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Bayesian optimization on FIFRELIN Monte-Carlo code to fit neutron and gamma multiplicities

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Abstract : FIFRELIN (Fission FRagments Evaporation moedLINg) is a Monte-Carlo code based on Hauser-Fesbach formalism [1]. Its purpose is to simulate the de-excitation process of fission fragments. Firstly, fission fragments are generated using a sampling over model and experimental data. Some models depend on free parameters that the user can adjust. After the fission fragments are generated, a cascade over a level scheme is simulated. The free parameters selected no longer interfere with this second step. Numerous quantities of interest are calculated (mass yields, prompt particle spectra, multiplicities ...). Up to now, the code relies on four free parameters which mainly control the initial excitation and total angular momentum of fission fragment. Up to now, the main limitation of the code is the capacity to explore the 4D input space. For instance, one FIFRELIN simulation takes seven minutes to get the uncertainties in the order of experimental precision for neutron and gamma multiplicities. It corresponds to 24h of computational time for barely 3 or 4 points in each dimension of the input space. Therefore, it is unrealistic to use a direct exploration of the input space, in order to find a solution that align with the experimental data [2] [3]. To do so, we propose to use Bayesian optimization, supported by the use of Gaussian Process [4]. An independent Gaussian Process models each physical observable, in order to reach global solution that minimize the distance between FIFRELIN response and the experimental target [5]. Starting from scratch, using 20 CPUs, we find inputs that correctly fit the neutron and gamma multiplicities in less than one hour. Neutron emission probability is well fitted also. Other observables can be added, such as the neutron multiplicity as a function of mass. This induces constraint on potential values of temperature ratios, defined for each fragmentation this time. Physical interpretation of this new input model of FIFRELIN will also be presented.

[1] O. Litaize, O. Serot, et L. Berge, « Fission modelling with FIFRELIN »

[2] V. Piau, O. Litaize, A. Chebboubi, S. Oberstedt, A. Göök, et A. Oberstedt, « Neutron and gamma multiplicities calculated in the consistent framework of the Hauser-Feshbach Monte Carlo code FIFRELIN »

[3] P. Santi et M. Miller, « Reevaluation of Prompt Neutron Emission Multiplicity Distributions for Spontaneous Fission »

[4] J. Snoek, H. Larochelle, et R. P. Adams, « Practical Bayesian Optimization of Machine Learning Algorithms »

[5] A. K. Uhrenholt et B. S. Jensen, « Efficient Bayesian Optimization for Target Vector Estimation »

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