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New Global Calculation of Nuclear Masses and Fission Barriers for Astrophysical Applications

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Abstract. The FRDM(1992) mass model [1] has an accuracy of 0.669 MeV in the region where its parameters were determined. For the 529 masses that have been measured since, its accuracy is 0.46 MeV, which is encouraging for applications far from stability in astrophysics. We are developing an improved mass model, the FRDM(2008). The improvements in the calculations with respect to the FRDM(1992) are in two main areas. (1) The macroscopic model parameters are better optimized. By simulation (adjusting to a limited set of now known nuclei) we can show that this actually makes the results *more* reliable in new regions of nuclei. (2) The ground-state deformation parameters are more accurately calculated. We minimize the energy in a four-dimensional deformation space ($\varepsilon_2, \varepsilon_3, \varepsilon_4, \varepsilon_6$) using a grid interval of 0.01 in all 4 deformation variables. The (non-finalized) FRDM (2008-a) has an accuracy of 0.596 MeV with respect to the 2003 Audi mass evaluation before triaxial shape degrees of freedom are included (in progress). When triaxiality effects are incorporated preliminary results indicate that the model accuracy will improve further, to about 0.586 MeV.

We also discuss very large-scale fission-barrier calculations in the related FRLDM (2002) model, which has been shown to reproduce very satisfactorily known fission properties, for example barrier heights from ^{70}Se to the heaviest elements, multiple fission modes in the Ra region, asymmetry of mass division in fission and the triple-humped structure found in light actinides. In the superheavy region we find barriers consistent with the observed half-lives. We have completed production calculations and obtain barrier heights for 5254 nuclei heavier than $A = 170$ for all nuclei between the proton and neutron drip lines. The energy is calculated for 5 009 325 different shapes for each nucleus and the optimum barrier between ground state and separated fragments is determined by use of an “immersion” technique.

Keywords: Nuclear Masses, Fission Barriers
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INTRODUCTION

We discuss a new global calculation of ground-state (gs) and fission-barrier nuclear-structure data. The gs calculation includes nuclear masses, deformation parameters, and spins of odd-even nuclei. We also give some details of a very large-scale calculation of fission barriers for 5254 heavy nuclei. Some aspects of the calculations were reported at the *International Conference on Nuclear Data and Technology, April 22–27, 2007, Nice* [2]. We present here additional results that are new since that meeting. We use the macroscopic-microscopic method; full details of the model are found in Refs. [1, 3, 4].

