Low fidelity covariances in the fast neutron region

M.T. Pigni[†], M. Herman, P. Obložinský
National Nuclear Data Center - Brookhaven National Laboratory
Upton, New York, 11973-5000, U.S.A.

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† Reference author : pigni@bnl.gov

Introduction

- ✓ Triggered by current interest in innovative energy systems (GNEP) and fuel cycles (AFCI), with strong demand for neutron cross section covariances.
- ✓ In the new ENDF/B-VII.0 library the number of files including covariances is limited to a very few materials (7% of the materials in the neutron sublibrary).
- ✓ Our method to estimate covariances is based on the BNL nuclear reaction model code EMPIRE and Bayesian code KALMAN (LANL).
- ✓ Essential point in our method is the estimate of model parameter uncertainties based on previous studies and our own experience.

Goal: Materials and reactions

List of materials provided by NNDC (BNL), namely ENDF/B-VII.0 neutron sublibrary:

- Structural nuclei (^{19}F - ^{nat}Zn). . . . . 57 materials
- Fission products (^{69}Ga - ^{170}Er). . . . . . 219 materials
- Heavy nuclei (^{175}Lu - ^{209}Bi). . . . . . .31 materials,

Elastic - MT=2

Inelastic - MT=4

(n,2n) - MT=16

Fission - MT=18

(n,γ) - MT=102

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Covariance procedure

- ✓ A bash script was written to prepare 18 default model parameters for 3 basic nuclear reaction models (spherical OM, Hauser-Feshbach, exciton pre-equilibrium) and sensitivity input to run *Empire* for 219 fission products.
- ✓ Cross sections and sensitivity matrices were calculated for main reaction channels at 30 energy mesh points (5 keV - 20 MeV).
- ✓ Procedure to run *Kalman* with no experimental data and to propagate model parameter uncertainties to covariance matrices according to the ENDF format (file 33).
- ✓ Stereographic plots of correlation matrices and pictures of cross section uncertainties were interactively generated.

Evaluation method: Bayesian update

$$\mathbf{X}^{(n+1)} = \mathbf{X}^{(n)} - \mathbf{X}^{(n)}\mathbf{A}^{\mathrm{T}}(\mathbf{W}+\mathbf{V})^{-1}\mathbf{A}\mathbf{X}^{(n)},$$

$$\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + \mathbf{X}^{(n)}\mathbf{A}^{\mathrm{T}}(\mathbf{W}+\mathbf{V})^{-1}(\boldsymbol{\eta}^{(n)} - \boldsymbol{\sigma}(\mathbf{x}^{(n)}))$$

Sensitivity Matrix: $a_{\ell,m} = \frac{\partial \sigma_\ell(\mathbf{x})}{\partial x_m}$

Set of model parameters: $\mathbf{x} = (x_1 \ldots x_m)$

Parameter matrix correlations: $\mathbf{X} \equiv \langle \Delta x_i \Delta x_j \rangle$

Experimental cross sections: $\boldsymbol{\eta} = (\eta_1, \ldots, \eta_k)$

Evaluated cross sections: $\boldsymbol{\sigma}(\mathbf{x}) = (\sigma_1(\mathbf{x}), \ldots, \sigma_k(\mathbf{x}))$

Correlation matrices, W and V, for $\boldsymbol{\sigma}$ and $\boldsymbol{\eta}$ respectively

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Sensitivity of model parameters

Effect of a given model parameter on cross sections is determined via the relation

$$\mathcal{S}_\rho(k) = \frac{\sigma_\rho^{(+)}(k) - \sigma_\rho^{(-)}(k)}{\sigma_\rho^{(0)}}\,, \quad (1)$$

