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

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LLNL-PRES-XXXXXX
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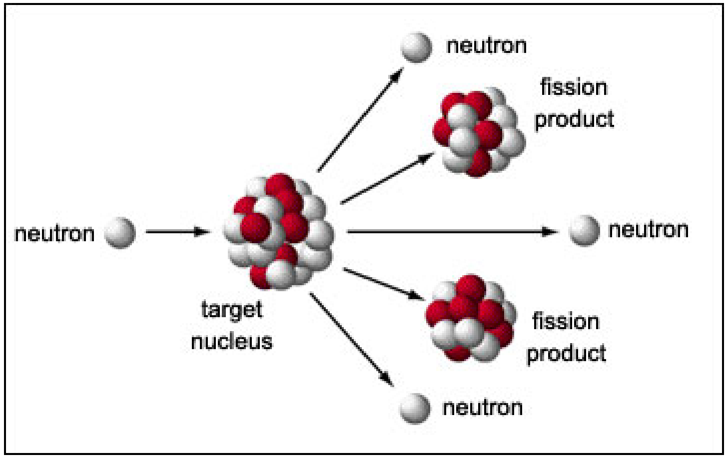
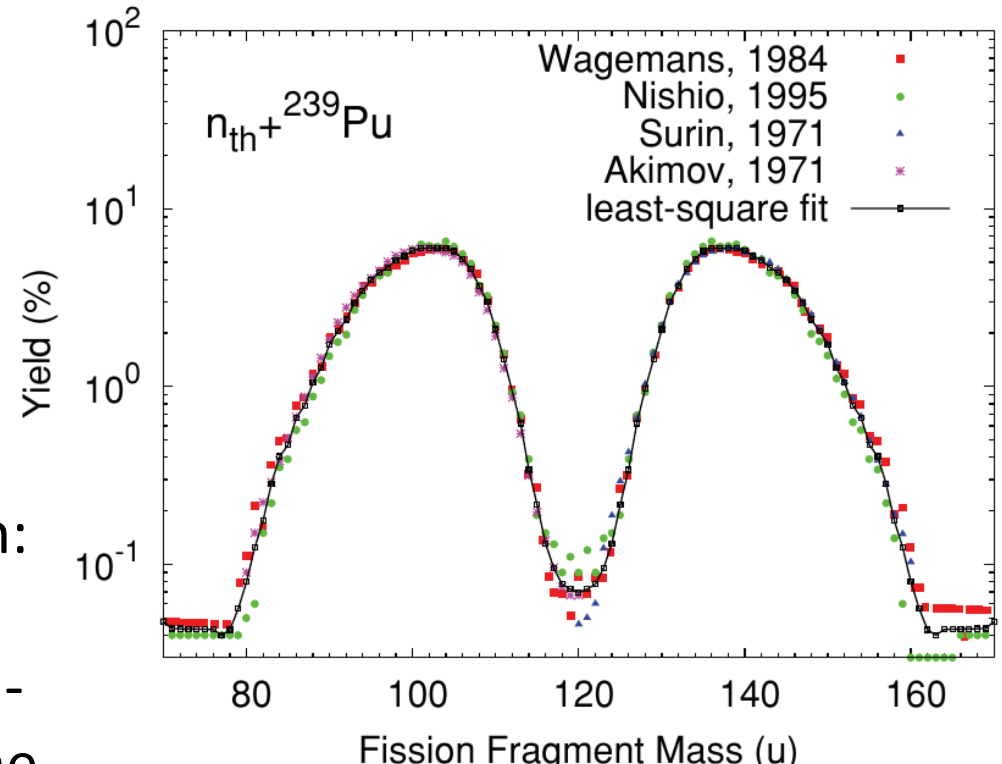
Neutron-Induced Fission

What it is and why we should try to measure/compute



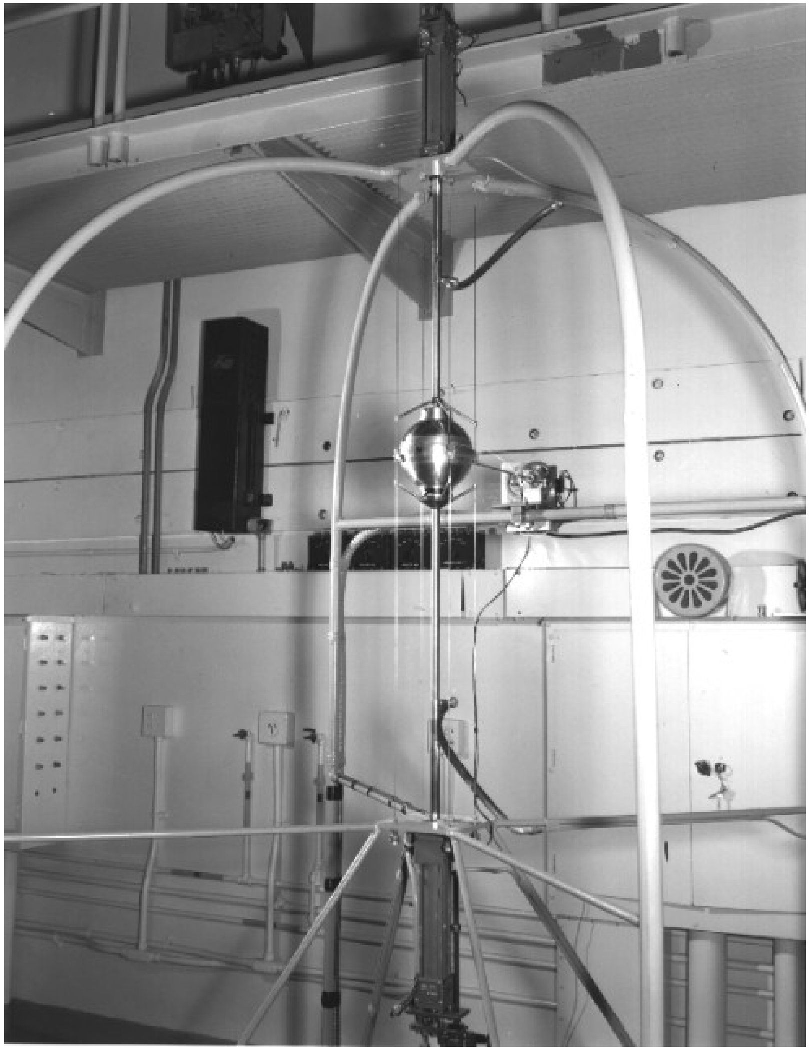


- Fission fragment distribution: probability (normalized to 200) to observe a given number of particles (=mass) in the fragments
- Depends on target, neutron incident energy

Applications of Induced Fission

Simulate reactor technology on a computer

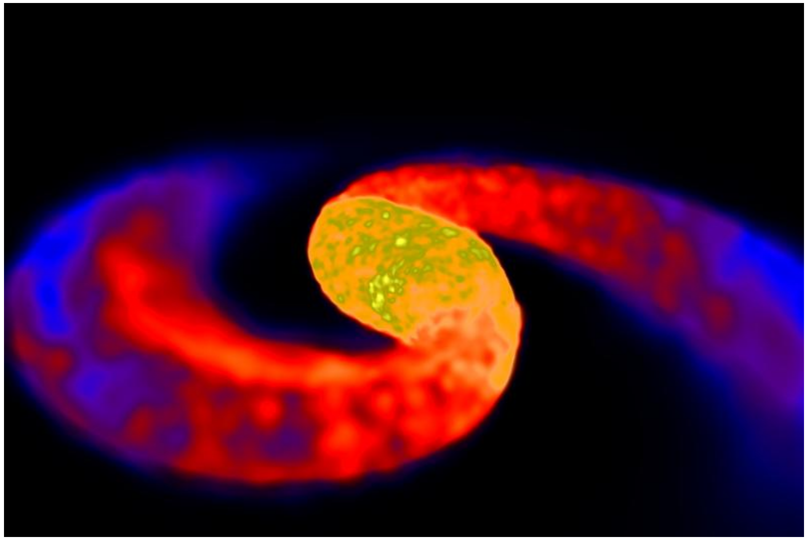
- Critical assembly is small amount of fissile material (= fission as soon as hit by neutrons)
- Criticality (neutrons out = neu-torns in) depends on geometry, composition, etc.
- Multi-physics problem
  - Material physics
  - Transport (of particles in material)
  - Nuclear physics
- Fission fragment distributions im-portant input

