Applications of Nuclear Data: GEF

ICTP-IAEA Workshop on the Evaluation of Nuclear Data for Applications

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IAEA International Atomic Energy Agency *Atoms for Peace*

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A wealth of theoretical and practical information is available from the main publications and references therein:

General Description of Fission Observables
K-H Schmidt, B. Jurado
NEA/DB/DOC(2014)1 JEFF Report 24
`www.khs-erzhausen.de/Preprints/db-doc2014-1.pdf`

General Description of Fission Observables: GEF Model Code
K-H Schmidt, B. Jurado, C. Amouroux, C. Schmitt
Nuclear Data Sheets 131 (2016) 107-221
`www.khs-erzhausen.de/Preprints/HAL-GEF-NDS.pdf`

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You will remember from the previous week that:

- Fission is a complex process and accurate prediction of most post-fission quantities requires empirical modeling

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You will remember from the previous week that:

- Fission is a complex process and accurate prediction of most post-fission quantities requires empirical modeling
- GEF is a nuclear fission simulation code that models a variety of important fission observables

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- Fission is a complex process and accurate prediction of most post-fission quantities requires empirical modeling
- GEF is a nuclear fission simulation code that models a variety of important fission observables
- GEF takes a 'general approach' that applies a selection of semi-empirical parameters and is valid for a wide range of targets and fissioning conditions

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- Fission is a complex process and accurate prediction of most post-fission quantities requires empirical modeling
- GEF is a nuclear fission simulation code that models a variety of important fission observables
- GEF takes a 'general approach' that applies a selection of semi-empirical parameters and is valid for a wide range of targets and fissioning conditions
- GEF is specifically engineered to allow parameter variation to better fit the model results to experiment and, as a consequence, can be used for uncertainty quantification

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- Open source and available from Karl-Heinz's website: `http://www.khs-erzhausen.de/GEF.html`

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- Open source and available from Karl-Heinz's website: `http://www.khs-erzhausen.de/GEF.html`
- GEF is a Monte-Carlo code running a series of simulations and treating these as samples of the true code predictions

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- GEF is a Monte-Carlo code running a series of simulations and treating these as samples of the true code predictions
- A set of 'reference' results are known as the GEFY (GEF Yields) in ENDF-6 format (`http://www.khs-erzhausen.de/GEFY.html`)

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- GEF is a Monte-Carlo code running a series of simulations and treating these as samples of the true code predictions
- A set of 'reference' results are known as the GEFY (GEF Yields) in ENDF-6 format (`http://www.khs-erzhausen.de/GEFY.html`)
- The code is written in FreeBASIC, requiring the `fbc` compiler (that is not available for OS X)

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- GEF can be run directly from the command line with `./GEF`, which prompts a series of terminal queries for input information

```
$ ./GEF
    Enter Z and A of fissioning nucleus:  92 236
    Chose the input option: EN
    Energy input is the incident neutron energy.
    Enter energy value (MeV):
```

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- Alternatively, provide an input file with the required information (omitted data is taken to be default)

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```
$ ./GEF
    Enter Z and A of fissioning nucleus:  92 236
    Chose the input option: EN
    Energy input is the incident neutron energy.
    Enter energy value (MeV):
```

- Alternatively, provide an input file with the required information (omitted data is taken to be default)
- This requires a file `file.in` that contains a list of files with input data

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The directory content could be: `file.in` and `U235_2.0MeV`:

```
$ head file.in
   U235_2.0MeV
$ head U235_2.0MeV
   1
   2.0
   Options(err,cor)
   92, 236, "EN"
```

Each of the lines in the input files must follow a specific format

- The `file.in` file has one file name per line (comments with `'` are ignored)

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The directory content could be: `file.in` and `U235_2.0MeV`:

```
$ head file.in
   U235_2.0MeV
$ head U235_2.0MeV
   1
   2.0
   Options(err,cor)
   92, 236, "EN"
```

Each of the lines in the input files must follow a specific format

- The `file.in` file has one file name per line (comments with ' are ignored)
- Each file defines a (set of) simulation(s) and requires a precisely defined type of input for each line

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```
1
2.0
Options(err,cor)
92, 236, "EN"
```

