TALYS, Monte Carlo and Covariances

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Introduction

Experimentalists:

- are well educated: give uncertainties with their results.
- But, not seldom:
    - wrong systematical errors (usually underestimated), or,
    - no systematical errors given at all
- Difficult to establish good covariance data file, especially for correlation between different reaction channels (usually obtained from different labs).

Introduction

Theoreticians:

- Good behaviour: some don't stop until all reaction channels are completely predicted.
- Bad behaviour: most of them say their models are good, but none of them says how good: x-y instead of x-y-dy

No excuse possible:

- the strong nucleon-nucleon force is not known,
- the exact many-body problem is not solved,
- $\longrightarrow$ all nuclear models are wrong
- so where are the uncertainties of the OMP, fission, capture, pre-equilibrium, etc. cross sections?

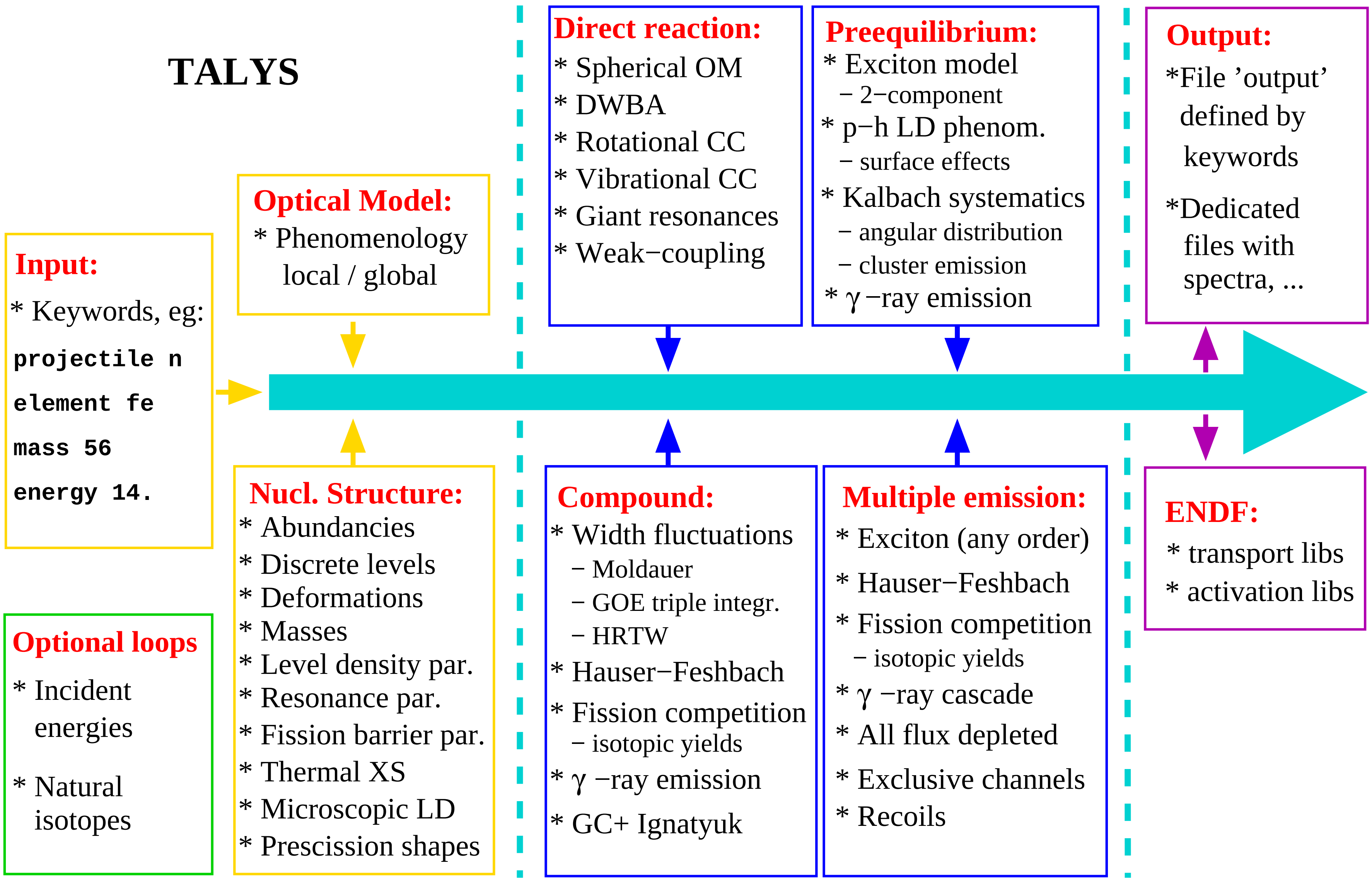
Approach

- Find a nuclear model code that predicts all open reaction channels, and is very flexible in input and output.
- Assess realistic uncertainties for the input, i.e. nuclear model, parameters.
- Propagate these uncertainties directly to the cross sections, angular distributions, gamma production, energy spectra, etc. using a Monte Carlo method (Don Smith, Eric Bauge).
- Obtain full covariance matrix (diagonal elements $\longrightarrow$ uncertainties).

TALYS

TALYS: nuclear reaction software by NRG Petten and CEA Bruyères-le-Châtel.

- Energy range 1 keV - 200 MeV.
- Neutrons, protons, deuterons, tritons, helions, alphas and photons.
- Many nuclear reaction models implemented.
- Continuous, smooth description over a wide energy and mass range.
- All open nuclear reaction channels covered.
- Appropriate for basic physics and applications.

