Implementation of PFNS in EMPIRE

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Outline

- Calculation of PFNS in EMPIRE
- Fitting cross sections with Kalman filter
- Differences between fitting cross sections and PFNS
- Extension of Kalman utility to accommodate PFNS fitting
- Results of PFNS fits
- Conclusion

PFNS Calculation in EMPIRE

- Only 1st chance fission implemented in EMPIRE
- Two prompt fission models:
  - Los Alamos (Madland-Nix) – though not the latest one!
  - Kornilov
- Four parameters:
  - PFNTKE – Scales the total kinetic energy of the fission fragments
  - PFNALP – Scales the energy of both the light and heavy fragments
  - PFNRAT – Adjusts the ratio of the kinetic energy of the light to heavy fragments
  - PFNERE – Scales the total fission energy release
- PFNS independent of and uncorrelated with cross section calculations (1st chance only – 2nd chance will correlate)

Cross-section sensitivity-matrix file

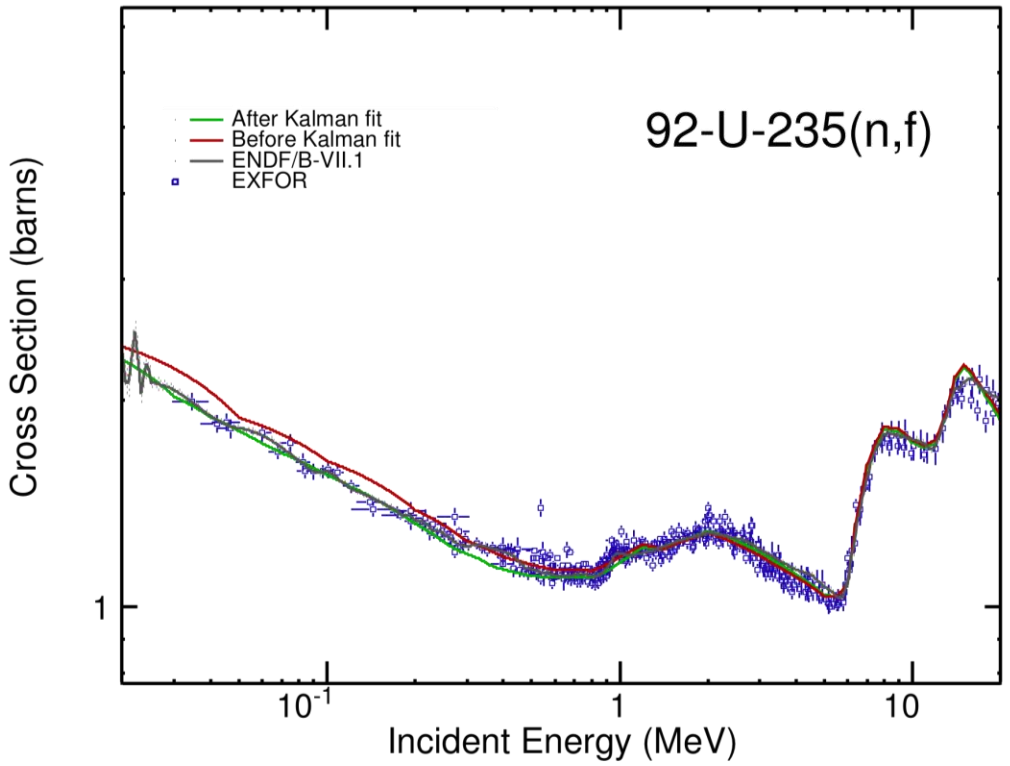
Reactions

Incident energies

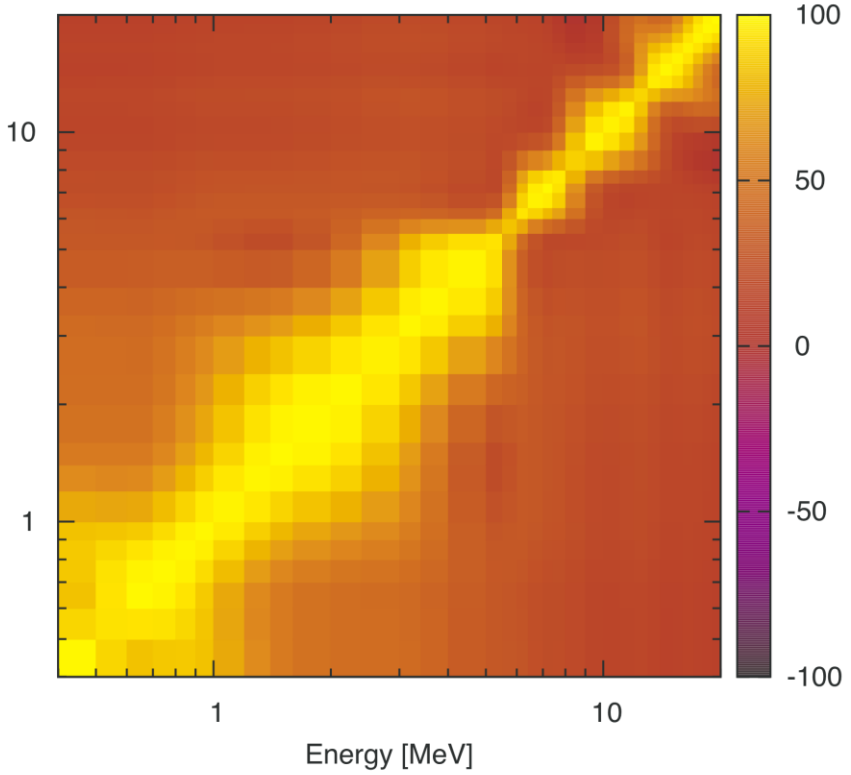
```
#  9      n +  92-U -235       Elastic* and Nonelast* modified for A>220 and En>3.5 MeV (Cross s
# Parameter: UOMPRV    0  1  1  0  variation: +-0.030      Sensitivity matrix
#  Einc        Total        Elastic*     Nonelast*    Fission      Mu-bar       Nu-bar     (z,gamma)
5.0001E-07  3.5332E-02 -2.1322E-01  3.9447E-02  3.9457E-02 -2.4309E-04  0.0000E+00  3.9414E-02
1.0000E-03 -9.5611E-02 -2.3413E-01  4.4698E-02  3.9920E-02 -6.4198E-02  0.0000E+00  6.4282E-02
2.0000E-03 -1.1392E-01 -2.3370E-01  5.6385E-02  4.6770E-02 -9.3706E-02  0.0000E+00  9.4539E-02
5.0000E-03 -1.2941E-01 -2.3121E-01  9.0488E-02  6.8420E-02 -1.1855E-01  0.0000E+00  1.7096E-01
1.0000E-02 -1.3038E-01 -2.2535E-01  1.3805E-01  1.0236E-01 -1.1107E-01  0.0000E+00  2.5428E-01
2.0000E-02 -1.1810E-01 -2.1046E-01  2.0214E-01  1.5066E-01 -7.8751E-02  0.0000E+00  3.2698E-01
