Covariances in EMPIRE code: capabilities, results and issues

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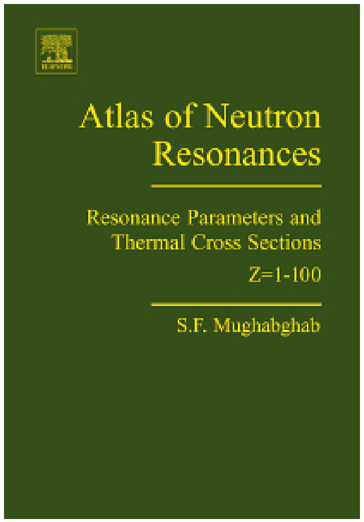
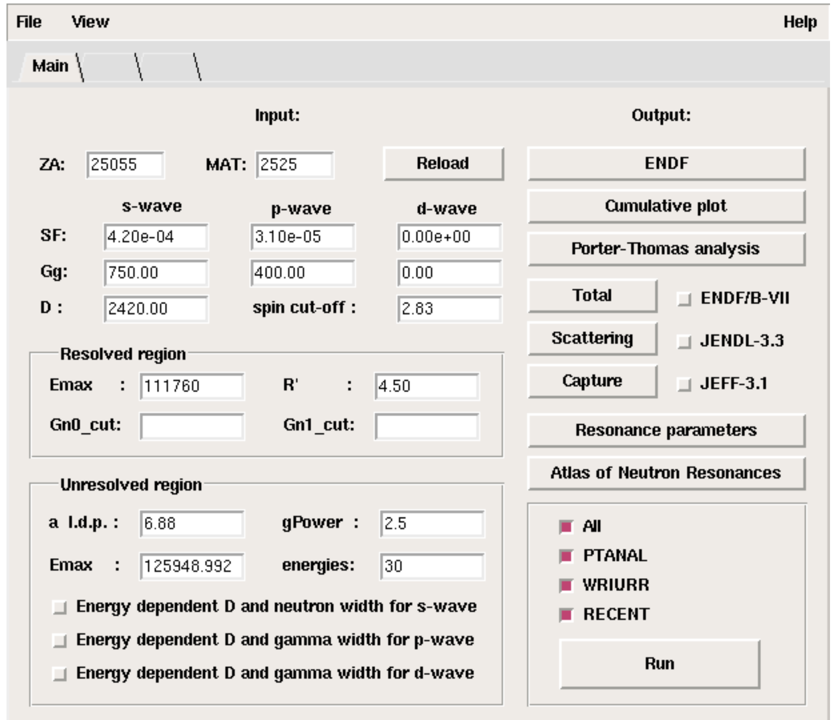
Approaches to covariances in EMPIRE

- Resolved Resonance Region
  - Atlas of Neutron Resonances (EMPIRE resonance module)
- Unresolved Resonance Region
  - Atlas of Neutron Resonances (EMPIRE resonance module)
  - any of the fast neutron methods below
- Fast neutron region
  - EMPIRE-KALMAN (model & model+experiment)
  - EMPIRE-Monte Carlo (MC) (model)
  - EMPIRE-MC-GANDR (model+experiment)
  - Unified Monte Carlo (model+experiment, not yet implemented)

Resonance Region

Atlas & EMPIRE resonance module





MF = 2

MF = 32

(compact format)

See poster by **Young-Sik Cho** for more details and results

See contribution by **S.F. Mughabghab** on ensuring consistency among thermal cross section uncertainty and uncertainties of resonance parameters

Fast neutron region

Kalman: Bayesian, Generalized Least Squares approach

update # — exp. n x-sec

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

model parameters — model x-sec

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

parameter covariance — exp. n covariance

$$\mathbf{Q} = (\mathbf{W} + \mathbf{V})^{-1}$$

error matrix

$$\mathbf{W} = \mathbf{A}\mathbf{X}\mathbf{A}^{\mathrm{T}}$$

sensitivity matrix

$$a_{i,j} = \frac{\partial\sigma(\mathbf{x}, E_i)}{\partial x_j}$$

Ingredients:

- model x-sections
- model parameter uncertainties
- x-sec. sensitivities to parameters
- experimental x-sections
- covariances for each experiment

