R-matrix school 2025:
SAMMY computer exercises for students

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R-matrix school 2025, Oak Ridge, TN, June 2–6, 2025

Basic information to run SAMMY

- Set up path for SAMMY executable
- SAMMY code runs as "`SAMMY < input`" where `input` contains list of filenames as

```
What is the name of the INPut file?
inputname.inp
>>> inputname.inp <<<
What is the name of the PARameter file?
parname.par
>>> parname.par <<<
What is the DATa file name? EMIN? EMAX? dataname.twenty
>>> dataname.twenty <<<
Emin and Emax = 0.0             1000.0
```

File Extensions are not mandatory but recommended. Important output files are `SAMMY.{LPT,LST}`. `inputname.inp` and `dataname.twenty` files are linked by experimental corrections: it is a common convention to have same names `inputname = dataname` with different extensions.

Plotting measured and calculated data

- `SAMMY.LST` contains the measured and calculated data for plotting
- Python scripts are used to plot data for all the test cases
- `SAMMY.LST` is composed by the following (optional $*$) sections or columns

Section	Contents and units
1	Energy in eV, keV, or MeV as specified in the input
2	Measured data (type)
3	Measured data (type) uncertainty
4	Prior (or 0^{th}) theoretical data
5$*$	Post (or final after n iterations) theoretical data
6$*$	Measured transmission (dimensionless)
7$*$	Measured transmission uncertainty (dimensionless)
8$*$	Prior Theoretical transmission (dimensionless)
9$*$	Post Theoretical transmission (dimensionless)
10$*$	Theoretical data uncertainty

data (types) = {[total, fission, capture, elastic] cross section (barn), transmission, [fission, capture] yield}

EX001: Input files structure

- Nucleus Xy with mass number $A = 10$ and spin $I = 0$
- Reaction type: neutron induced capture $\equiv{}^{10}$Xy(n, γ)

```
Example # 001
10xy          10.000  8.0       12.0
do not solve bayes equations
ev
fgm
twenty
generate odf file automatically
quantum numbers are in parameter file

      300.
    2.9080
capture

nuclide masses and abundances follow
 10.00000   0.999999  0.000010 0 1
```

```
PARTICLE PAIR DEFINITIONS
Name=n+10xy       Particle a=neutron       Particle b=10xy
     Za= 0        Zb= 1         Pent=1     Shift=0
     Sa=  0.5     Sb=   0.0     Ma=   1.008664920000000     Mb=  10.000000000000

SPIN GROUPS
  1      1    0  0.5 0.9999990
    1  n+10xy      0  0.5

RESONANCES are listed next
10.0       1.         0.5                             0 0 0 0 0 1

.100000000
Channel radii in key-word format
Radii=  2.908000,  2.908000    Flags=0, 0
   Group=  1   Chan=  1,
```

- Separation between experimental conditions (.inp file on the left) and R-matrix parameters (.par file on the right)

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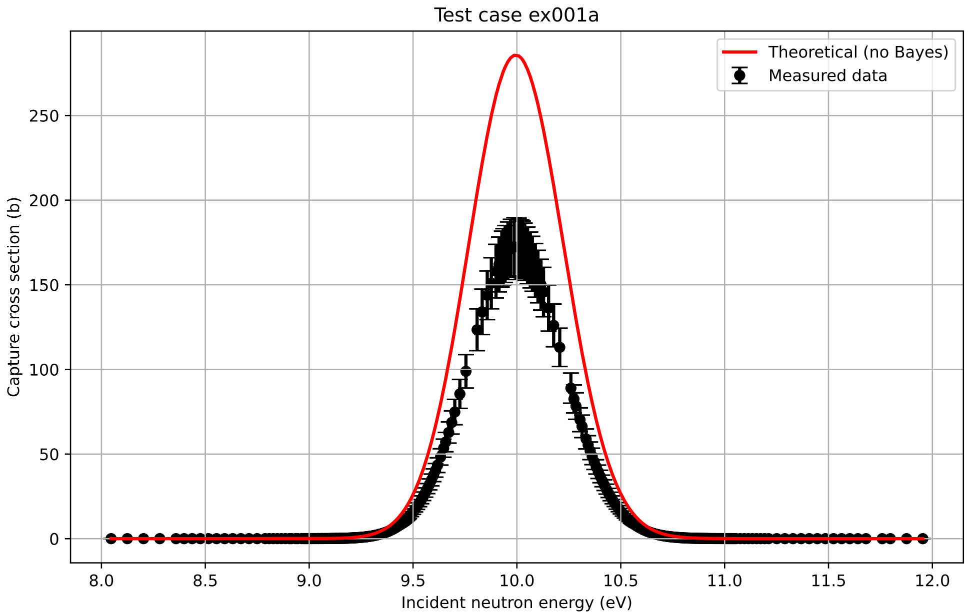
EX000: Auxiliary code SAMQUA (two cases)

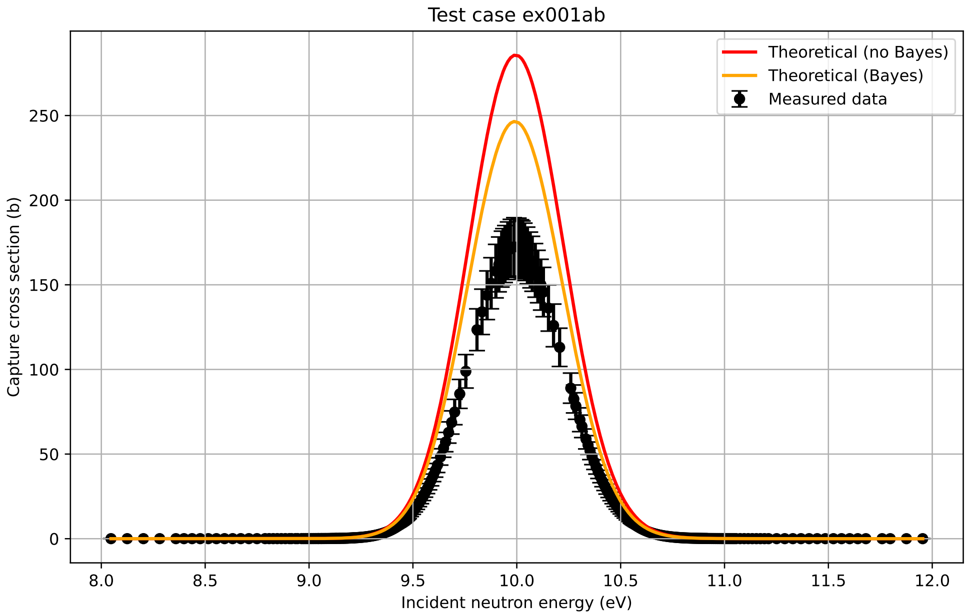
- Two input files `ex000{a,b}.inp` plus `README.FIRST`
  - `ex000.e` dependency of `ex000a.inp`: energy list to compute penetrability factors
- Output files: `ex000*.{quantum*,quanpar,table}`
- Two format options: “Particle-pair” with `ex000a.inp` and “Cadarache” with `ex000b.inp`
- Goal: generation of SAMMY quantum number information for
  - (a) outgoing reactions for incident partition n+^{16}O
  - (b) outgoing reactions for incident partition α+^{18}O
  - Discussion on the results