5.0000E-02 -7.4618E-02 -1.6311E-01  2.8541E-01  2.2013E-01 -8.7413E-03  0.0000E+00  2.9836E-01
0.10000    -1.6379E-02 -1.1750E-01  3.9162E-01  1.1281E-01  7.9176E-02  0.0000E+00  6.0355E-02
0.20000     6.1469E-02 -5.1821E-02  4.4432E-01 -1.0416E-01  1.8407E-01  0.0000E+00 -9.5418E-02
                                                                                    .
                                                                                    .
                                                                                    .
18.000      4.0722E-02  1.6951E-02  6.5864E-02 -9.8206E-03 -6.7892E-03  0.0000E+00  4.0305E-02
19.000      4.9946E-02  3.4349E-02  6.6790E-02 -4.9435E-03 -4.6205E-03  0.0000E+00  4.6762E-02
20.000      5.9446E-02  5.2243E-02  6.7334E-02  2.1019E-04 -2.8310E-03  0.0000E+00  4.7065E-02
#  9      n +  92-U -235       Elastic* and Nonelast* modified for A>220 and En>3.5 MeV (Cross s
# Parameter: UOMPVV    0  1  1  0  variation: +-0.030      Sensitivity matrix
#  Einc        Total        Elastic*     Nonelast*    Fission      Mu-bar       Nu-bar     (z,gamma)
5.0001E-07  3.2431E-01 -1.4557E-01  3.3211E-01  3.3219E-01 -2.1843E-04  0.0000E+00  3.3175E-01
1.0000E-03  4.7272E-02 -2.1113E-01  3.0902E-01  3.1035E-01 -1.7912E-02  0.0000E+00  3.0354E-01
2.0000E-03 -9.1586E-04 -2.1442E-01  3.0267E-01  3.0377E-01 -2.3164E-02  0.0000E+00  2.9829E-01
5.0000E-03 -5.5802E-02 -2.1883E-01  2.9634E-01  2.9602E-01 -1.9886E-02  0.0000E+00  2.9731E-01
1.0000E-02 -8.5742E-02 -2.2060E-01  2.9544E-01  2.9369E-01 -5.1391E-03  0.0000E+00  3.0123E-01
2.0000E-02 -1.0198E-01 -2.1724E-01  2.9764E-01  2.9489E-01  1.8438E-02  0.0000E+00  2.9835E-01
5.0000E-02 -9.7564E-02 -1.9504E-01  2.9905E-01  2.9776E-01  5.3491E-02  0.0000E+00  2.4659E-01
0.10000    -7.1001E-02 -1.6958E-01  3.2671E-01  2.4234E-01  9.1152E-02  0.0000E+00  1.2211E-01
0.20000    -2.1156E-02 -1.3262E-01  3.5552E-01  1.0872E-01  1.3753E-01  0.0000E+00 -1.0026E-03
```