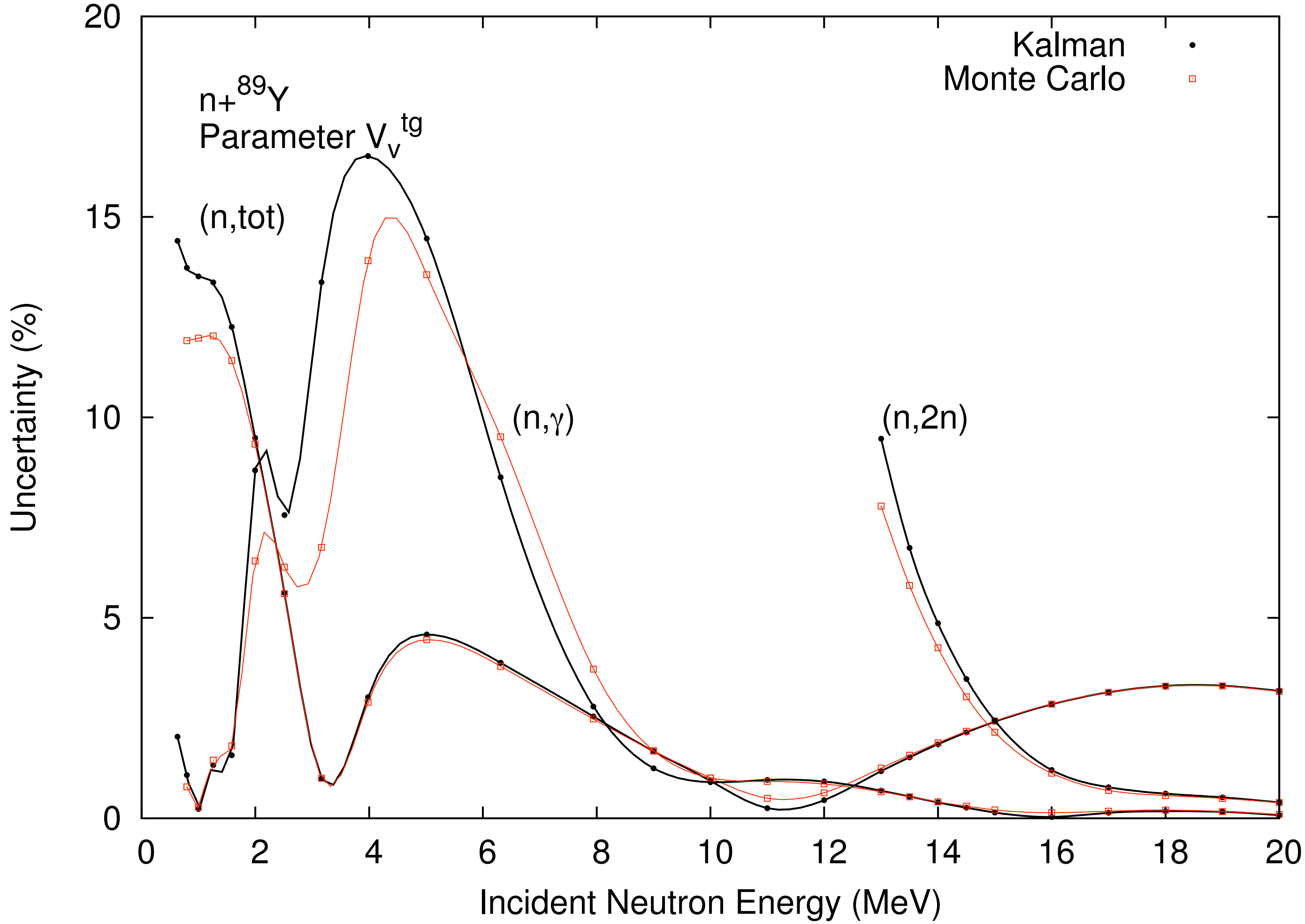
Unifies model parameters, experiments, x-sections, covariances

Comparison
KALMAN versus Monte Carlo

- Object of comparison
  - EMPIRE-KALMAN versus EMPIRE-MC (model covariances)
  - EMPIRE-KALMAN versus EMPIRE-MC-GANDR (model+exp. Covar.)
- Reactions
  - total
  - capture
  - (n,2n)
- Varied: full set of parameters as well as independently the four selected below
  - Mean free path in the exciton model (PCROSS)
  - γ-emission strength in the compound
  - OM volume depth of the real potential
  - OM real diffuseness