- Exercise: to run multiple isotope test case `ex000x.inp` in “Particle-pair” format option

EX001: Simple one-resonance nonfissile nucleus

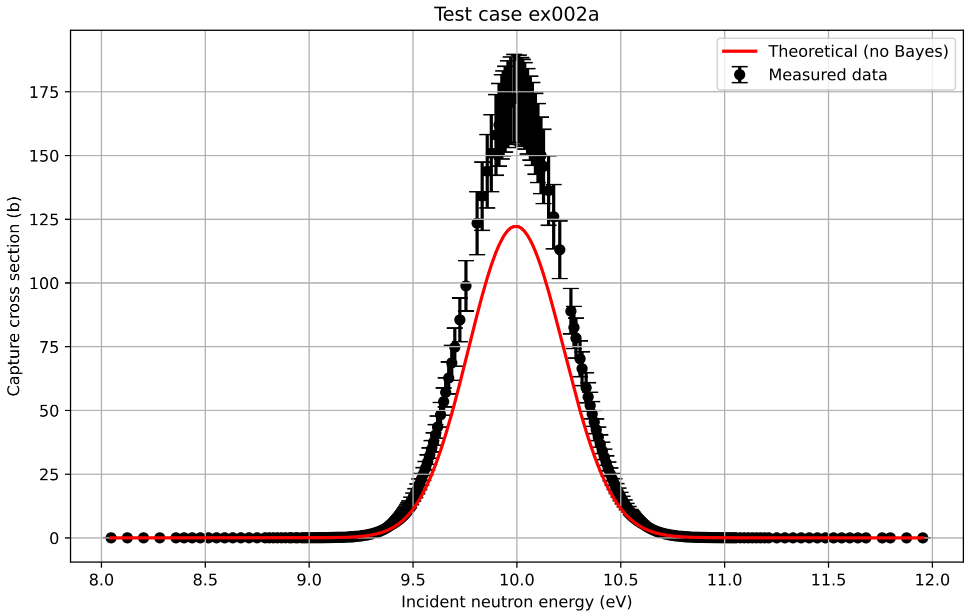
- One input file `ex001a.inp`
- Reaction type: capture$\equiv$ ^{10}Xy(n,γ)
- Run with (`ex001x.inp`) or without (`ex001a.inp`) Bayesian option
- Change `ITMAX` in `ex001x.inp` file to see convergence of the fit

