Uncertainties of MC calculations

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Outline

Objectives

Can we trust models?

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The good question: How much can we trust the models?

Uncertainties should answer this question.

But uncertainties can be badly treated!
(Typically: only statistical uncertainties, systematics 10% as default, etc.)

INCL-ABLA

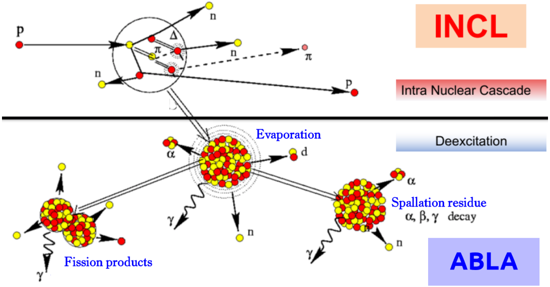
Spallation reaction (20 MeV - 20 GeV)

IntraNuclear Cascade (INC)

- Degrees of freedom: Hadron N, Δ, π, η, ω, K, Λ, Σ, ...
- Binary collision
- Hundreds of cross sections

Deexcitation

- DOF: n, p, d, α, ...
- Evaporation, Fission, Multi Fragmentation



INCL-ABLA

- **Models are not perfect**
- **There are many "free" parameters**

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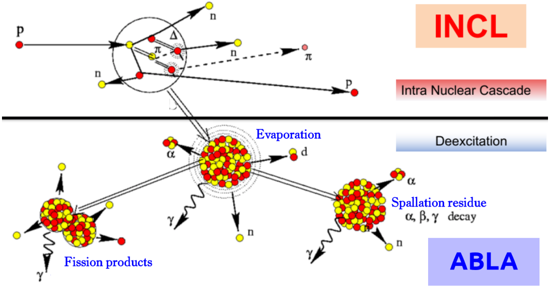

Our objectives

- Model bias
- Model uncertainties
- Optimal parameters
  Parameter uncertainties

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  Parameter uncertainties → How the errors propagate through the model?
  What is the impact of such parameter?
  Can we constrain parameter value based on exp. data?

Methodology

A Bayesian approach: Generalised Least Square

Bias/optimal parameters and their uncertainties can both be estimated with the same tool:
the GLS formula:

$$\rho(\underbrace{y_1}_{\text{Observables of interest}} \mid \underbrace{y_2}_{\text{Exp. data}}) = \mathcal{N}\left(\underbrace{\mu_1}_{\text{prior}} + \Sigma_{12}\Sigma_{22}^{-1}(\underbrace{y_2}_{\text{Exp. data}} - \underbrace{\mu_2}_{\text{Model prediction}}),\ \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right)$$

Σ_{11}: Covariance matrix between the obs. of interest
Σ_{22}: Covariance matrix between the exp. data and the model

Hypotheses:
Linear model (False) $\rightarrow$ need of iterations
Gaussian process
(if false: Gibbs sampling: Hirtz et al. EPJA 60:149 (2024))

GLS: Hypothesis implications

Not a linear model

Risk of local minimum

The model has to be realistically able to reproduce data

A Gaussian process

$$\pi_0(y_1) \propto \exp\left(-\frac{1}{2}(y_1-\mu_1)^T\Sigma_{11}^{-1}(y_1-\mu_1)\right)$$
$$= \exp\left(-\frac{1}{2}\chi^2_{11}\right)$$

The χ^2 is the natural figure of merit for this approach.
Other figures of merit could show different results.