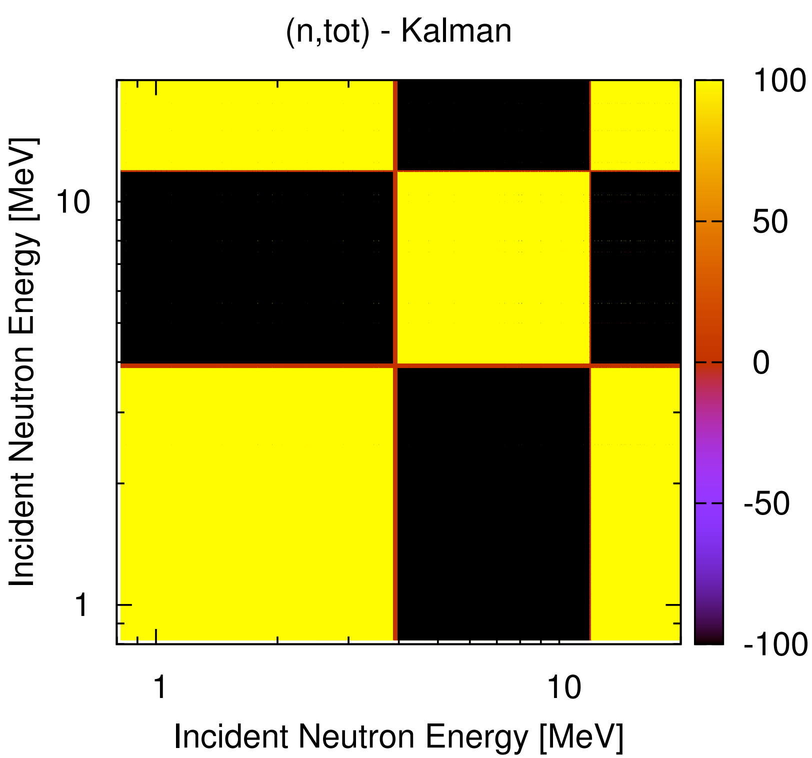
n + ^{89}Y

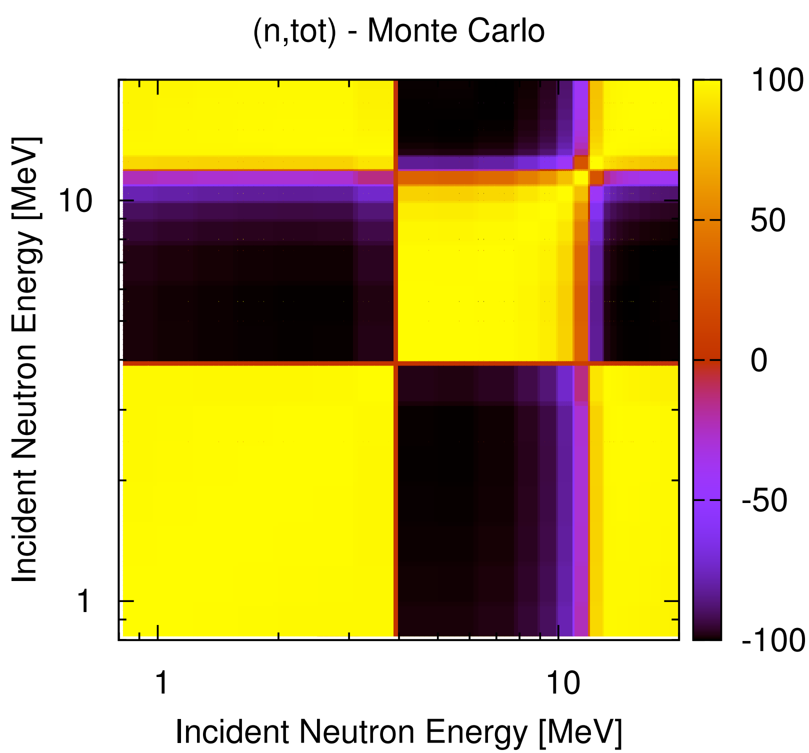
comparison of uncertainties due to OMP real volume depth