- First line controls the number of events sampled and must be a number N
- The number of simulated events is $100,000 \times N$
- $N = 1$ takes <10 seconds, but options will multiply this!
- Second line is the energy (multiple types) in MeV, can also be a list, e.g.:

```
1
1.0, 2.0, 3.0, 4.0, 5.0
Options(err,cor)
92, 236, "EN"
```

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```
1
2.0
Options(err,cor)
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```

- Third line switches on various options:

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```
1
2.0
Options(err,cor)
92, 236, "EN"
```

- Third line switches on various options:
  - **err**: calculation with perturbed parameters (taken from internal distributions with pre-defined variances)

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```
1
2.0
Options(err,cor)
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```

- Third line switches on various options:
  - **err**: calculation with perturbed parameters (taken from internal distributions with pre-defined variances)
  - **ptb**: prints outputs of perturbed parameter calculations

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```
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```

- Third line switches on various options:
  - **err**: calculation with perturbed parameters (taken from internal distributions with pre-defined variances)
  - **ptb**: prints outputs of perturbed parameter calculations
  - **random**: (for random ENDF file generation, not in this version)

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Options(err,cor)
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- Third line switches on various options:
  - **err**: calculation with perturbed parameters (taken from internal distributions with pre-defined variances)
  - **ptb**: prints outputs of perturbed parameter calculations
  - **random**: (for random ENDF file generation, not in this version)
  - **cov**: print out covariance matrices

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  - **cor**: print out correlation matrices

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  - **ptb**: prints outputs of perturbed parameter calculations
  - **random**: (for random ENDF file generation, not in this version)
  - **cov**: print out covariance matrices
  - **cor**: print out correlation matrices
  - **lmd**: print a 'list-mode' output with summary of all simulated events
    - Not all quantities are output in the 'list-mode' file. You will run examples and parse them

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```
1
2.0
Options(err,cor)
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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:

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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state

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```
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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission

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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission
  - **ISx**: nucleus in isomeric state *x* and energy above that state

Inputs
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1
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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission
  - **ISx**: nucleus in isomeric state *x* and energy above that state
  - **EN**: incident neutron energy

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  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission
  - **ISx**: nucleus in isomeric state *x* and energy above that state
  - **EN**: incident neutron energy
  - **EP**: incident proton energy

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```

- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission
  - **ISx**: nucleus in isomeric state *x* and energy above that state
  - **EN**: incident neutron energy
  - **EP**: incident proton energy
  - **ENx**: as with EN but target in isomeric state *x*

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- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
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  - **ISx**: nucleus in isomeric state *x* and energy above that state
  - **EN**: incident neutron energy
  - **EP**: incident proton energy
  - **ENx**: as with EN but target in isomeric state *x*
  - **EB**: energy above the outer fission barrier

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- The last line gives the charge and baryon number of the fissioning system, as well as the type of fission:
  - **GS**: energy above the ground state
  - **FC**: as with GS, but allowing *only* first change fission
  - **ISx**: nucleus in isomeric state *x* and energy above that state
  - **EN**: incident neutron energy
  - **EP**: incident proton energy
  - **ENx**: as with EN but target in isomeric state *x*
  - **EB**: energy above the outer fission barrier
  - **ES**: reads excitation energy spectrum from `Espectrum.in` and calculates weighted set of first chance fission for spectrum

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- GEF uses a set of semi-empirical parameters to control the relative contributions of the various shell effects, the charge distribution, etc.

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- GEF uses a set of semi-empirical parameters to control the relative contributions of the various shell effects, the charge distribution, etc.
- Each has its own internal 'uncertainty' value and automatic pertubation with the `err` option unlocks this

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- GEF uses a set of semi-empirical parameters to control the relative contributions of the various shell effects, the charge distribution, etc.
- Each has its own internal 'uncertainty' value and automatic pertubation with the `err` option unlocks this
- Users can manually adjust these using the terminal-provided options:

```
Enter scaling factor for even-odd effect in Z and N yields (default = 1): 1.2

Shell effect in the symmetric channel is assumed to be  0.3 MeV.
You may enter another guess value if you want to change it: 0.4

Use locally adjusted model parameters, if available (0 or 1): 1
```

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Enter scaling factor for even-odd effect in Z and N yields (default = 1): 1.2

Shell effect in the symmetric channel is assumed to be  0.3 MeV.
You may enter another guess value if you want to change it: 0.4

Use locally adjusted model parameters, if available (0 or 1): 1
```

