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Fission in R-processes Elements (FIRE) - Annual Report: Fiscal Year 2017

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Fission in R-processes Elements (FIRE)

Annual Report: Fiscal Year 2017

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Project Summary

The goal of the FIRE topical collaboration in nuclear theory is to determine the astrophysical conditions of the rapid neutron capture process (r-process), which is responsible for the formation of heavy elements. This will be achieved by including in r-process simulations the most advanced models of fission (spontaneous, neutron-induced, beta-delayed) that have been developed at LLNL and LANL. The collaboration is composed of LLNL (lead) and LANL for work on nuclear data (ground-state properties, fission, beta-decay), BNL for nuclear data management, and the university of Notre Dame and North Carolina State University for r-process simulations. Under DOE/NNSA agreement, both universities receive funds from the DOE Office of Science, while national laboratories receive funds directly from NA221.

Project Achievements: FY2017

Microscopic Approach to Nuclear Data (LLNL)

The goal for this part of the project is to lay the foundations of a consistent description of nuclear data properties within nuclear density functional theory (DFT). The same energy density functional (EDF) used to compute ground-state properties can also be used to determine beta-decay rates within the QRPA approach; spontaneous fission probabilities by multidimensional quantum tunneling through large-scale potential energy surfaces at the WKB approximation; fission fragment distributions from the time-dependent generator coordinate method (TDGCM).

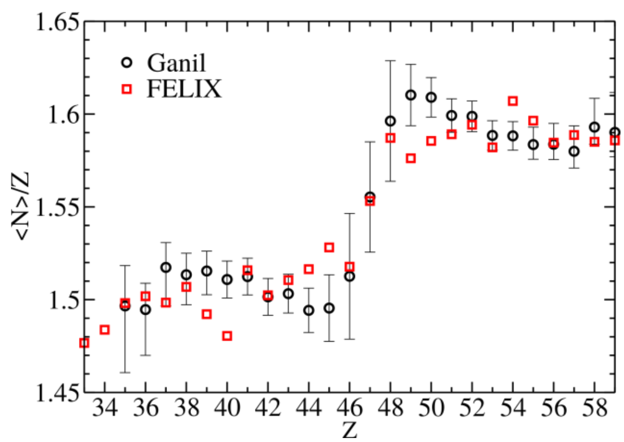

Figure 1 – Average number of neutrons per element among the fission fragments in the neutron-induced fission of ^{239}Pu. Calculations (red squares) were obtained with the SkM oarametrization of the Skyrme energy density functional.*

FIRE PI Nicolas Schunck has used the newly released versions of the DFT solvers HFBTHO and HFODD, and of the TDGCM solver FELIX to validate and benchmark fission product yields in actinides, see Figure 1. FIRE summer student Evan Ney (UNC Chapel Hill, supervisor: Jon Engel) has developed a workflow (written in Python) to generate efficiently potential energy surfaces calculations with HFBTHO. This workflow is being tested and will be used starting in FY18 to initiate the calculation of two-dimensional potential energy surfaces for all nuclei larger than Lead that are involved in the r-process.

Nuclear Data and Applications (LANL)

The goal for this part of the project is to generate global tables of nuclear data usable in r-process simulations. Nuclear data include ground-state properties (proton and neutron separation energies, Q-values for α- and β-decay), fission rates, spectrum and fragment distributions, and beta-decay rates. The overall theoretical approach for nuclear structure is based on the macroscopic-microscopic model. Fission fragment distributions are computed from a semi-microscopic approach derived from Langevin dynamics. The fission spectrum is computed in the Hauser-Feshbach theory. β-decay rates are computed in the QRPA approach with a phenomenological residual interaction.

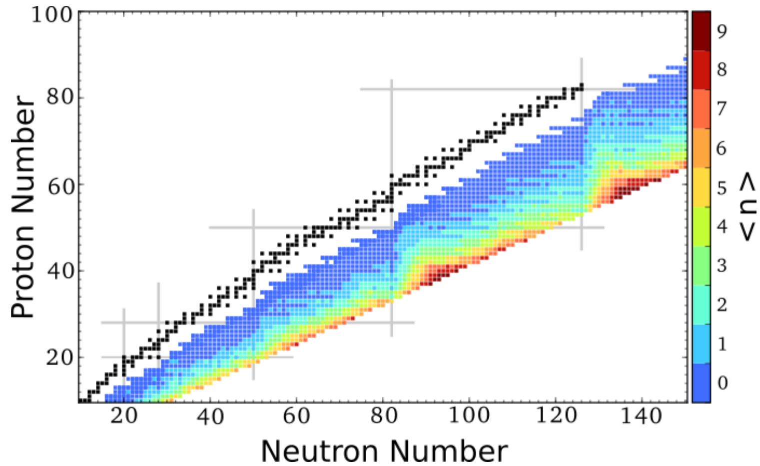

Figure 2 – Realistic calculation based on QRPA+Hauser-Feshbach formalism of the average number of neutrons emitted after β-decay for all elements in the nuclear chart.