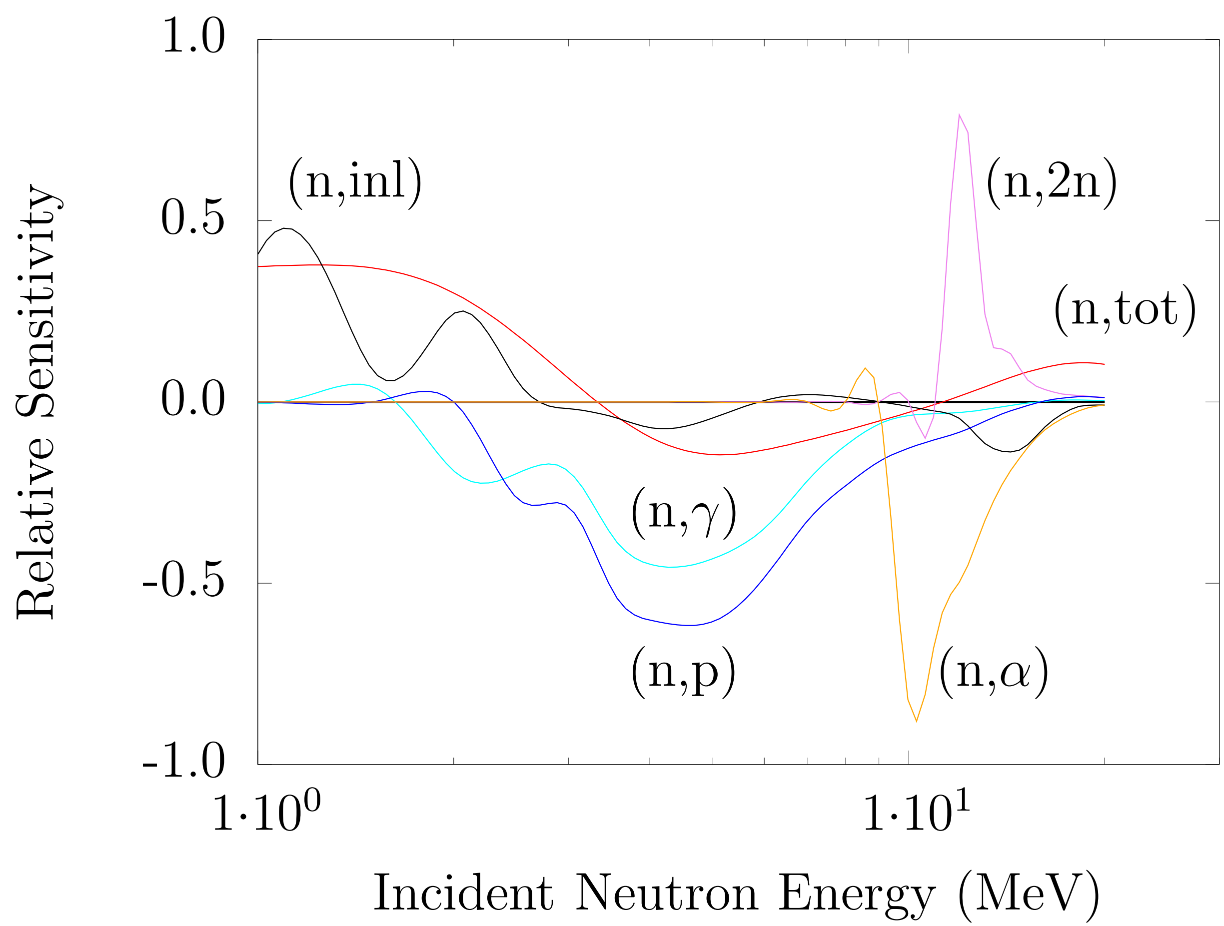
where,

$$\sigma_\rho^{(0)} = \sigma_\rho(E; x_1, \ldots, x_j)$$

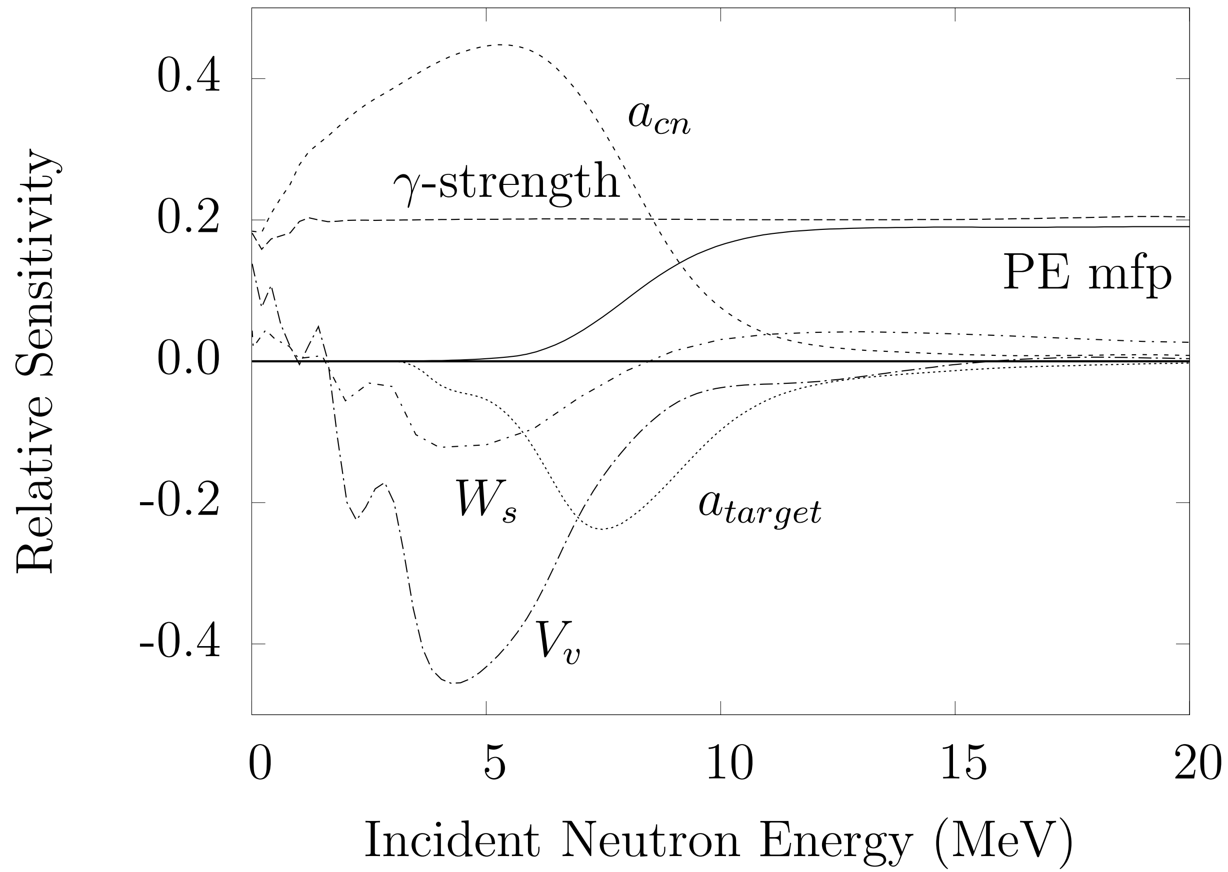
is the value of the cross section calculated for the best or default set of parameters $\mathbf{x} = (x_1, \ldots, x_j)$ for a specific reaction channel ρ, while

$$\sigma_\rho^{(\pm)}(k) = \sigma_\rho^{(\pm)}(E; x_1, x_2, \ldots, x_k \pm \delta x_k, \ldots, x_j)\,.$$

Sensitivity of model parameters



Sensitivity of model parameters



Model parameter uncertainties

	Δr_s	Δr_v	Δr_w	ΔV_v	ΔW_s	ΔW_v	Δa_s	Δa_v	ΔV_v	ΔW_s
%	±3.0	±3.0	±3.0	±3.0	±5.0	±5.0	±3.0	±3.0	±3.0	±3.0

Table 1: Uncertainties for optical model parameters for neutrons and protons. These values are based on the analysis performed by A.J. Koning (2003) for a simplified set of the global neutron OMP parameters.

	Δa_{cn}	Δa_{tg}	Δa_{n2n}	Δa_{np}	Δg_{np}	Δg_{tg}	$\Delta(\gamma\text{-}str.)$	Δ(PE mfp)
%	±10	±10	±10	±10	±10	±10	±20	±20

Table 2: Uncertainties for level densities and pre-equilibrium emissions. The values are based on M. Herman's analysis.