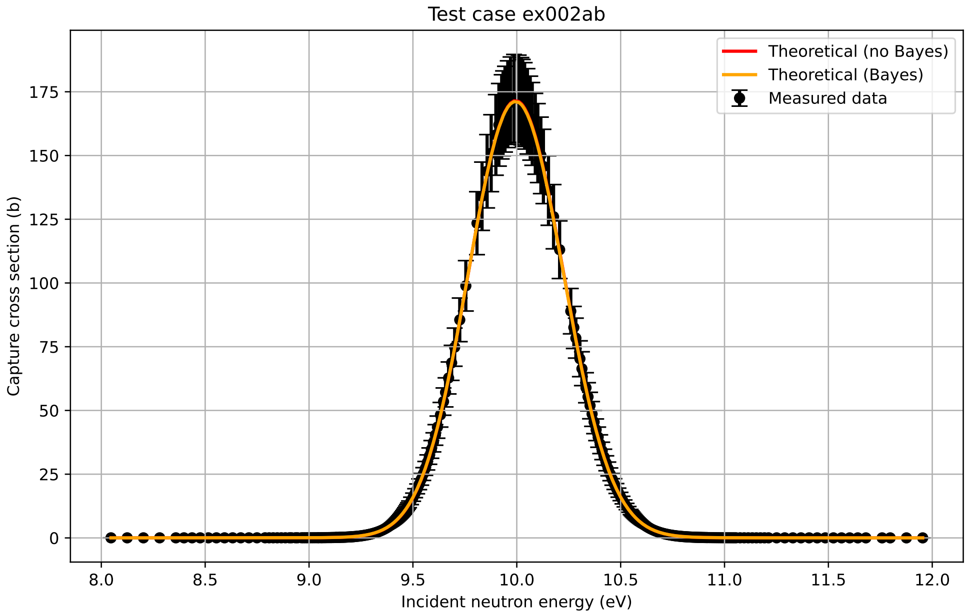




EX002: Simple one and several resonances fissile nucleus

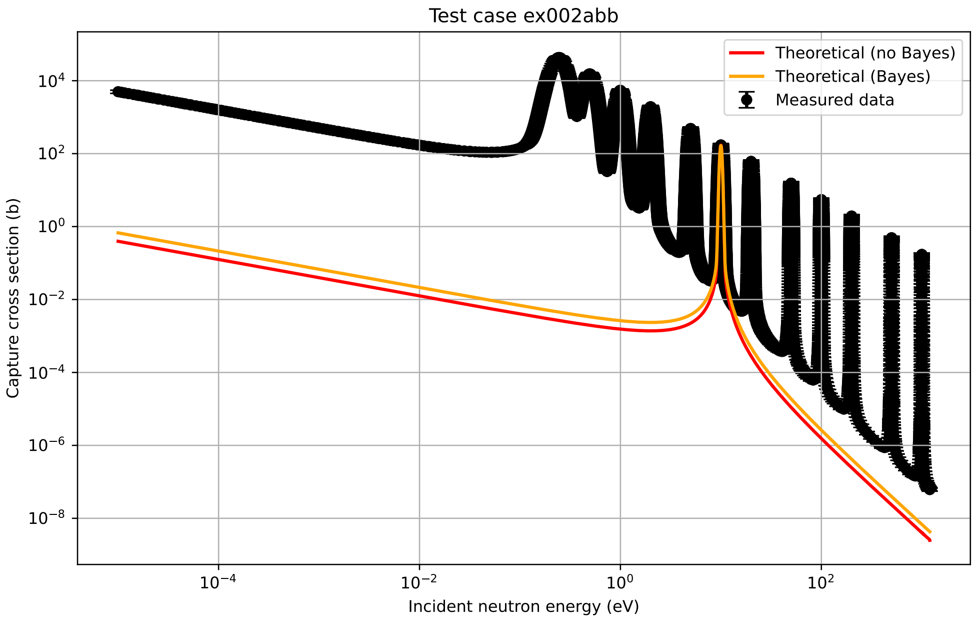
- One input file `ex002a.inp`
- Reaction type: capture$\equiv$ ^{10}Xy(n, γ)
- Run with (`ex002b.inp`) or without (`ex002a.inp`) Bayesian option
- Impact of adding fission widths on capture reaction channel

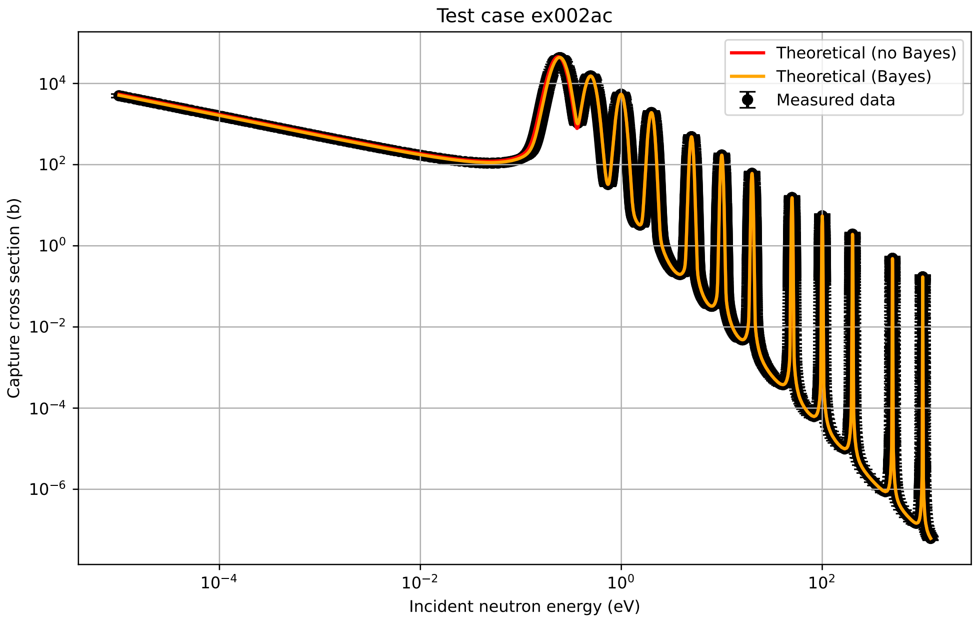




EX002: Simple one and several resonances fissile nucleus

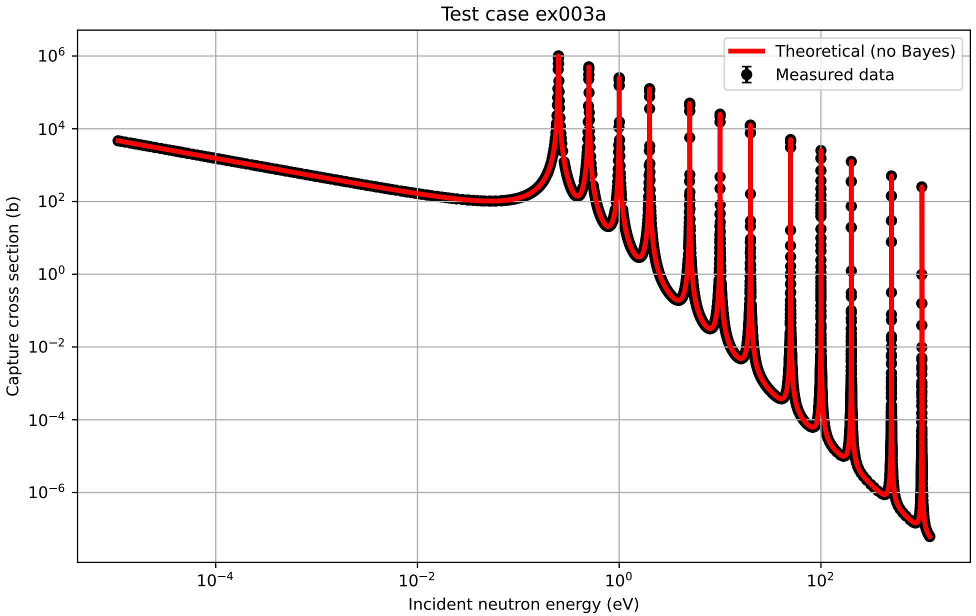
- Changing energy limits from 8-12 eV to 0-1200 eV
- Including several resonances (`ex002c.par`)
- log-log plots