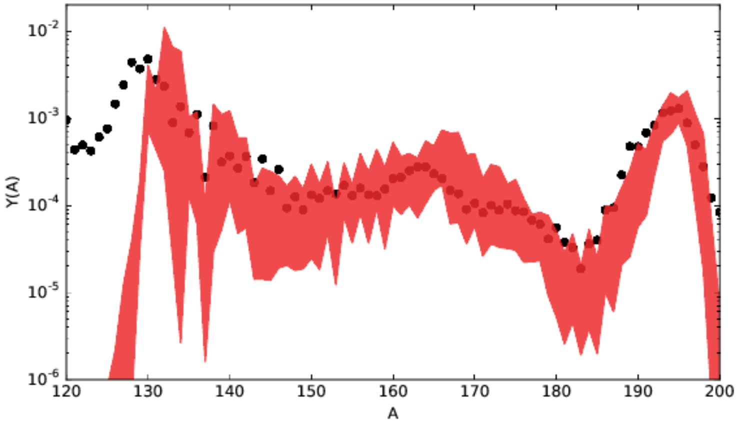


Fission in Basic Science

Fission determines the relative proportion of elements in the universe

- 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





Theory of Induced Fission

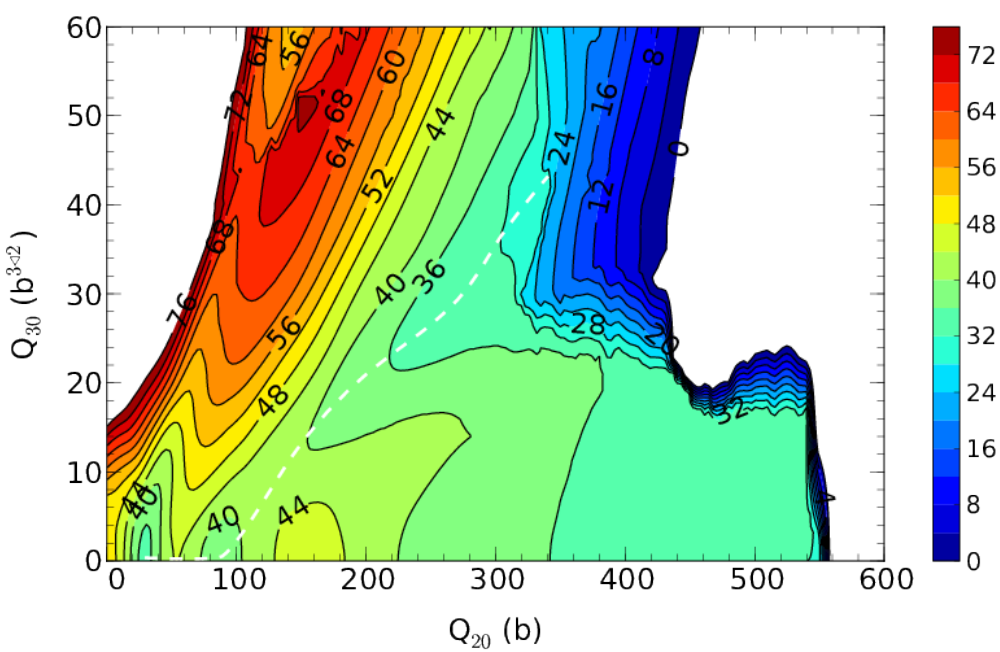
Basic Concepts

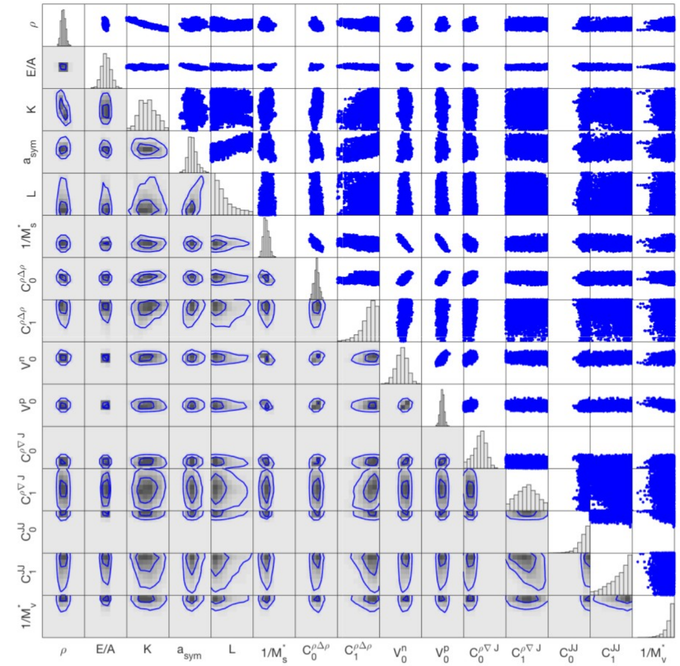
- Simple idea (Bohr and Wheeler, 1939): Nucleus deforms itself until it breaks into two fragments
- Theorist's job:
  - Predict how energy of the nucleus changes with deformation(s)
  - Predict the probability for the nucleus to have a given deformation
  - Relate characteristics of the fragments with 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

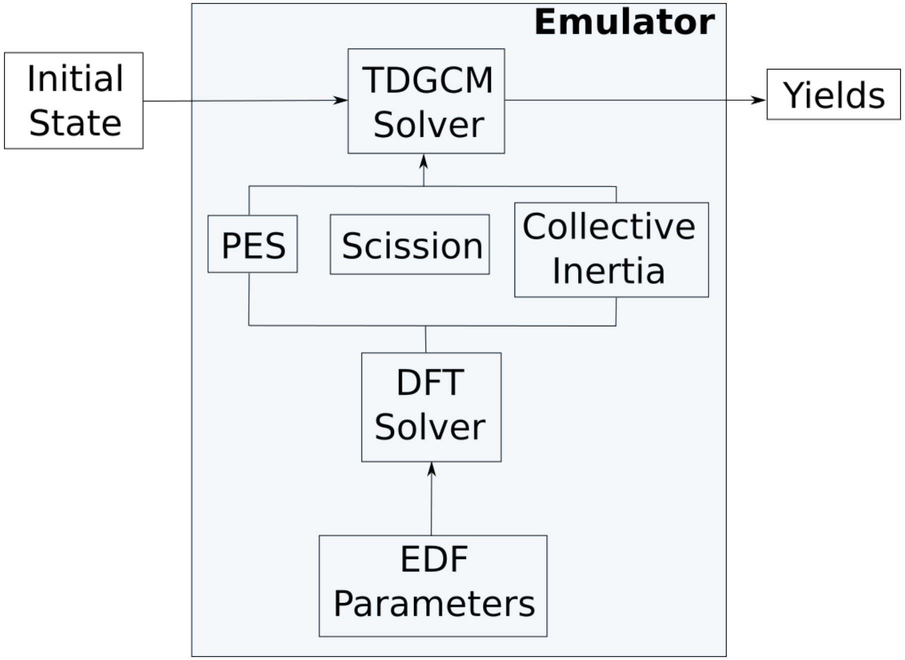
- Parameters of the energy density functional (about a dozen)
- Size of collective space = how many deformations (or other indicators) do you need to characterize fission?
- Recipe to compute collective inertia: most popular method relies on additional approximations
- Scission lines = the point/line/surface 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