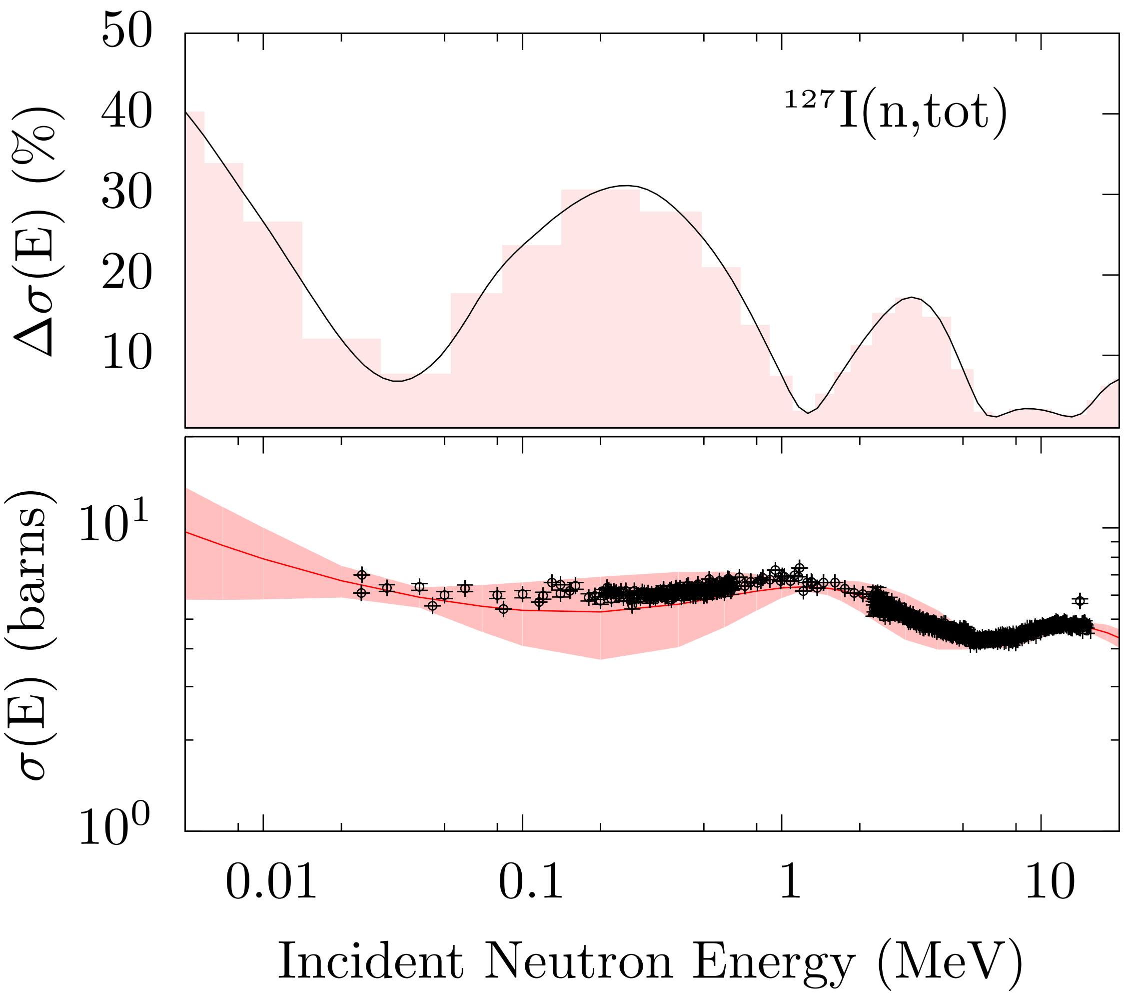
File 33 for ^{127}I - Example


```
5.312700+4 1.258140+2          0          0          0          1532533102    1
0.000000+0 0.000000+0          0        102          0          1532533102    2
0.000000+0 0.000000+0          1          5        465         30532533102    3
1.000000-5 5.000000+3 1.000000+4 2.000000+4 4.000000+4 7.000000+4532533102    4
1.000000+5 2.000000+5 4.000000+5 6.000000+5 8.000000+5 1.000000+6532533102    5
1.200000+6 1.500000+6 1.700000+6 2.000000+6 2.500000+6 3.000000+6532533102    6
4.000000+6 5.000000+6 6.000000+6 7.000000+6 8.000000+6 9.000000+6532533102    7
1.000000+7 1.200000+7 1.400000+7 1.600000+7 1.800000+7 2.000000+7532533102    8
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0532533102    9
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0532533102   10
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0532533102   11
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0532533102   12
0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 1.239167-2532533102   13
9.530548-3 6.604117-3 6.822294-3 9.211948-3 1.130562-2 1.410545-2532533102   14
1.499138-2 1.450047-2 1.620528-2 1.668101-2 1.654551-2 1.643345-2532533102   15
1.667016-2 1.672637-2 1.695897-2 1.652111-2 1.387125-2 1.163917-2532533102   16
1.043459-2 1.098256-2 1.210384-2 1.294047-2 1.343959-2 1.416787-2532533102   17
1.551862-2 1.729264-2 1.845796-2 1.052189-2 1.223082-2 1.319760-2532533102   18
1.382761-2 1.377143-2 1.316591-2 1.317981-2 1.316359-2 1.348341-2532533102   19
1.340080-2 1.345759-2 1.340915-2 1.322289-2 1.302107-2 1.258390-2532533102   20
1.241250-2 1.291808-2 1.388655-2 1.487396-2 1.525050-2 1.537540-2532533102   21
1.553999-2 1.579322-2 1.626316-2 1.647718-2 1.643124-2 1.630409-2532533102   22
1.958827-2 2.153970-2 2.016022-2 1.757636-2 1.286703-2 1.182688-2532533102   23
1.232449-2 1.100807-2 1.025067-2 1.048176-2 1.045473-2 9.721625-3532533102   24
```

$$\approx$$

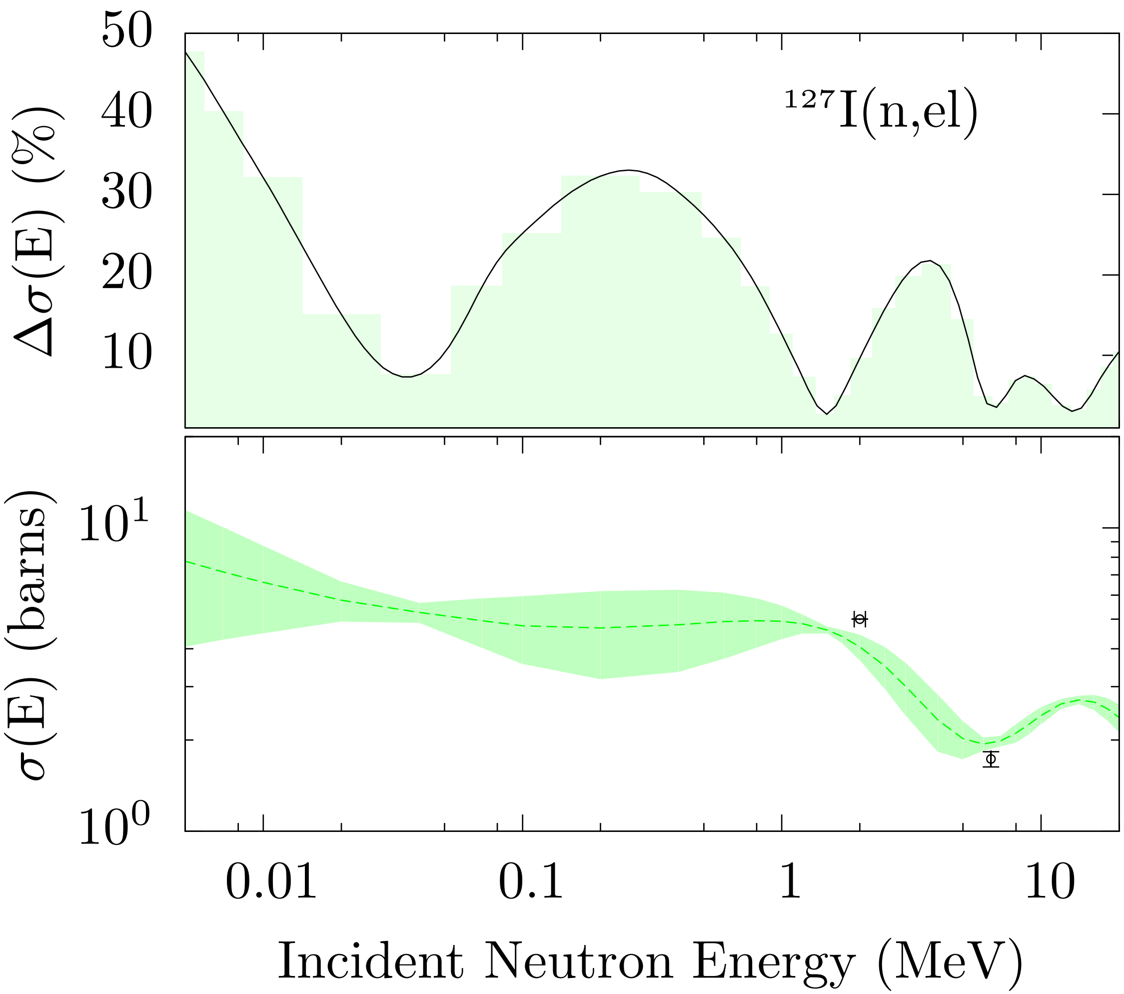
```
3.200676-2 6.389377-3 9.428953-2 1.165153-1 1.290957-1 1.304407-1532533102   72
1.216254-1 1.101687-1 8.584736-2 6.132215-2 3.059810-2 8.823635-4532533102   73
1.580825-1 1.834349-1 1.913991-1 1.843823-1 1.720093-1 1.424090-1532533102   74
1.082675-1 6.225419-2 1.697629-2 2.183085-1 2.324826-1 2.288497-1532533102   75
2.178526-1 1.879664-1 1.501457-1 9.660517-2 4.297398-2 2.529737-1532533102   76
2.559019-1 2.505308-1 2.289483-1 1.959753-1 1.450110-1 9.237348-2532533102   77
2.687540-1 2.734768-1 2.690805-1 2.492536-1 2.103229-1 1.674478-1532533102   78
2.890849-1 3.039011-1 2.995450-1 2.756972-1 2.456236-1 3.534225-1532533102   79
3.779839-1 3.834490-1 3.788355-1 4.281608-1 4.611511-1 4.810248-1532533102   80
5.253057-1 5.735303-1 6.478680-1                                  532533102   81
                                                                  532533102   82
```