^{89}Y(n,tot) correlation matrix

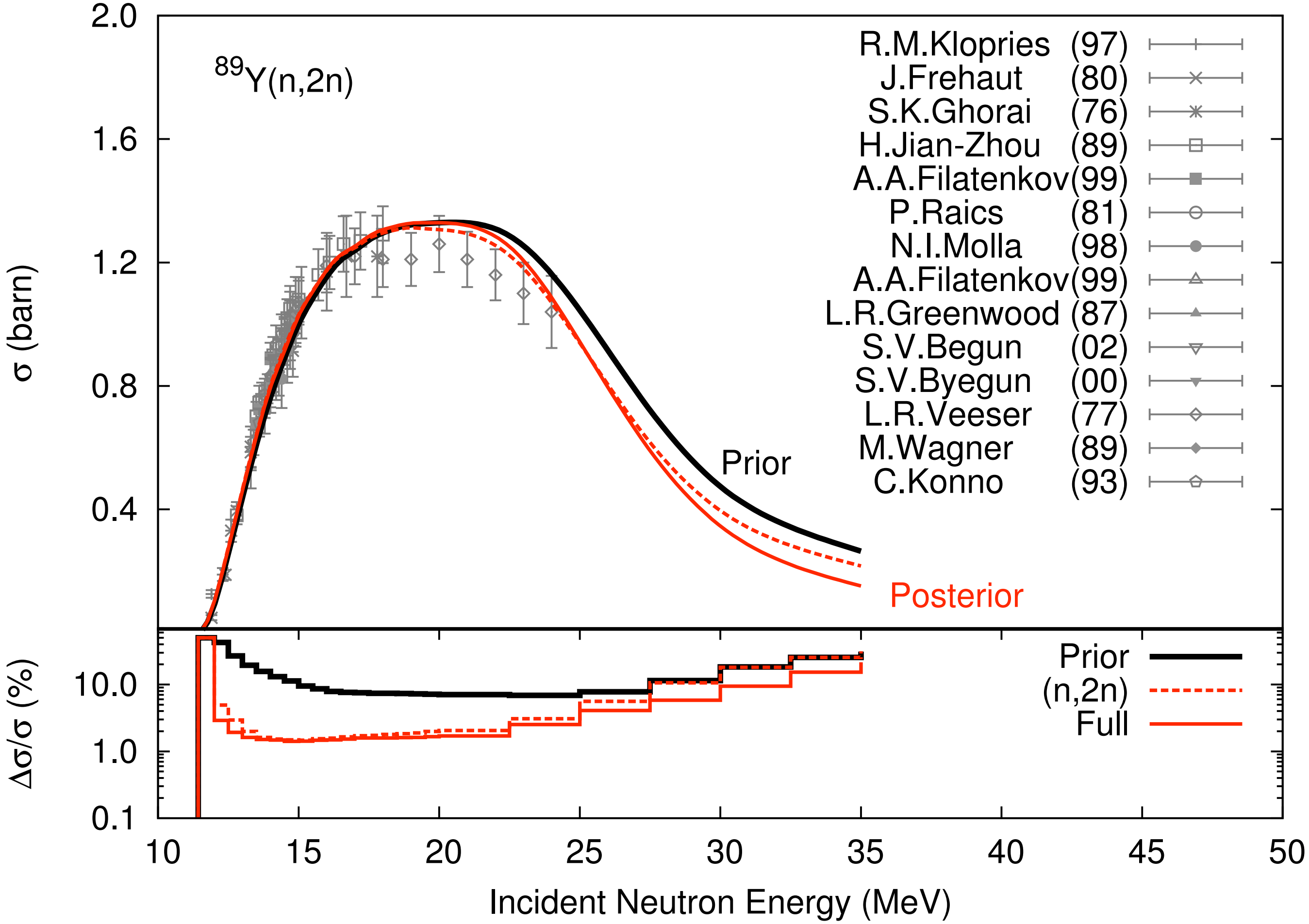
no experimental data





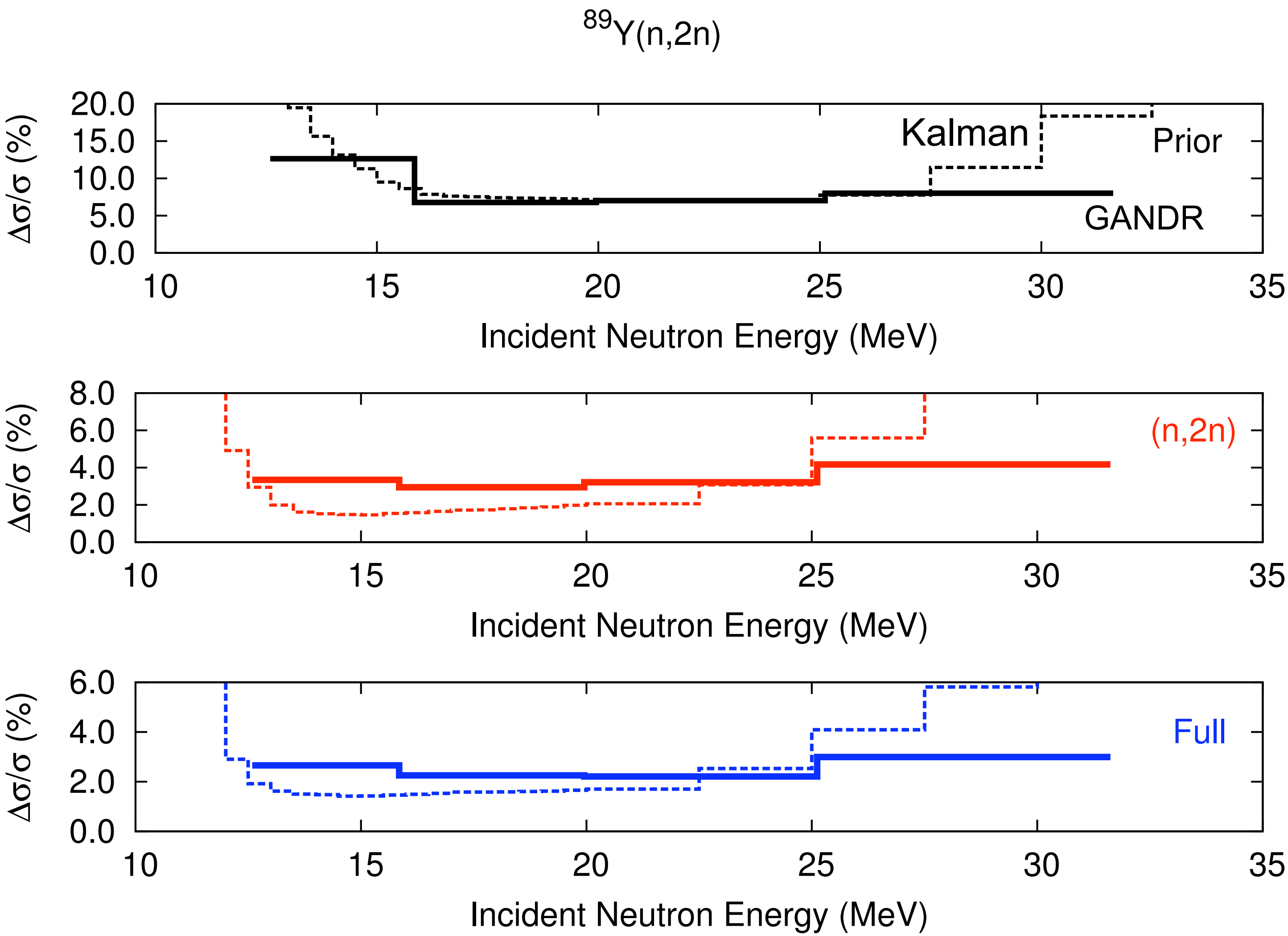
^{89}Y(n,2n) cross sections and uncertainties