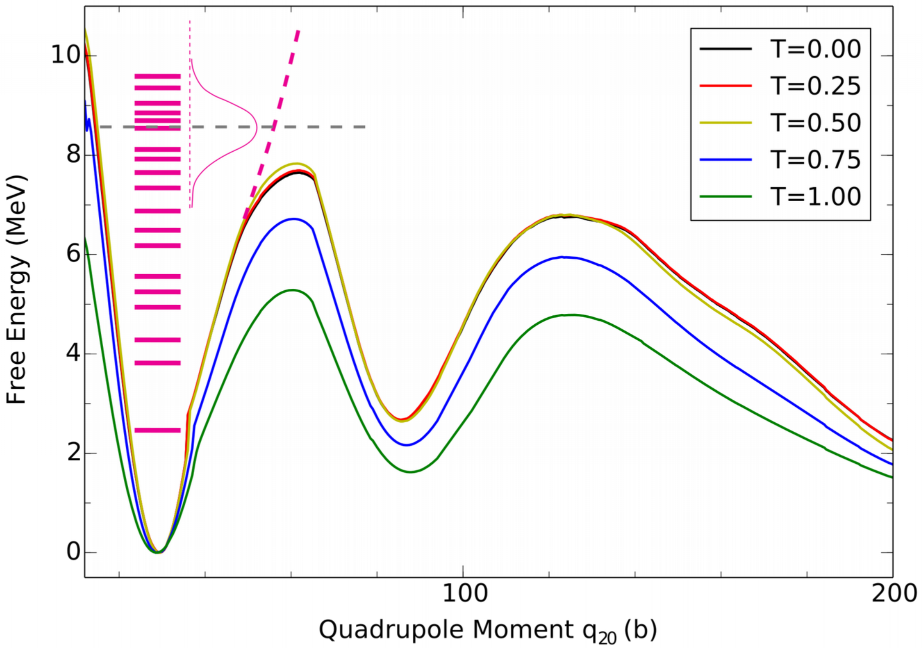
Initial State

A Simple One-Parameter Problem

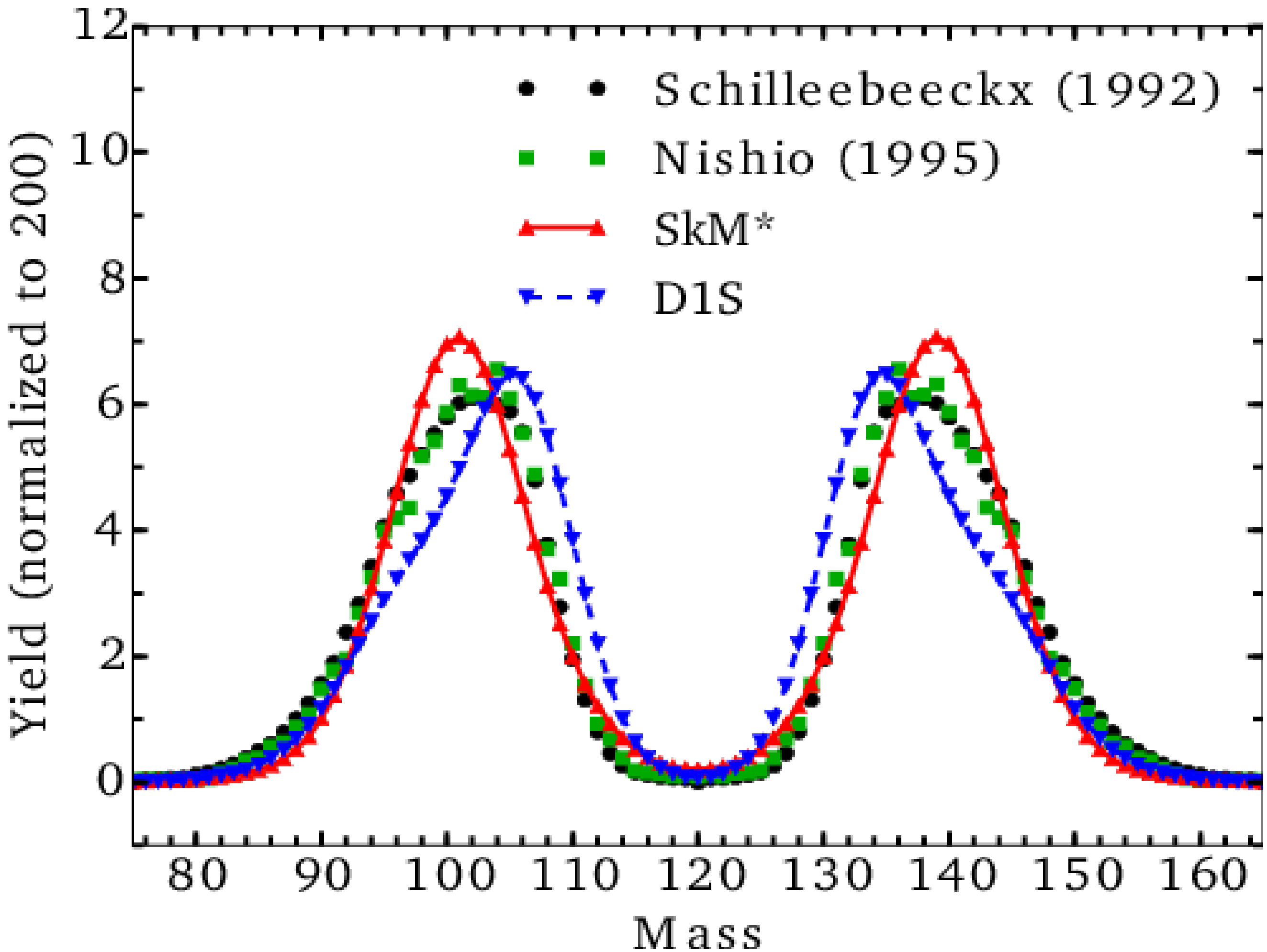
- Model the initial probability distribution as a weigted sum of eigenvalues (known)

$$g(q_2,q_3;t=0)=\sum_k e^{-\frac{1}{2}\left(\frac{E_k-\bar{E}}{\sigma}\right)^2} g_k(q_2,q_3)$$