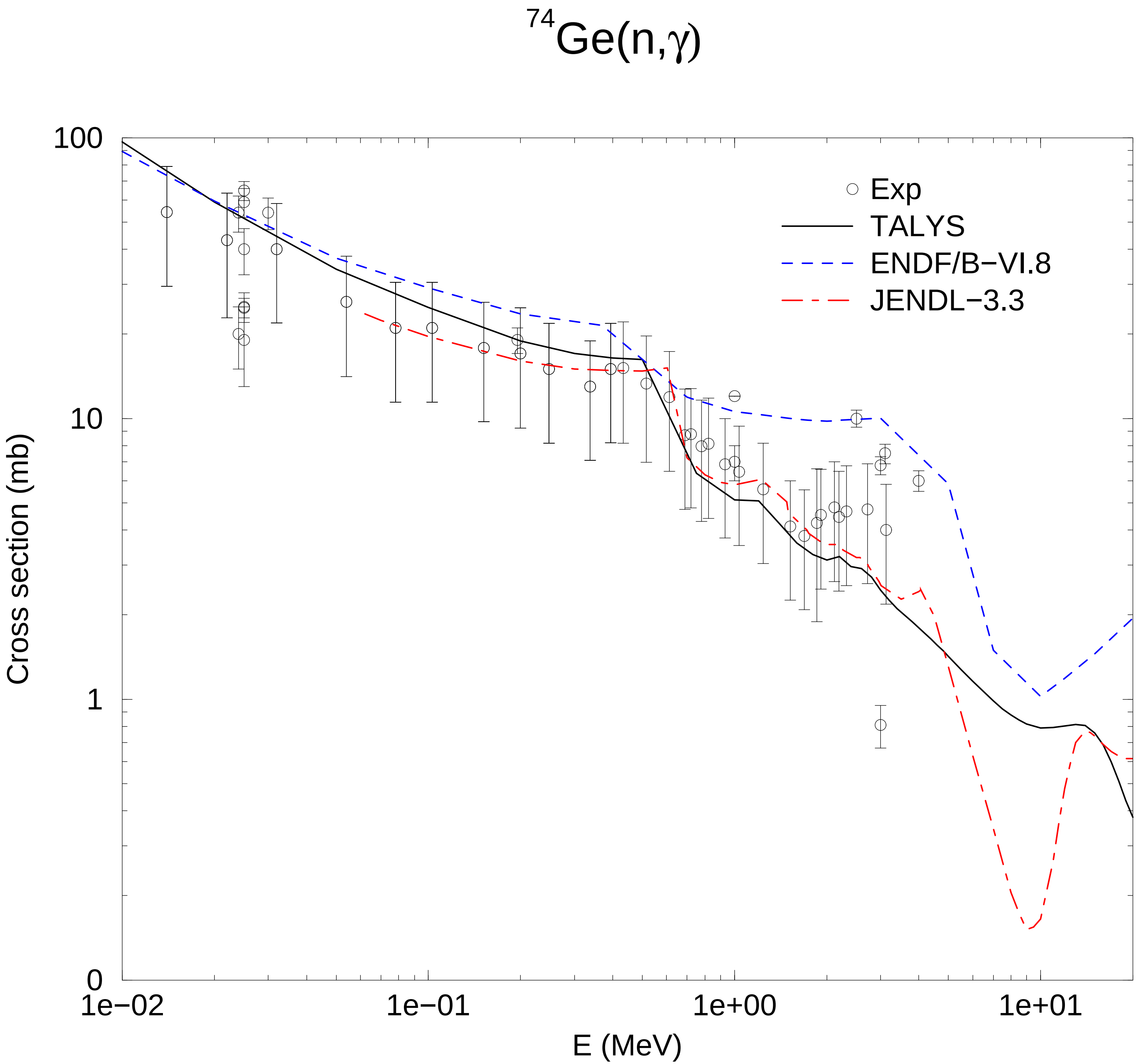

TALYS
Input:
* Keywords, eg:
projectile n
element fe
mass 56
energy 14.
Optional loops
* Incident energies
* Natural isotopes
Optical Model:
* Phenomenology local / global
Nucl. Structure:
* Abundancies
* Discrete levels
* Deformations
* Masses
* Level density par.
* Resonance par.
* Fission barrier par.
* Thermal XS
* Microscopic LD
* Prescission shapes
Direct reaction:
* Spherical OM
* DWBA
* Rotational CC
* Vibrational CC
* Giant resonances
* Weak−coupling
Compound:
* Width fluctuations
− Moldauer
− GOE triple integr.
− HRTW
* Hauser−Feshbach
* Fission competition
− isotopic yields
* γ −ray emission
* GC+ Ignatyuk
Preequilibrium:
* Exciton model
− 2−component
* p−h LD phenom.
− surface effects
* Kalbach systematics
− angular distribution
− cluster emission
* γ −ray emission
Multiple emission:
* Exciton (any order)
* Hauser−Feshbach
* Fission competition
− isotopic yields
* γ −ray cascade
* All flux depleted
* Exclusive channels
* Recoils
Output:
*File ’output’ defined by keywords
*Dedicated files with spectra, ...
ENDF:
* transport libs
* activation libs