Results - Uncertainties for ^{127}I



Reaction channel: Total...Elastic...Inelastic...(n,2n)...(n,γ)

Results - Uncertainties for ^{127}I



Reaction channel: Total...Elastic...Inelastic...(n,2n)...(n,γ)

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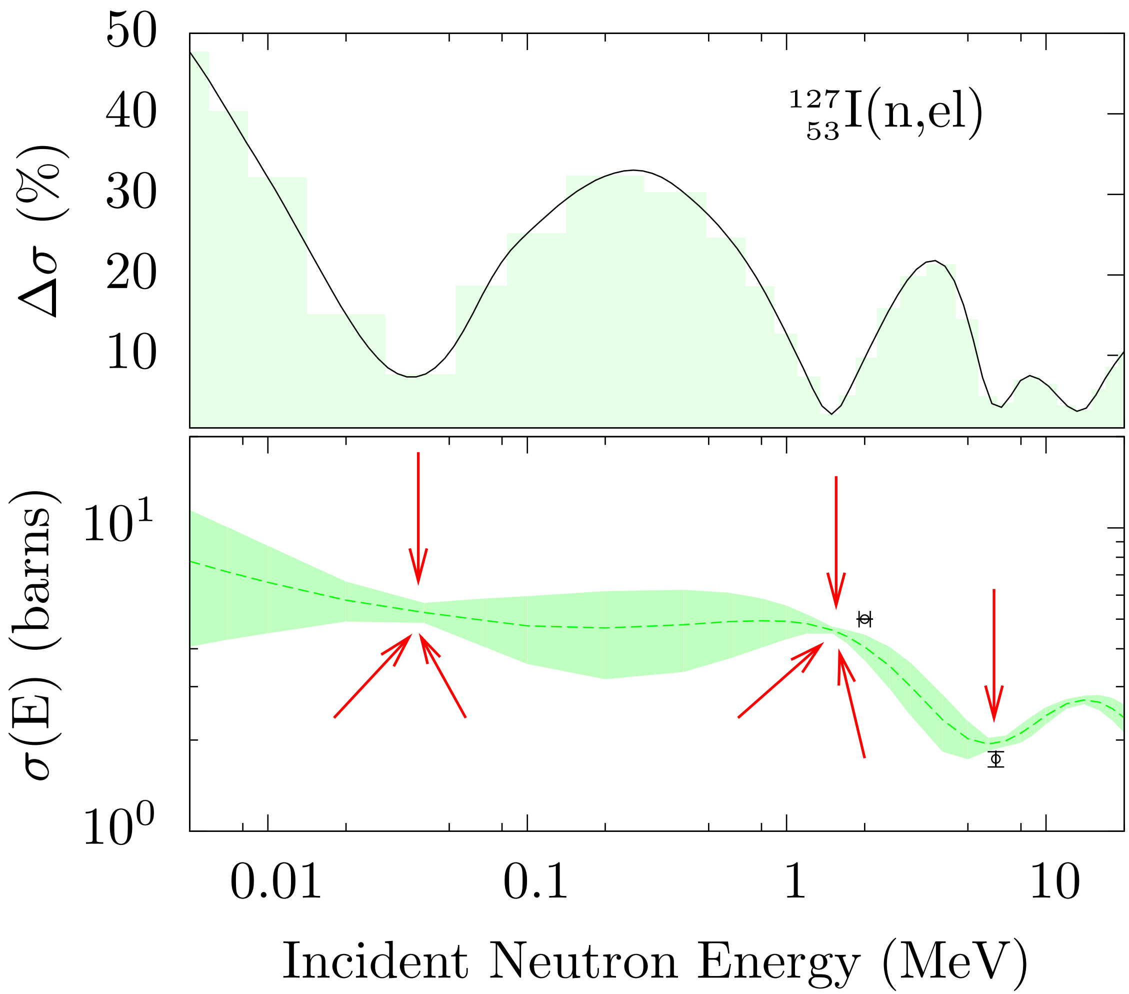

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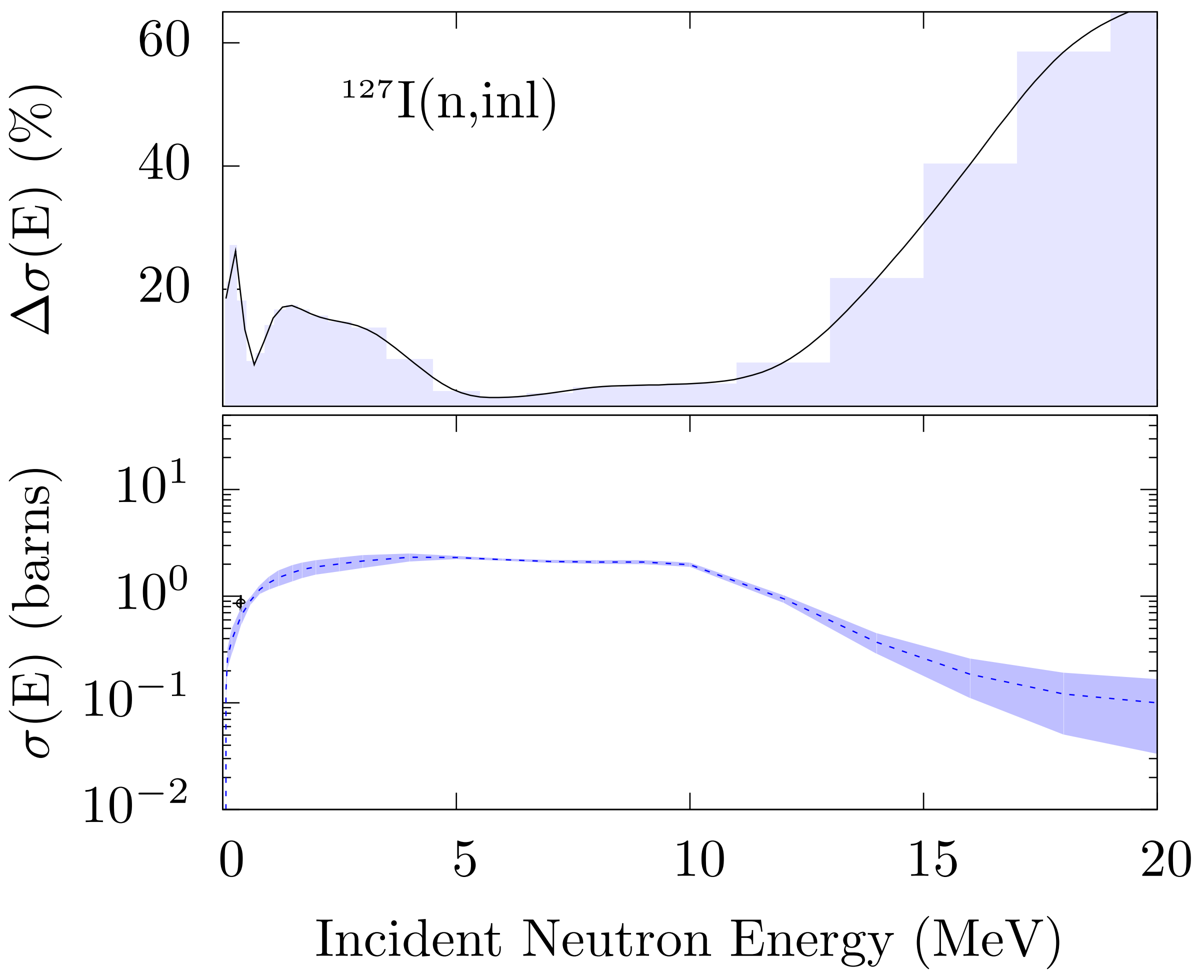