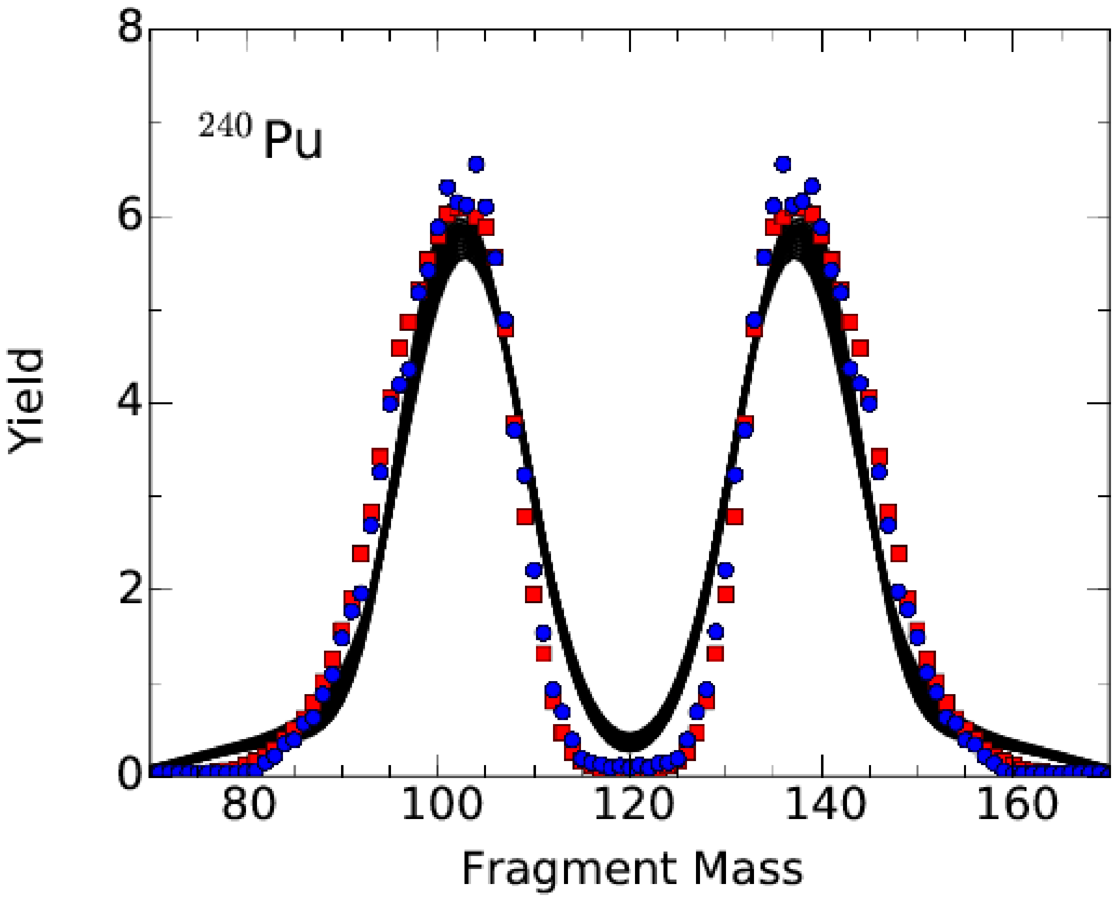


Baseline Calculation
We use the SkM* EDF



Design Runs
Sources of Uncertainties

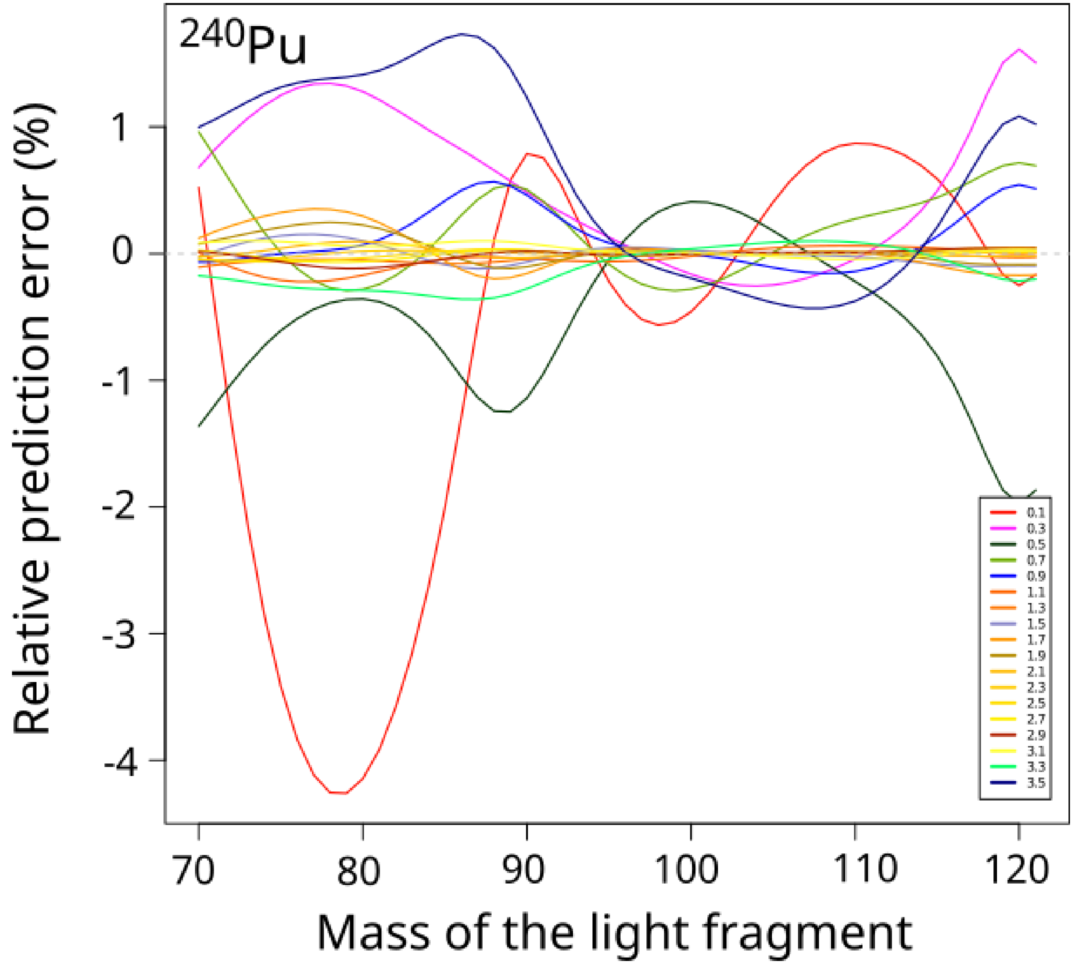
- Vary σ from 0.1 to 3 by step of 0.1



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

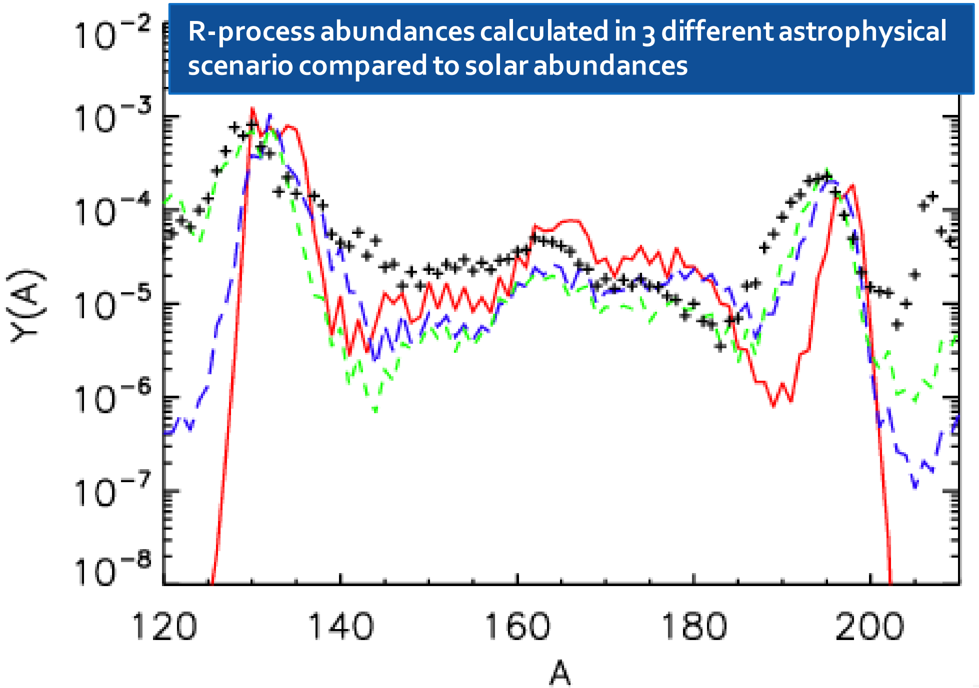


Conclusions

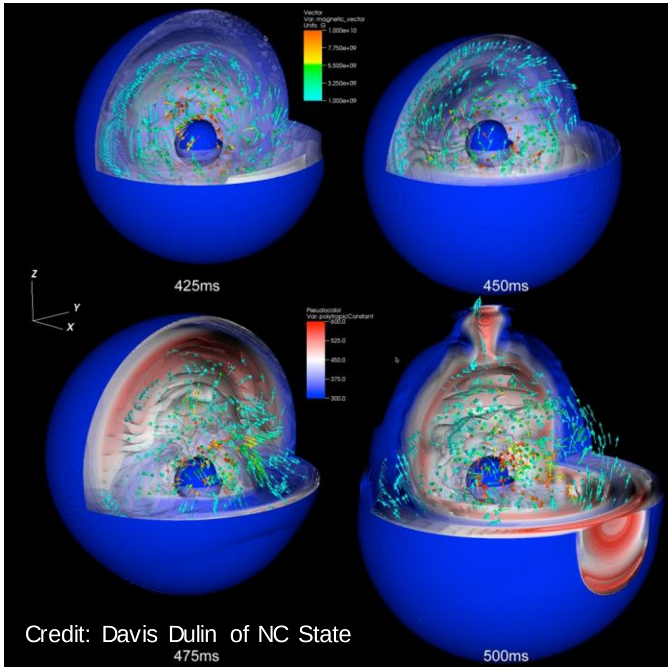
- Fission product yields are outputs of complex workflows (2 different codes, computationally expensive PES, different sources of uncertainties)
- Short term outlook
  - Calibration phase requires likelihood function: how to define it?
  - Take experimental discrepancies into account?
- Longer-term outlook
  - 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