effect of including experimental data in KALMAN



$^{89}Y(n,2n)$ uncertainties

effect of including experimental data

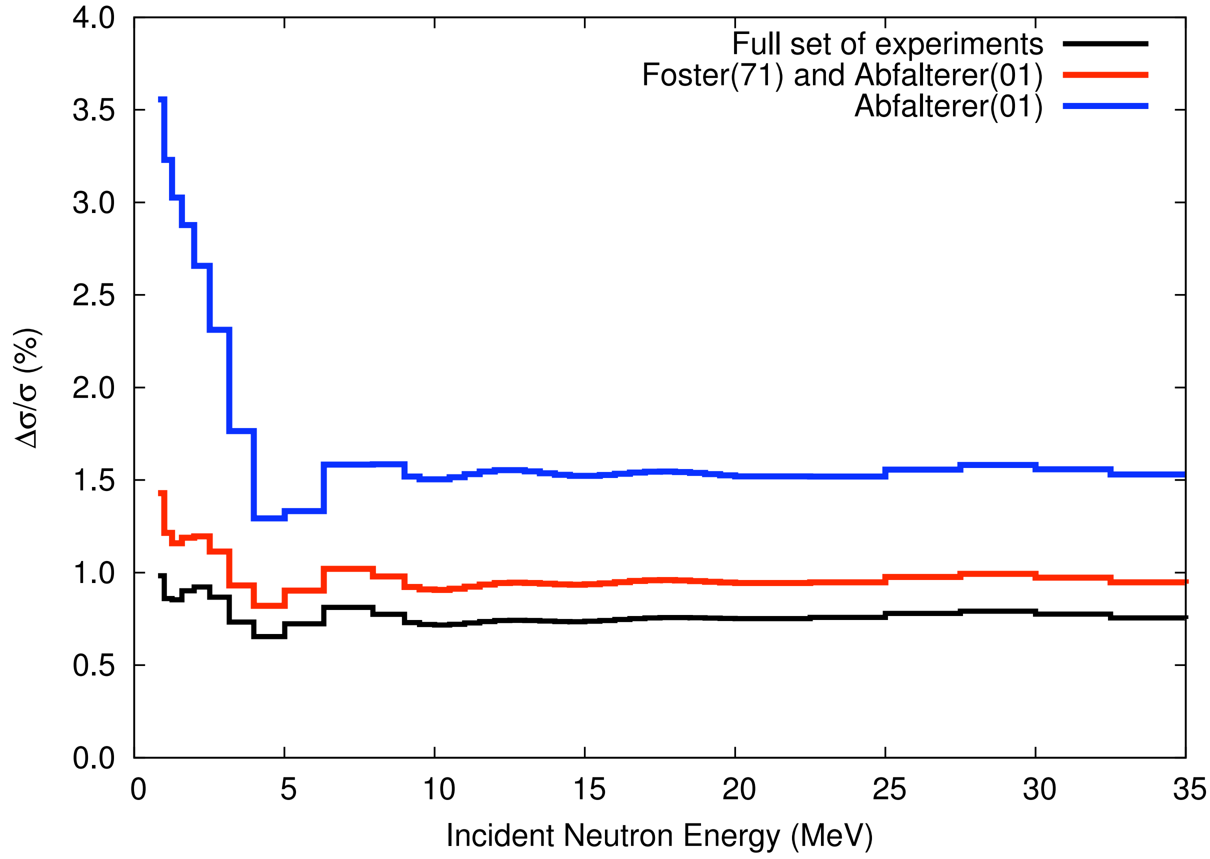


^{89}Y(n,total) uncertainties

effect of adding experimental data

EMPIRE-KALMAN

- Systematic error 2.8% for all measurements
- More data - smaller errors
- Generally, increased experimental correlations increase slightly uncertainties and considerably χ^2



Lesson learned from the comparison

- Model based uncertainties and correlations obtained with KALMAN and MC are equivalent.
- To minimize nonlinearity effects in KALMAN sensitivity matrix should be calculated using perturbation close to the final parameter uncertainty.
- Inclusion of experimental data (GANDR in MC) reduces uncertainties in both approaches (although more in KALMAN). However, cross-experiment correlations were included in GANDR but not in KALMAN.
- In KALMAN, systematic errors in experimental data increase uncertainties only slightly, while Chi**2 increases considerably.
- If number of experimental points is not excessive both methods give comparable results, otherwise...

Unreasonably low uncertainties

Is KALMAN over optimistic? No, it isn't!

Perturbo: KALMAN uncertainties can be much lower than experimental systematic uncertainties

Ergo: there is no limit for lowering uncertainties!

Voco in dubium: are such uncertainties trustworthy?