Reaction channel: Total...Elastic...**Inelastic...**(n,2n)...(n,γ)

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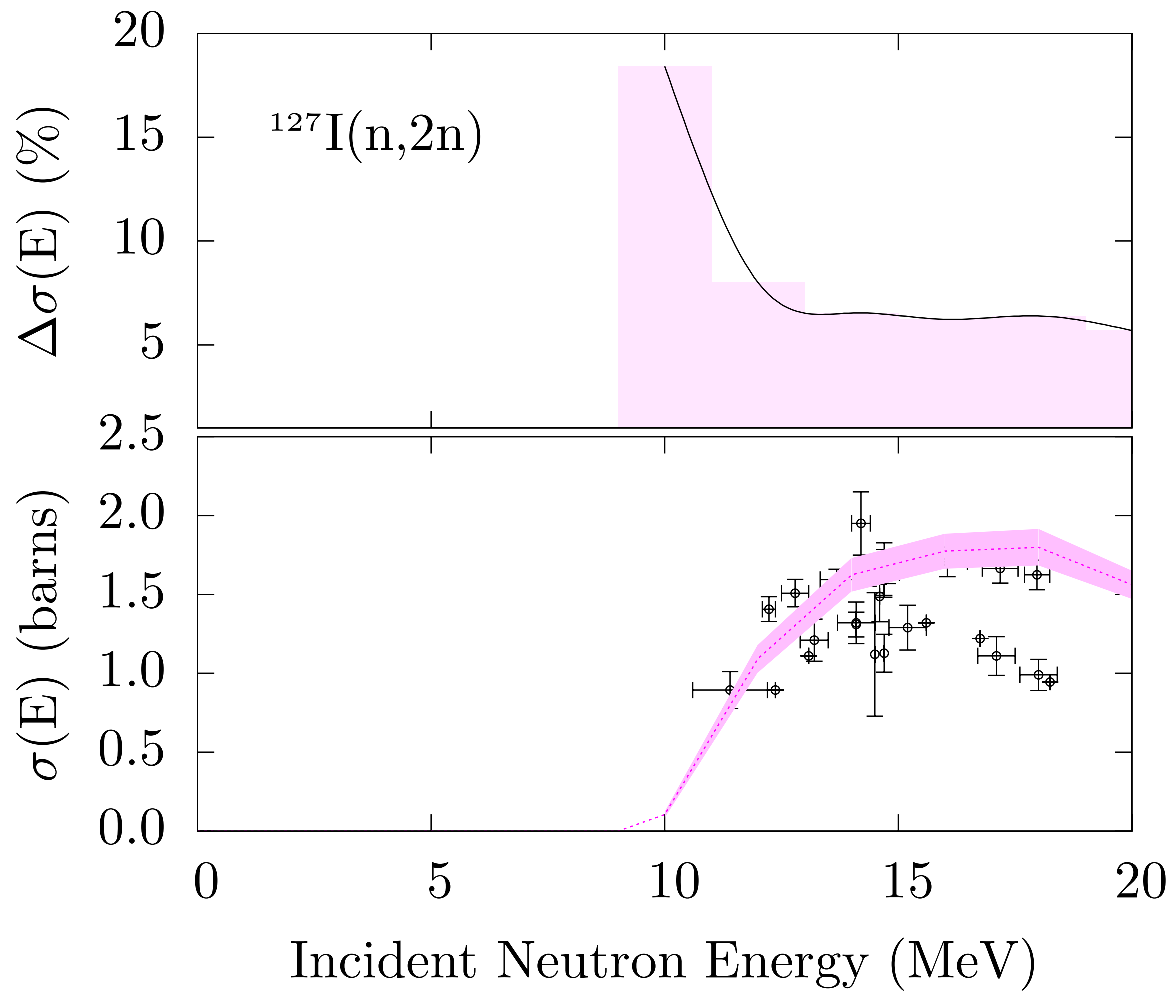