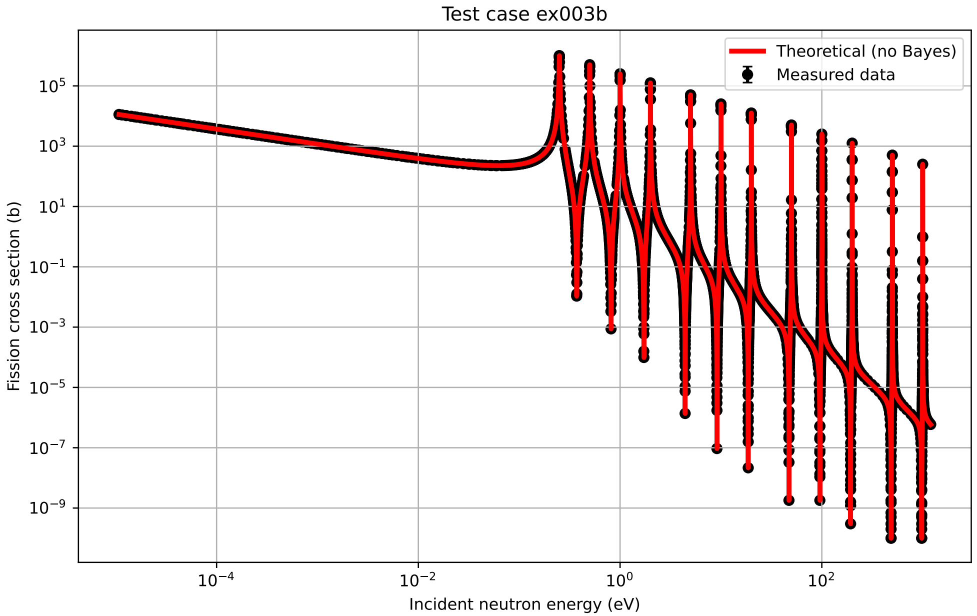




EX003: Different kinds of cross sections

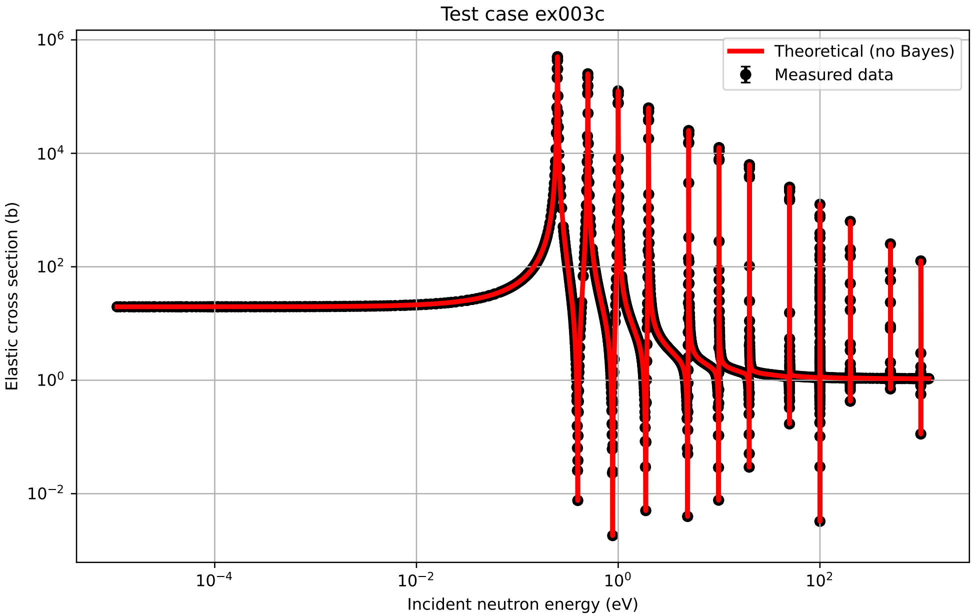
- Several input files `ex003{a,b}.inp`
- Reaction types: (a) capture$\equiv$ ^{10}Xy(n,γ), (b) fission$\equiv$ ^{10}Xy(n,f)

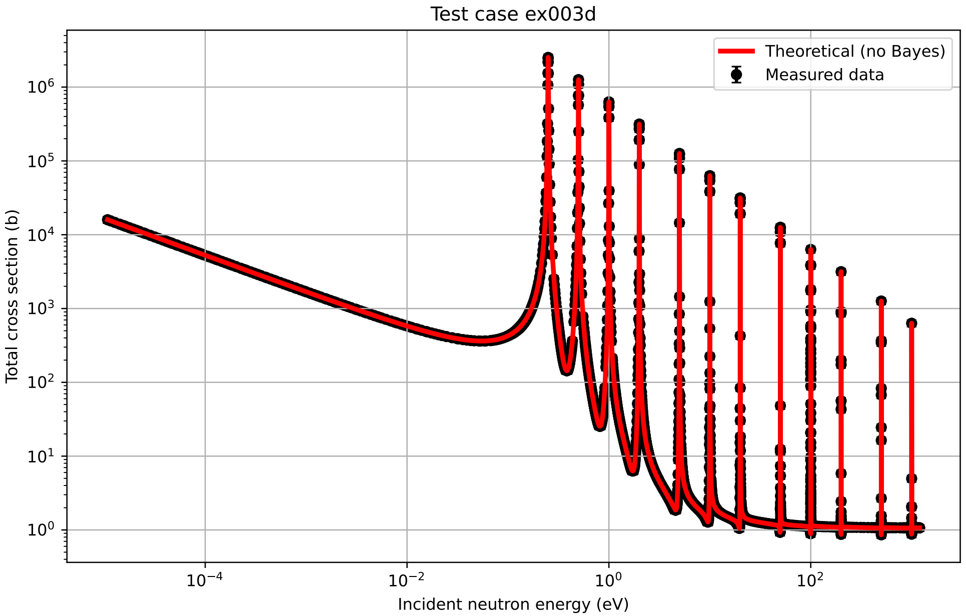




EX003: Different kinds of cross sections

- Several input files `ex003{c,d}.inp`
- Reaction types: (c) elastic$\equiv{}^{10}$Xy$(n,$el$)$, (d) total$\equiv{}^{10}$Xy$(n,$tot$)$