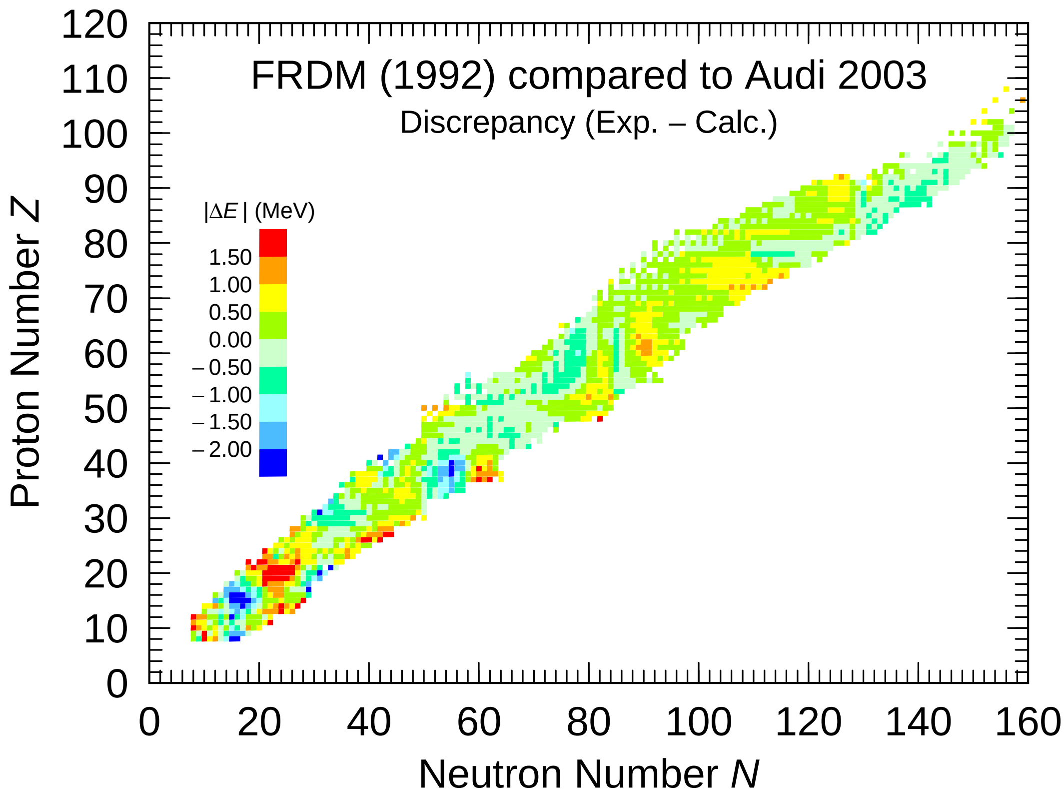

FIGURE 1. Difference between the Audi 2003 mass evaluations and the FRDM (1992) mass table. No systematic divergence far from stability is observed.

MASS AND FISSION-BARRIER CALCULATIONS

A goal for a theory of nuclear masses is that it be able to accurately predict masses of nuclei for which no measured values are available. Data for unknown nuclei are needed in many simulations; one example is simulations of the r-process. Our FRDM (1992) which was finalized in 1992 and published in 1995 [1], was adjusted to a 1989 data base of nuclear masses [5]. We have since compared it to nuclear masses measured after 1989. There are 529 such masses in the Audi 2003 mass evaluation [6]. The model accuracy for these *predicted* nuclear masses is 0.46 MeV; much better than in the region where the model parameters were adjusted, see discussion in [2]. In Fig. 1 we compare calculated masses to the *entire* Audi 2003 evaluation, that is the 529 nuclei measured since 1989 are also included. They are mainly located along the upper and lower edges of the plotted region, that is towards the neutron and proton drip lines. In Fig. 2 we show a similar plot for the HFB-8 mass model [7]. This model exhibits larger staggering between odd and even nuclei (a problem that may have been improved in later model versions) and, in the heavy regions, a more systematic variation in the error between the proton and neutron drip lines.