FIRE postdoc Matthew Mumpower (LANL) studied the competition between the various decay modes of the very neutron-rich nuclei involved in the r-process. For the first time, all decay channels (neutron emission, γ emission, β-decay rate and β-delayed fission, spontaneous and neutron-induced fission) were considered simultaneously. This was possible thanks to advanced modeling of nuclear decay with Hauser-Feshbach theory, which can predict the average number of neutrons emitted in each decay; see Figure 2. Mumpower showed that for typical r-process in a neutron star merger scenario, β-delayed fission plays a critical role in determining the decay of heavy elements; see Figure 3. This work will be submitted to PRL.

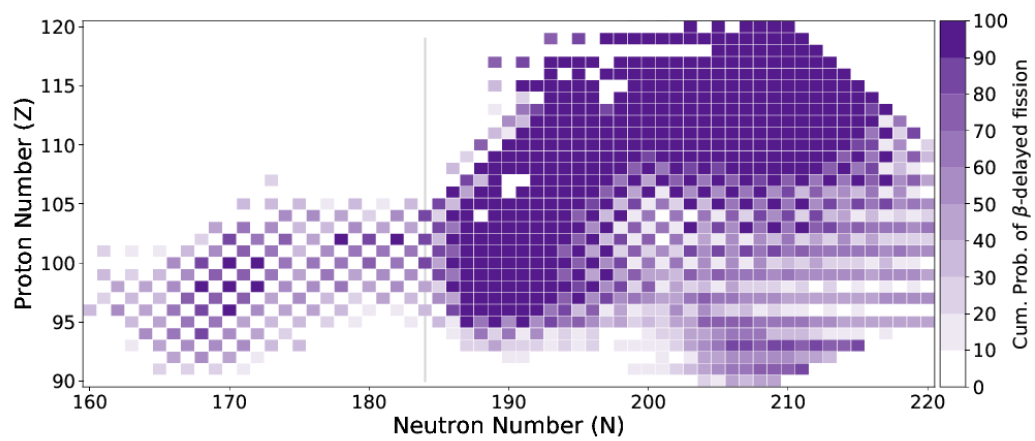

Figure 3 - Fission probability of heavy, neutron-rich elements after being formed by β-decay (β-delayed fission)

FIRE staff Anna Hayes-Sterbenz (LANL) quantified the uncertainty in the fission antineutrino spectra due to the uncertainty in the one-body weak magnetism correction to nuclear β-decay rates. This work is an important step in determining if the neutrino reactor anomaly is caused by physics beyond the standard model or by incorrect evaluations of β-decay of fission fragments.

Astrophysical Simulations (ND, NCSU)

FIRE postdoc Nicole Vassh (ND) has begun extensions of the nuclear physics reverse-engineering work (see J. Phys. G **44**, 034003 (2017)). The goal is to use the features of the rare-earth peak of the solar r-process abundance pattern to deduce the (still unknown) nuclear masses required to produce it, given a particular set of astrophysical conditions. Vashh validated her approach by comparing the predictions of nuclear masses from this reverse-engineer approach to standard mass evaluations and recent measurements at the CARIBU facility at ANL, see Figures 4 and 5. She demonstrated that this method can produce reliable constraints on the value of nuclear masses for nuclei far from stability. In a second, related project, Vashh and ND graduate student Erika Holmbeck have incorporated various mass models as well as empirical and semi-empirical fission yield models to analyze the influence of fission yields on r-process abundance patterns. They identified nuclei that provide a robust fission flow.

