Benchmarking Nuclear Fission Theory

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We suggest a small set of fission observables to be used as test cases for validation of theoretical calculations. The purpose is to provide common data to facilitate the comparison of different fission theories and models. The proposed observables are chosen from fission barriers, spontaneous fission lifetimes, fission yield characteristics, and fission isomer excitation energies.

I. MOTIVATION

Nuclear fission is a very complex process and its theory presents an enormous challenge. As Bohr and Wheeler stated in their 1939 pioneering paper [1], theoretical progress in the theory of fission would in all likelihood take time to resolve: “An accurate estimate for the stability of a heavy nucleus against fission in its ground state will, of course, involve a very complicated mathematical problem”. Indeed, even in the present era of extensive computer resources, a comprehensive microscopic explanation of nuclear fission rooted in interactions between protons and neutrons still eludes us. Consequently, it remains difficult for both experimentalists and theorists to assess various models of fission and their predictions. To address this situation, it would be very useful if different theoretical approaches could be easily compared. Most importantly, such reporting should promote a closer interaction between theorists and experimentalists to stimulate new experiments that can differentiate between models or unveil new phenomena.

To that end, we would like to suggest a list of experimental observables, or evaluated empirical quantities, that are well established, and could serve as benchmarks of the accuracy of a theoretical approach. Our recommendation for future model development work is to present along with predictions of a theory, the results when applied to this small set of data. The benchmark cases we have selected are basic fission observables in nuclei that are well known experimentally. The observables in the benchmark are: fission barriers, fission mass distributions, total kinetic energies of fission fragments, spontaneous fission lifetimes, and fission isomer excitation energies. This leaves out a rich variety of interesting phenomena that includes kinetic energy distributions of fission yields, scission neutrons, and barrier state spectroscopy. The theory for these quantities is not as well developed. Hopefully, candidate theories for the more complex phenomena would be sufficiently general to apply them to the basic benchmarks.

It is also important that the results be reported in a way that makes comparisons easy. In particular, we would like to know how the theory performs on average for the data set, if the parameters of the theory have not been adjusted to the data. We would also like to know how well the theory describes the fluctuations of individual data.

We understand that a large community of experimentalists, theorists, and evaluators has been working for a long time on developing standards and benchmarks related to fission data. The purpose of the present contribution is not to reproduce, or even attempt to reproduce, this large body of work, but instead to select from it a subset of well-known fission data that can be readily used by fission theorists to guide and test their work.

When dealing with fission data, it is important to realize that what is considered “experimental data” is often the result of a more or less complicated deconvolution process related to a physical observable. This caveat will be repeated and illustrated wherever it applies.

Finally, as the purpose of these notes is to stimulate benchmarking rather than provide critical evaluation of various models of fission, we choose not to provide specific examples of theoretical calculations. Here, we would like to draw the reader’s attention to the talks presented at the INT Program 13-3, posted online [2], which contain a wealth of useful information about the current status of fission theory.

II. THE BENCHMARKS

A. Fission Barrier Heights

The concept of a fission barrier height is fraught with ambiguity [2]. A theoretical definition is the energy difference between the ground state and the highest saddle point in a shape-constrained potential energy surface (PES) that has the lowest energy for all possible paths leading to fission from the ground state. If the theory treats the angular momentum of the nucleus, the benchmark should be for the PES corresponding to the angular momentum of the ground state. We have chosen 15 examples for the benchmarks, including the well-known nu-
TABLE I. Fission barrier parameters for the even-even actinides. $E_A$ and $E_B$ are the empirical heights of the inner and outer fission barrier, respectively. The uncertainty on the empirical barrier heights ranges from 0.3 MeV to 1 MeV.

