Quantification of Uncertainties for Predictions of Fission Fragment Distributions

... and a few other things

Information and statistics in nuclear experiment and theory (ISNET-5)
York, UK
November, 8th 2017

Nicolas Schunck
Neutron-Induced Fission
What it is and why we should try to measure/compute

- Fission fragment distribution: probability (normalized to 200) to observe a given number of particles (=mass) in the fragments
- Depends on target, neutron incident energy
Applications of Induced Fission
Simulate reactor technology on a computer

- Critical assembly is small amount of fissile material (= fission as soon as hit by neutrons)
- Criticality (neutrons out = neutrons in) depends on geometry, composition, etc.
- Multi-physics problem
  - Material physics
  - Transport (of particles in material)
  - Nuclear physics
- Fission fragment distributions important input
Heavy elements are formed in nuclear reactions in neutron-rich environments

Various astrophysical scenarios:
- Recent LIGO-VIRGO observations confirm neutron star mergers option
- Other options (supernovae, black holes, etc.) not ruled out yet

Nuclear reaction networks combined with astrophysical models predict observed abundances
- Fission terminates r-process
- Fission cycling

Fission in Basic Science
Fission determines the relative proportion of elements in the universe
Theory of Induced Fission

Basic Concepts

- Simple idea (Bohr and Wheeler, 1939): Nucleus deforms itself until it breaks into two fragments

- Theorist’s job:
  - Predict how energy of the nucleus changes with deformation(s)
  - Predict the probability for the nucleus to have a given deformation
  - Relate characteristics of the fragments with deformation

- What makes it complicated
  - Ideally, only use basic constituents of nucleus (neutrons and protons) and their interaction
  - System is ruled by quantum mechanics, process is time-dependent, and other niceties
Theory of Induced Fission

A Few More Technical Details

- Theoretical framework is nuclear density functional theory
- Same energy functional gives potential energy surface and collective inertia (=resistance to motion in collective space)
- Time-dependent theory on top of DFT gives probability as function of time – and thus fragment yields
Theory of Induced Fission
Sources of Uncertainties

- Parameters of the energy density functional (about a dozen)
- Size of collective space = how many deformations (or other indicators) do you need to characterize fission?
- Recipe to compute collective inertia: most popular method relies on additional approximations
- Scission lines = the point/line/surface that separates the whole nucleus from split configurations
- Numerical precision of calculations at large deformations
- Initial probability in the collective space
  - No theory whatsoever about that
  - Focus on this talk
Model the initial probability distribution as a weighted sum of eigenvalues (known)

\[ g(q_2, q_3; t = 0) = \sum_{k} e^{-\frac{1}{2} \left( \frac{E_k - \bar{E}}{\sigma} \right)^2} g_k(q_2, q_3) \]
Baseline Calculation
We use the SkM* EDF
Design Runs
Sources of Uncertainties

- Vary $\sigma$ from 0.1 to 3 by step of 0.1
Emulator
Gaussian Process Model Trained on 18 Design Runs

- Relative error less than 2% (except at the boundary)
- Example for a yield of 5: 5.0±0.1
  - Smaller than experimental uncertainties
  - Smaller than numerical precision
Conclusions

- Fission product yields are outputs of complex workflows (2 different codes, computationally expensive PES, different sources of uncertainties)

- Short term outlook
  - Calibration phase requires likelihood function: how to define it?
  - Take experimental discrepancies into account?

- Longer-term outlook
  - Propagate uncertainties of EDF parameters
  - Size of design runs could be huge
  - Set up GPM for PES itself and plug in to emulator for time evolution
    - See talk by M. Shelley
    - Challenge: emulate discontinuities
We do not know how the heaviest elements are formed

- Heavy elements are formed by nuclear reactions involving rapid neutron capture (r-process) in stellar environments
- Exact astrophysical conditions of the r-process (neutron star merger? core-collapse supernova?) remain unknown must be tested by nucleosynthesis simulations

R-process abundances calculated in 3 different astrophysical scenario compared to solar abundances
r-process Sensitivity to Mass Models

- 10 mass models: DZ33, FRDM95, FRDM12, WS3, KTUY, HFB17, HFB21, HFB24, SLY4, UNEDF0

- Two distinct sets of astrophysical conditions:
  - **Cold** – n-rich merger outflow (Just 2015)
  - **Reheating** – n-rich “slow” ejecta from merger (Mendoza-Temis 2015)
Measured Decay Rates and Masses

NUBASE 2016
\(\beta\)-decay, \(\alpha\)-decay, and spontaneous fission

AME 2016 / Jyväskylä / CPT at CARIBU
Reverse Engineering r-process calculation

Astrophysical conditions
Fission Yields
Rates (n capture, $\beta$-decay, fission....)

Nucleosynthesis code (PRISM)

Markov Chain Monte Carlo (MCMC)
Likelihood function

Nuclear masses

Abundance prediction
MCMC evolution of a single run

- Monte Carlo mass corrections
  \[ M(Z, N) = M_{DZ}(Z, N) + a_N e^{-(Z-c)^2/2f} \]

- Check
  \[ \sigma^2_{\text{rms}}(M_{\text{AME12}}, M) \leq \sigma^2_{\text{rms}}(M_{\text{AME12}}, M_{DZ}) \]

- Update nuclear quantities and rates

- Perform nucleosynthesis calculation

- Calculate \( \chi^2 \)
  \[ \chi^2 = \sum_{A=150}^{180} \frac{(Y_{\odot,r}(A) - Y(A))^2}{\Delta Y(A)^2} \]

- Update parameters OR revert to last success
  \[ \mathcal{L}(m) = \exp \left( -\frac{\chi^2(m)}{2} \right) \quad \alpha(m) = \frac{\mathcal{L}(m)}{\mathcal{L}(m-1)} \]

- Black – solar abundance data
- Grey – AME 2012 data
- Red – values at current step
- Blue – best step of entire run
Rare Earth Peak with MCMC solutions
Results

- Astrophysical trajectory: hot, low entropy wind such as in a merger accretion disk
- 50 parallel, independent MCMC runs
- 21 runs in red band, 7 runs in orange band
- Average $\chi^2 \sim 20$ for red and orange solutions

Uncertainties in UNEDF1

- Uncertainty Quantification
  - Estimate model errors
  - Define predictive power
  - Extrapolate beyond experiment
- Bayesian inference methods
  - Posterior distribution available
    McDonnell et al. PRL 114 (2015) 122501
- Statistical uncertainties can be propagated
  - Inputs for r-process with UQ
  - Requires High Performance Computing
Abundance Patterns

- Neutron star merger
- 50 calculations of the same process
- Solar abundances
- Systematic uncertainties

Martin et al, PRL 116 (2016) 121101
The r-process informs DFT

Astrophysical data can constrain DFT parameters
DFT informs the r-process

UQ allows to discriminate between astrophysical scenarios
Effect of new data on uncertainties

- Upcoming neutron rich measurements
  - CERN, TRIUMF, GSI, RIKEN, FRIB, ...
- Two-fold reduction of uncertainty
  - Measured masses
  - Improving mass models
- Simulated mass tables assuming FRIB data
Anticipated improvements

Mass model, AME2016, Simulated FRIB