Quantification of Uncertainties for Predictions of Fission Fragment Distributions

Information and statistics in nuclear experiment and theory (ISNET-5)
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LLNL-PRES-XXXXXX
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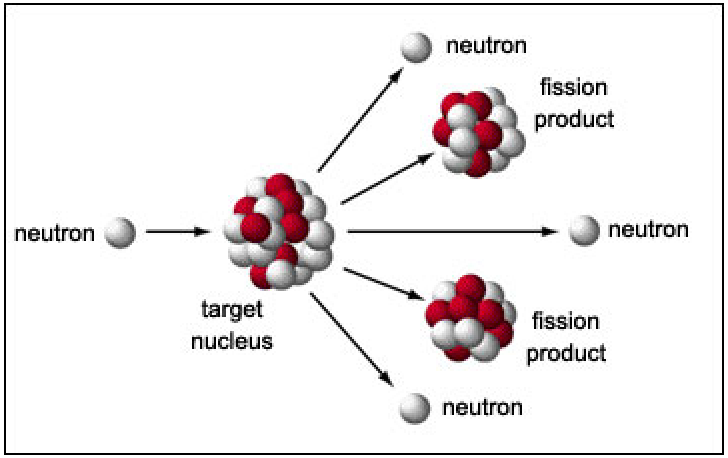
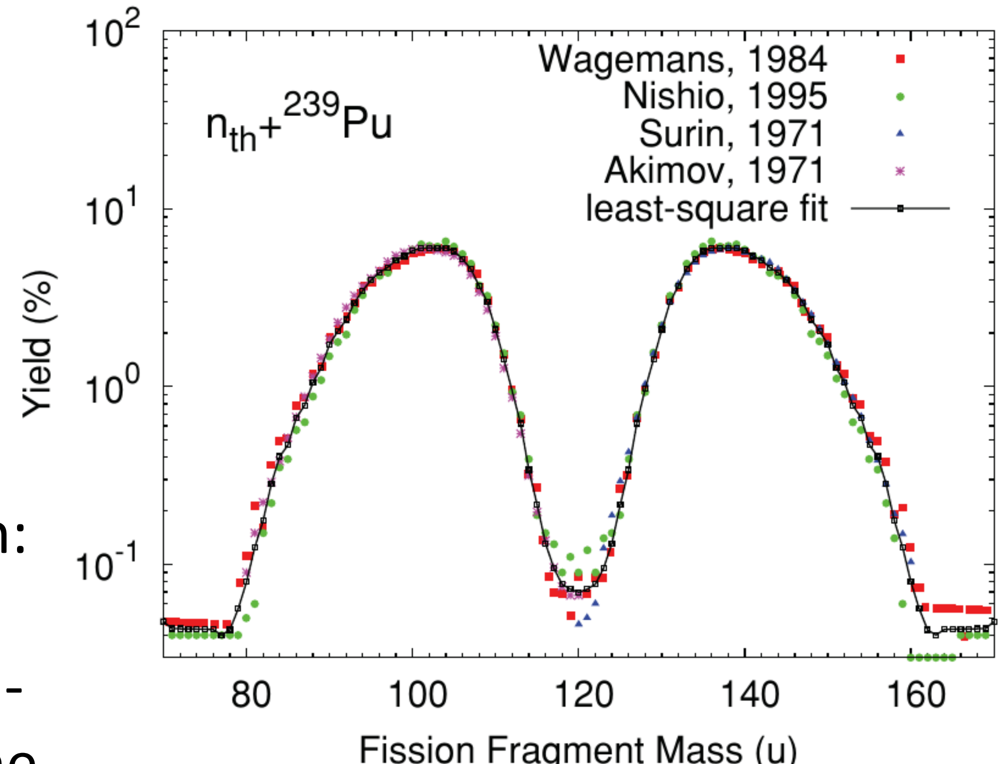
Neutron-Induced Fission