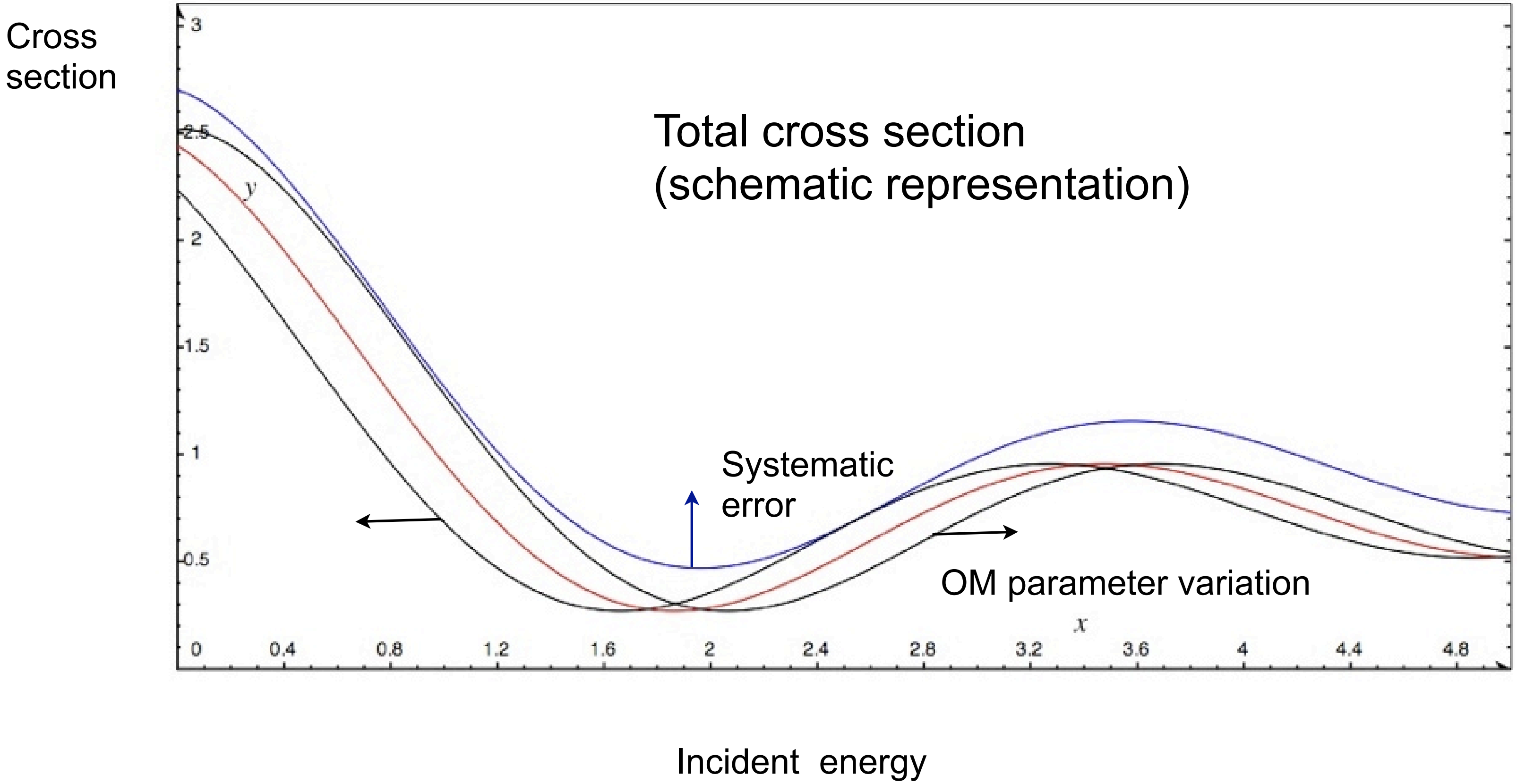
Judicium: no, they are not!

So... what are we missing?

- Example: uncertainties for total cross sections
  - often very many experimental points
  - well defined quantum-mechanical model - spherical optical model (CC or DWBA for deformed nuclei)
  - not affected by level densities, gamma-ray strength functions, preequilibrium emission, etc. ...