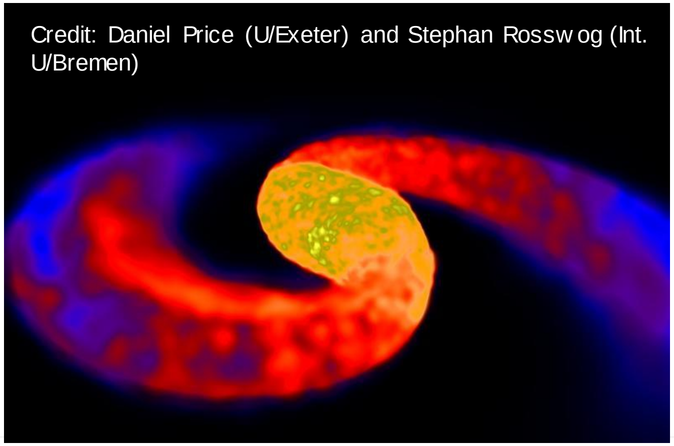
We do not know how the heaviest elements are formed

- 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





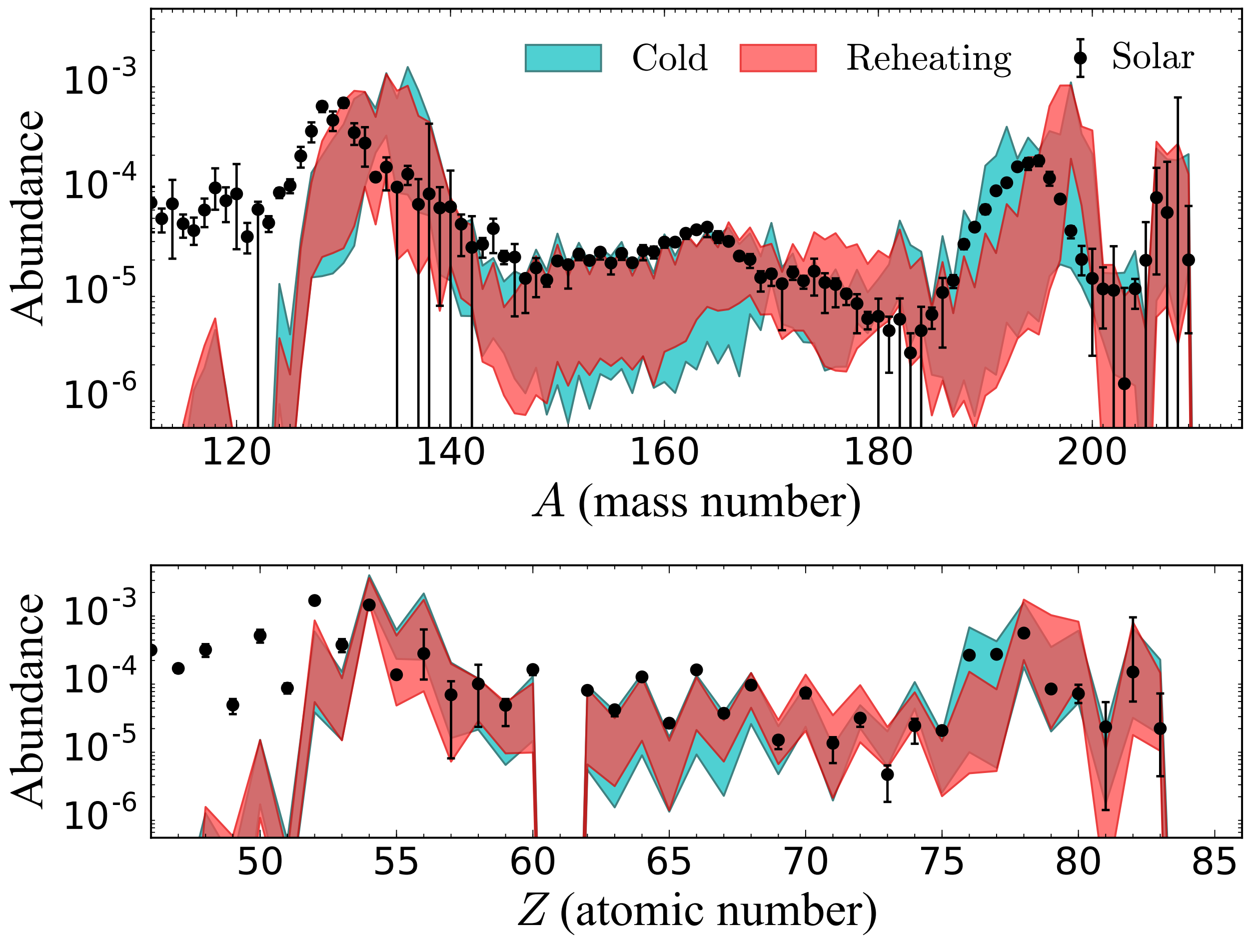
r-process Sensitivity to Mass Models

- 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)