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



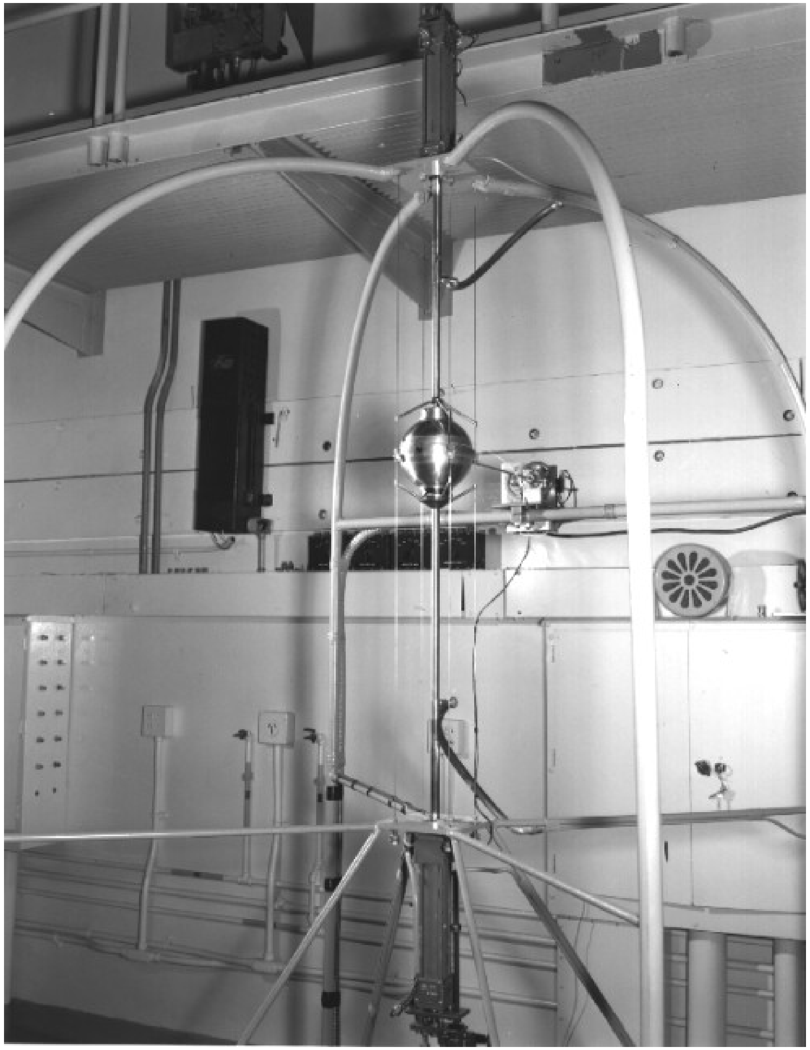


- Fission fragment distribution: probability (normalized to 200) to observe a given number of particles (=mass) in the fragments
- Depends on target, neutron incident energy

Applications of Induced Fission

Simulate reactor technology on a computer

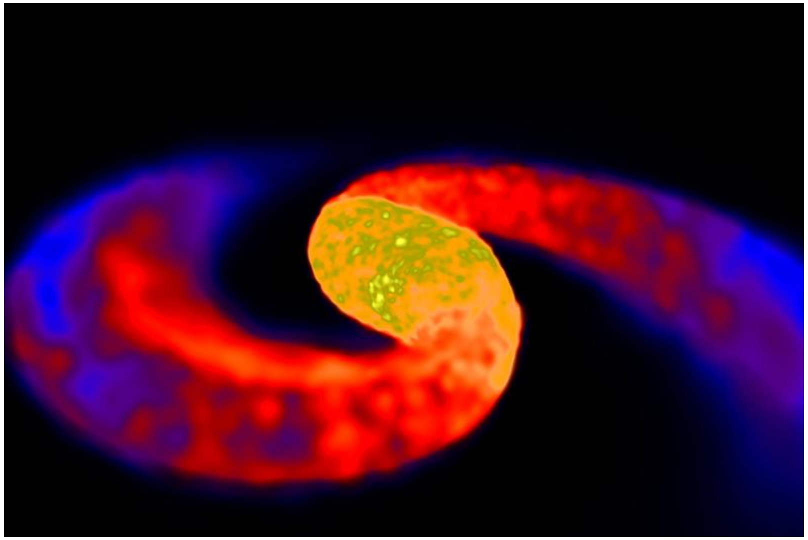
- Critical assembly is small amount of fissile material (= fission as soon as hit by neutrons)
- Criticality (neutrons out = neu-torns in) depends on geometry, composition, etc.
- Multi-physics problem
  - Material physics
  - Transport (of particles in material)
  - Nuclear physics
- Fission fragment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