We have now improved the FRDM (1992) mass model. Successive improvements are

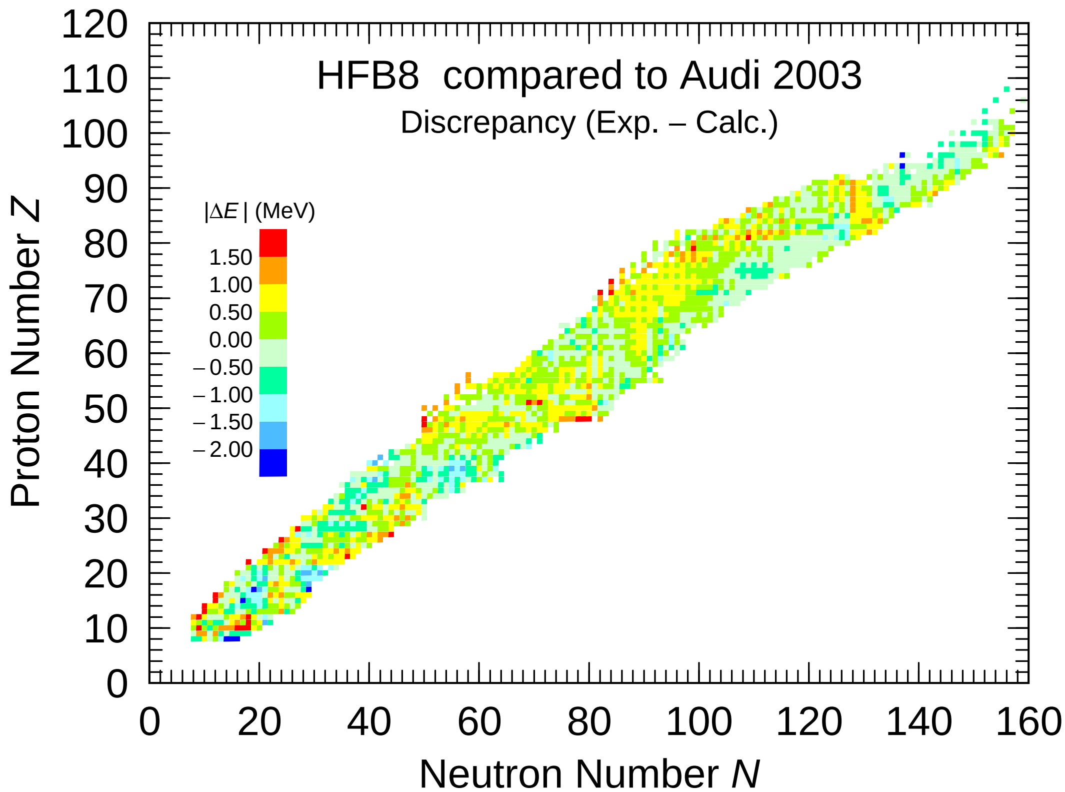

FIGURE 2. Difference between the Audi 2003 mass evaluations and the HFB-8 mass table.

listed in table 1. The first three lines show the published FRDM (1992) compared to the data set to which it was adjusted (Audi 1989, labeled "1"), the totality of masses in the most recent mass evaluation (Audi 2003, labeled "2") and new masses in A2003 relative to A1989 (labeled "3"). Because of a 100 000 fold increase in computer power since the FRDM (1992) calculation was carried out we can now considerably refine the calculation. On line 4 (92-a) we show the result of a better optimization of the constants to the 1989 data set. Line 5 compares this better optimized model to the 529 new masses. It is interesting to note that the better optimized model has better predictive power (0.42 MeV versus 0.46 MeV)! Line 6 compares to the entire 2003 data set. The next three lines (92-b) differ only in that fission barriers are not included in the adjustment. We have earlier [8, 3, 4] observed that the FRDM should not be applied to fission barriers. The next line (06-a) shows the effect of adjusting the model parameters to the 2003 data set. The model is extraordinarily stable, its accuracy only changing by 0.0017 MeV.

In our 1992 mass calculation [1] the determination of the ground-state deformation was carried out by interpolation in a coarsely spaced grid in the two deformation coordinates ε_2 and ε_4; ε_3 and ε_6 were studied only approximately (see [1]). Here we considerably refine this calculation, by studying the stability of *all* minima found in the limited-space potential-energy-surface calculations in a full 4D deformation space in the coordinates ε_2, ε_3, ε_4 and ε_6. We use a grid with a grid interval 0.01 in all 4

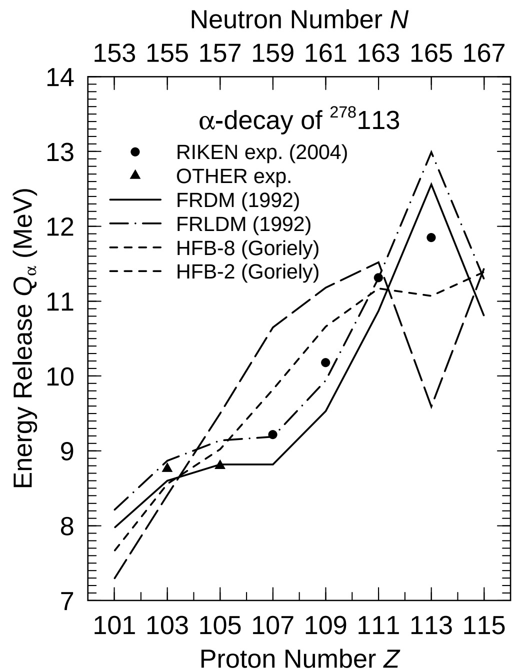

FIGURE 3. Calculated and observed Q_α values in the α-decay of element ^{278}113. See the discussion in the text.