Cross-section fit, an example

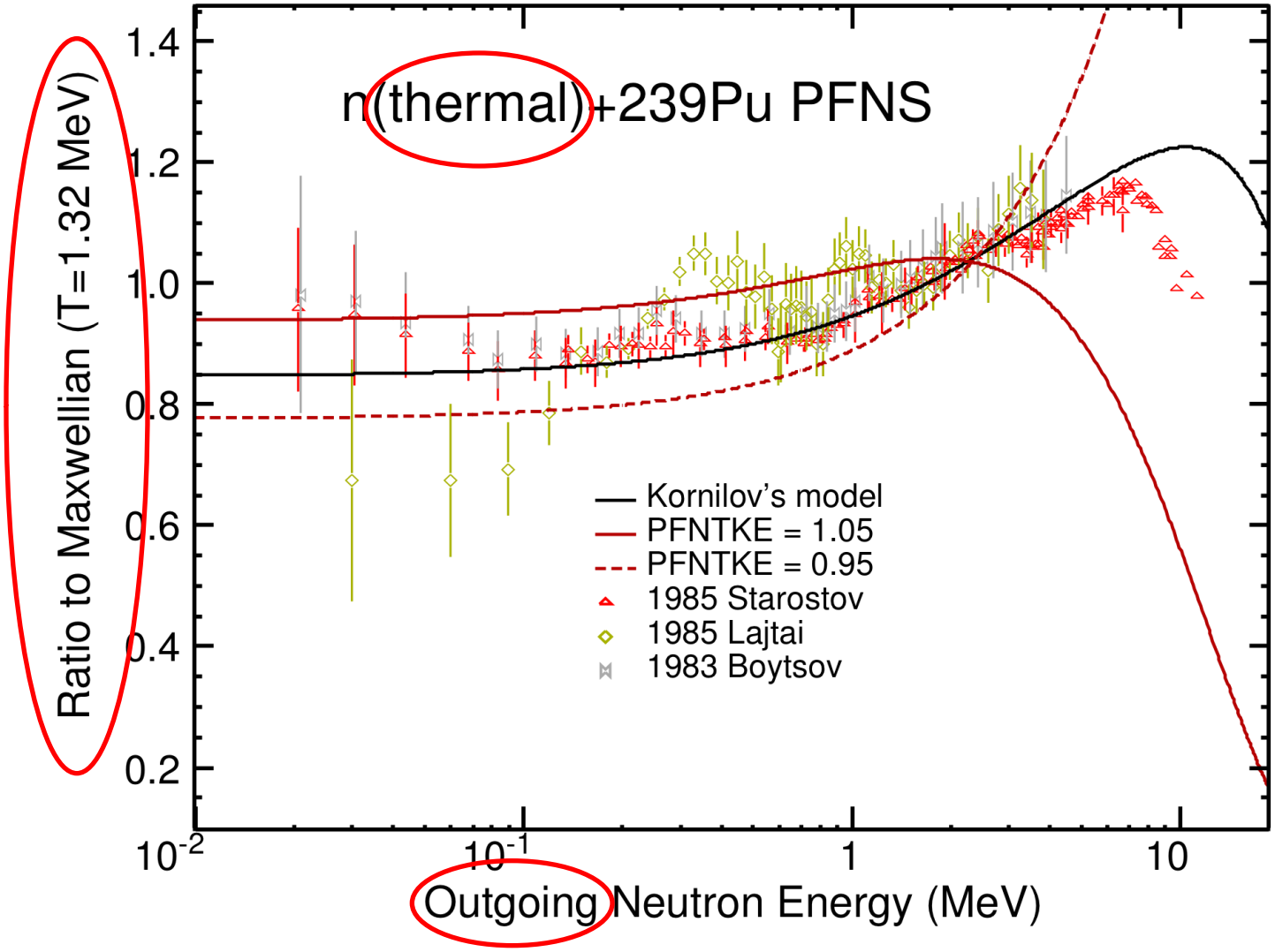
Improvement of the agreement of fission cross sections with experimental data by fitting through Kalman filter



Corresponding correlation matrix



PFNS calculation



Default calculation of PFNS (Kornilov) for ^{239}Pu and effect of changing total kinetic energy of the fragments by 5% in both directions.

There are differences from the case of cross sections!