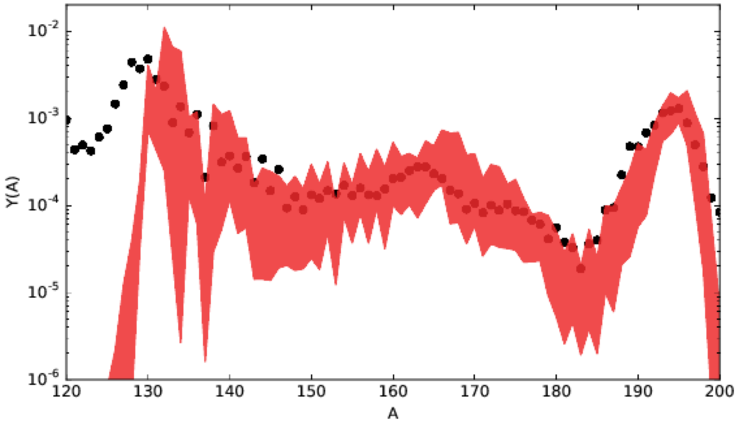


Fission in Basic Science

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

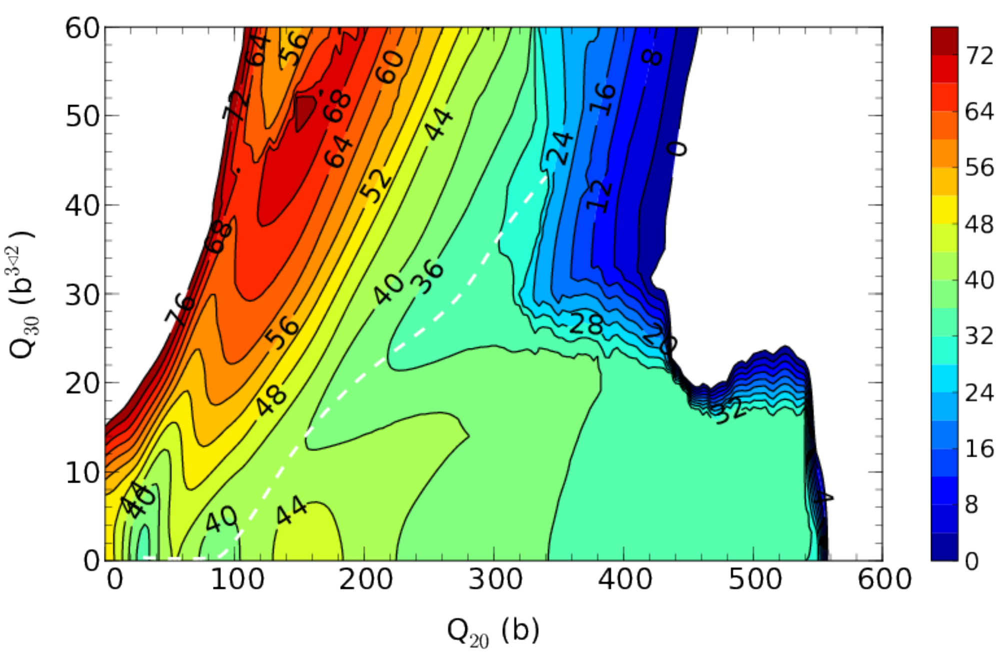
Basic Concepts

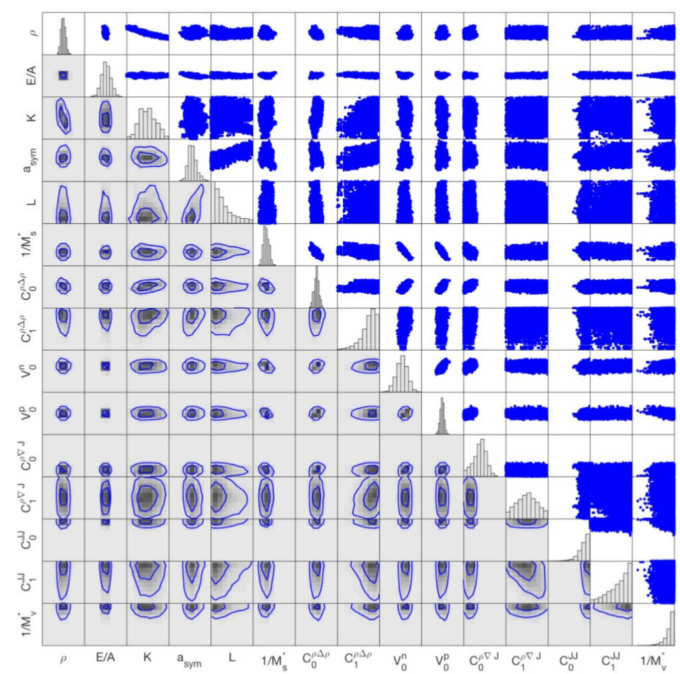
- Simple idea (Bohr and Wheeler, 1939): Nucleus deforms itself until it breaks into two fragments
- Theorist's job:
  - Predict how energy of the nucleus changes with deformation(s)
  - Predict the probability for the nucleus to have a given deformation