- The local adjusted parameters are held in the source code `GEF.bas` (this version has some parameters for Z=90, but you could add others)

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- GEF generates a few output folders including:

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- GEF generates a few output folders including:
  - **out**/ contains the pseudo-xml `.dat` files containing summaries of all data

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- GEF generates a few output folders including:
  - **out**/ contains the pseudo-xml `.dat` files containing summaries of all data
  - **dmp**/ contains many `.dmp` 'dump' files separated by intuitive file names
  - **tmp**/ contains some temporary files such as the multivariate distribution data
  - **ctl**/ contains some files specific to multi-threading

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- The `.dat` file contains many quantities such as:

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- The `.dat` file contains many quantities such as:
  - nuclide distributions,

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- The `.dat` file contains many quantities such as:
  - nuclide distributions,
  - gamma spectra,

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- GEF generates a few output folders including:
  - **out**/ contains the pseudo-xml `.dat` files containing summaries of all data
  - **dmp**/ contains many `.dmp` 'dump' files separated by intuitive file names
  - **tmp**/ contains some temporary files such as the multivariate distribution data
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  - gamma spectra,
  - neutron yields and spectra,
  - kinetic energies, J of fragments,
  - many derived quantities and multi-parameter distributions

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- Adding the various options to the input file also generates data made with sampled input model parameters.

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- Adding the various options to the input file also generates data made with sampled input model parameters.
  - The `.mvd` multi-variate distribution file contains the nuclide yields from each set with different, sampled input parameters

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- Adding the various options to the input file also generates data made with sampled input model parameters.
  - The `.mvd` multi-variate distribution file contains the nuclide yields from each set with different, sampled input parameters
  - The `.ptb` pertubation files within `out/` contains a series of standard, full outputs for each of the calculations with sampled input parameters

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  - The `.mvd` multi-variate distribution file contains the nuclide yields from each set with different, sampled input parameters
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  - The `.ptb` pertubation files within `out/` contains a series of standard, full outputs for each of the calculations with sampled input parameters
  - The standard `.dat` file contains all of the standard information, plus a variety of covariance matrices
- GEF calculates covariances between mass, charge and nuclide distributions, but with low-statistics calculations for each of the perturbed sets. Various other correlations may be calculated using the full, perturbed output files

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- The `.lmd` contains a history of all the individual events that were simulated by GEF. These allow users to calculate any of a large range of outputs, correlations, etc.

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- The `.lmd` contains a history of all the individual events that were simulated by GEF. These allow users to calculate any of a large range of outputs, correlations, etc.
- Depending on the input options (within the terminal, request the extra outputs), the data will be expanded or simple.

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- Depending on the input options (within the terminal, request the extra outputs), the data will be expanded or simple.
  - First lines are always populated with the data from the pre- and post-neutron fragments:
    - Charge and baryon numbers
    - Spins and excitation energies
    - Neutron emission
    - Kinetic energies

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  - First lines are always populated with the data from the pre- and post-neutron fragments:
    - Charge and baryon numbers
    - Spins and excitation energies
    - Neutron emission
    - Kinetic energies
  - Subsequent lines are optional and contain information on the emitted neutron and gamma yields, energies and angles

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Exercises

- `/home/nfs1/smr3151/scripts/install_GEF.sh`
- Run GEF directly with terminal prompts
- Run GEF for U235 with input files over an energy range for neutron-incident simulations and compare the mass distributions – check the range 5-7 MeV for novel features
- Run GEF using the perturbation options for covariance data
- Run GEF in 'list mode'. For those seeking a challenge, process the data for correlations

Lecture break for exercises

UK Atomic Energy Authority

The Abdus Salam International Centre for Theoretical Physics
www.ictp.it

IAEA
International Atomic Energy Agency
Atoms for Peace

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- GEF can calculate several quantities that can be contained within the ENDF-6 file format, for example average prompt neutron emission and neutron spectra

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- GEF can calculate several quantities that can be contained within the ENDF-6 file format, for example average prompt neutron emission and neutron spectra
- For use with FISPACT-II, we will be interested in the fission yields