Using Kalman to fit PFNS

Initial obstacles:

- Different quantities
- Maxwellian normalization of experimental data
- Function of E_{out} vs. function of E_{inc}
- Outgoing energy instead of incident energy
- Incident energy instead of reaction

Solutions:

- KALMAN does not know
- Andrej Trkov improved PFNS data extraction from EXFOR file
- KALMAN does not know – Reformatting: Transposing the sensitivity matrix!

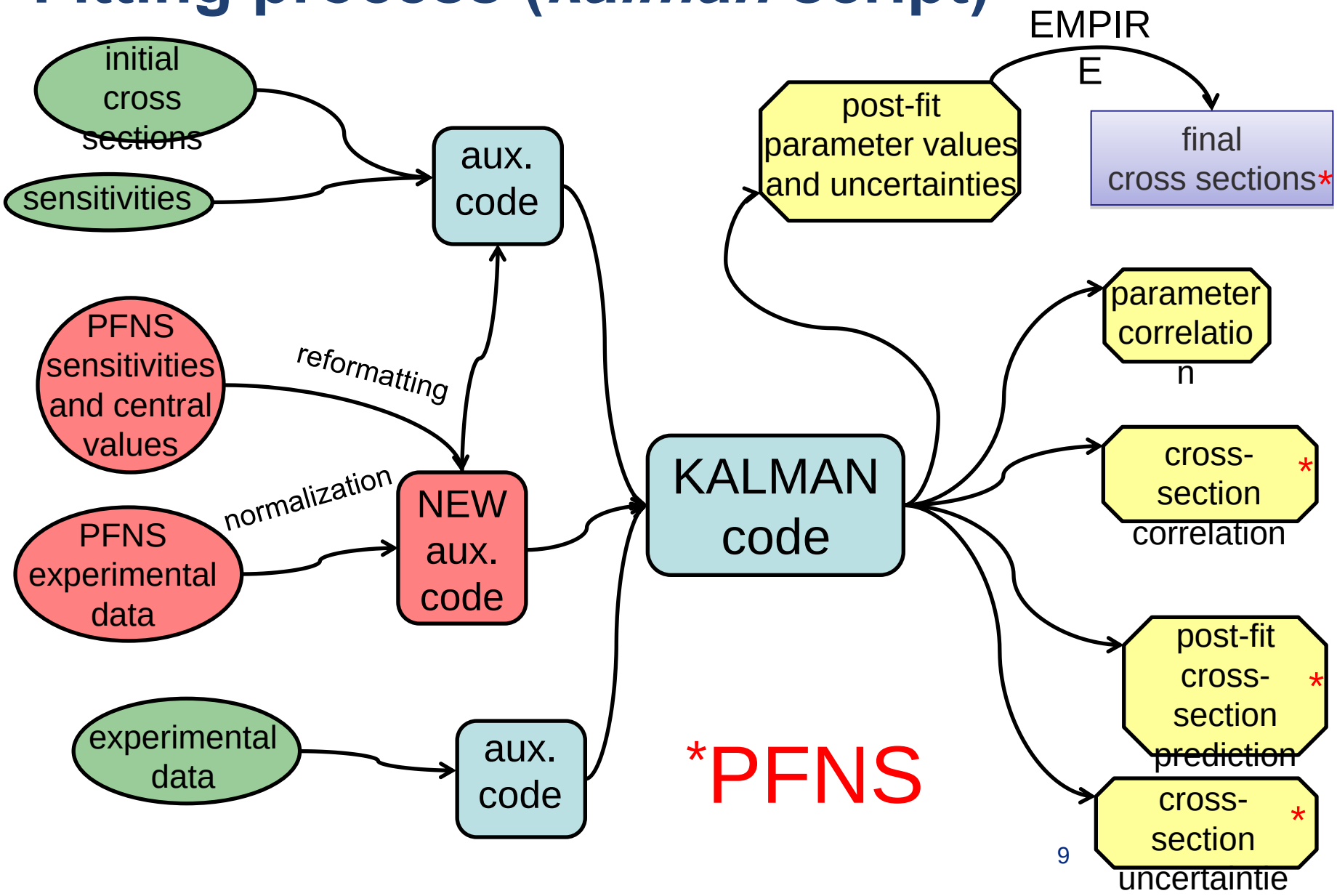
Reformatting PFNS Sensitivity-matrix file