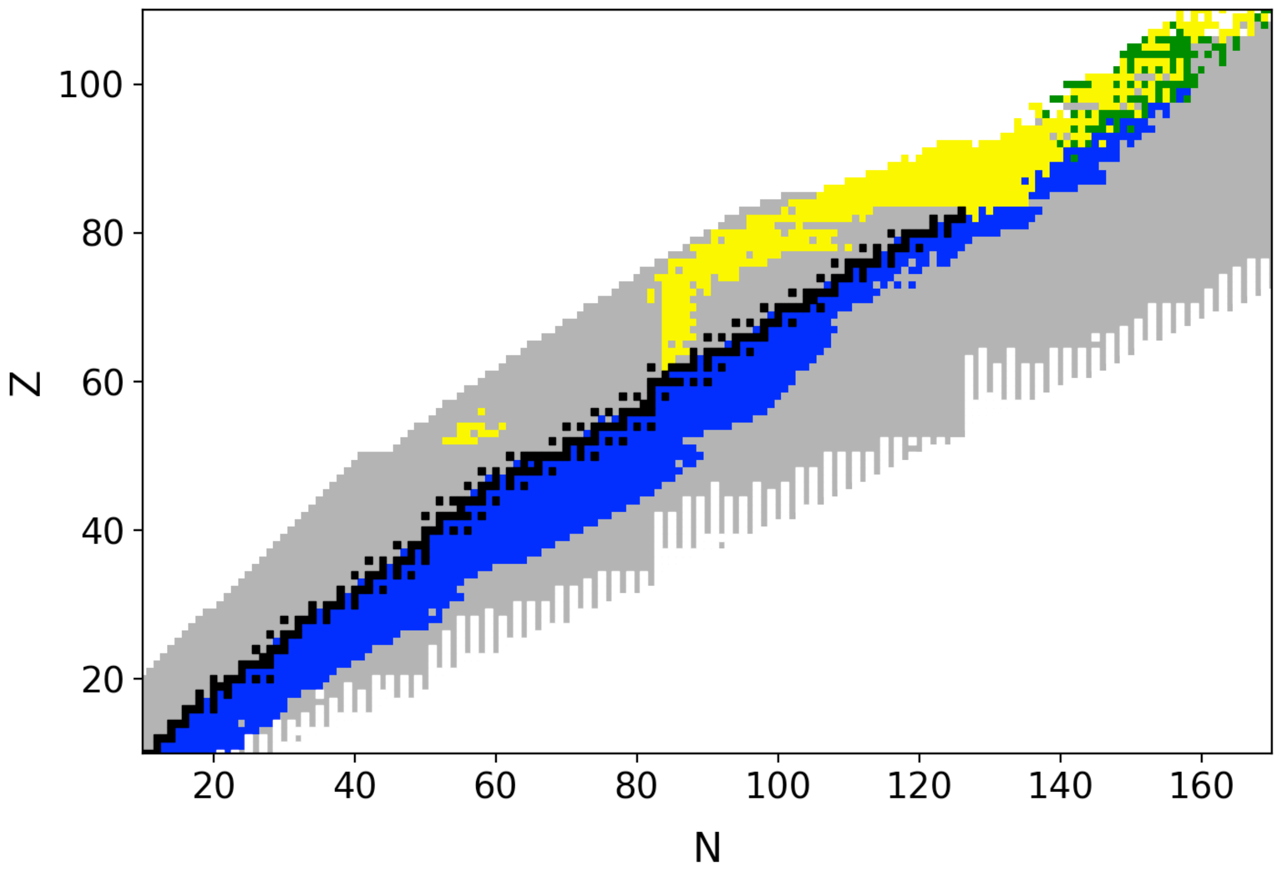


Côté et al (2017)

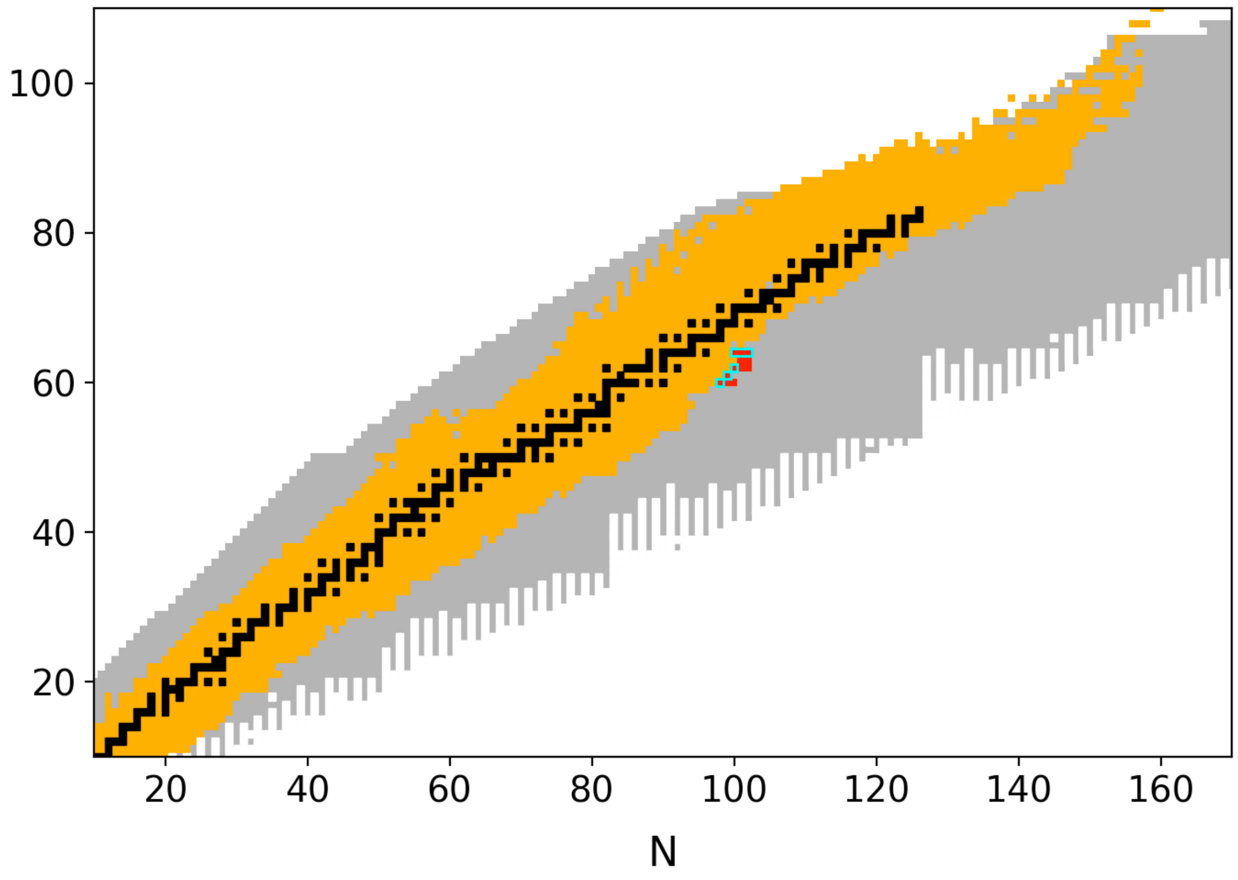
Measured Decay Rates and Masses

NUBASE 2016

β-decay, α-decay, and spontaneous fission



AME 2016 / Jyväskylä / CPT at CARIBU



Reverse Engineering r-process calculation

Astrophysical conditions

Fission Yields

Rates (n capture, β-decay, fission….)

Nucleosynthesis code

(PRISM)

Abundance prediction

Markov Chain Monte Carlo (MCMC)

Likelihood function

Nuclear masses

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

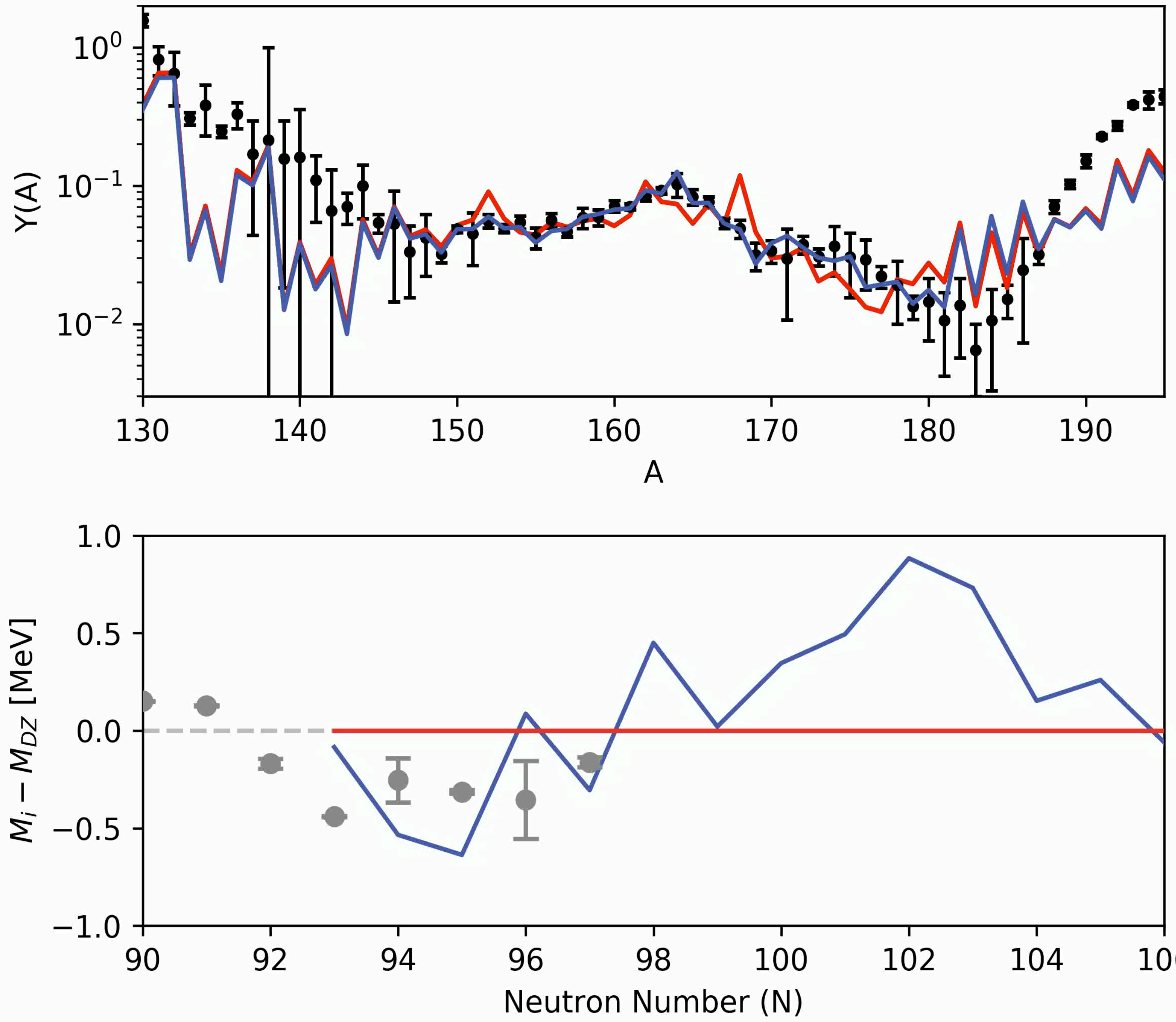
$$\sigma^2_{\mathrm{rms}}(M_{\mathrm{AME12}}, M) \le \sigma^2_{\mathrm{rms}}(M_{\mathrm{AME12}}, M_{DZ})$$