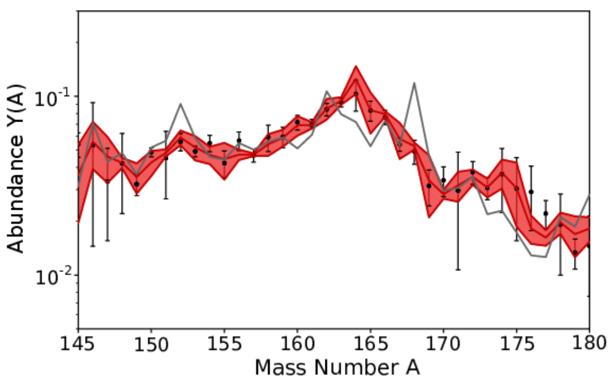

Figure 4 - Abundances of elements near the rare-earth peak obtained with the Duflo-Zuker mass formula (in grey) and for the reversed-engineered masses (red band).

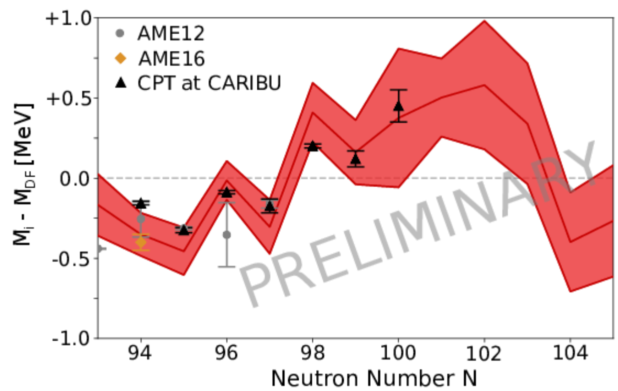

Figure 5 - Deviations between reverse-engineered masses and Duflo-Zuker mass formula for Nd (Z=60) isotopes. Comparisons with Atomic Mass Evaluations from 2012 and 20016 and recent measurements at CARIBU are also shown

FIRE graduate student Yonglin Zhu has begun studying how the matter-neutrino resonance (MNR) effect affects the r-process in neutrino-driven winds occurring during a neutron-star merger. Due to the considerable number of neutrinos and electrons present during the merger, large numbers of neutrino-electron interactions can occur resulting in flavor oscillations of neutrinos, hence changes in electron fraction Ye. This, in turns, affect the abundance pattern in r-process simulations.

R-process simulations in the FIRE collaboration are performed with the recently completed version 1.0 of PRISM (Portable Routines for Nucleosynthesis Modeling). PRISM is a new nuclear reaction network code that can include in r-process simulations full information on the charge and mass distributions of fission fragments. Development of PRISM is led by Matthew Mumpower and ND graduate student Trevor Sprouse.

Data Management and Web Interface (BNL)

FIRE member Alejandro Sonzogni has designed and implemented a website for the FIRE collaboration, http://www.nndc.bnl.gov/fire/. The website features public pages describing the collaboration, its structure and its members, and giving access to standard metrics (publications, talks). The website also contains a password-protected section for internal use by members of the collaboration. This internal section is used as a repository of talks given at the annual meeting, of quarterly and annual reports, and provide web forms to populate the publication and talks database.

Metrics

Publications (Cumulative)

1. M.R. Mumpower, T. Kawano, J.L. Ullmann, M. Krtička, and T. M. Sprouse, "*Estimation of M1 scissors mode strength for deformed nuclei in the medium- to heavy-mass region by statistical Hauser-Feshbach model calculations*," In press in Phys. Rev. C [arXiv:1706.07504]
2. X. B. Wang and A. C. Hayes, "*Weak magnetism correction to allowed β-decay for reactor antineutrino spectra*", Phys. Rev. C **95**, 064313 (2017)
3. M. Mumpower, T. Kawano, P. Möller, "*Neutron-gamma competition for β-delayed neutron emission*", Phys. Rev. C **94**, 064317 (2016)

Talks (Cumulative)