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- GEF can calculate several quantities that can be contained within the ENDF-6 file format, for example average prompt neutron emission and neutron spectra
- For use with FISPACT-II, we will be interested in the fission yields
- Fission yields have an exceptionally simple structure, as described in section 8.3 of the manual:

  `https://www-nds.iaea.org/exfor/x4guide/manuals/endf-manual.pdf`

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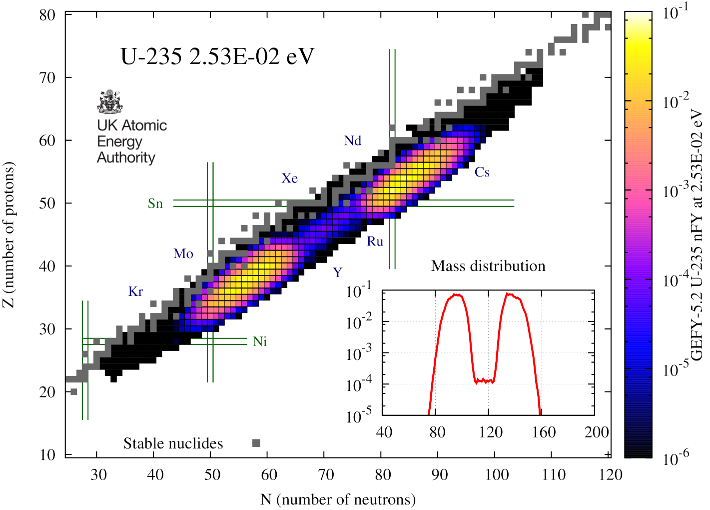