| Z  | A    | Symbol | $E_A$ (MeV) | $E_B$ (MeV) |
|----|------|--------|-------------|-------------|
| 90 | 230  | Th     | 6.1         | 6.8         |
| 90 | 232  | Th     | 5.8         | 6.7         |
| 92 | 232  | U      | 4.9         | 5.4         |
| 92 | 234  | U      | 4.8         | 5.5         |
| 92 | 236  | U      | 5           | 5.67        |
| 92 | 238  | U      | 6.3         | 5.5         |
| 94 | 238  | Pu     | 5.6         | 5.1         |
| 94 | 240  | Pu     | 6.05        | 5.15        |
| 94 | 242  | Pu     | 5.85        | 5.05        |
| 94 | 244  | Pu     | 5.7         | 4.85        |
| 96 | 241  | Cm     | 7.15        | 5.5         |
| 96 | 242  | Cm     | 6.65        | 5           |
| 96 | 244  | Cm     | 6.18        | 5.1         |
| 96 | 246  | Cm     | 6           | 4.8         |
| 96 | 248  | Cm     | 5.8         | 4.8         |

TABLE II. Table of (even-even) Fission isomer excitation energies $E_{II}$.

| Nuclide | $E_{II}$ (keV) | $T_{1/2}$ |
|---------|---------------|-----------|
| $^{236}\text{U}$ | 2750 | 120 ns |
| $^{238}\text{U}$ | 2557.9 | 280 ns |
| $^{238}\text{Pu}$ | ~2400 | 0.6 ns |
| $^{240}\text{Pu}$ | ~2800 | 3.7 ns |
| $^{242}\text{Pu}$ | ~2000 | 28 ns |
| $^{242}\text{Cm}$ | ~3000 | 55 ns |
| $^{242}\text{Cm}$ | ~1900 | 40 ps |
| $^{244}\text{Cm}$ | ~2200 | ≤5 ps |

C. Spontaneous Fission Lifetimes

The examples chosen in Table III are for illustrative purposes only. Many more spontaneous fission half-lives have been measured and analyzed, as reported in Ref. [9]. For the examples we have chosen the well-known $^{240}\text{Pu}$ lifetime together with two cases among heavier actinide elements that exhibit extreme variations in lifetimes.

It is worth noting that when dealing with quantities that can vary by many orders of magnitude, it makes sense to compare not the differences between theory and experiment but rather the logarithm of the ratio of theory...
to experiment,
\[ R_x = \log \left( \frac{x_{th}}{x_{exp}} \right). \]  
(1)

The target performance measures are then the mean value of \( R_x \),
\[ \bar{R}_x = \frac{1}{N_d} \sum_i R_{x,i} \]  
(2)
and the variance about the mean
\[ \sigma = \frac{1}{N_d} \left( \sum_i (R_{x,i} - \bar{R}_x)^2 \right)^{1/2}. \]  
(3)

Here \( N_d \) is the number of data points in the benchmark set. We note that these measures are in common use, for example in reporting the performance of theories of the nuclear level density [10]. Of course, if the model makes use of a parameter to fit benchmark data or data of the same kind, only the \( \sigma \) value provides an interesting test of the theory.

D. Mass Distributions

Fission fragment yields are commonly characterized by independent, cumulative and chain mass yields. Establishing meaningful benchmarks is complicated by the fact that there is no direct relation between what theories predict and what experiments measure.

Experimentally, the best-known mass yields are for the thermal neutron-induced fission reactions of \(^{235}\text{U}\) and \(^{239}\text{Pu}\). Precise measurements (1–2%) have often been made using radiochemical techniques, in which cumulative yields are measured. Inferring the independent yields from those measurements therefore requires some modeling. Finally, fission theories will predict pre-neutron emission fission fragment yields, while experimental data always correspond to post-neutron emission yields.

However, for benchmarking purposes, we just recommend only two quantities that should be easier to compute and reflect the coarsest features of the distribution.

We first determine the average mass \( A_m \) as
\[ A_m = \frac{1}{P} \sum_A AP(A) \]  
(4)
where \( P = \sum_A P(A) \) is the total probability. Note that \( P = 1 \) is not precisely satisfied in the evaluated data tables. The experimental \( A_m \) comes out a few units less than half the mass number of the original nucleus.