1. G. C. McLaughlin, "*Neutrino flavor transformation in compact object mergers and reverse engineering the rare earth peak*", INT, Seattle, August 2017
2. R. Surman, "*Nuclear physics inputs for nucleosynthesis*", review talk, INT-17-2b Electromagnetic Signatures of r-Process Nucleosynthesis in Neutron Star Binary Mergers, Institute of Nuclear Theory, Seattle, WA, July 2017
3. P. Jaffke, "*Implementing and testing theoretical fission fragment yields in a Hauser-Feshbach statistical decay framework*", Scientific Workshop on Nuclear Fission Dynamics and the Emission of Prompt Neutrons and Gama Rays, Varna, Bulgaria, June 20-22, 2017
4. R. Surman, "*Nuclear masses and the site of r-process nucleosynthesis*", invited talk, Nuclear Physics in Astrophysics VIII, Catania, Sicily, June 2017
5. G. C. McLaughlin, "*Theory Initiatives*", NSAC Meeting, June 2017
6. R. Surman, "*Astrophysical Alchemy*", colloquium, Ball State University, Muncie, IN, April 2017
7. R. Surman, "*Astrophysical alchemy*", colloquium, Department of Physics, University of Washington in St. Louis, St. Louis, MO, March 2017
8. R. Surman, "*Neutron capture rates and r-process nucleosynthesis*", workshop talk, INT Program INT-17-1a: Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart, Seattle, WA, March 2017
9. G. C. McLaughlin, "*Stellar Explosions and Nucleosynthesis*", Colloquium, University of Tennessee, Knoxville, TN, February 2017
10. G. C. McLaughlin, "*Stellar Explosions and Nucleosynthesis*", Colloquium, Kent State, Kent, OH, February 2017
11. R. Surman, "*Nucleosynthesis and neutrino physics in compact object mergers*", invited talk, APS April Meeting, Washington, D.C, January 2017

Outlook for FY2018

During the annual meeting, the collaboration has decided to establish a benchmark for nuclear data calculations. The collaboration identified ^{270}Pu (Z=94, N=186) as a heavy, very neutron-rich nucleus with very robust fission channels in current r-process simulations. For this single nucleus, we will use both fully-microscopic and macroscopic-microscopic models to compute separation energies, spontaneous fission half-lives, spontaneous and neutron-induced fission fragment distributions, fission cross-sections, neutron spectrum and beta-decay rates. Work on this benchmark will start during FY17-Q4. One of the primary goals is compare predictions from fully microscopic and semi-microscopic calculations where both these methods are applicable. Another important benefit from using such a benchmark is to interface semi-microscopic models with DFT, and to obtain fixed-points for fully empirical fits.

Project Management

Administrative Summary

Under the call for proposal for topical collaborations, DOE requires an unincorporated consortium business model for the distribution of funds. The subcontract with ND was signed on 02/07/2017 and with NCSU on 03/13/2017. As of August 9, 2017, all funds from DOE were received by LLNL. Both ND and NCSU have begun billing LLNL for work performed under FIRE. As a reminder, FIRE supports a postdoc at the University of Notre Dame, a postdoc at LANL, a graduate student at NCSU and a summer student at LLNL. The remainder of the money is used to support staff in each of the participating institutions

The collaboration hired Nicole Vassh for the ND postdoc position, Marc Verriere for the LANL postdoc position, Yonglin Zhu as the NCSU graduate student and Evan Ney as the LLNL summer intern. Due to delays in establishing subcontracts, Vashh started work in February and Zhu only in May. Ney stayed at LLNL from May 29 to Aug. 12. Verriere will start work at LLNL in September 2017.

An initial kick-off meeting was organized at the University of Notre Dame Dec. 12-13, 2016. The goal of this kick-off meeting was for members of the collaboration to know each other and their respective research. LLNL hosted the first annual collaboration meeting between June 26-28, 2017. 14 participants from all 5 institutions attended.

Performance Summary

The milestones for FY2017 listed in the FIRE proposal are recalled below, together with a comment about their status

Milestone	Comment
Assemble and run nucleosynthesis estimates for a wide range of astrophysical models; Consider the impact of current nuclear data uncertainties on the r-process patterns produced and look for distinguishing characteristics of the patterns that stand out over the uncertainties.	Mostly done, manuscript in preparation. Collaborative work between ND and NCSU
Benchmark DFT+TDGCM calculation of neutron-induced FPY and fission rates for the ^{239}Pu(n,f) (even-mass compound nucleus) and ^{238}U(n,f) (odd-mass compound nucleus) reactions; initiate the DFT calculation of two-dimensional potential energy surfaces for all nuclei with Z > 82 from ground-state to scission with the UNEDF1 functional as reference.	Mostly done. Work by LLNL. Calculations of odd-mass nuclei require extension of the collective inertia formalism which is not finalized yet.
Study nuclear reactor anti-neutrino, especially discrepancies between calculations and experiments.	Done. Work by LANL
Benchmark macroscopic-microscopic β-decay calculations	Done. Work by LANL.

against decay heat and reactor neutrino calculations.	
Extend model of β-delayed fission to all fissioning systems.	Done. Work by LANL
Produce database of β-delayed neutron yields and validate it in calculations of r-process abundance patterns	Done. Collaborative work between LANL/ND/NCSU