Data produced by TALYS

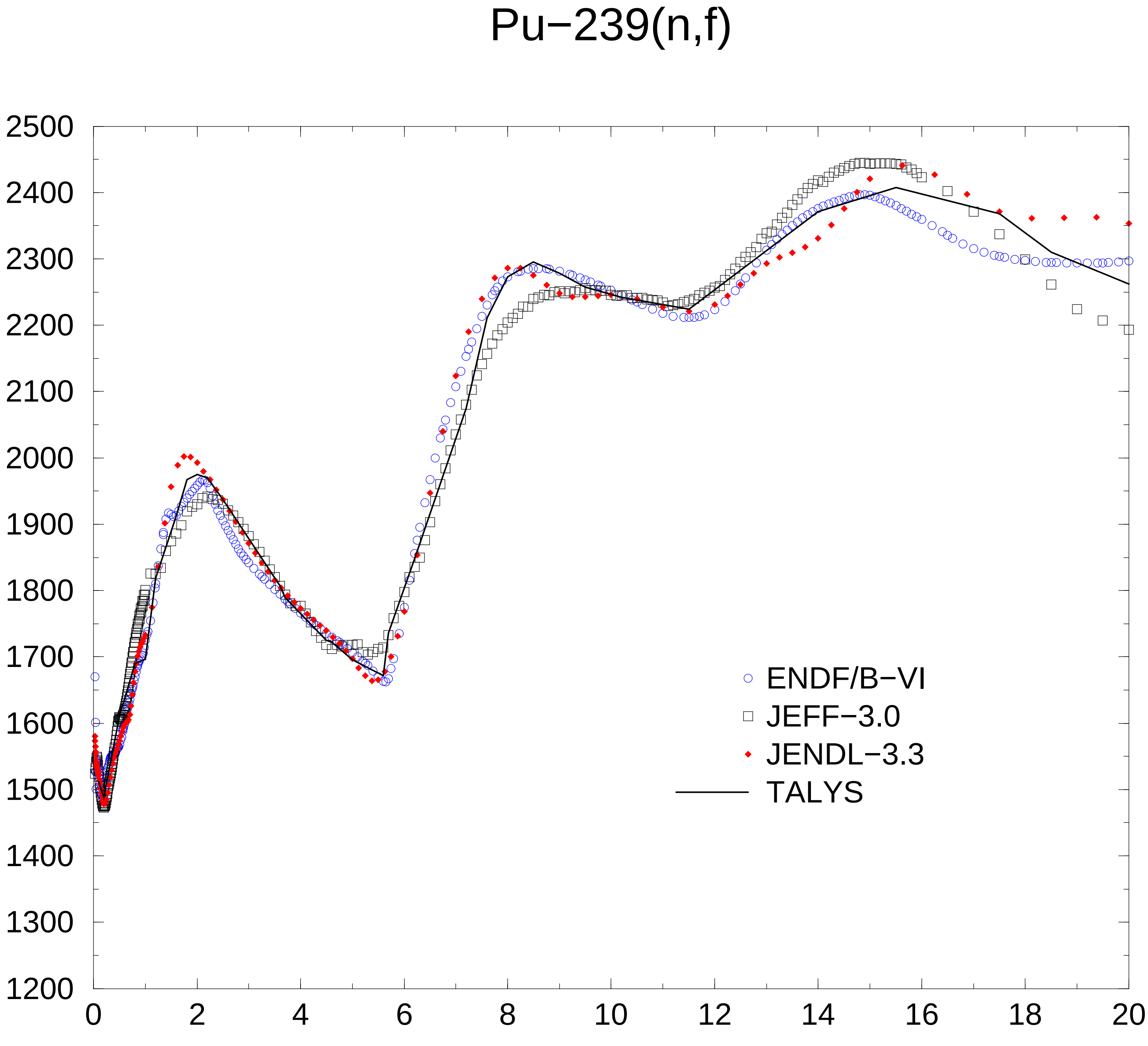
- Total, elastic and reaction cross sections.
- Inelastic cross sections (per level $+$ total).
- Elastic and inelastic angular distributions.
- Exclusive reaction channels, e.g. (n,p), (n,np).
- Exclusive double-differential spectra.
- Exclusive isomeric production cross sections.
- Exclusive discrete and continuum gamma-ray production cross sections.
- Photonuclear reactions.

Data produced by TALYS

- Reactions on isomeric targets.
- Fission cross sections.
- Fission yields.
- Recoils.
- Total particle production cross sections, e.g. (n,xn).
- Total particle production double-differential spectra.
- Residual production cross sections (including isomers).
- Activation libraries in ENDF-6 and EAF format.
- Transport libraries in ENDF-6 format.