The benchmarks are the following two moments of the distribution for the higher mass fragments:
\[ S_\sigma = \frac{1}{P} \sum_{A>A_m} P(A) (A - A_m), \]  
(5)
\[ \sigma^2 = \frac{1}{P} \sum_{A>A_m} P(A) (A - A_m)^2 - S_\sigma^2. \]  
(6)
Here \( P_{\sigma} \) is the total probability of producing fission fragments of mass higher than \( A_m \):
\[ P_{\sigma} = \sum_{A>A_m} P(A). \]  
(7)

In simple models \( P_{\sigma} \) will be equal to one, but the experimental value differs from that by a small amount.

For the experimental cases, we include the thermal neutron-induced fission of \(^{235}\text{U}\), \(^{239}\text{Pu} \) and \(^{255}\text{Fm} \). The first two have the classic asymmetric mass yields and the latter has a more centered yield curve. Also we consider an example of spontaneous fission of \(^{252}\text{Cf} \). The moments in Table IV were extracted from the experimental \( P(A) \) data compiled in Refs. [11, 12]. The Table also gives the values of \( A_m \) and \( P_{\sigma} \) for the data, although these are not part of the benchmark. The full tables for \( P(A) \) are provided in the Appendix.

E. Total Kinetic Energies

The total kinetic energy (TKE) of the fission fragments is an important quantity for several reasons. It is an indicator for the shape of the fission fragments near their scission configurations: the higher the TKE value, the more compact the nascent fragments are. This quantity also directly influences the excitation energy left in the initial fragments, which is released through the evaporation of neutrons and photons. It also represents an important benchmark for fission theories to compute.

The average pre-neutron evaporation total kinetic energy \( \langle \text{TKE} \rangle \) for \(^{252}\text{Cf} \) spontaneous fission and thermal neutron-induced fission of \(^{233,235}\text{U} \) and \(^{239,241}\text{Pu} \) are considered as energy standards [13]. To a first-order, the evolution of \( \langle \text{TKE} \rangle \) follows the Coulomb parameter \( Z^2/A^{1/3} \).
TABLE V. Recommended \[13\] average pre-neutron evaporation total kinetic energies of the fission fragments.

| Reaction      | ⟨T KE⟩ (MeV) |
|---------------|--------------|
| $^{233}$U ($n_{th}$, f) | 170.1 ± 0.5  |
| $^{235}$U ($n_{th}$, f) | 170.5 ± 0.5  |
| $^{239}$Pu ($n_{th}$, f) | 177.9 ± 0.5  |
| $^{252}$Cf (sf) | 184.1 ± 1.3  |

III. CONCLUDING REMARKS

This document provides a small set of fission data that can be used to test the validity of theoretical calculations. Obviously the fission process is very complex and rich, and many more data exist beyond this very small sample. One should view these notes as a living document, which will need to be updated as more useful information becomes available, and as fidelity of fission theory improves.

IV. ACKNOWLEDGMENT

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V. APPENDIX

This Appendix contains the tabulated information on individual mass yield distributions for the cases listed in Table IV (From Ref. [11] and ie.lbl.gov/fission.html.)

TABLE VI: Fission Product Yields per 100 Fissions for $^{235}$U: thermal neutron induced fission.

| A Chain Yield (%) | Average Z |
|-------------------|-----------|
| 66                | 7.22E-08  |
| 67                | 3.61E-07  |
| 68                | 7.16E-07  |
| 69                | 1.57E-06  |
| 70                | 3.62E-06  |
| 71                | 8.39E-06  |
| 72                | 2.65E-05  |
| 73                | 1.02E-04  |
| 74                | 3.39E-04  |
| 75                | 1.07E-03  |

