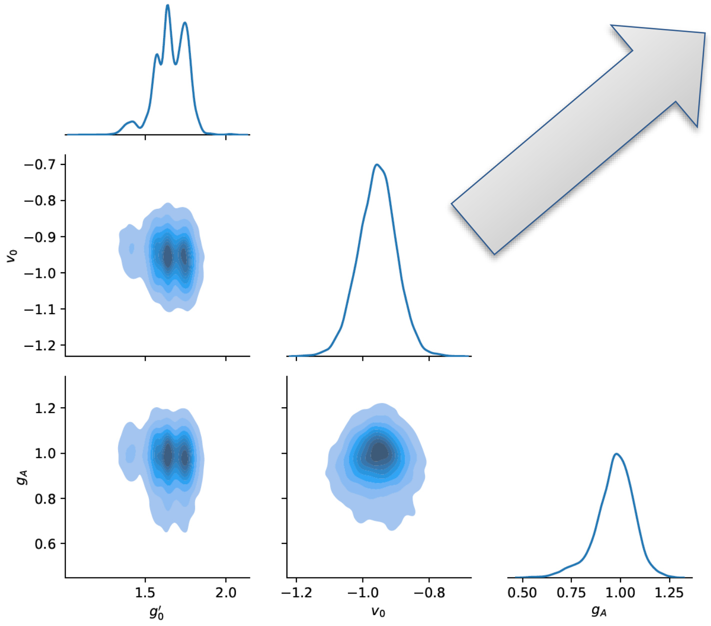
Integrated method

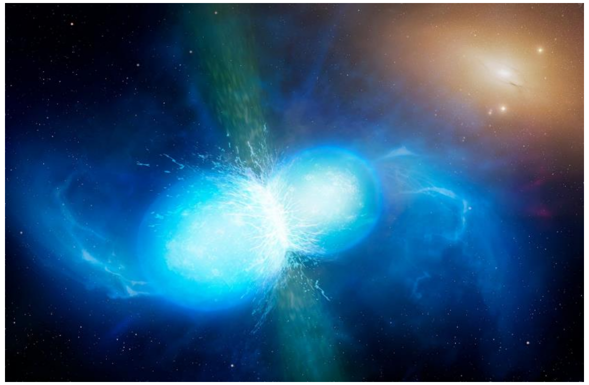


Conclusions and outlook



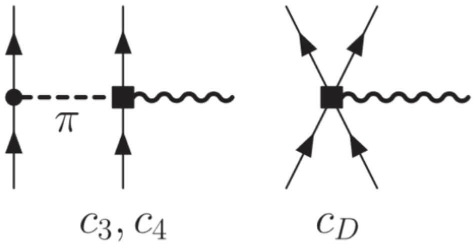


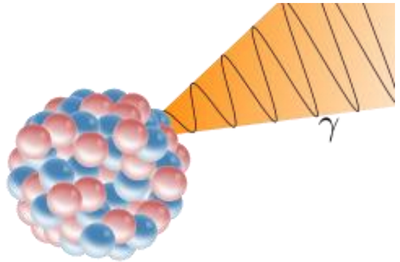




Conclusions and outlook

- Astrophysical simulations may help us on the selection of fit targets.
- The FAM with two-body currents is ready to use, which eliminates the necessity to fit g_A but introduces new unknown parameters.
  We can use the current framework to calibrate these new parameters.
- We will also extend our framework for other nuclear observables, such as the gamma decay.
- We are going to explore the application of the reduced basis method for better emulators of FAM codes.
- Statisticians are exploring the variational Bayesian method to totally remove the MCMC sampling in our framework.
- Bayesian model mixing can help us build models that vary with *Z* and *N* and provide best results in various regions.





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Backup Slides

Additional remarks on the χ^2 optimization

No.	Nucleus	E_{GTR}	Error	No.	Nucleus	E_{GTR}	Error
1	^{208}Pb	15.6	0.2	3	^{90}Zr	8.7	–
2	^{132}Sn	16.3	0.6	4	^{112}Sn	8.94	0.25

- POUNDERS (Practical Optimization Using No Derivatives for sums of Squares) in PETSc/TAO is the numerical tool for the optimization.
- It was first used in the fits of UNEDF functionals (Phys. Rev. C **82**, 024313 (2010)).