  - Relate characteristics of the fragments with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

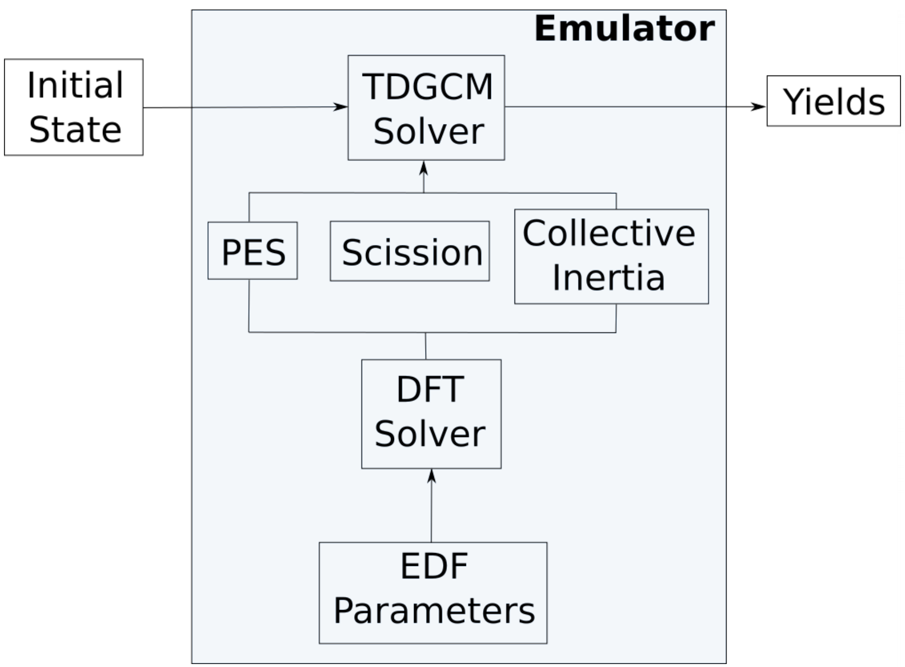
- Parameters of the energy density functional (about a dozen)
- Size of collective space = how many deformations (or other indicators) do you need to characterize fission?
- Recipe to compute collective inertia: most popular method relies on additional approximations
- Scission lines = the point/line/surface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