- Update nuclear quantities and rates
- Perform nucleosynthesis calculation
- Calculate χ^2

$$\chi^2 = \sum_{A=150}^{180} \frac{\left(Y_{\odot,r}(A) - Y(A)\right)^2}{\Delta Y(A)^2}$$

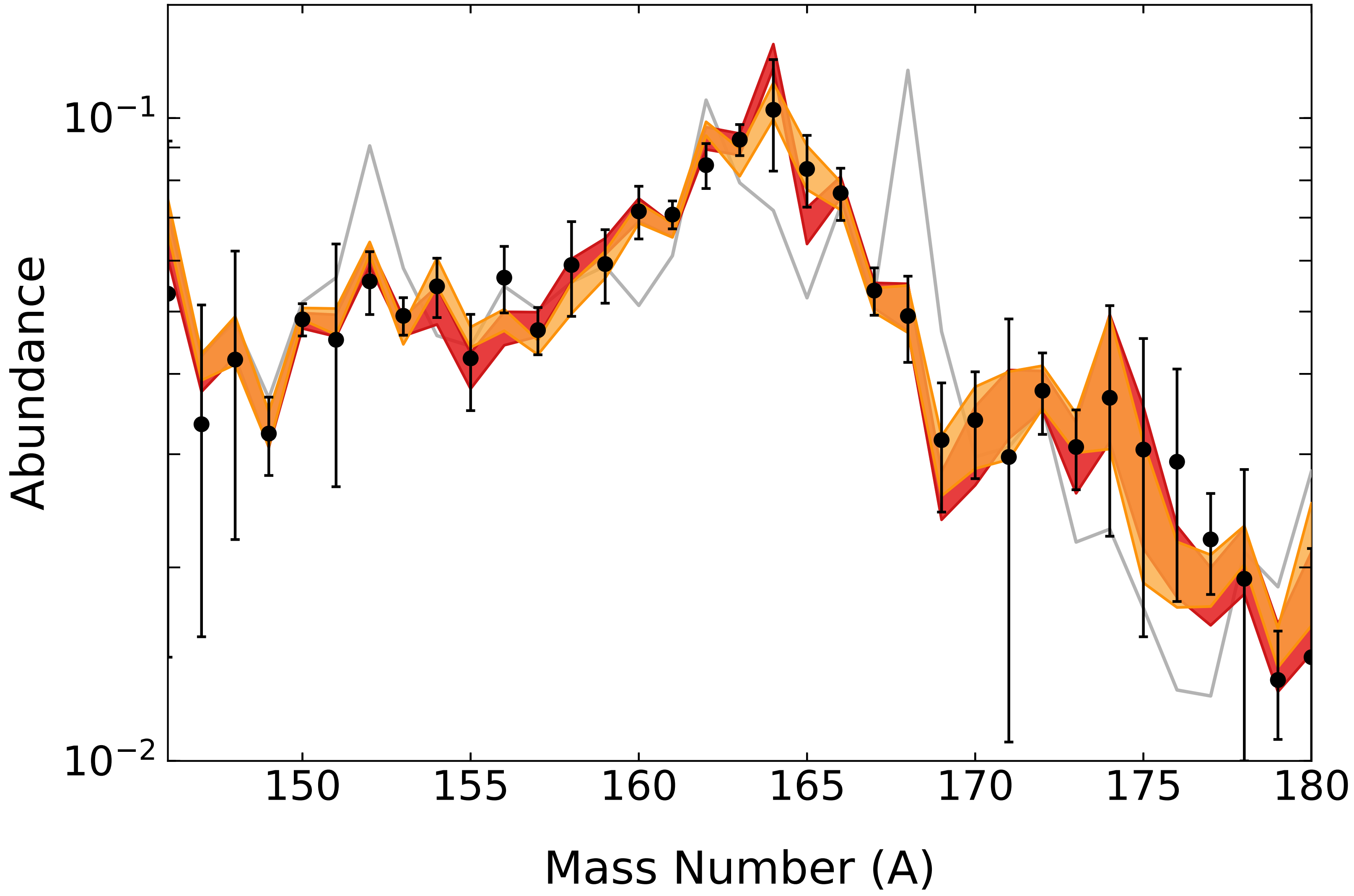
- Update parameters OR revert to last success

$$\mathcal{L}(\mathrm{m}) = \exp\left(-\frac{\chi^2(\mathrm{m})}{2}\right) \longrightarrow \alpha(\mathrm{m}) = \frac{\mathcal{L}(\mathrm{m})}{\mathcal{L}(\mathrm{m}-1)}$$



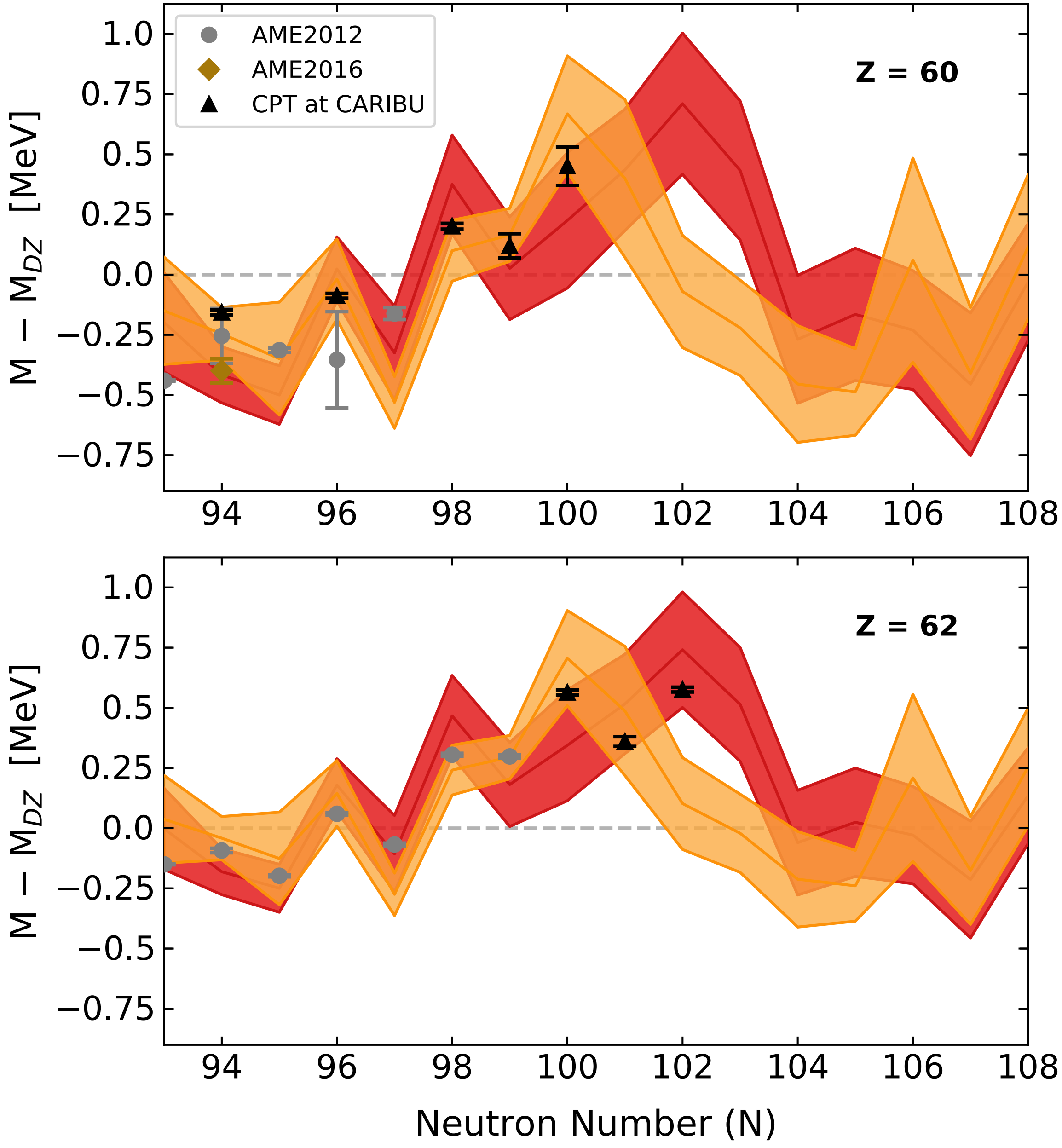
Black – solar abundance data
Grey – AME 2012 data
Red – values at current step
Blue – best step of entire run