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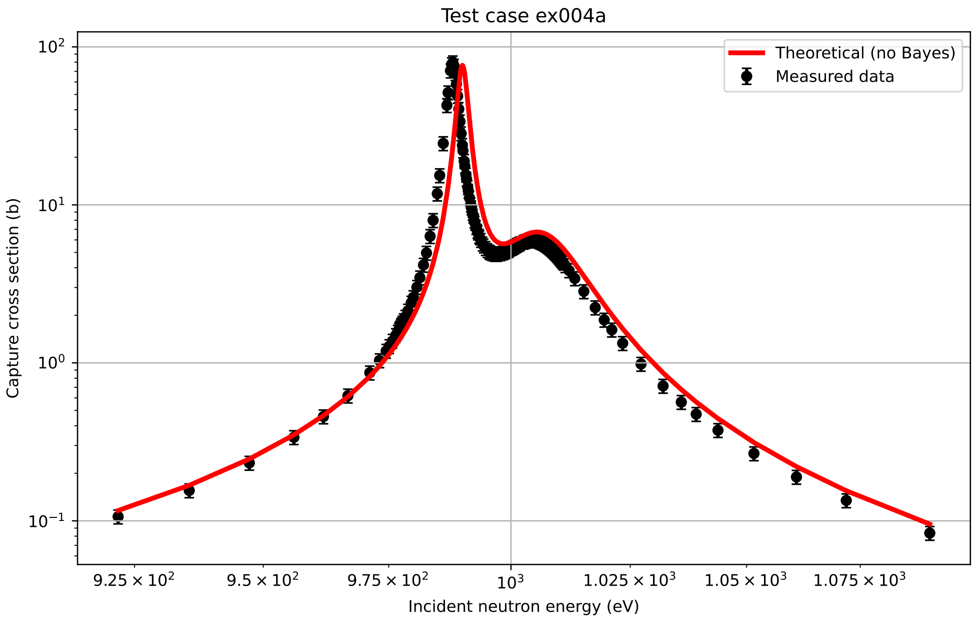
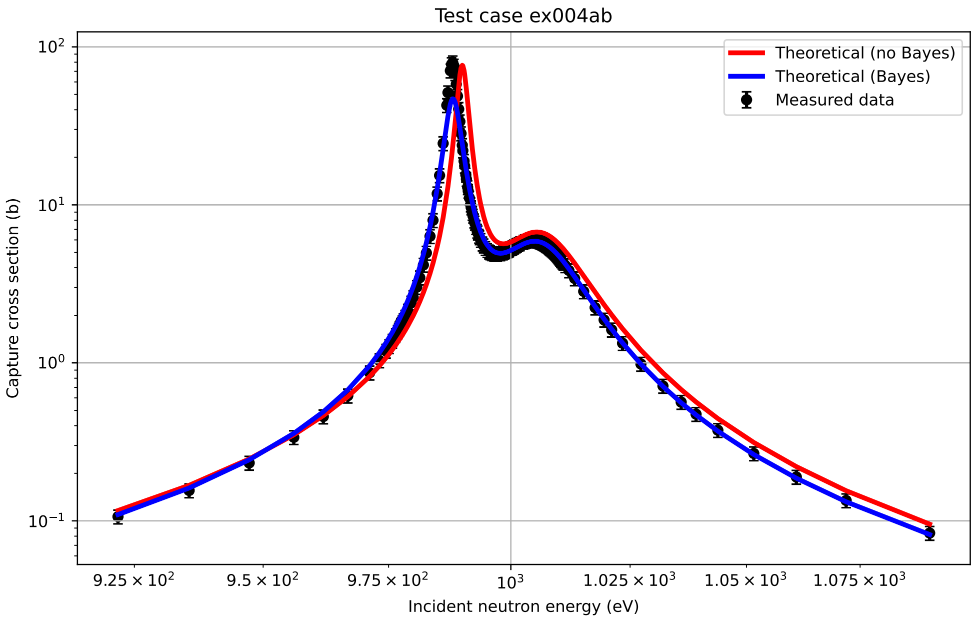
EX004: $\ell \geq 0$ (s, p, d waves); I$\geq$0

- Input files `ex004{a,b}.inp`
- Reaction type: capture$\equiv$ ^{10}Xy(n,γ)
- Noticing different resonance shapes (target spin $I = 0$ and partial waves $\ell = 0, 1$)





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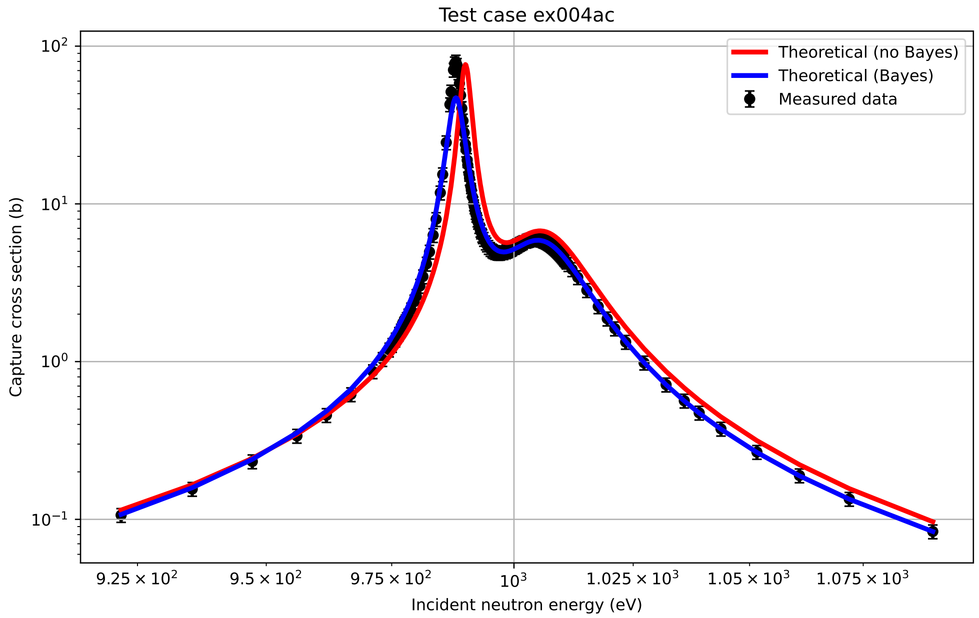
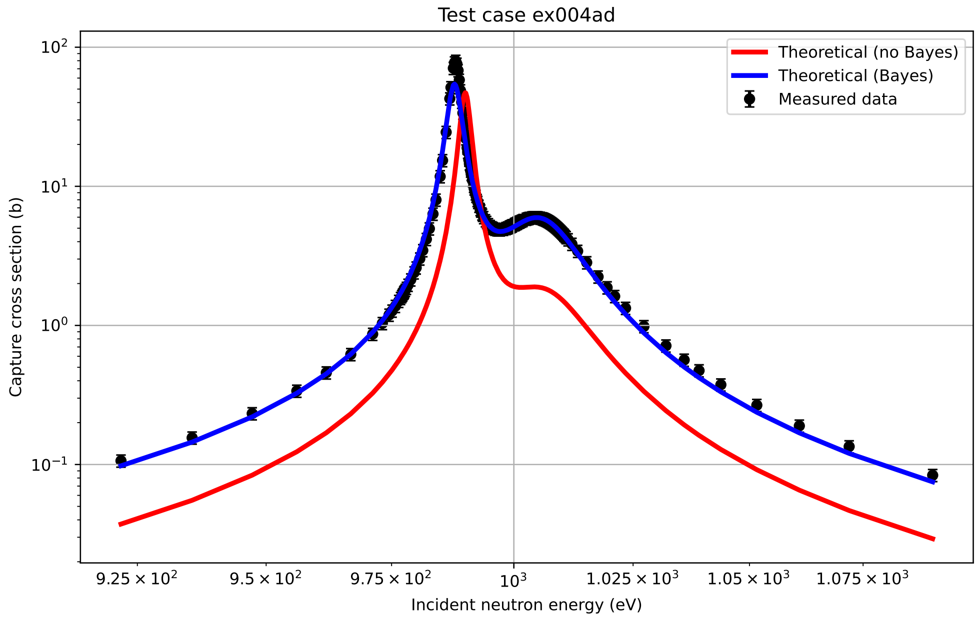
EX004: $\ell \geq 0$ (s, p, d waves); I$\geq$0