Incident energies

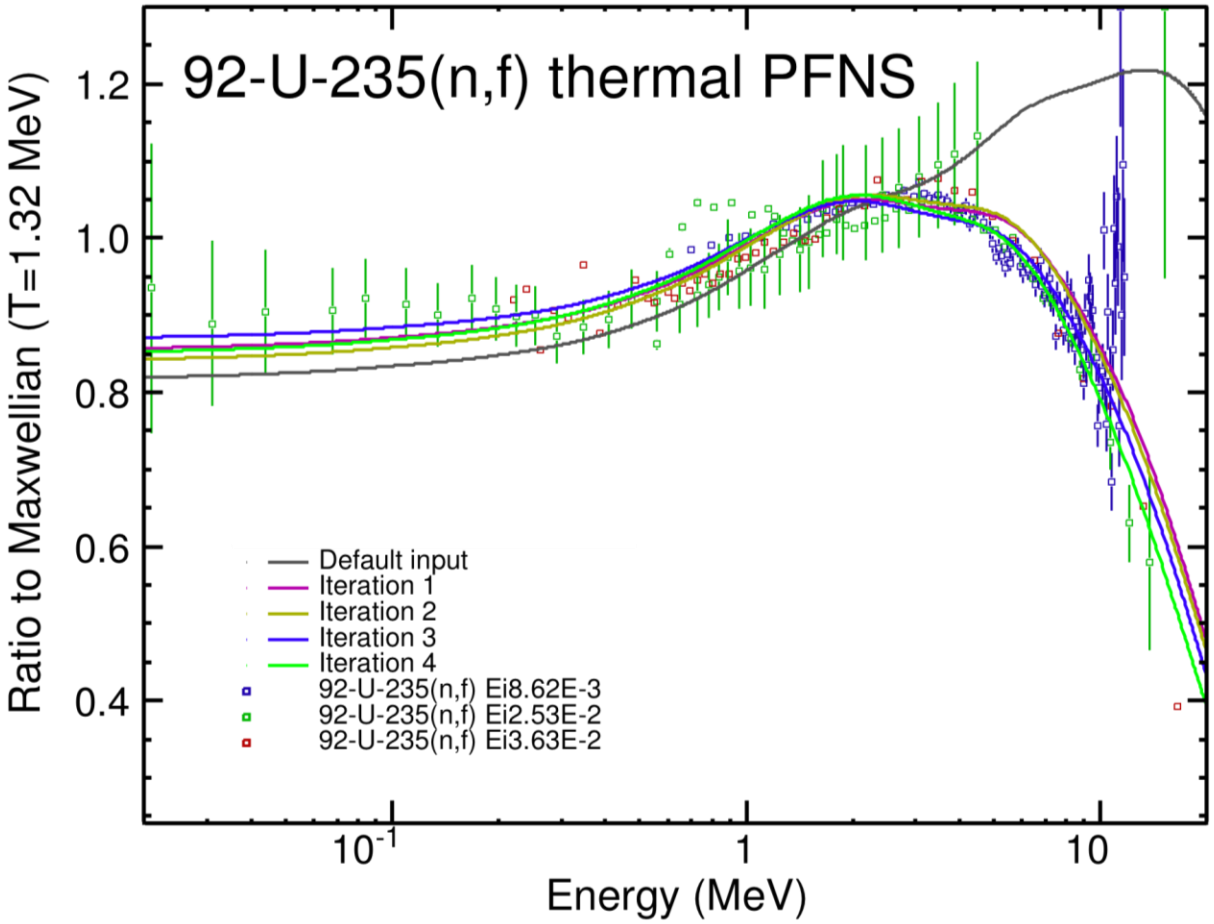
Outgoing energies

```
# 44            92-U -236
# Parameter: PFNTKE    0  0  0  0  variation: +-0.050     Sensitivity matrix
#  Eemit     5.000E-07   1.000E-03   2.000E-03   5.000E-03   1.000E-02   2.000E-02   5.000E-02
1.0000E-11  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
4.0000E-11  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
7.0000E-11  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
1.0000E-10  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
4.0000E-10  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
7.0000E-10  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
1.0000E-09  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
4.0000E-09  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
7.0000E-09  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
1.0000E-08  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01
4.0000E-08  1.9068E-01  1.9067E-01  1.9068E-01  1.9067E-01  1.9063E-01  1.9059E-01  1.9044E-01

24.500      -6.8575E+00 -6.8565E+00 -6.8557E+00 -6.8529E+00 -6.8487E+00 -6.8404E+00 -6.8152E+00
24.600      -6.9303E+00 -6.9294E+00 -6.9286E+00 -6.9261E+00 -6.9218E+00 -6.9131E+00 -6.8875E+00
24.700      -7.0040E+00 -7.0031E+00 -7.0022E+00 -6.9997E+00 -6.9954E+00 -6.9866E+00 -6.9606E+00
24.800      -7.0787E+00 -7.0777E+00 -7.0768E+00 -7.0742E+00 -7.0699E+00 -7.0610E+00 -7.0344E+00
24.900      -7.1542E+00 -7.1531E+00 -7.1522E+00 -7.1495E+00 -7.1450E+00 -7.1360E+00 -7.1092E+00
25.000      -7.2304E+00 -7.2294E+00 -7.2286E+00 -7.2257E+00 -7.2211E+00 -7.2119E+00 -7.1847E+00

# 44            92-U -236
# Parameter: PFNALP    0  0  0  0  variation: +-0.050     Sensitivity matrix
#  Eemit     5.000E-07   1.000E-03   2.000E-03   5.000E-03   1.000E-02   2.000E-02   5.000E-02
1.0000E-11 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
4.0000E-11 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
7.0000E-11 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
1.0000E-10 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
4.0000E-10 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
7.0000E-10 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
1.0000E-09 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
4.0000E-09 -7.0954E-02 -7.0967E-02 -7.0956E-02 -7.0949E-02 -7.0943E-02 -7.0932E-02 -7.0888E-02
```