Continued
| A Chain Yield (%) | Average Z |
|-------------------|-----------|
| 137               | 6.34E+00  | 53.44 |
| 138               | 6.76E+00  | 53.84 |
| 139               | 6.48E+00  | 54.1  |
| 140               | 6.76E+00  | 54.46 |
| 141               | 5.86E+00  | 55.07 |
| 142               | 5.83E+00  | 55.47 |
| 143               | 5.96E+00  | 55.82 |
| 144               | 5.51E+00  | 56.13 |
| 145               | 3.95E+00  | 56.51 |
| 146               | 3.00E+00  | 56.89 |
| 147               | 2.25E+00  | 57.66 |
| 148               | 1.68E+00  | 57.82 |
| 149               | 1.08E+00  | 58.21 |
| 150               | 6.53E-01  | 58.42 |
| 151               | 4.19E-01  | 58.95 |
| 152               | 2.67E-01  | 59.47 |
| 153               | 1.58E-01  | 59.8  |
| 154               | 7.44E-02  | 60.09 |
| 155               | 3.21E-02  | 60.45 |
| 156               | 1.48E-02  | 60.88 |
| 157               | 6.15E-03  | 61.38 |
| 158               | 3.29E-03  | 61.79 |
| 159               | 1.01E-03  | 62.05 |
| 160               | 3.19E-04  | 62.92 |
| 161               | 8.53E-05  | 62.79 |
| 162               | 1.59E-05  | 63.31 |
| 163               | 6.10E-06  | 63.67 |
| 164               | 1.88E-06  | 63.99 |
| 165               | 9.32E-07  | 64.29 |
| 166               | 3.62E-07  | 64.64 |
| 167               | 2.47E-07  | 65.16 |
| 168               | 5.70E-08  | 65.64 |
| 169               | 2.39E-08  | 65.92 |
| 170               | 5.01E-09  | 66.18 |
| 171               | 2.35E-09  | 66.58 |
| 172               | 7.69E-10  | 67.06 |

TABLE VII: Fission Product Yields per 100 Fissions for $^{239}$Pu: thermal neutron induced fission.
| A Chain Yield (%) | Average Z |
|-------------------|-----------|
| 147               | 2.01E+00  |
| 148               | 1.64E+00  |
| 149               | 1.22E+00  |
| 150               | 9.67E-01  |
| 151               | 7.38E-01  |
| 152               | 5.76E-01  |
| 153               | 3.61E-01  |
| 154               | 2.60E-01  |
| 155               | 1.66E-01  |
| 156               | 1.24E-01  |
| 157               | 7.42E-02  |
| 158               | 4.14E-02  |
| 159               | 2.06E-02  |
| 160               | 9.68E-03  |
| 161               | 4.85E-03  |
| 162               | 2.60E-01  |
| 163               | 9.17E-04  |
| 164               | 5.26E-08  |
| 165               | 1.44E-07  |
| 166               | 6.02E-06  |
| 167               | 1.47E-05  |
| 168               | 3.18E-07  |
| 169               | 1.57E-07  |
| 170               | 4.94E-08  |

Continued
| A Chain Yield (%) | Average Z |
|-------------------|-----------|
| 157               | 5.38E-01 | 6.16E+01 |
| 158               | 4.70E-01 | 6.22E+01 |
| 159               | 3.40E-01 | 6.24E+01 |
| 160               | 2.86E-01 | 6.30E+01 |
| 161               | 1.94E-01 | 6.32E+01 |
| 162               | 1.20E-01 | 6.36E+01 |
| 163               | 7.58E-02 | 6.40E+01 |
| 164               | 4.72E-02 | 6.43E+01 |
| 165               | 2.87E-02 | 6.47E+01 |
| 166               | 1.84E-02 | 6.51E+01 |
| 167               | 9.57E-03 | 6.55E+01 |
| 168               | 5.25E-03 | 6.59E+01 |
| 169               | 1.67E-03 | 6.63E+01 |
| 170               | 1.40E-03 | 6.66E+01 |
| 171               | 7.09E-04 | 6.70E+01 |
| 172               | 4.65E-04 | 6.74E+01 |

