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Optimizing GEF code parameters with GEFTuner to enhance fission product yield predictions

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1. Introduction

The General Description of Fission Observables (GEF) code [1] is pivotal in predicting various fission observables, including the mass distribution of fission products. Accurate and reliable predictions of fission product yields are essential for applications in reactor physics, nuclear security, and spent fuel management. Traditional methods often utilize empirical models such as the 5 Gaussian model [2] to describe the mass distribution of fission products. However, these models rely on a limited set of parameters and may not fully capture the complexities of the fission process.

The developers of the GEF code have used the "eye-fit" method for parameter fitting due to the complexity of the problem which made developing an automatic fit procedure challenging [3]. This approach relies on intuition obtained from experience and physical knowledge regarding the relations between GEF parameters and observables. However, given that the GEF code encompasses approximately 100 parameters, an efficient method is necessary to handle such a large number of parameters effectively.

To address this need, this study introduces GEFTuner, a specialized program developed to optimize the numerous parameters of the GEF code. GEFTuner employs a unique algorithm to efficiently find the optimal parameter set, offering greater efficiency compared to traditional methods. Applying GEFTuner to experimental data from U^{233}, U^{235} and Pu^{239} fissions yielded optimized parameters that significantly improved agreement with experimental data compared to initial parameters. Our findings highlight the improvements in the accuracy and robustness of fission product yield descriptions when using parameters obtained with GEFTuner.

2. Methods and Results

2.1 GEF subroutine

The GEF code is an essential tool for predicting various aspects of nuclear fission. However, to better isolate and study the nuclear fission process itself, and to simplify the complexity, we utilized the GEF subroutine version rather than the stand-alone version of the GEF code.

The stand-alone version of the GEF code simulates the spontaneous or neutron-induced fission of a specific nucleus using the Monte-Carlo method. This version includes processes that occur after the compound nucleus undergoes "scission," where it splits into two fragments. After the scission, the highly excited fission fragments emit prompt neutrons, a process that involves additional physics beyond nuclear fission. To focus solely on the nuclear fission process and to simplify our study, we considered the processes only up to the scission point.

The GEF subroutine is specifically designed to be used in combination with other nuclear-reaction codes such as TALYS and EMPIRE. It handles the fission process from the formation of the compound nucleus up to the point of scission, excluding the subsequent emission of prompt neutrons and gamma rays. This approach allows us to examine the nuclear fission process in isolation, thereby providing clearer insights and reducing complexity.

In this work, we utilized the GEF subroutine version 2022-V2-2 to calculate the fission product yields. By focusing on the pre-scission dynamics, we aimed to enhance our understanding of the fundamental nuclear fission process and refine the predictive capacity of the GEF code. The results calculated by the GEF subroutine are the fission fragment yields at the scission point, specifically the pre-neutron emission fission fragment yields.

Such experimental data are extremely rare due to the difficulty of directly measuring these yields, often requiring several assumptions for deduction. For parameter fitting of the GEF subroutine, we used the most accurate pre-neutron emission fission fragment yield experimental data available, obtained by P. Geltenbort [4]. This dataset includes data for the thermal neutron induced fission U^{233}, U^{235} and Pu^{239}, and is considered one of the most reliable. Using this high-quality data, we aimed to achieve better optimization and more accurate predictions of fission product yields.

2.2 GEFTuner

Figure 1 shows the schematic flow of our automated model parameter tuning process. The tuning tool creates a GEFSUB input file, invokes the code, compares the calculated results with the experimental data, computes $\chi 2$, and repeats this procedure until user-provided convergence criteria are satisfied by using the gradient search technique, grid search, and/or random search. To reduce the computational time, multiple CPUs are employed simultaneously using MPI (Message Passing Interface). The whole process is terminated after a user-specified number of loops is completed. We can monitor the current status of fitting by checking automatically generated plots at each iteration.

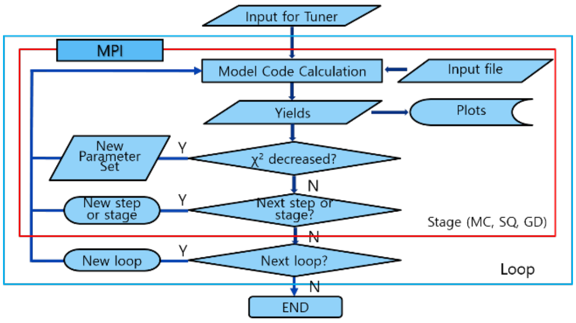

Fig. 1. Schematic flow of the automated model parameter tuning process

2.3 Method

This study focused on optimizing 28 key parameters of the GEF code, which are essential for describing the fission channels. These parameters were modified to fit the calculated results with the experimental data. The optimization process employed two distinct algorithms: gradient search and a combination of gradient search with grid search. Gradient search iteratively minimizes a function by moving in the direction of the steepest descent. Grid search, on the other hand, systematically searches for optimal hyperparameters by evaluating a defined parameter space, leading to better convergence and model accuracy.

The parameter adjustment range was set between 50% to 150% of their initial values. During each loop, the parameters were adjusted up to 10%, requiring five loops to span the entire adjustment range. However, to ensure thorough parameter search and better optimization, an additional loop was conducted, making a total of six loops performed.

2.4 Results

The optimization of the 28 parameters in the GEF code led to improvements in the predicted fission product yields. By comparing the initial and optimized parameter sets, we evaluated the model's predictive performance against experimental data.