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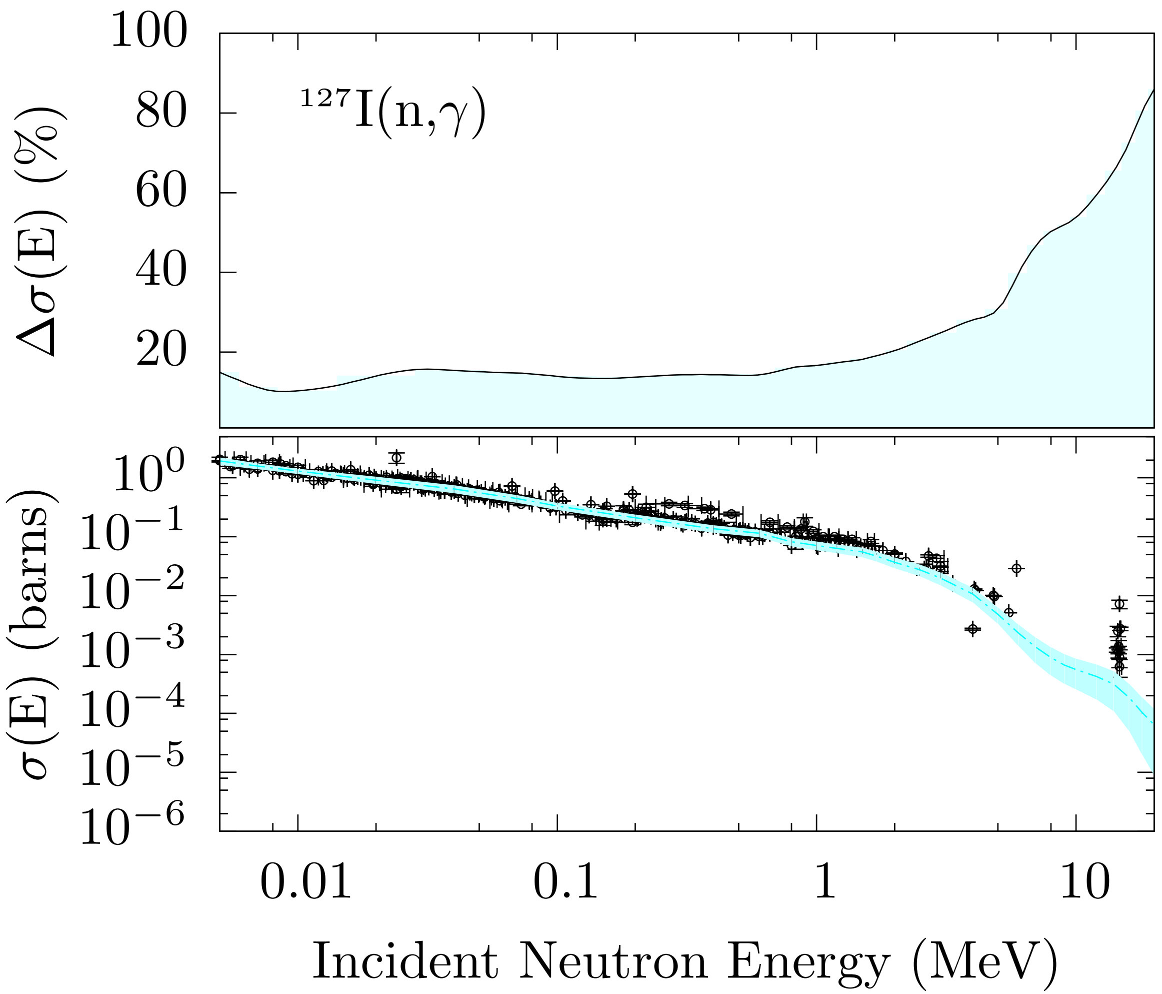
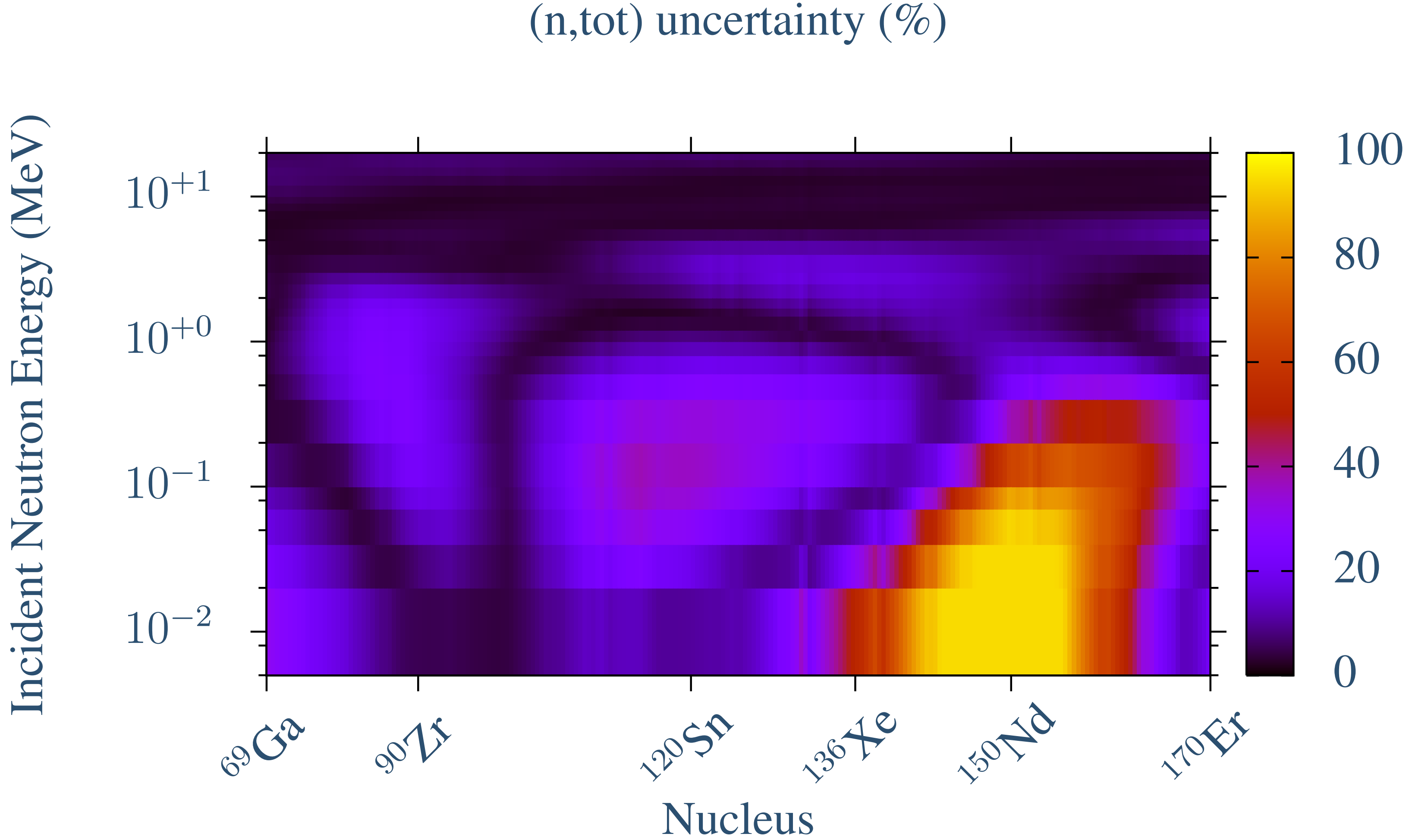


Reaction channel: Total...Elastic...Inelastic...(n,2n)...(n,γ)

Compact results ("BNL plot")

Fission products - MT=1



Compact results (“BNL plot”)