fispact.ukaea.uk/nuclear-data/fission-yields

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ENDF fission yields

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```
9.4239E+04 2.3700E+02         37          0          0          03586 8454     1
1.0000E-05 0.0000E+00         36          0       6144       15363586 8454     2
2.1060E+04 0.0000E+00 0.0000E+00 0.0000E+00 2.2060E+04 0.0000E+003586 8454     3
0.0000E+00 0.0000E+00 2.2061E+04 0.0000E+00 0.0000E+00 0.0000E+003586 8454     4
2.2062E+04 0.0000E+00 0.0000E+00 0.0000E+00 2.2063E+04 0.0000E+003586 8454     5
0.0000E+00 0.0000E+00 2.3060E+04 0.0000E+00 1.2381E-15 1.2379E-133586 8454     6
2.3061E+04 0.0000E+00 1.0550E-15 1.0549E-13 2.3062E+04 0.0000E+003586 8454     7
3.8392E-16 3.2184E-14 2.3063E+04 0.0000E+00 9.7240E-17 5.6010E-153586 8454     8
2.3064E+04 0.0000E+00 0.0000E+00 0.0000E+00 2.3065E+04 0.0000E+003586 8454     9
0.0000E+00 0.0000E+00 2.4060E+04 0.0000E+00 2.1660E-14 2.1658E-123586 8454    10
2.4061E+04 0.0000E+00 4.9592E-14 4.9587E-12 2.4062E+04 0.0000E+003586 8454    11
9.3808E-14 7.8536E-12 2.4063E+04 0.0000E+00 7.2610E-14 4.1286E-123586 8454    12
```

- First line, column is the target

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```

- First line, column is the target
- Second line, first column is the incident energy in eV

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```
9.4239E+04 2.3700E+02         37          0          0          03586 8454    1
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```

- First line, column is the target
- Second line, first column is the incident energy in eV
- Remaining lines are sets of 4 numbers in sequence:

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- First line, column is the target
- Second line, first column is the incident energy in eV
- Remaining lines are sets of 4 numbers in sequence:
  - **ZAFP** identifier = (1000Z + A)
  - **FPS** isomeric state identifier (e.g. 0, 1, 2...)
  - **Y(I/C)** yield (independent or cumulative)
  - **DY(I/C)** 1 σ uncertainty (independent or cumulative)

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- The independent yields $IY(nuc)$ are the standard outputs that you would expect: an appropriately normalised probability of producing each nuclide (nuc = isotope and state)

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Independent vs cumulative

- The independent yields $IY(nuc)$ are the standard outputs that you would expect: an appropriately normalised probability of producing each nuclide (nuc = isotope and state)
- Cumulative yields $CY(nuc)$ are a derived quantity:

$$CY(nuc) = IY(nuc) + \sum_{nuc'} B(nuc' \to nuc) CY(nuc')$$

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- Cumulative data are inherently *dependent on decay data evaluations*

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Independent vs cumulative

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- Independent and cumulative data are distinguished by `mt` numbers 454 and 459, respectively
- Cumulative data are inherently *dependent on decay data evaluations*
- *Note* that it is common to treat only 100 products with remaining as 'psuedo-products'

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- Use of the independent yields requires complete knowledge of the decay processes

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- Use of the independent yields requires complete knowledge of the decay processes
- FISPACT-II utilises the full, energy-dependent (and reaction-rate weighted) fission yield data

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- Use of the independent yields requires complete knowledge of the decay processes
- FISPACT-II utilises the full, energy-dependent (and reaction-rate weighted) fission yield data
  - This requires *matching* decay data evaluations

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  - This requires *matching* decay data evaluations
- There is no agreed ENDF-6 format for covariance matrices of fission products, so at present FISPACT-II cannot utilise any of this data (even though GEF can calculate it)

If you build it, they will come!

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- An alternative is to use *Total Monte-Carlo*

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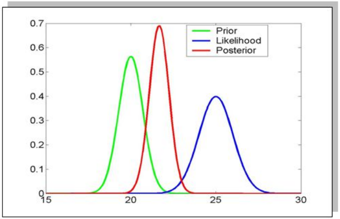
Bayesian statistics

new data $\quad$ prior knowledge

$$p(y\,|\,\theta) \qquad p(\theta)$$

$$p(\theta\,|\,y) \propto p(y\,|\,\theta)\,p(\theta)$$

posterior $\propto$ likelihood • prior

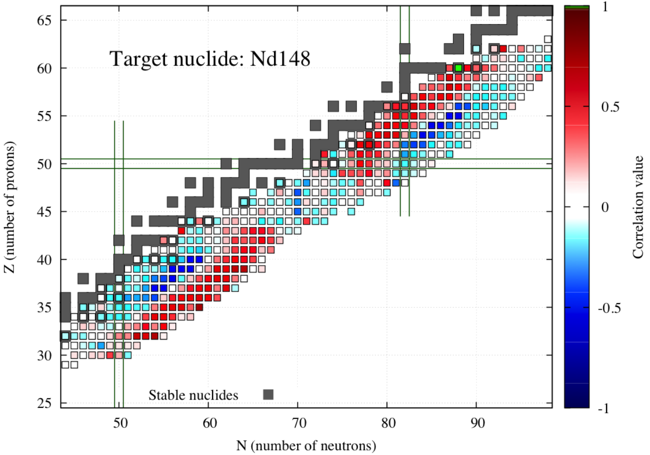


Bayes theorem allows one to formally incorporate prior knowledge into computing statistical probabilities.

Priors can be of different sorts: empirical, principled or shrinkage priors.

The "posterior" probability of the parameters given the data is an optimal combination of prior knowledge and new data, weighted by their relative precision.

- Sampling of the input parameters with posterior distributions generated from a Bayesian process, we can obtain files with *fully correlated* yield variation



ENDF/applications

Bayesian files

[12]ATI, [13]IRMM, [14]NNL.

Random files

1. Random fission yields
2. Random thermal scattering
3. Random ENDF-6 files
4. Random ACE files

Sub-library files

1. neutron

TENDL-2015: (release date: 18 January 2016)

Last update: 5 October 2016

TENDL is a nuclear data library which provides the output of the **TALYS** nuclear model code system for direct use in both basic physics and applications. The 8th version is **TENDL-2015**, which is based on both default and adjusted **TALYS** calculations and data from other sources (previous releases can be found here: 2008, 2009, 2010, 2011, 2012, 2013, and 2014).

- Thankfully, Dmitri has done the work and it is available to the public!
  `https://tendl.web.psi.ch/tendl_2015/randomYields.html`
- For data, reference ENDF-6 data files are used in the Bayesian analysis

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- You have calculated decay heat from fission pulses with FISPACT-II (or will)

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- Plot the results and compare with libraries and experimental data
- For those seeking a challenge, download the TENDL nFY files for another system - ask me for experimental data

Lecture break for exercises

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