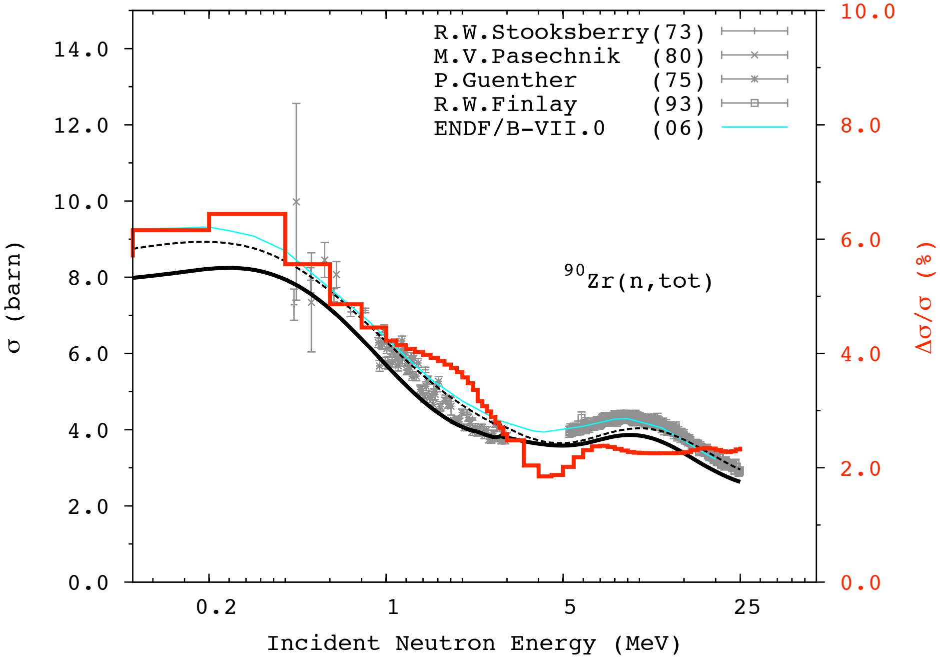
Adjusting OMP parameters

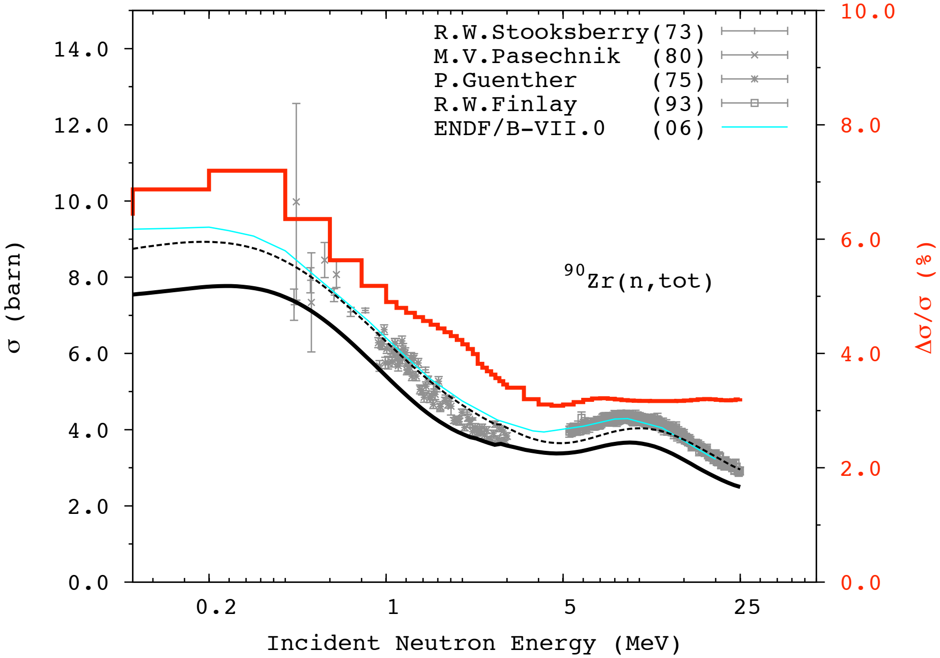
there is no OM parameter to scale x-sections!



Simulating intrinsic OM uncertainty

adding fake parameter to scale cross sections





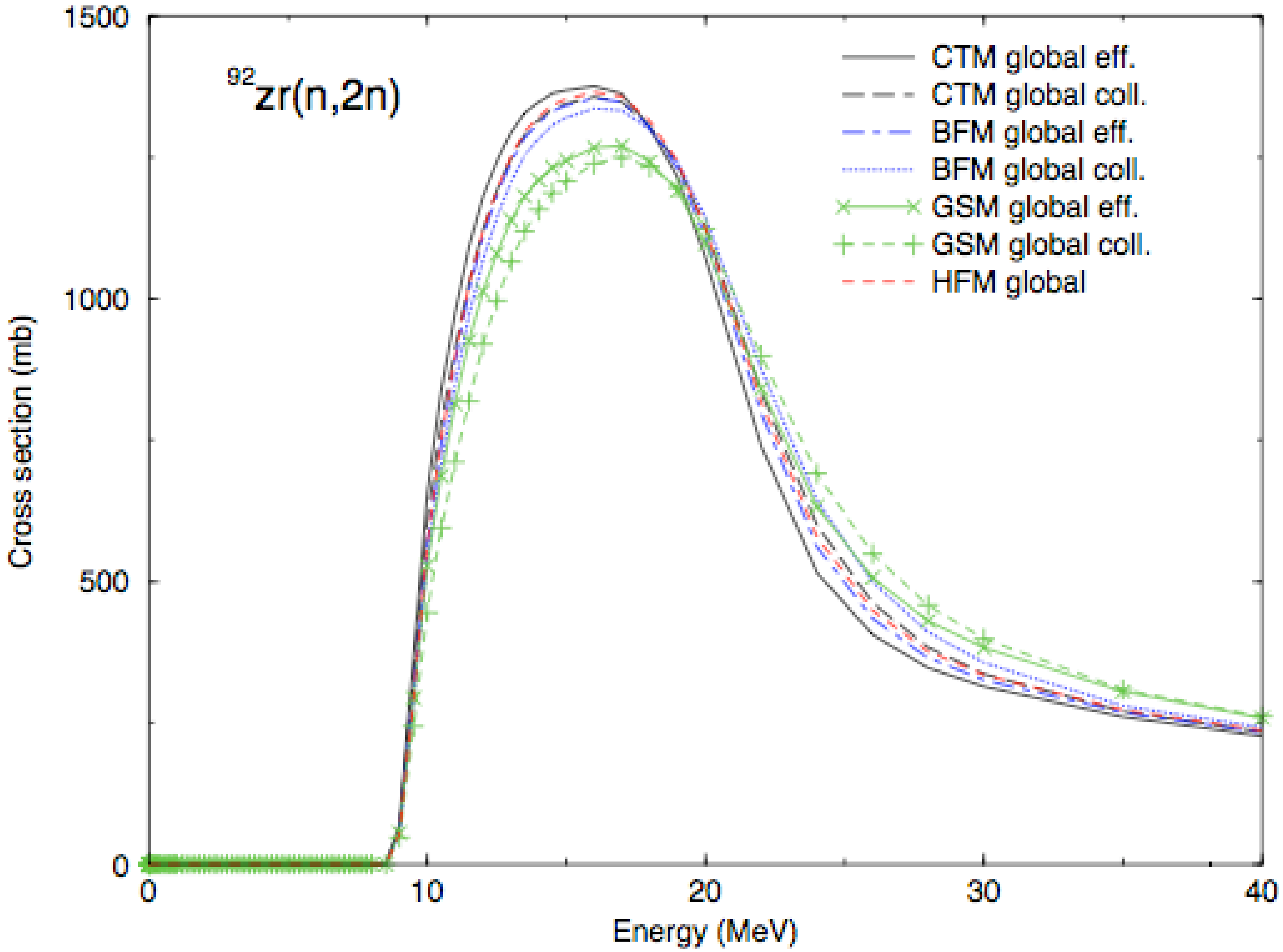
- Systematic experimental error 3%
- Lowest KALMAN predicted uncertainties ~2%

- Fake, scaling parameter added to the sensitivity matrix
- KALMAN predicted uncertainties >3%

experimental systematic error is respected!