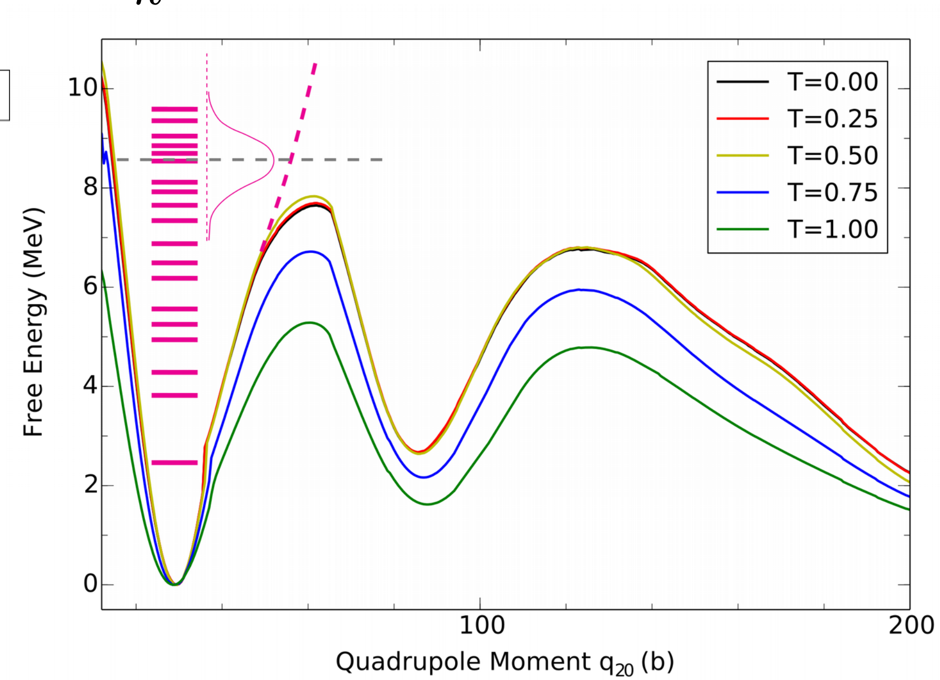
Initial State

A Simple One-Parameter Problem

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

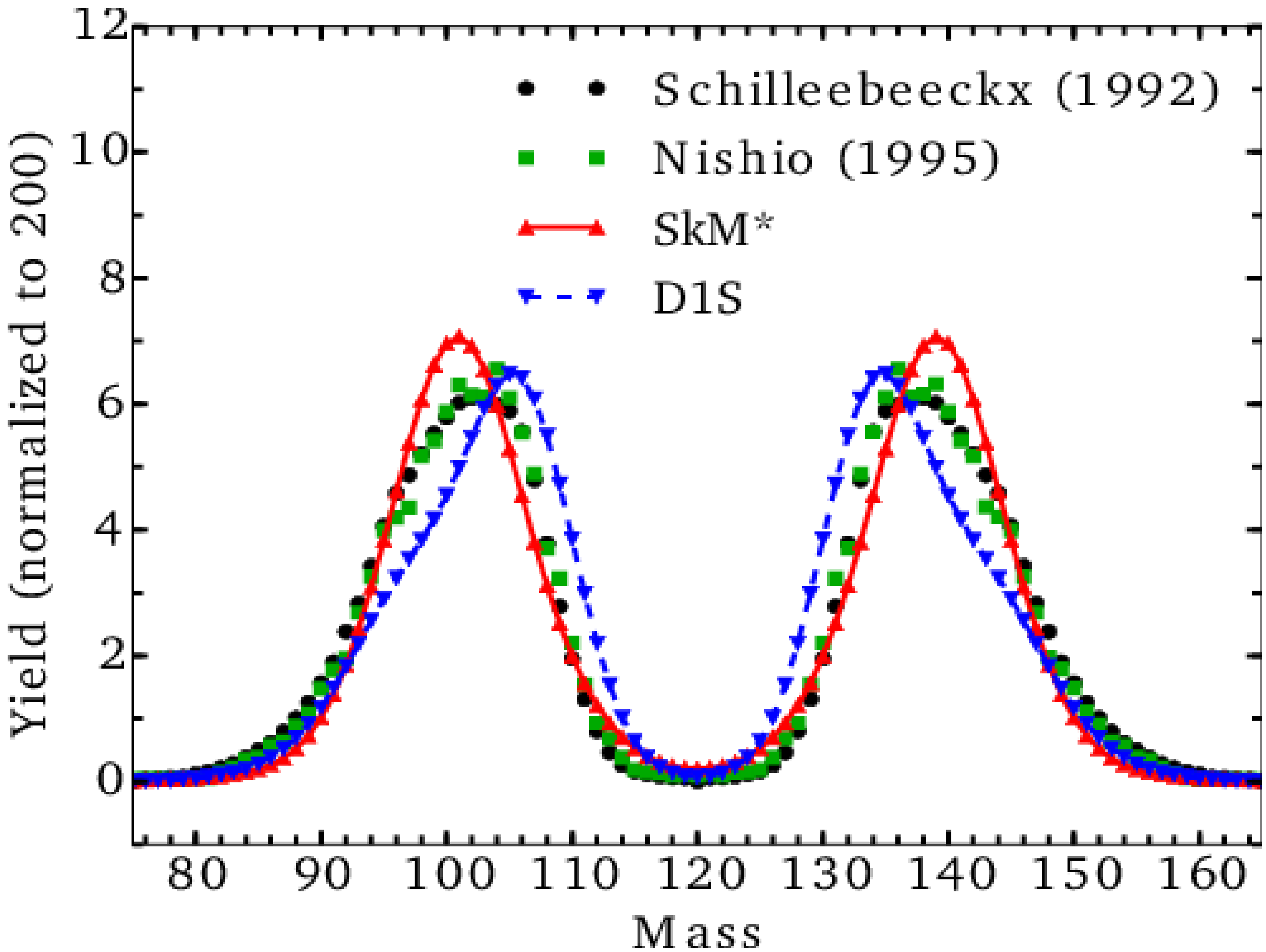
$$g(q_2, q_3; t = 0) = \sum_k e^{-\frac{1}{2}\left(\frac{E_k - \bar{E}}{\sigma}\right)^2} g_k(q_2, q_3)$$