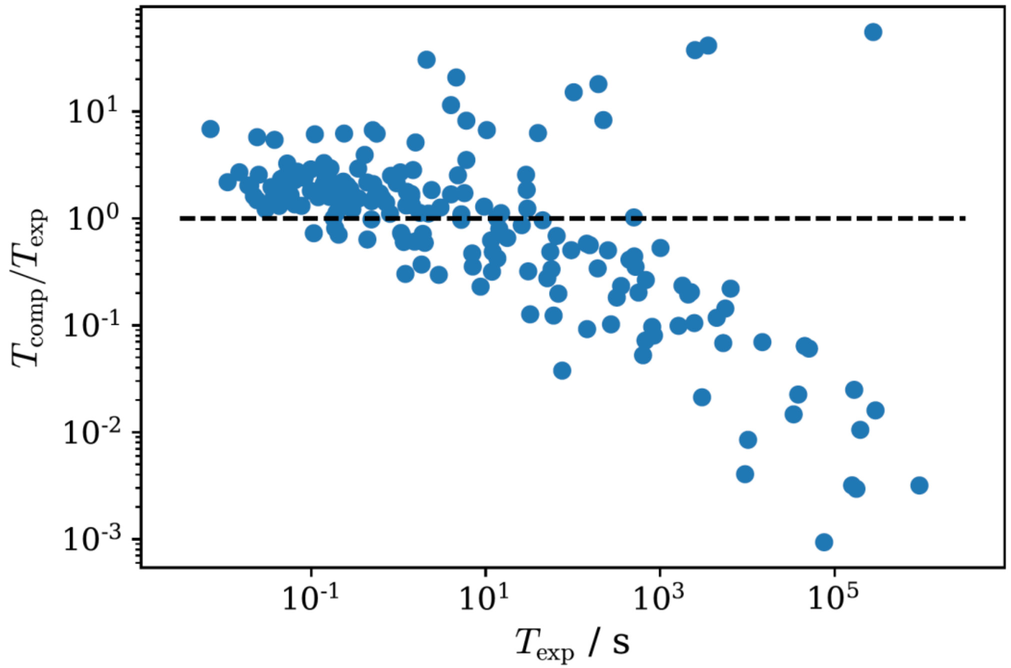
- The χ^2 optimization is based on the assumption that all the normalized residuals are independently Gaussian distributed: $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 I_{n_d})$.
- The probability distribution of $\boldsymbol{x}$ is $P(\boldsymbol{x}) \propto \exp\left[-\frac{\chi^2(\boldsymbol{x})}{2\sigma^2}\right] \approx C\exp\left[-\frac{1}{4\sigma^2}(\boldsymbol{x}-\hat{\boldsymbol{x}})^T H(\boldsymbol{x}-\hat{\boldsymbol{x}})\right]$, where $\hat{\boldsymbol{x}}$ is the minimum point of χ^2 , H is the Hessian matrix (proportional to the covariance matrix of $\boldsymbol{x}$).
- Approximate formula for the covariance matrix $\mathrm{Cov}(\hat{\boldsymbol{x}}) \approx \chi^2(\hat{\boldsymbol{x}})[G^T(\hat{\boldsymbol{x}})G(\hat{\boldsymbol{x}})]^{-1}$, where Jacobian matrix G is defined as $G_{ij} = \frac{\partial \varepsilon_i}{\partial x_j}$.

Results with the tensor term included (χ^2 optimization)

Fit	g'_0	g'_1	v_0	g_A
A	1.59560 (0.039)	0 (fixed)	−0.99993 (0.178)	1 (fixed)
B	1.59184 (0.034)	0 (fixed)	−1.19745 (0.179)	0.50345 (0.143)
C	1.73245 (0.820)	−0.37034 (2.143)	−0.99920 (0.183)	1 (fixed)
D	2.72206 (0.422)	−2.54125 (0.781)	−1.23511 (0.179)	0.41168 (0.132)