deformation parameters. We start by calculating a 4D "cube" around a minimum found in the previous mass calculation in 2D ε_2-ε_4 space [1]. Such a cube consists of 81 grid points, 80 of them on the surface of the cube. The lowest energy will be for a point on the surface of this cube, unless the initial point determined from the limited 2D calculation

TABLE 1. FRDM (1992) and successive enhancements, compared to different data sets. The first column indicates a model designation, the second which data set the model was Adjusted/Compared to, and the last two columns the mean deviation and the model accuracy. In column 2 "1", "2", and "3" stand for the Audi 1989 mass evaluation [5], the Audi 2003 mass evaluation [6], and masses that are in the 2003 evaluation but not in the 1989 evaluation ("new" masses), respectively. The model constants are given in the middle section. The top line gives the original model constants [1].

Model	A/C	a_1	a_2	J	Q	a_0	c_a	C	γ	μ_{th}	$\sigma_{th;\mu=0}$
(92)	1/1	16.247	22.92	32.73	29.21	0.00	0.436	60	0.831	0.0156	0.6688
(92)	1/3									0.1755	0.4617
(92)	1/2									0.0607	0.6314
(92)-a	1/1	16.245	23.02	32.22	30.73	−2.24	0.465	104	0.927	0.0000	0.6614
(92)-a	1/3									0.0174	0.4208
(92)-a	1/2									0.0114	0.6180
(92)-b	1/1	16.286	23.37	32.34	30.51	−5.21	0.468	179	1.027	0.0000	0.6591
(92)-b	1/3									0.0031	0.4174
(92)-b	1/2									0.0076	0.6157
(06)-a	2/2	16.274	23.27	32.19	30.64	−5.00	0.450	169	1.000	0.0000	0.6140
(07)-a	2/2	16.231	22.96	32.11	30.83	−3.33	0.460	119	0.907	0.0000	0.5964

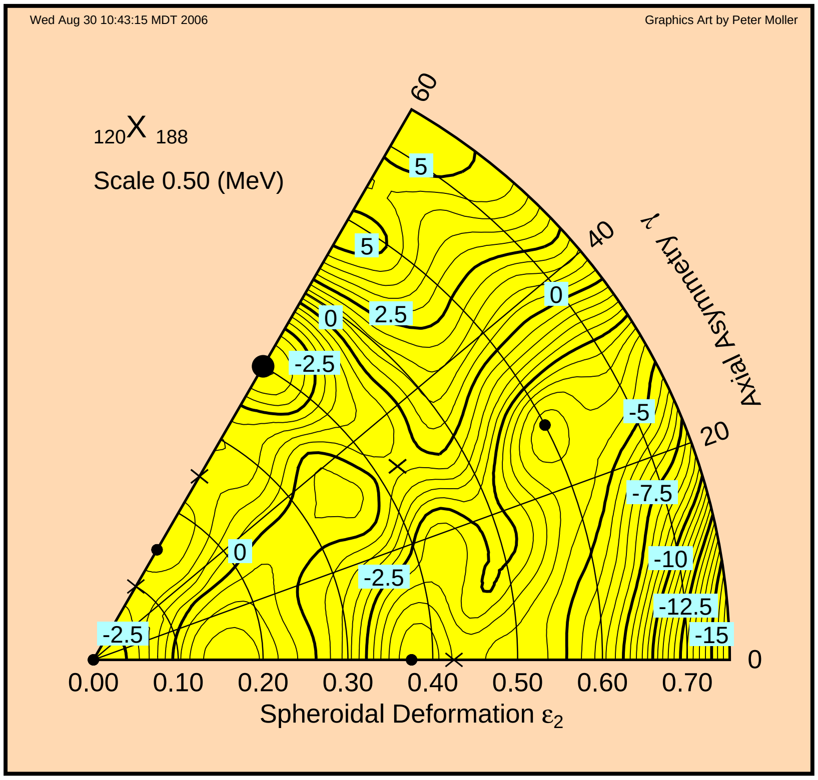

FIGURE 4. Calculated potential-energy surface for $^{308}120$. The filled dots indicate local minima, the x symbols significant saddles. The large filled dot designates the ground state. Although this minimum is not the lowest minimum it has the highest saddle with respect to fission and is therefore considered to be the ground-state minimum.