Model uncertainties
case of various level density approaches

Koning, Hilaire, Gorieli, RIPL-3 and submitted to Nucl. Phys.



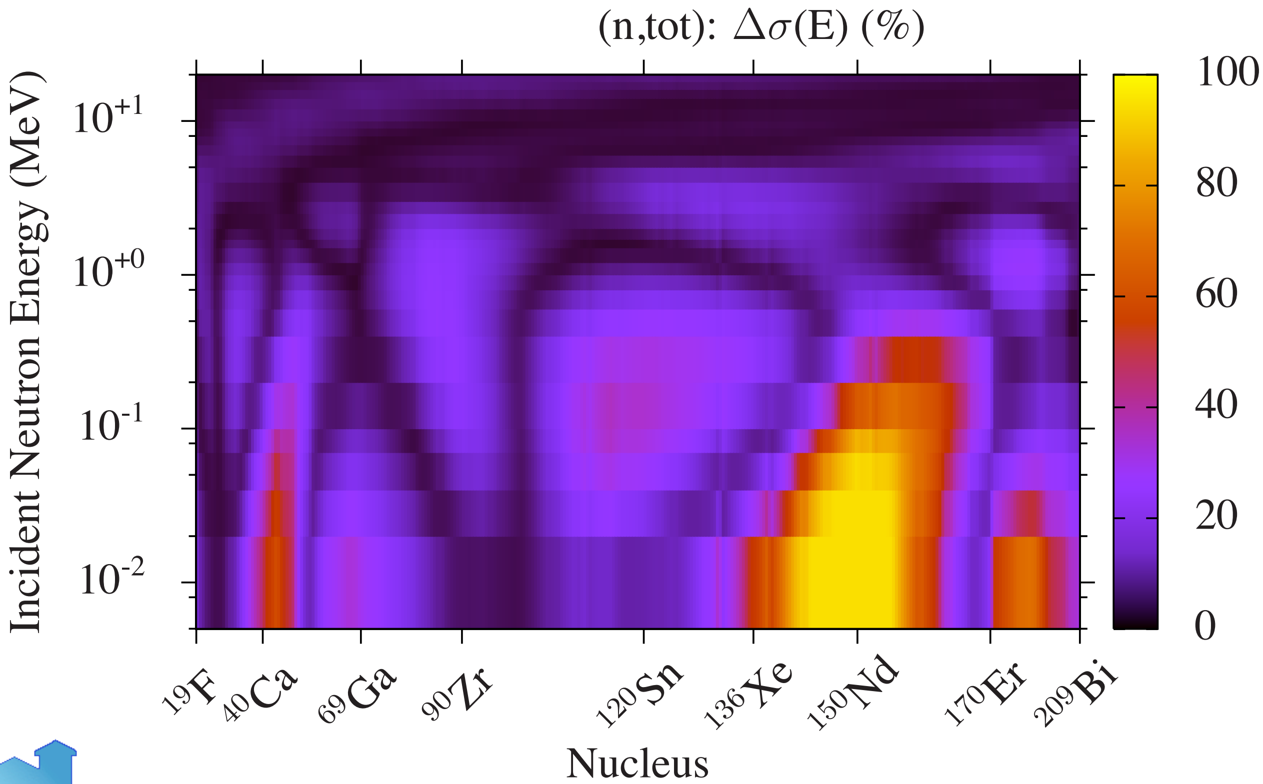
Use of different models for level densities, gamma-ray strength functions, different optical potentials, etc... can indicate intrinsic model uncertainties.

In MC one could even sample from the models.

'Low-fidelity' project

substantial EMPIRE's contribution (other: SG26, ENDF/B-VII.0)

Simple estimates of cross section covariances (5 keV - 20 MeV) generated with EMPIRE for 307 materials in the neutron sublibrary of ENDF/B-VII.0



Intriguing structure in the energy-mass plane: valleys of low uncertainties predicted by the optical model. (see contribution by M.Pigni)

R. Capote: deviations of experimental data in these valleys might indicate intrinsic model uncertainties.

Conclusions

- Covariance capabilities in resonance and fast neutron range implemented and operative in the EMPIRE code
- Intensive effort dedicated to covariance estimation (SG26, ‘low-fidelity’ and individual ‘high-fidelity’ evaluations for Criticality Safety, ENDF/B-VII.0 adjustment for GNEP)
- Model based covariances using KALMAN and MC are equivalent
- Model+experiment covariances using KALMAN and MC are similar if number of experimental points is modest
- Inclusion of experimental data reduces KALMAN results slightly more than MC-GANDR results (attention: cross experiment correlations!)
- Inflexibility of the model is responsible for the very low uncertainties. There is nothing wrong with the methods for estimating covariances!
- Open problems:
  - intrinsic model uncertainties
  - procedures for calculating covariances
  - practical implementation of the UMC (non-linear cases)