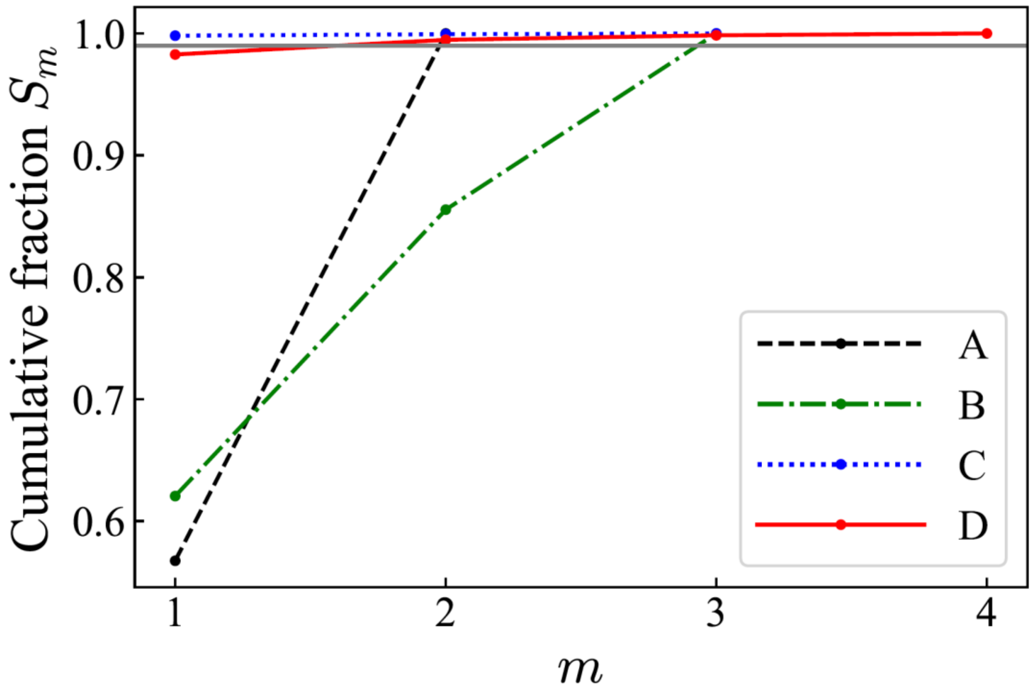
Strong correlation between g'_0 and g'_1 is seen in Fits C and D.