accidentally turns out to be the location of the local minimum. If not, we construct a new 4D cube around the point corresponding to the lowest energy on the surface of the initial cube, taking care not to recalculate energies that are already calculated. We continue in this fashion until the lowest-energy point is *not* on the surface of the last cube investigated. It is then the interior point in this last cube that is the minimum in the full 4D space. We investigate all the minima found in the 2D space in this fashion. However, we found that sometimes there exists one minimum for $\varepsilon_3 = 0$ and another at $\varepsilon_3 \approx 0.1$. separated by a low ridge. We therefore repeat the search for minima with the above starting points, except $\varepsilon_3 = 0.1$ in all the starting points. The lowest of the 4D minima is the optimum choice for the ground state, with the exception that for heavy nuclei the stability with respect to fission needs to be investigated as discussed below.

This refined calculation improves the accuracy of our original study to 0.596 MeV, (07)-a in Table 1. We can anticipate that including axial asymmetry effects [9] will further improve the accuracy to about 0.586 MeV. In our work we include essential refinements that in practice are not possible to consider in self-consistent Hartree-Fock calculations. To illustrate one issue, we show in Fig. 3 a comparison of calculated and observed Q_α values for the first $^{278}113$ decay chain that was observed at RIKEN. The cusp at $N = 165$ in the FRDM and FRLDM models occurs because of a change in gs deformation from deformed to spherical. In the HFB-8 calculation the cusp occurs because of a deformation change from $\beta_2 = 0.21$ to $\beta_2 = 0.42$ However, although the more deformed minimum is the lowest found in the HFB-8 calculation, our experience tells us that it will have a very low barrier with respect to fission. Therefore the higher-energy, less deformed minimum should be tabulated as the "ground state". We illustrate further this issue in Fig. 4 in a potential-energy plot for $^{308}120$. The deepest axially symmetric minimum is at $\varepsilon_2 = 0.375$ with $E \approx -4.7$ MeV. However, the barrier is only about 1 MeV high; the saddle is nearby at $\varepsilon_2 = 0.425$. Instead we need to designate the minimum with the highest barrier with respect to fission as the ground-state (an even more sophisticated approach would be to calculate the half-life with respect to all decay modes for all minima, but we do not take this step here). This model leads us to assign the minimum at $\varepsilon_2 = 0.40$ and $\gamma = 60$ and $E \approx -4.1$ MeV as the ground state. Equivalently, the ground state is oblate with $\varepsilon_2 = -0.40$. The saddle is at $\varepsilon_2 = 0.425$ and $\gamma = 32.5$ and $E \approx -0.25$ MeV. The barrier with respect to fission is about 3.9 MeV. We have for all nuclei in our mass studies (and fission-barrier studies) used a water-immersion technique to assign the ground-state to the correct minimum. So far HFB mass calculations do not use such techniques and must therefore be considered unreliable for heavy nuclei.

We have calculated fission potential-energy surfaces for 5254 nuclei from $A = 170$ to $A = 330$. For each nucleus the energy is calculated for 5 009 325 different shapes in a 5-dimensional deformation space. From these calculations we can determine all minima, saddle points between minima, valleys leading to different scission configurations (that is, different fission *modes*), ridge heights between valleys, and the distinctly different saddle points that provide the entry doorways to the different fission modes. Triaxial shapes were studied in the vicinity of the first barrier peak in a 3D calculation. We are in the process of tabulating these results. Our calculations agree well with various observed fission properties in the heavy- and superheavy-element regions. For example, we obtain 4 to 6 MeV barriers for the new elements between $Z = 107$ and $Z = 113$ that were observed in cold-fusion reactions. Barriers of this magnitude are required so that the fission half-lives are sufficiently long to be compatible with the observed half-lives, which are in the range μs to ms. This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

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