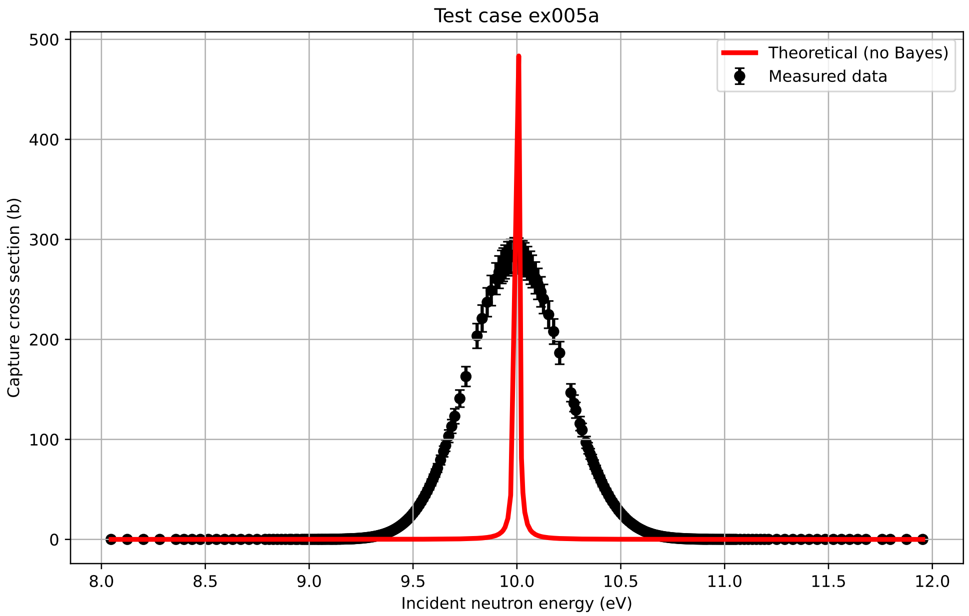
- Input files `ex004{c,d}.inp`
- Reaction type: capture
- Changing target spin to half-integer ($I = 1/2$) and adding partial waves $\ell = 0, 1, 2$

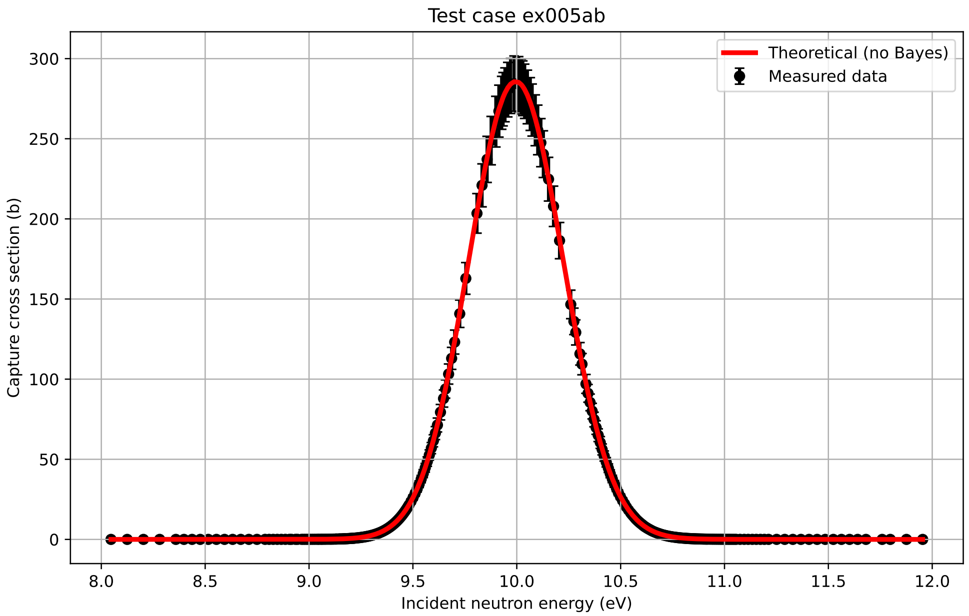




EX005: Doppler broadening

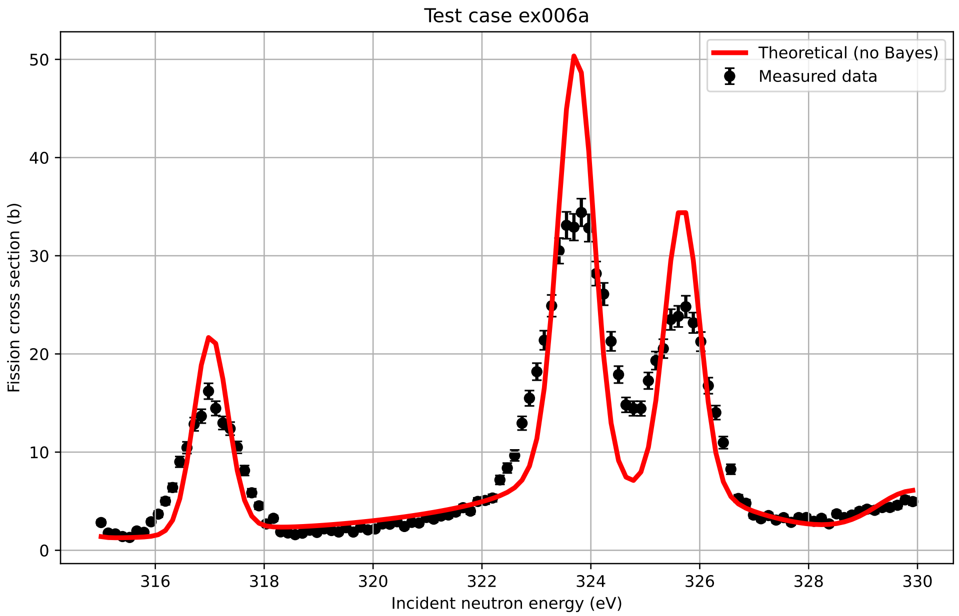
- Input files `ex005{a,b}.inp`
- Reaction type: capture
- Doppler Broadening switched on