Fitting process (*kalman* script)



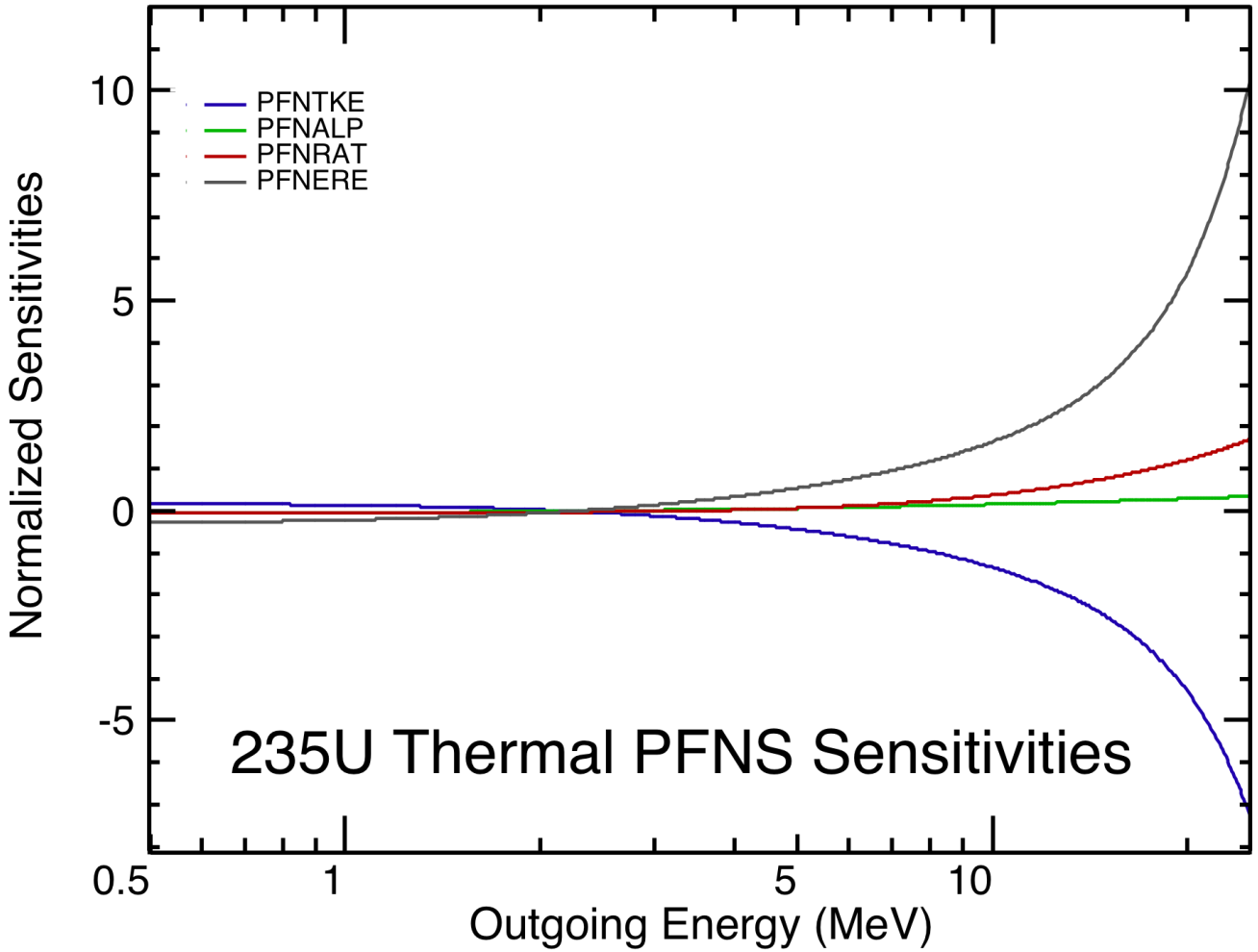
PFNS fit – Los Alamos model



Each KALMAN-EMPIRE iteration* improves agreement of calculated PFNS with experimental data!