Figures 2 present the mass distributions of thermal neutron induced fission of U^{233}, U^{235} and Pu^{239}. The gray dots represent the experimental data, while the initial parameter results are shown as black solid lines. The results obtained using only gradient search technique are represented by red solid lines, and the com1bination of gradient search and grid search results are shown as blue solid lines.

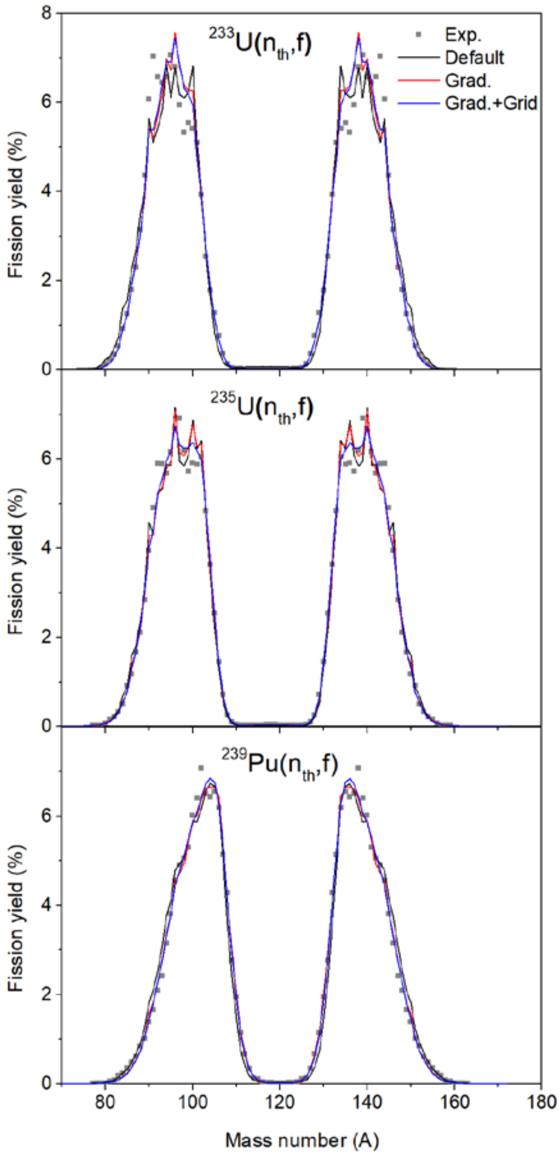

Fig. 2. Experimental data and calculated results from the GEF code using default parameters and optimized parameters for fission product yields of U^{233}, U^{235} and Pu^{239}.

To quantify the improvement, we calculated the chi-square χ^2 as follows:

$$\chi^2 = \frac{1}{n}\sum_i \left(\frac{Y_i^{cal} - Y_i^{exp}}{\Delta Y_i^{exp}}\right)^2$$

where Y_i^{cal} is the calculated yield, Y_i^{exp} is the experimental yield, ΔY_i^{exp} is the uncertainty in the experimental yield, and n is the number of experimental data.

We analyzed the chi-square values χ^2 across each optimization loop. Figure 3 illustrates the reduction in χ^2

values over the six optimization loops for both algorithms.

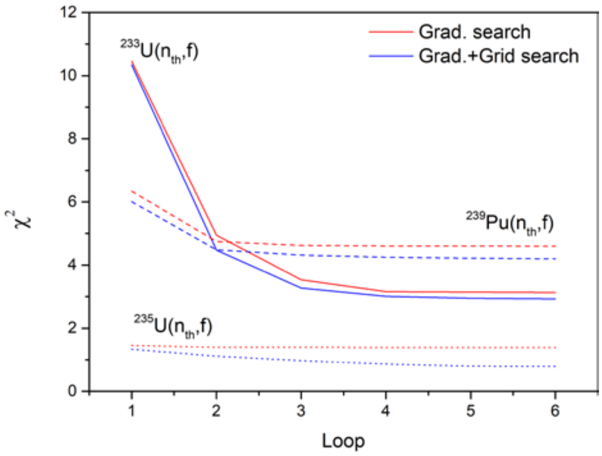

Fig. 3. Chi-square reduction over optimization loops.

Each data set contains results from both the gradient search and the combined gradient search + grid search approaches. Gradient search provided results similar to those obtained using the combined gradient search + grid search approach, even with reduced computing time. This indicates that for some nuclei, gradient search alone can be sufficient. However, in the case of $^{235}U(n_{th},f)$, the chi-square values do not decrease further with gradient search alone, suggesting that the algorithm may have been trapped in a local minimum. In contrast, the combined approach showed continued reduction in chi-square values, indicating more effective convergence.

The results revealed that the combined optimization approach enhanced the GEF code's ability to accurately predict fission product yields.

3. Conclusions

In this work, we aimed to optimize the parameters of the GEF code using a specialized program called GEFTuner. By focusing on the fission process up to the scission point, we utilized the GEF subroutine to isolate and better understand the nuclear fission process.

Two distinct optimization techniques were employed: gradient search and a combination of gradient search with grid search. The analysis demonstrated that both methods significantly improved the predictive performance of the GEF code. The optimized parameters achieved a substantial reduction in chi-square values, indicating better alignment with the experimental data. This study highlights the effectiveness of GEFTuner and the importance of using advanced optimization techniques to handle complex parameter spaces in nuclear models. Future work can extend these findings by exploring additional parameters and incorporating more diverse experimental data sets.

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