The difficulties

CPU limitations

- Number of experimental data taken into account
  The method requires the inversion of the Σ_{22}, which scales with N^3
- Running time of the model
  Need to run the model many time (iteration, Jacobian)

Covariance matrix limitations

$$\Sigma = \Sigma_{physics} + \Sigma_{exp} + \Sigma_{model}$$

- Understand the correlation between the observables (MLO)
- Understand the systematics of an experiment
- Experimental uncertainties can be poorly evaluated
  $\rightarrow$ need to double check

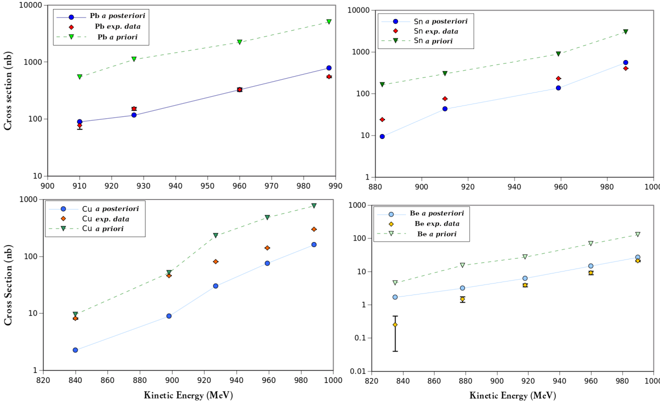
Parameters optimisation

Far subthreshold K^+ production (J. Hirtz et al. EPJA 60:149 (2024))

Study of a very specific phenomenon (proof of feasibility)

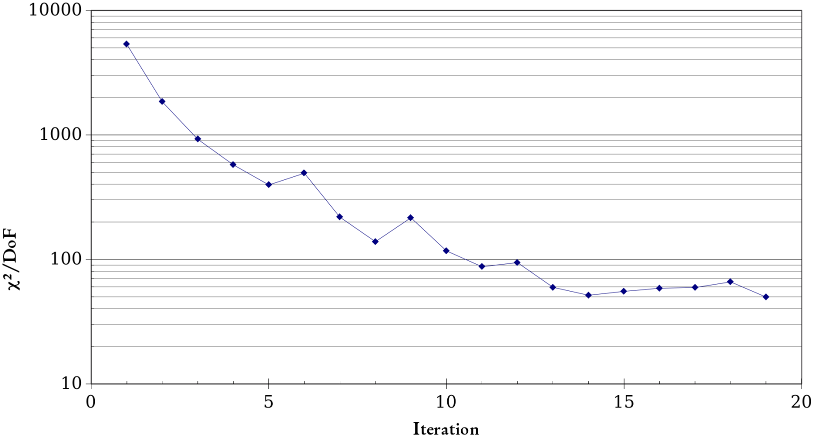
Parameters:

- $\sigma(NN \rightarrow K + X)$ (new = old x1.5)
- $\sigma(\pi N \rightarrow K + X)$ (new = old x0.26)
- $\sigma(\Delta N \rightarrow K + X)$ (new = old x0.43)
- Fermi momentum (new = 232 MeV/c)



Data: V. Koptev et al. Zh. Eksp. Teor. Fiz., 94:1-14, (1988)

Far subthreshold K^+ production: figure of merit



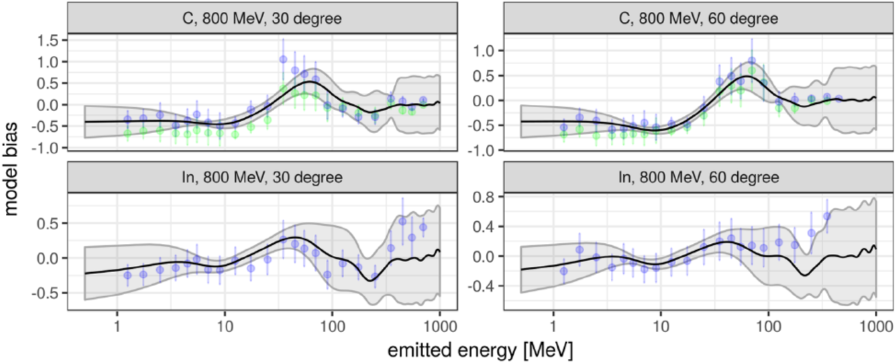
A lot of improvement but we started from far and we are still at $\chi^2/DoF \sim 50 \gg 1$

The model is still biased and/or the error bars are too small.