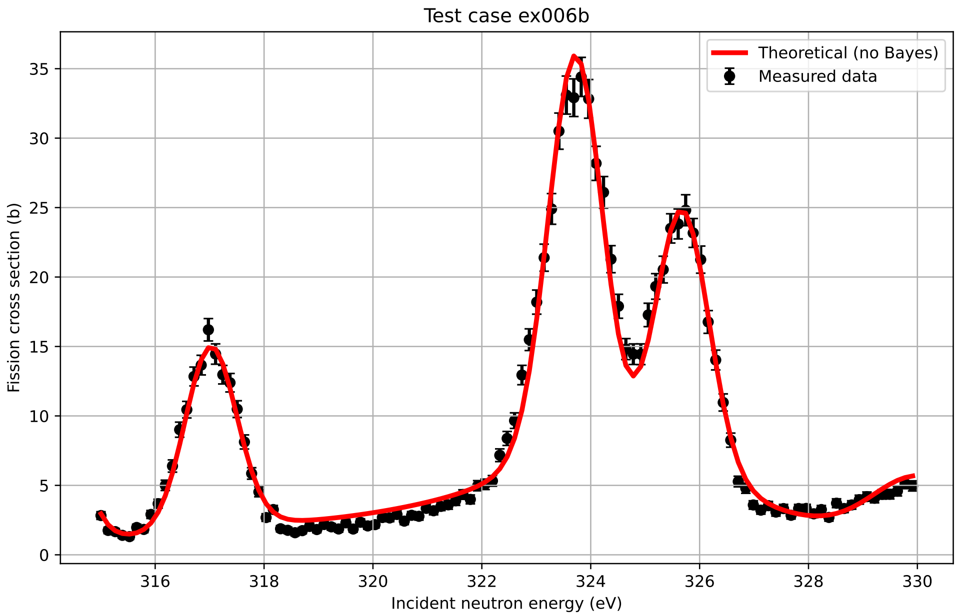




EX006: Resolution broadening (Gaussian)

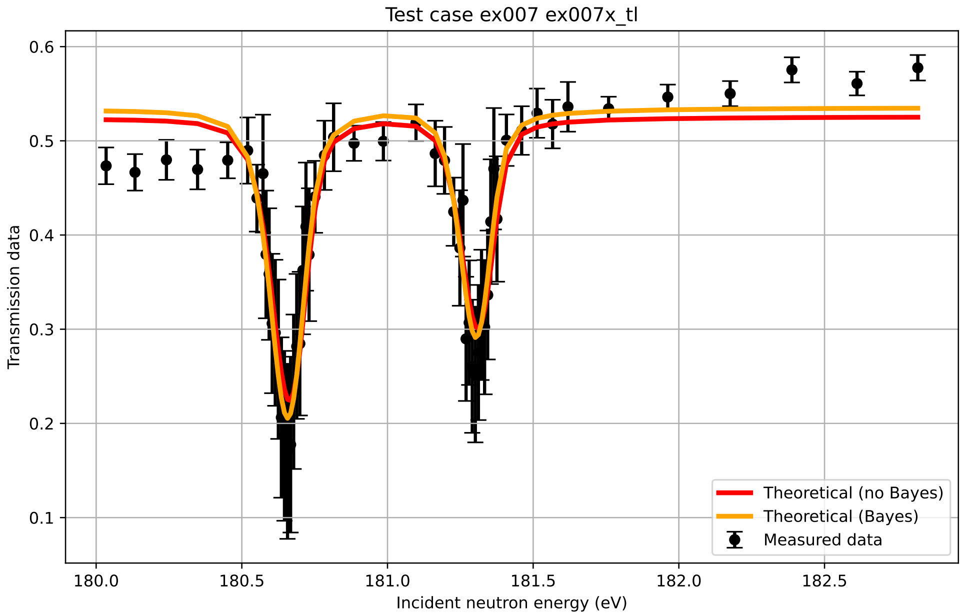
- Input files `ex006{a,b,c}.inp`
- Reaction type: Fission$\equiv {}^{239}$Pu(n,f)
- Gaussian resolution broadening: energy dependent channel width

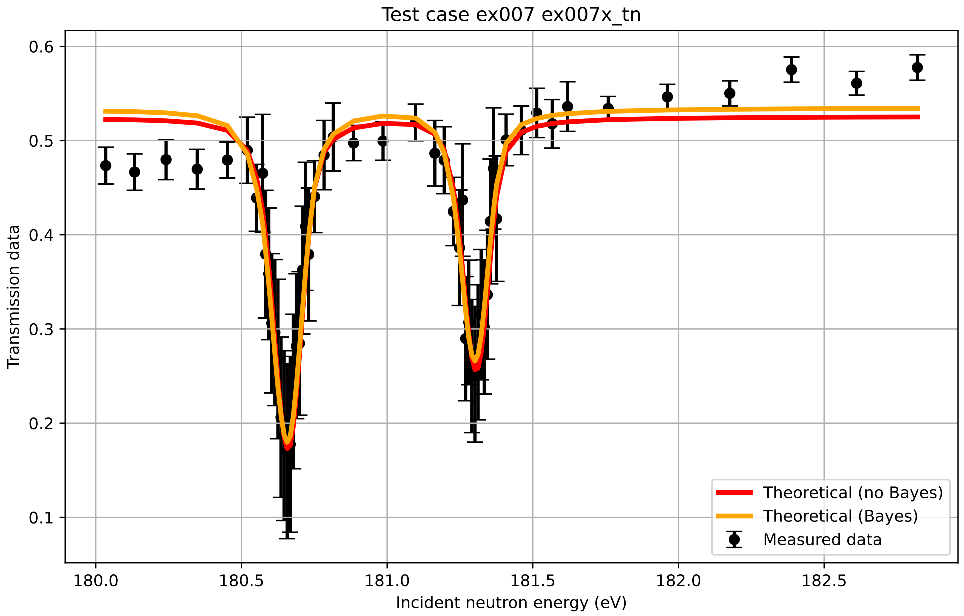




EX007: Resolution broadening (ORR)