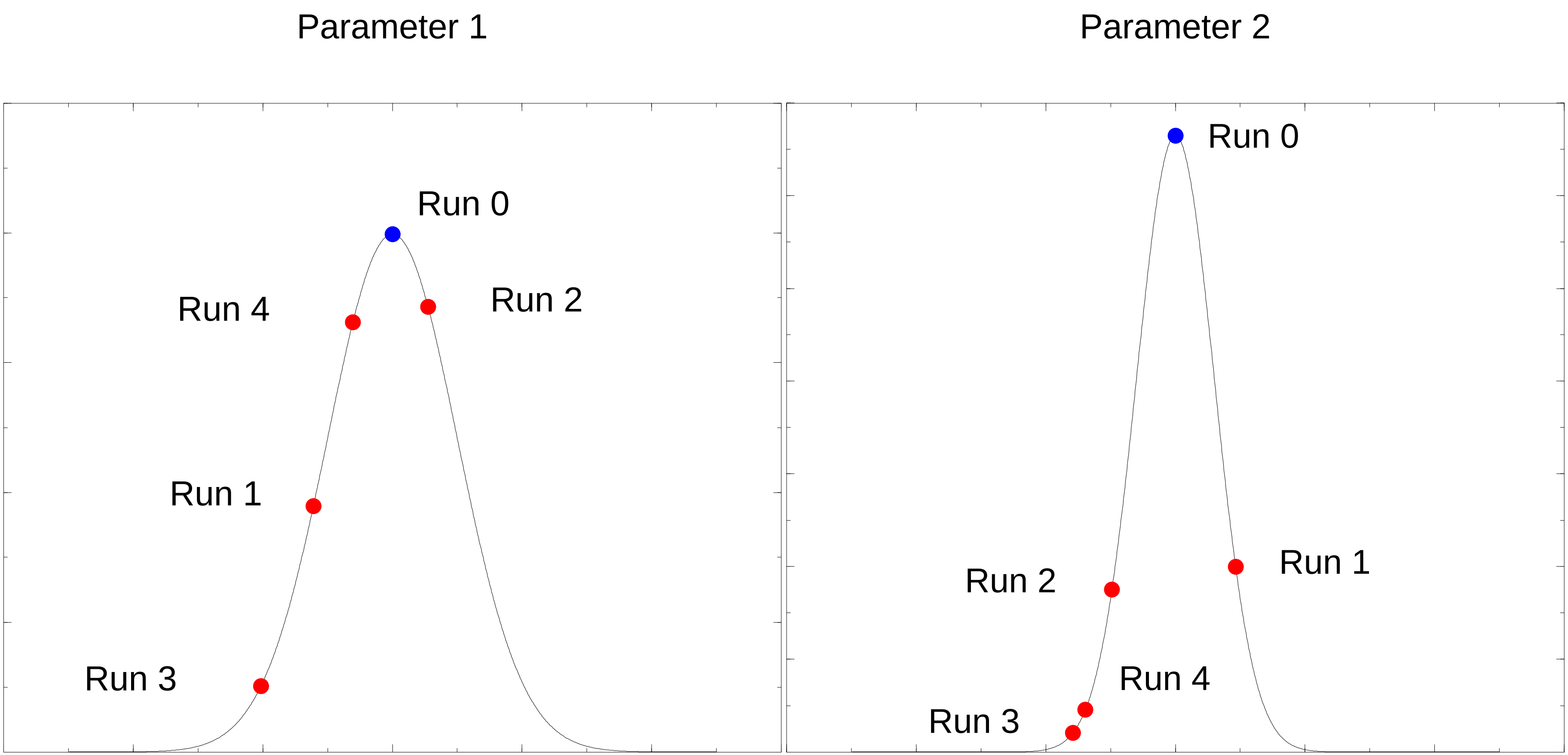
$^{74}Ge(n,\gamma)$
Exp
TALYS
ENDF/B−VI.8
JENDL−3.3
100
10
1
0
Cross section (mb)
1e−02
1e−01
1e+00
1e+01
E (MeV)