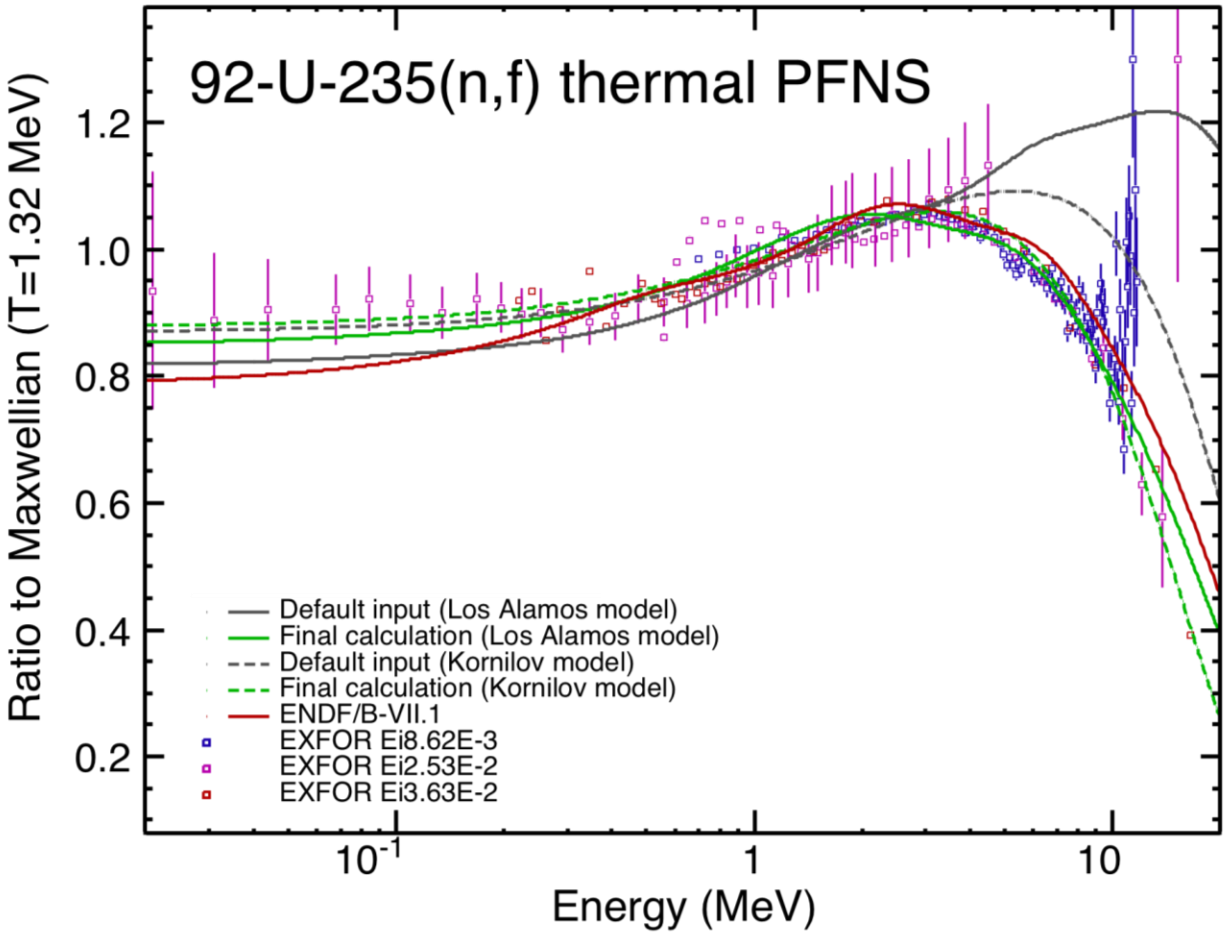
*For iterations 3 and 4, some spurious data points were removed from the fitting process.

PFNS sensitivity plot – Los Alamos model



- Parameters were varied 5%
- PFNS normalized to T_{maxw} = 1.32 MeV
- Crossing point
- Strong correlation / anticorrelation among PFNS parameters

PFNS fits – Los Alamos and Kornilov models



Fitting PFNS through Kalman filter enabled to improve description of experimental data for both models!

PFNS parameter correlation – ^{235}U

- Final values for the parameters

Parameter	Los Alamos model	Kornilov model
PFNTKE	1.0084E+0	1.1315E+0
PFNALP	9.3971E-1	8.9950E-1
PFNRAT	8.5436E-1	9.4934E-1
PFNERE	1.0157E+0	1.1129E+0

- Parameter correlations for both models:

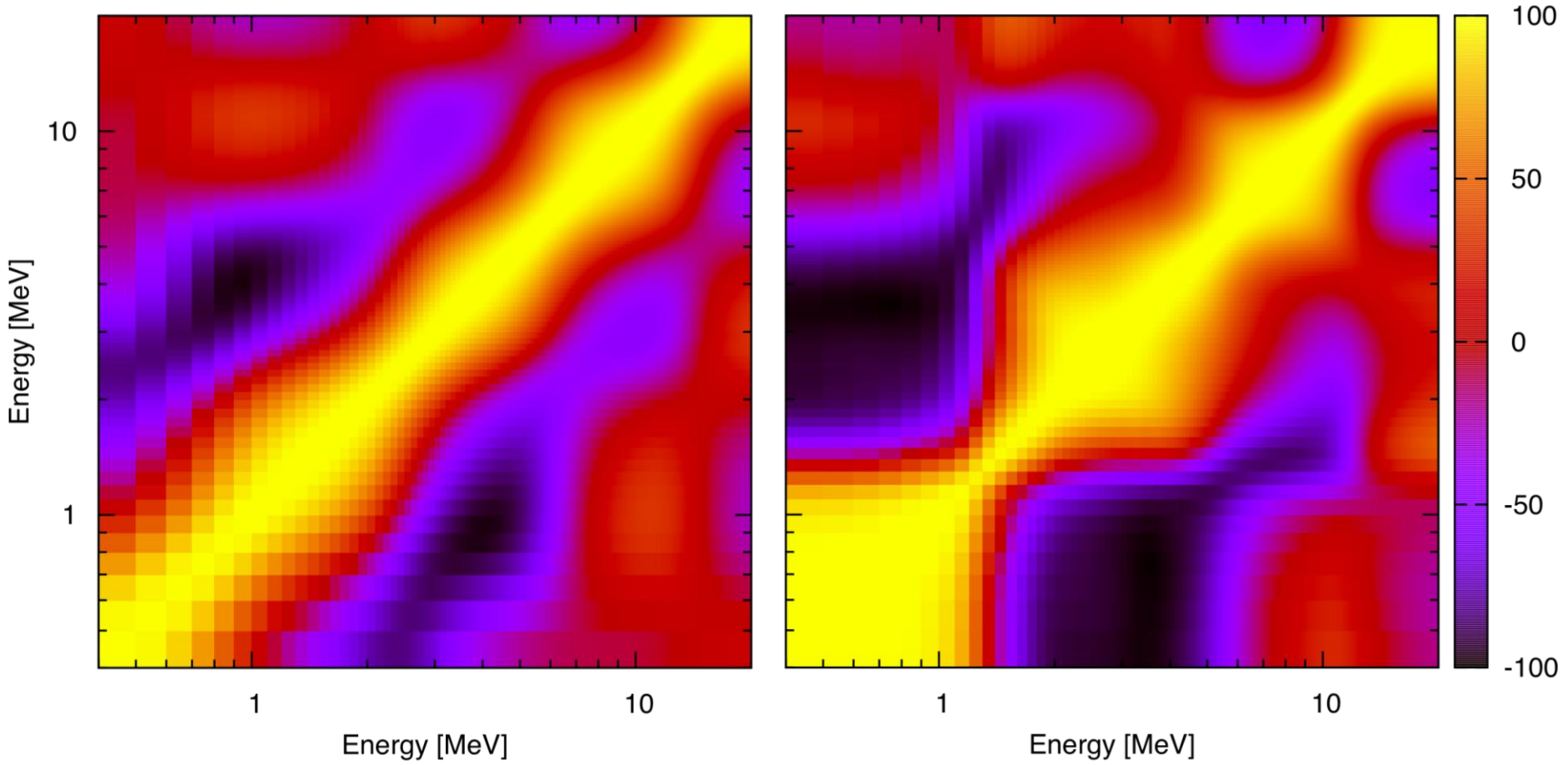
```
                          1    2    3    4
1PFNTKE000000 1.03E+00 1000
2PFNALP000000 9.88E-01 -740 1000
3PFNRAT000000 9.56E-01  779 -223 1000
4PFNERE000000 1.03E+00  963 -877  585 1000
```

Parameter correlations for the Los Alamos model

```
                          1    2    3    4
1PFNTKE000000 1.13E+00 1000
2PFNALP000000 8.99E-01 -526 1000
3PFNRAT000000 9.49E-01  298  612 1000
4PFNERE000000 1.11E+00  948 -766  -13 1000
```

Parameter correlations for the Kornilov model

PFNS correlations – ^{235}U



Correlations for the Los Alamos model

Correlations for the Kornilov model

Conclusion

- Calculation of 1st chance prompt fission spectra was incorporated in EMPIRE
- Two models were implemented:
  - Los Alamos model
  - Kornilov model
- We are now able to fit PFNS parameters to experimental data, for any Maxwellian normalization, for either model
- This allowed also to obtain:
  - Sensitivities to PFNS parameters
  - Correlations and covariances (both for parameters and PFNS)
  - Uncertainties (both for parameters and PFNS)
- Still independent from cross sections calculations