Model bias

DDNXS: Data used for training (G. Schnabel: EPJNST 4:33 (2018))

Estimation of the model bias and uncertainties on the bias:
With the training data: $\chi^2/DoF \sim 1$

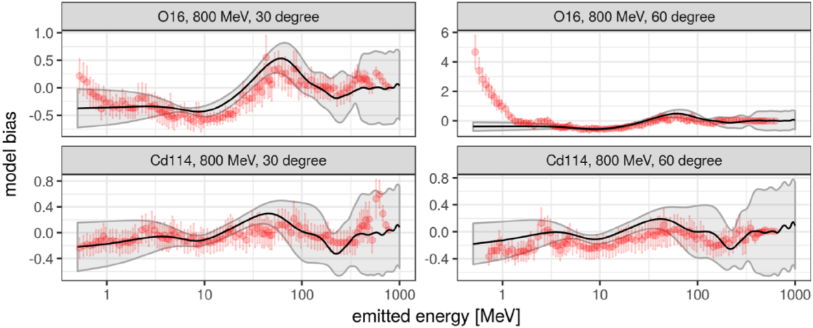


Experimental data:

W.B. Amian et al., NSE 112, 78 (1992); T. Nakamoto et al., JNST 32, 827 (1995)

DDNXS: Data not used for training

With the data not used for training: $\chi^2/DoF \sim 1$ in most cases but some pathological case unexplained.



Experimental data:

K. Ishibashi et al., JNST 34, 529 (1997)

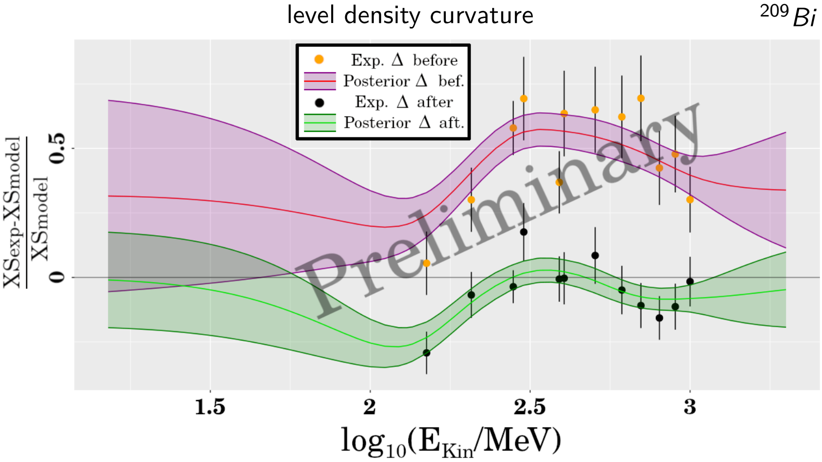
Complementarity: proton induced fission xs (Ho, Ta, Au, Pb, Bi, Th, U, Np, Pu)

Bias alone vs parameter optimisation → bias estimation

Improved:

fission dissipation coefficient

level density curvature



Results

- Application of GLS to Nuclear models
  - → Estimation of best parameters
  - → Estimation of parameters uncertainties (acceptable range, constraints)
  - → Estimation of model bias
  - → Estimation of model uncertainties

  We improved the model prediction (parameter optimisation), we are able to correct model predictions (model bias), and we can provide realistic uncertainties on our predictions (not just the statistical uncertainties).

- Future: application to various observable
  - → fission rate (ongoing)
  - → alpha induced XS
  - → etc.

Limits

Limits

- Prior knowledge (Partially compensated by MLO)
- Experimental covariance matrix
- Number of data to take into account (Pseudo inputs might help)
- Model CPU cost

Forces

- Adaptability
- Excellent interpolation power
- Realistic extrapolation
  - ▷ Projectile type
  - ▷ Projectile energy
  - ▷ Target mass
  - ▷ etc.

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