Pu−239(n,f)
2500
2400
2300
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
1200
0
2
4
6
8
10
12
14
16
18
20
ENDF/B−VI
JEFF−3.0
JENDL−3.3
TALYS

Covariances

- Nuclear model parameter vector $\mathbf{p}$, e.g.
  - $p^1 = a_{ld}(26, 56)$
  - $p^2 = a_{ld}(26, 57)$
  - $p^3 = r_V$, etc.
- Physical quantity vector σ of length N, e.g.
  - $\sigma^1 = \sigma_{n\gamma}(E_1)$
  - $\ldots$
  - $\sigma^i = d\sigma_{el}/d\Omega(E_1, \Theta_1)$
  - $\ldots$
  - σ^N
- $\sigma = T(\mathbf{p})$, where the function T stands for TALYS.
- Perform $k = 0, K$ (=1000) TALYS calculations with $\mathbf{p}$ drawn from a Gaussian random distribution.



Parameter 1
Run 0
Run 4
Run 2
Run 1
Run 3
Parameter 2
Run 0
Run 2
Run 1
Run 4
Run 3

Sample input file

AN ECN KEMA COMPANY

Input file 0 (Central values)

```
projectile n
element fe
mass 56
energy energies
channels y
filechannels y
#
#General parameters
M2constant 1.
#
# Parameters for  57Fe
a          26  57   6.77226
gammald    26  57   0.11927
gamgam     26  57   0.92000
sgr        26  57  83.976 E1
...........................
```

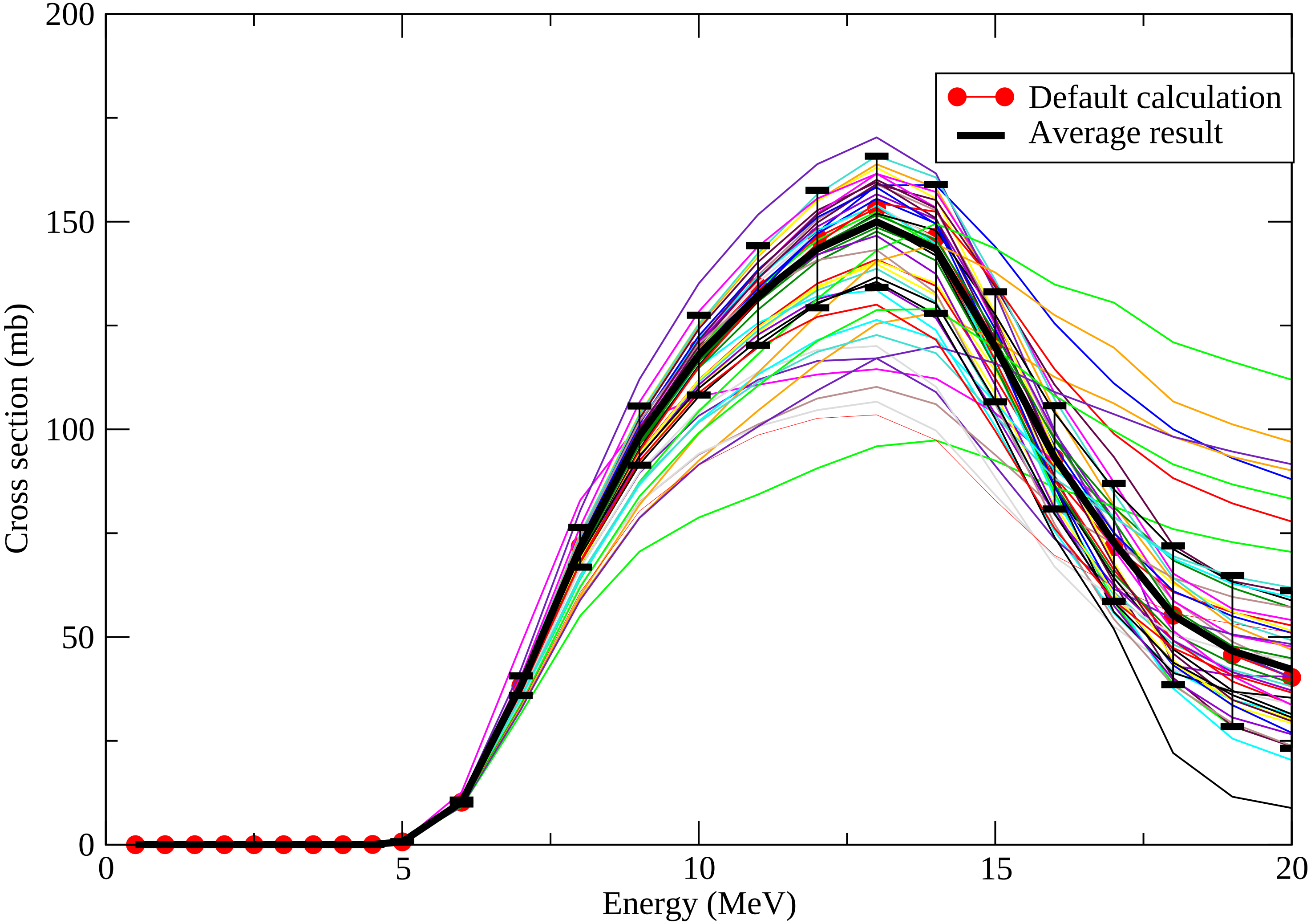
Input file 1

```
projectile n
element fe
mass 56
energy energies
channels y
filechannels y
#
#General parameters
M2constant 1.19515
#
# Parameters for  57Fe
a          26  57   6.29336
gammald    26  57   0.17733
gamgam     26  57   0.69751
sgr        26  57 102.600 E1
...........................
```