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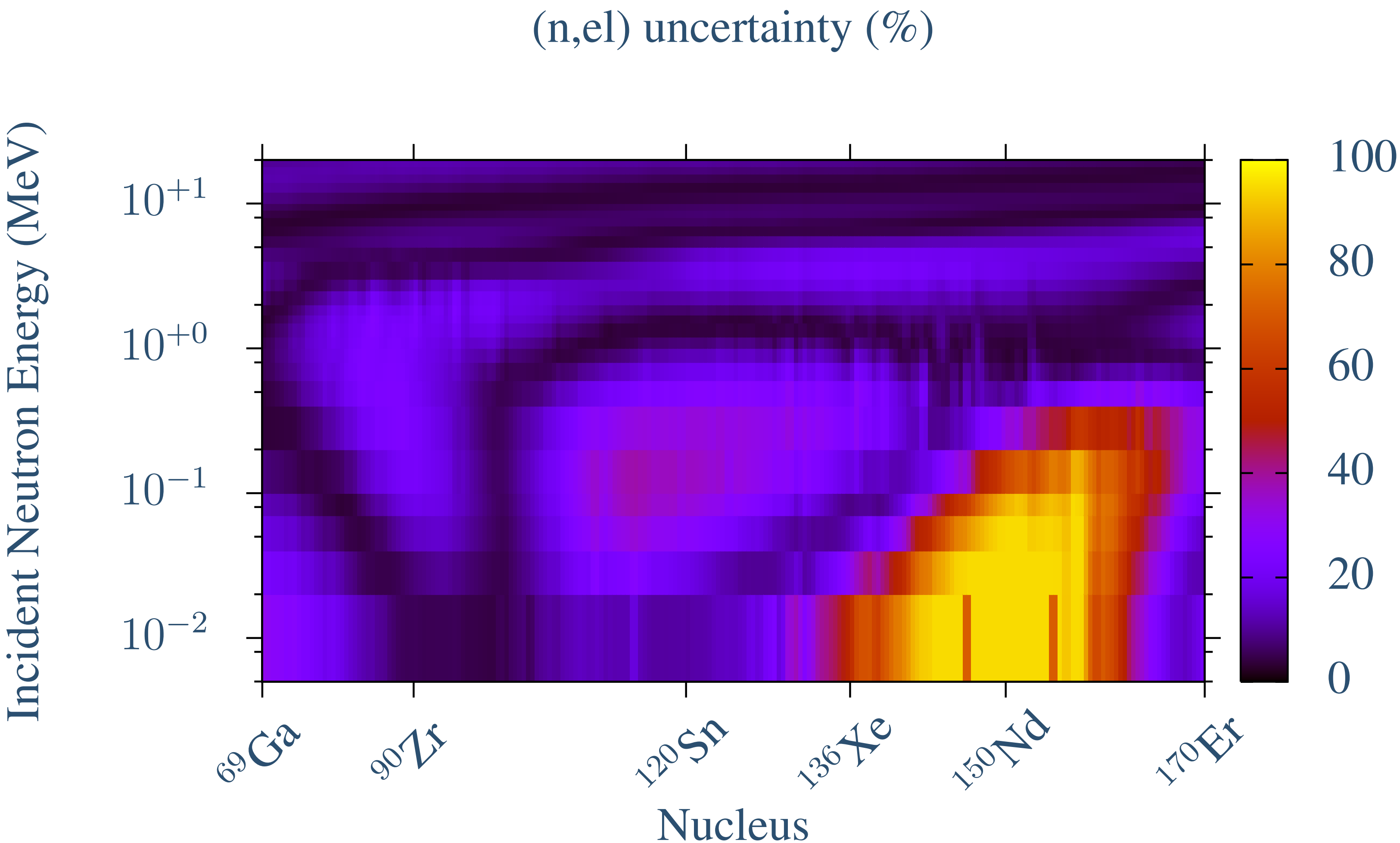
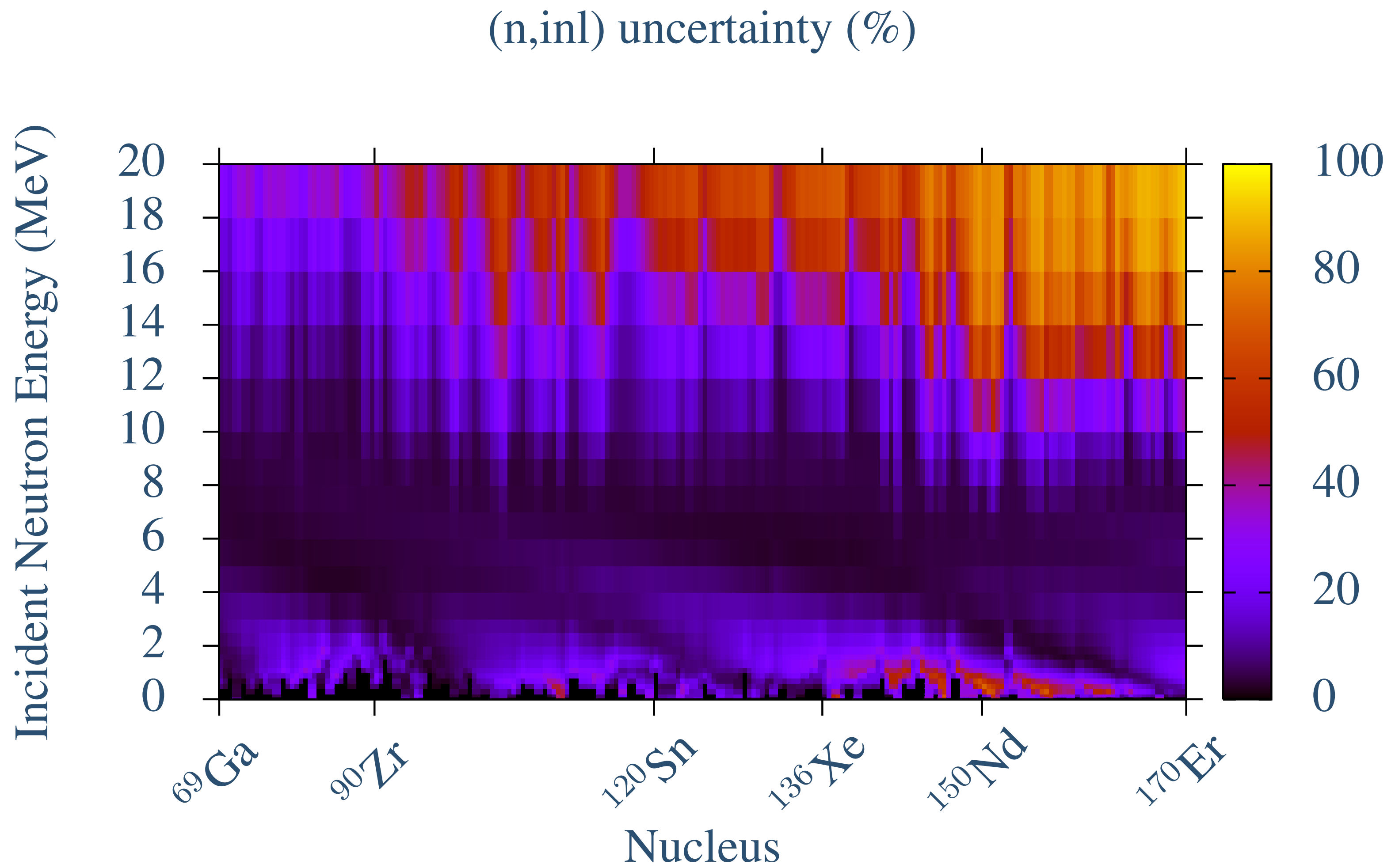
▷ Compact results (“BNL plot”)
Conclusions: results, issues and outlook