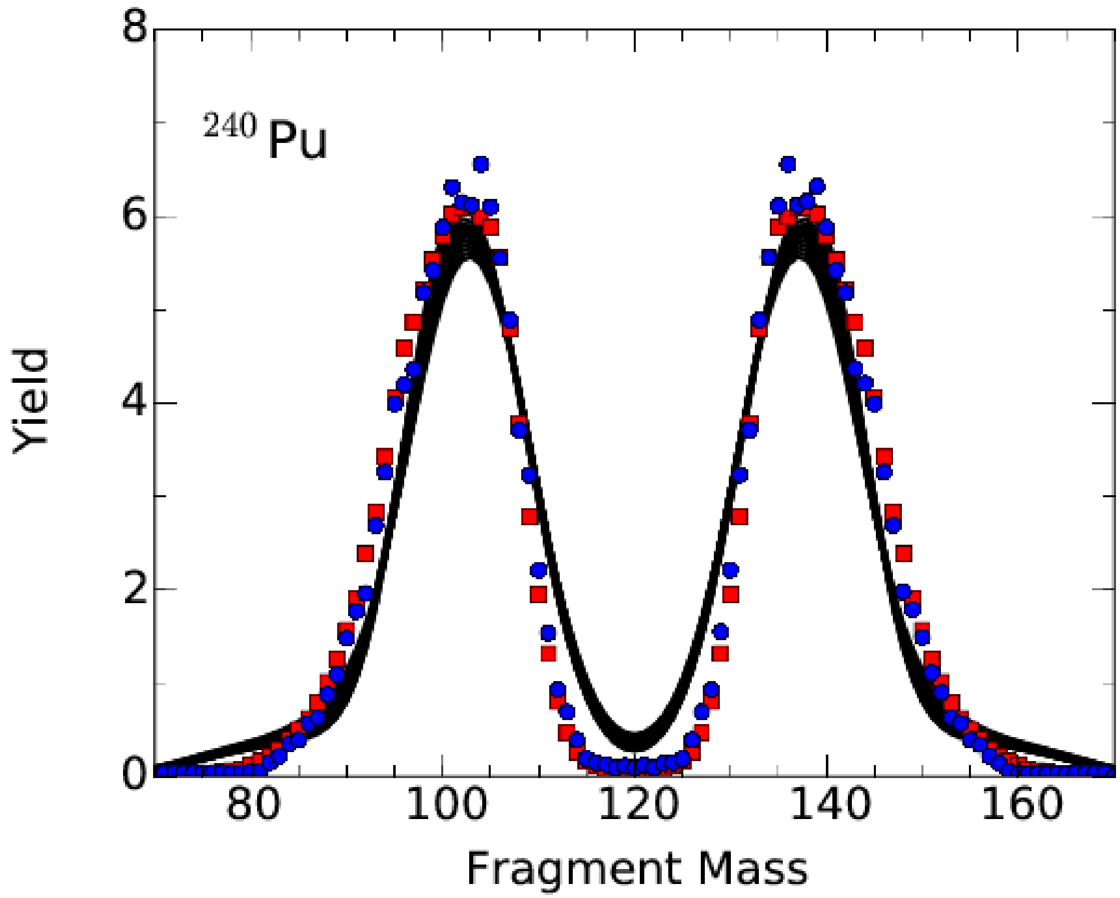
Baseline Calculation

We use the SkM* EDF



Design Runs
Sources of Uncertainties

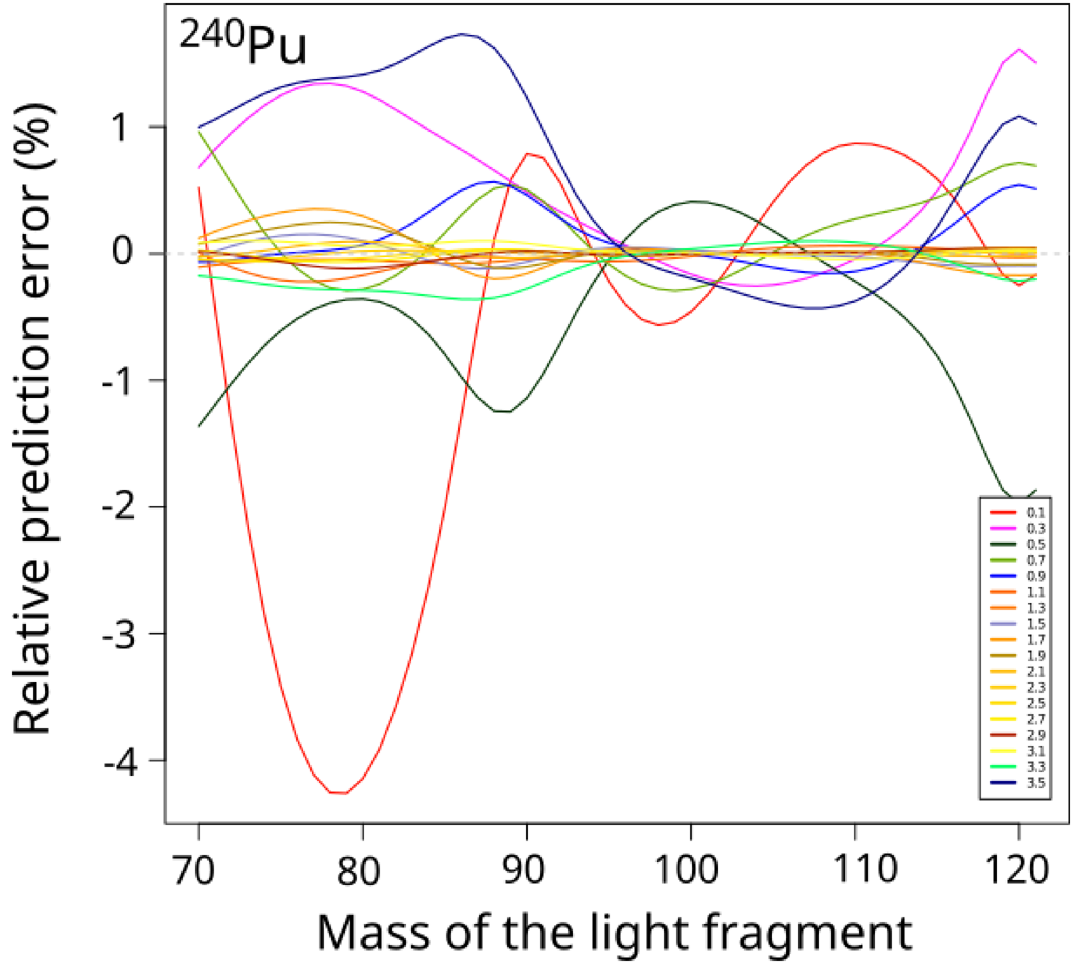
- Vary σ from 0.1 to 3 by step of 0.1



Emulator

Gaussian Process Model Trained on 30 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
- Lab-specific concerns: how to store emulators?

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