Predictions of Fit B

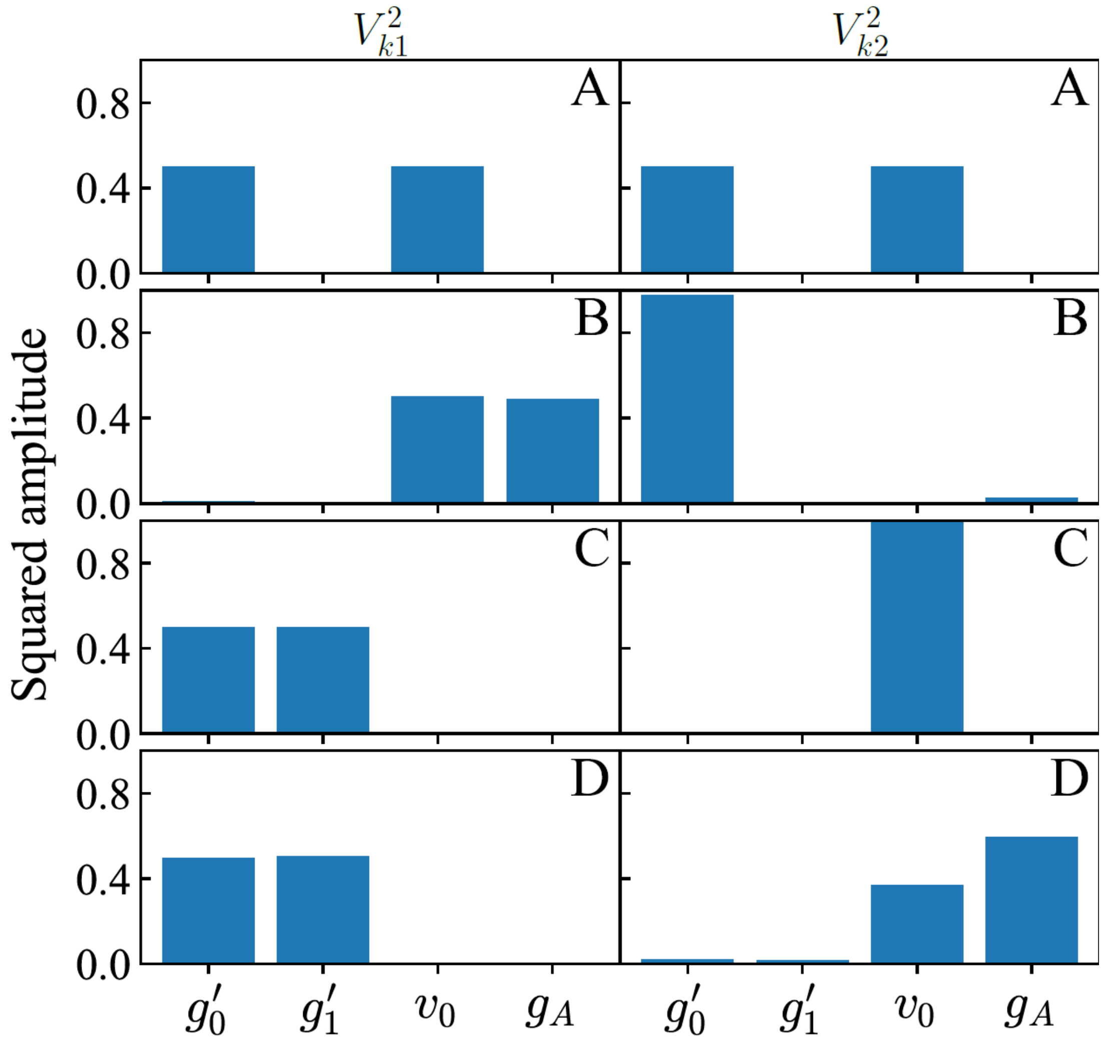


- For even-even nuclei with known β^--decay half lives, the figure shows ratios between calculated (with optimal parameter values) and experimental half lives.
- The error is typical for beta-decay calculations.
- Errors are larger for nuclei with longer half lives, primarily due to the leptonic phase-space factor.

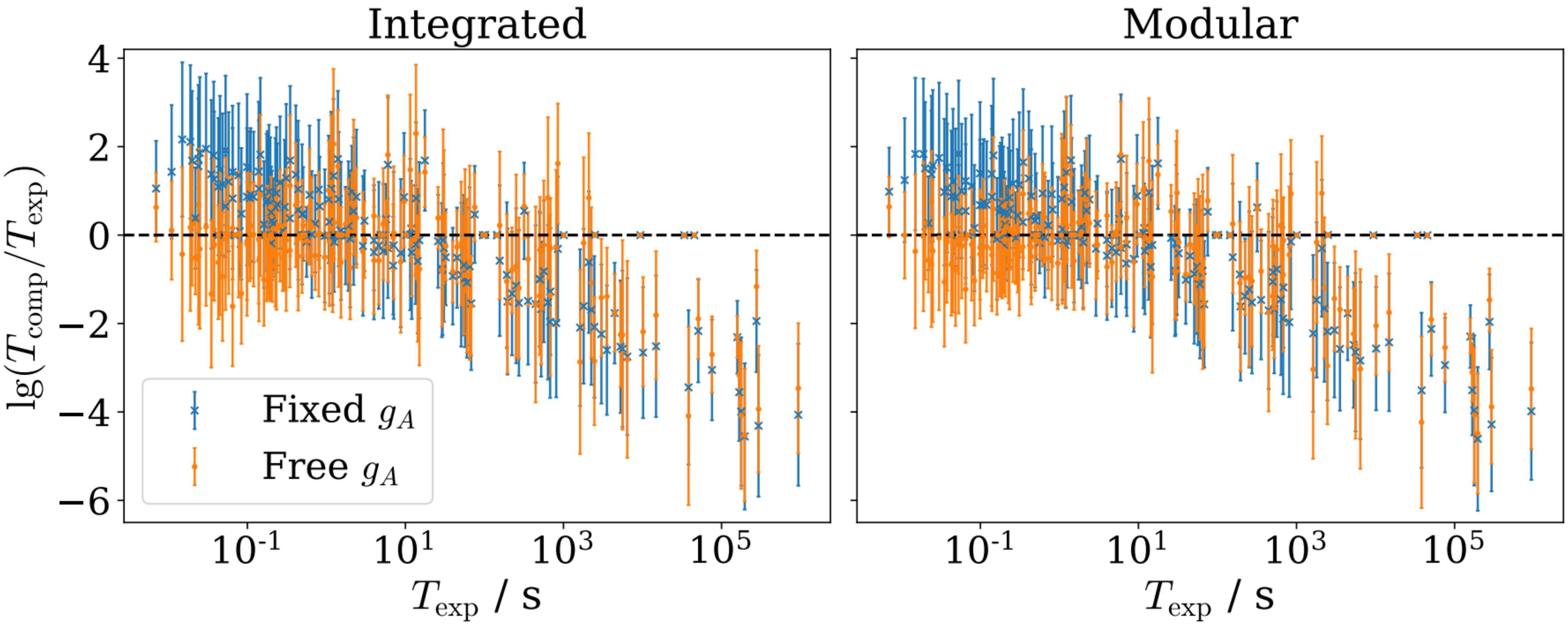
Number of effective parameters (PCA, χ^2 optimization)



Scheme	Free parameters	Fixed parameters
A	g_0', v_0	$g_A = 1$, $g_1' = 0$
B	g_0', v_0, g_A	$g_1' = 0$
C	g_0', g_1', v_0	$g_A = 1$
D	g_0', g_1', v_0, g_A	None



Predictions by the KOH model after calibration



g_A free to vary

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