Rare Earth Peak with MCMC solutions



Results

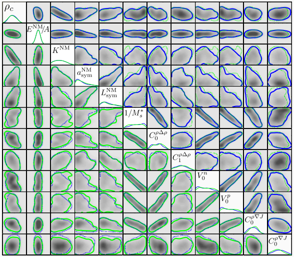
- Astrophysical trajectory:
  hot, low entropy wind such as in a merger accretion disk
- 50 parallel, independent MCMC runs
- 21 runs in red band, 7 runs in orange band
- Average $\chi^2 \sim 20$ for red and orange solutions

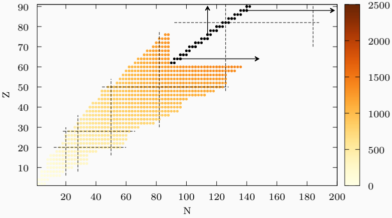


R. Orford, N. Vassh, et al (in preparation)

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

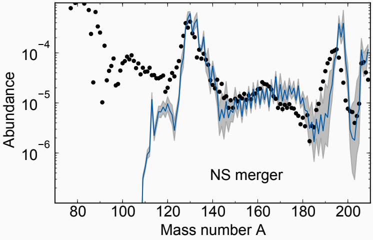


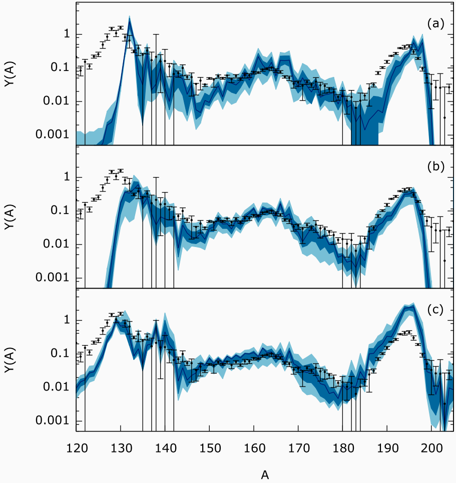


Abundance Patterns

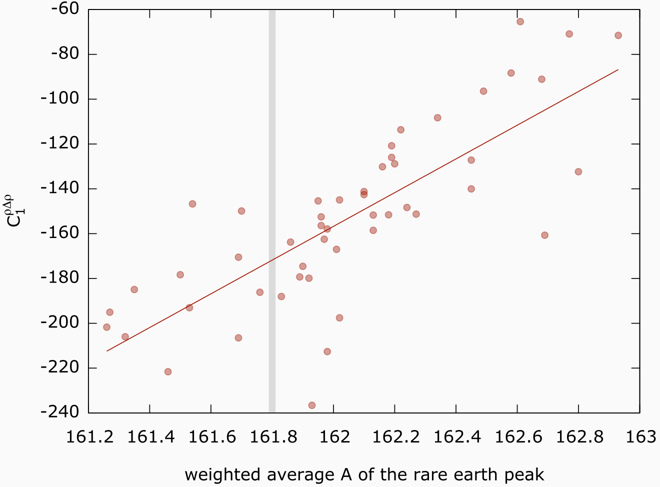
- Neutron star merger
- 50 calculations of the same process
- Solar abundances
- Systematic uncertainties

Martin et al, PRL 116 (2016) 121101



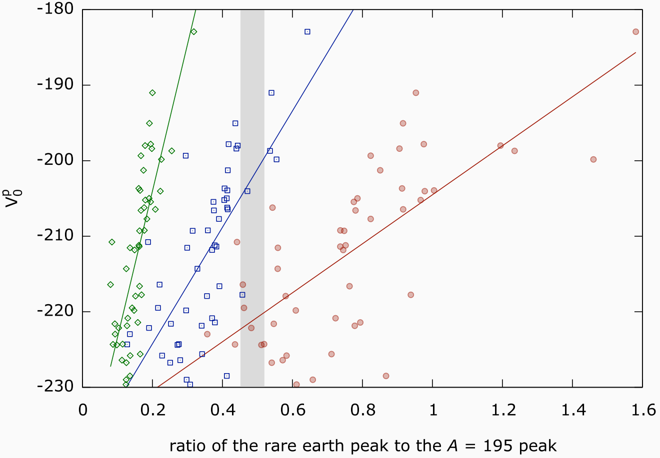


The r-process informs DFT



Astrophysical data can constrain DFT parameters

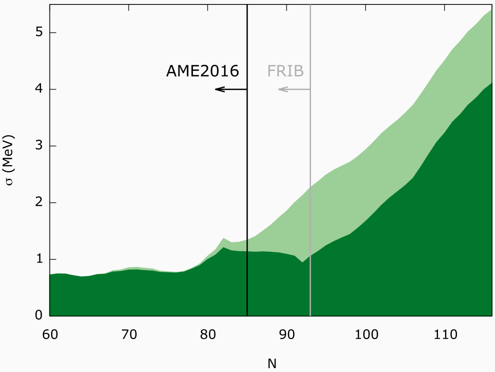
DFT informs the r-process



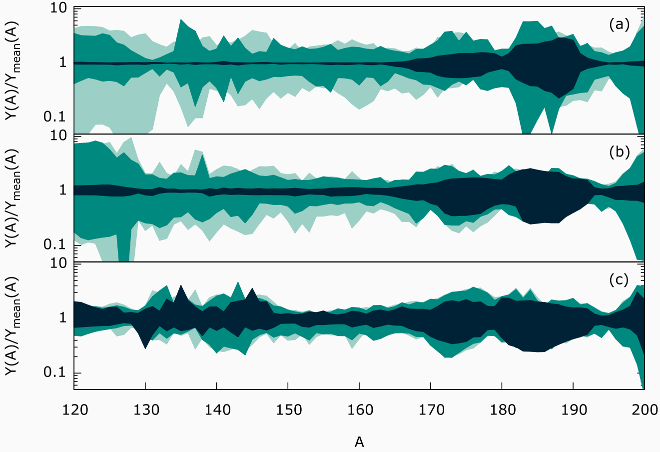
UQ allows to discriminate between astrophysical scenarios

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