Fission products - MT=2



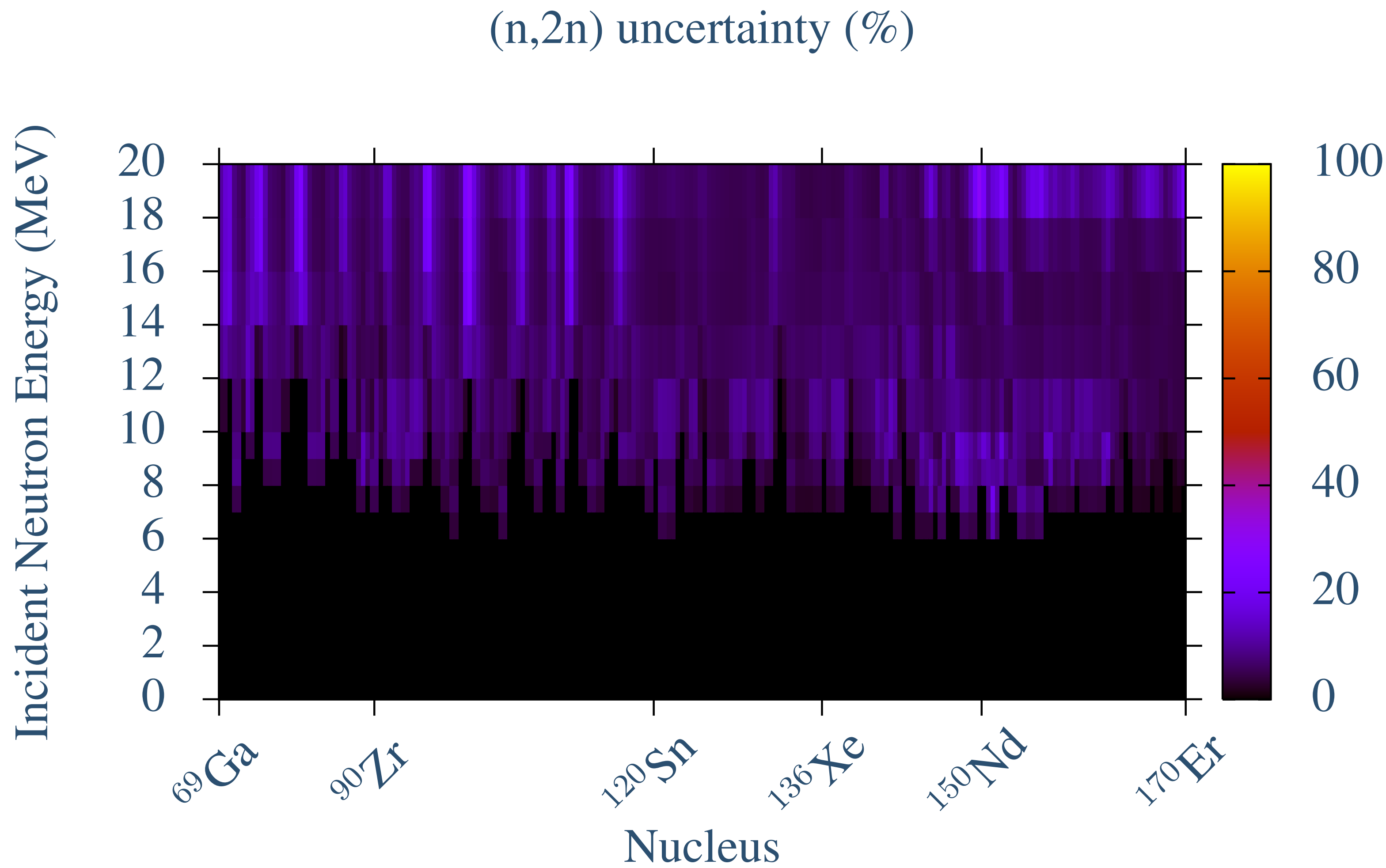
Compact results ("BNL plot")

Fission products - MT=4



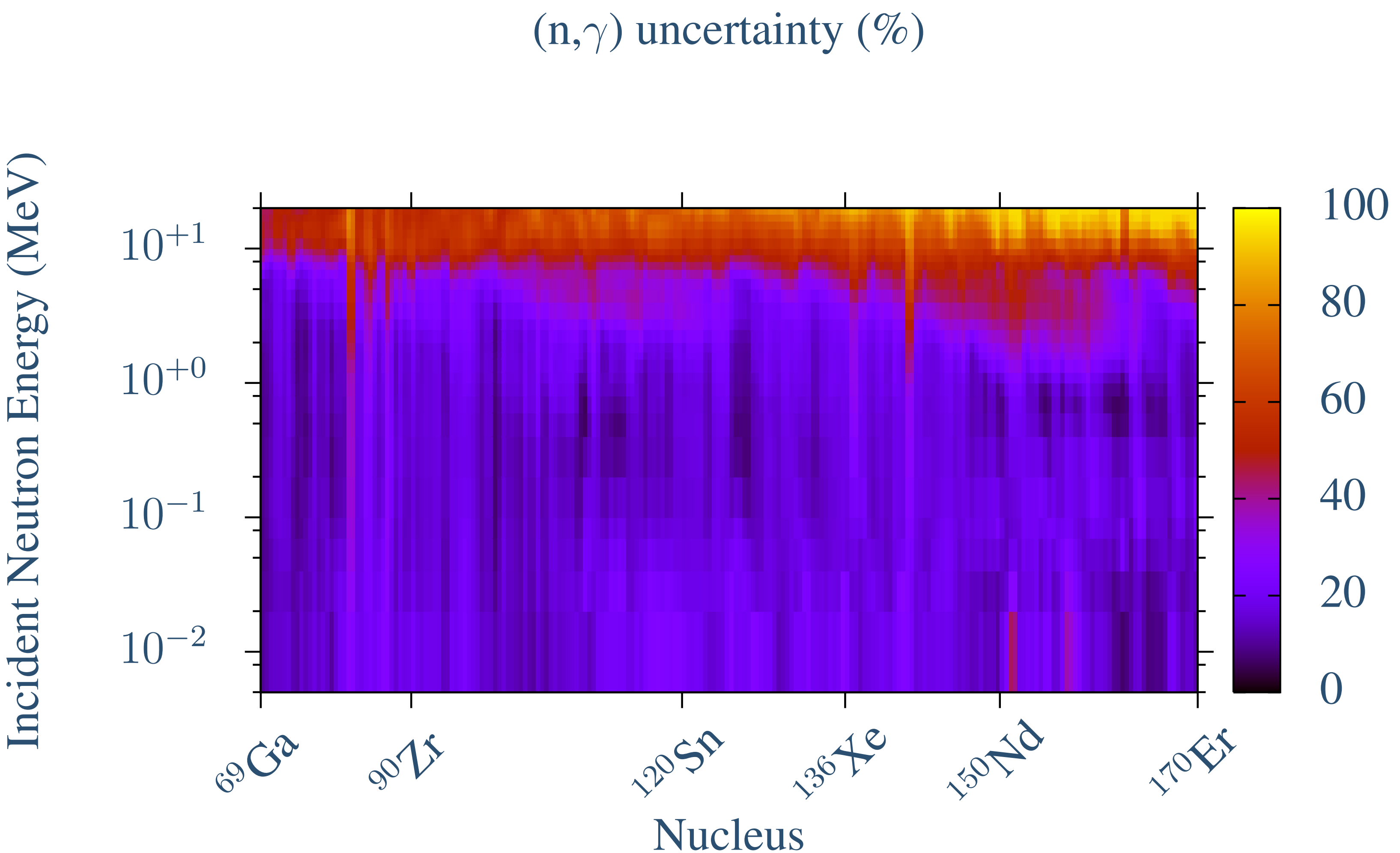
Compact results ("BNL plot")

Fission products - MT=16



Compact results ("BNL plot")

Fission products - MT=102



Conclusions: results, issues and outlook

- ✓ Results: Low-fidelity covariances (covariance estimates) were produced for 219 fission products in the fast neutron region (5 keV - 20 MeV)
- ✓ Issue: high uncertainties of (n,tot) at $E_n \lesssim 3$ MeV.
- ✓ Issue: Very high (n,tot) uncertainties at $E_n \lesssim 100$ keV for nuclei between Xe and Eu.
- ✓ Outlook: The method should be extended to more complex nuclear reaction models (deformed OM, multistep direct, ...)
- ✓ Outlook: A more rigorous choice of parameter uncertainties should be established, including their uncertanties (RIPL-3 project?).