| A Chain Yield (%) | Average Z |
|-------------------|-----------|
| 106               | 2.41E+00 | 42.68 |
| 107               | 2.61E+00 | 43.07 |
| 108               | 2.71E+00 | 43.46 |
| 109               | 2.90E+00 | 43.86 |
| 110               | 3.28E+00 | 44.25 |
| 111               | 3.19E+00 | 44.64 |
| 112               | 3.63E+00 | 45.03 |
| 113               | 4.25E+00 | 45.41 |
| 114               | 4.84E+00 | 45.81 |
| 115               | 5.59E+00 | 46.2 |
| 116               | 5.66E+00 | 46.58 |
| 117               | 5.85E+00 | 46.97 |
| 118               | 5.89E+00 | 47.35 |
| 119               | 5.97E+00 | 47.74 |
| 120               | 5.80E+00 | 48.14 |
| 121               | 5.70E+00 | 48.54 |
| 122               | 5.31E+00 | 49.14 |
| 123               | 4.92E+00 | 49.49 |
| 124               | 3.88E+00 | 49.8 |
| 125               | 3.02E+00 | 49.91 |
| 126               | 2.41E+00 | 50.13 |
| 127               | 2.32E+00 | 50.07 |
| 128               | 2.17E+00 | 51.4 |
| 129               | 2.27E+00 | 50.34 |
| 130               | 2.48E+00 | 50.46 |
| 131               | 3.21E+00 | 50.84 |
| 132               | 4.18E+00 | 51.24 |
| 133               | 5.42E+00 | 51.64 |
| 134               | 5.81E+00 | 52.06 |
| 135               | 6.19E+00 | 52.48 |
| 136               | 5.28E+00 | 52.73 |
| 137               | 6.47E+00 | 53.32 |
| 138               | 6.11E+00 | 53.73 |
| 139               | 5.72E+00 | 54.15 |
| 140               | 4.83E+00 | 54.58 |
| 141               | 4.62E+00 | 55.01 |
| 142               | 4.33E+00 | 55.45 |
| 143               | 3.14E+00 | 55.88 |
| 144               | 3.21E+00 | 56.3 |
| 145               | 2.84E+00 | 56.71 |
| 146               | 2.48E+00 | 57.11 |
| 147               | 2.02E+00 | 57.52 |
| 148               | 1.74E+00 | 57.92 |
| 149               | 1.47E+00 | 58.31 |
| 150               | 1.29E+00 | 58.7 |
| 151               | 1.29E+00 | 59.1 |
| 152               | 1.10E+00 | 59.5 |
| 153               | 9.98E-01 | 59.88 |
| 154               | 7.10E-01 | 60.27 |
| 155               | 5.31E-01 | 60.65 |
| 156               | 4.43E-01 | 61.04 |
| 157               | 3.65E-01 | 61.43 |
| 158               | 2.66E-01 | 61.81 |
| 159               | 1.95E-01 | 62.19 |
| 160               | 1.51E-01 | 62.57 |
| 161               | 1.15E-01 | 62.95 |
| 162               | 8.86E-02 | 63.34 |
| 163               | 7.09E-02 | 63.71 |
| 164               | 5.31E-02 | 64.09 |
| 165               | 4.39E-02 | 64.47 |
| 166               | 3.54E-02 | 64.85 |

TABLE IX: Fission Product Yields per 100 Fissions for $^{255}$Fm: thermal neutron induced fission.
| A  | Chain Yield (%) | Average Z |
|----|-----------------|-----------|
| 167| 2.66E-02        | 65.23     |
| 168| 1.77E-02        | 65.61     |
| 169| 1.51E-02        | 65.99     |
| 170| 1.24E-02        | 66.37     |
| 171| 8.86E-03        | 66.75     |
| 172| 7.08E-03        | 67.13     |

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