Covariances

- Let $\mathbf{p}_0, \sigma_0$ be the best parameter/quantity set.
- Covariance matrix $V_{ij} = \frac{1}{K}\sum_{k=1,K}(\sigma_k^i - \sigma_0^i)(\sigma_k^j - \sigma_0^j)$ for i,j=1,N
- Relative covariance matrix: $R_{ij} = V_{ij}/(\sigma_0^i \sigma_0^j)$ for i,j=1,N.
- One entire 0-20 MeV calculation for Fe-56 takes about 30 sec. on a 1 GhZ PC $\longrightarrow$ full covariance calculation takes one night.

Fe-56(n,p)



Default calculation
Average result
Cross section (mb)
Energy (MeV)
0
50
100
150
200
0
5
10
15
20

Outlook/Conclusions

- Given a flexible nuclear model code, covariances based on Monte Carlo $+$ nuclear modelling are intellectually simple and possible with current-day computer power.
- Main theoretical problem: disentangling parameter uncertainty from nuclear model uncertainty (Leeb)
- Proper inclusion of experimental data will of course complicate the situation.
- Comparison with Bayesian, linear approaches (Kawano, Vonach-Tagesen) not yet studied.
- Full sensitivity matrix information also available ($\longrightarrow$ physical insight).

Outlook/Conclusions

- Similar scheme (simulated annealing) now used for automated fitting of all partial cross sections.
- MF33 format finally understood by TALYS author (Vonach LB5 approach).
- Too much covariance information available, every possible correlation is included.
- Systematic filling of MF33/34 in data files foreseen.
- As holds for the central values, a nuclear model approach should not replace experimental approaches (GLUCS, etc.) when high-quality measurements are available.
- Method will be tuned to the three experimentally best known nuclides: Si-28, Fe-56, Ni-58 (x-y-dy tables from Vonach-Tagesen evaluations).