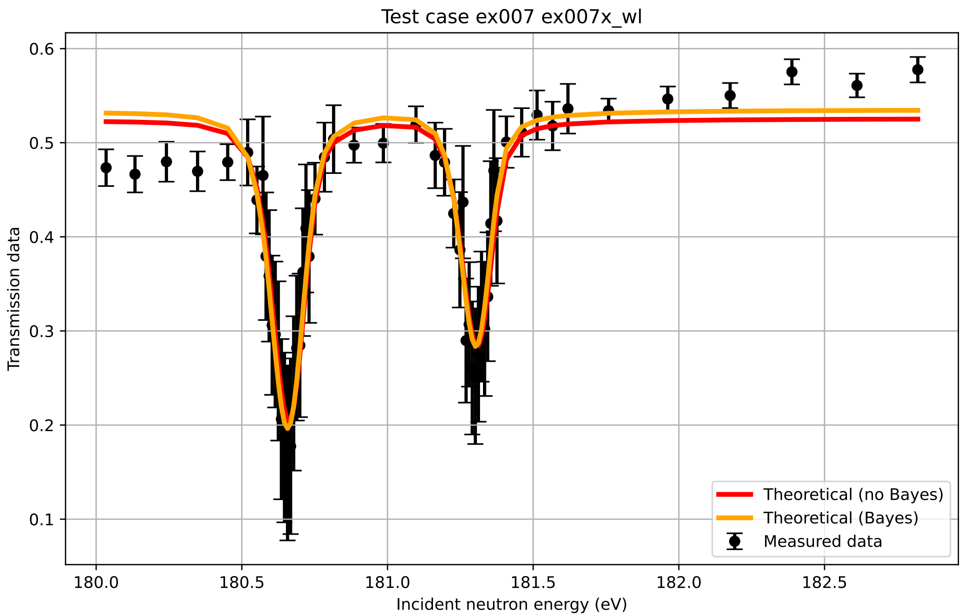
- Input files `ex007{tl,tn}.inp`
- Reaction type: Transmission data on n+^{58}Ni

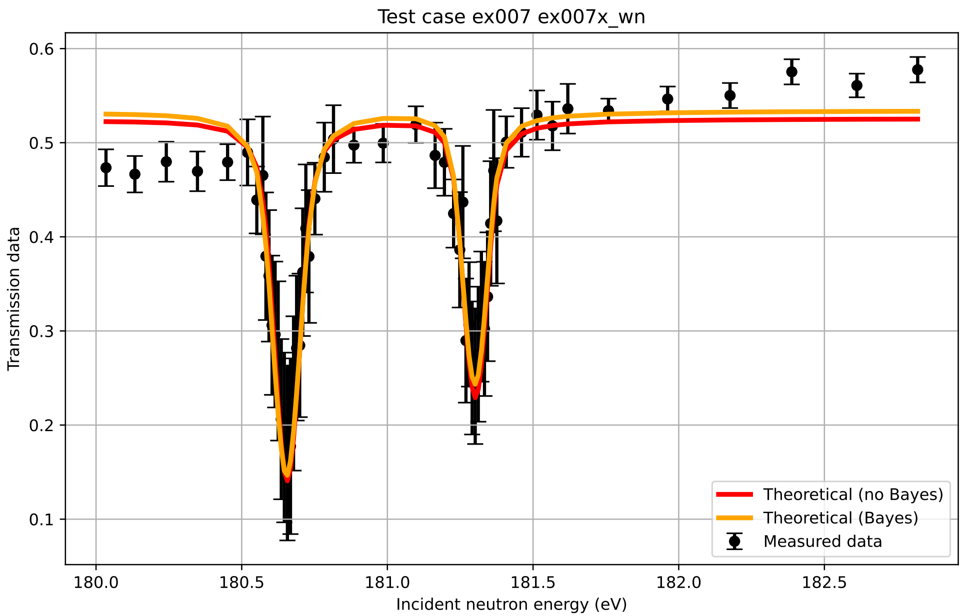




EX007: Resolution broadening (ORR)

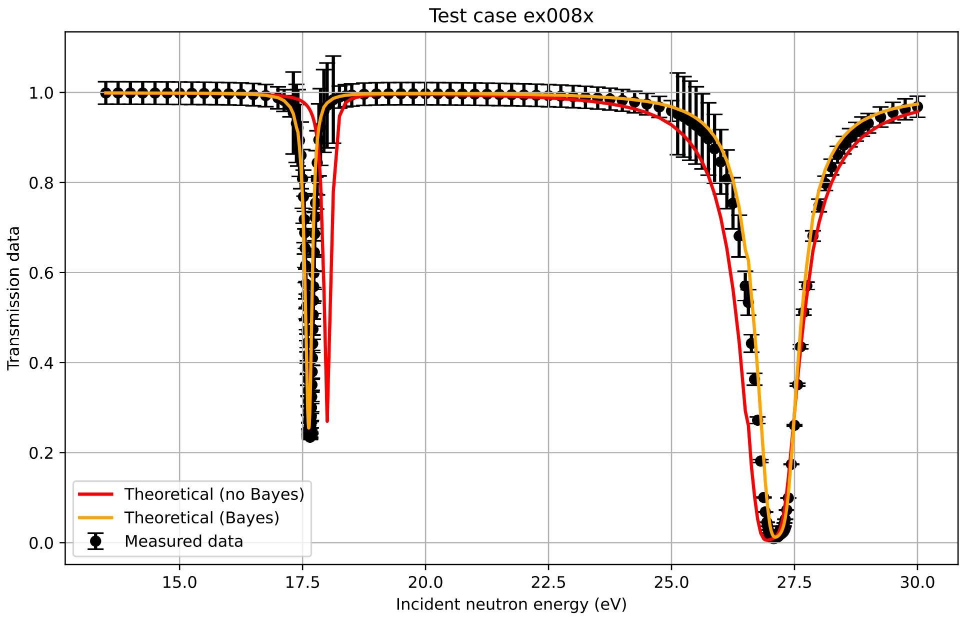
- Input files `ex007{wl,wn}.inp`
- Reaction type: Transmission data on n+^{58}Ni





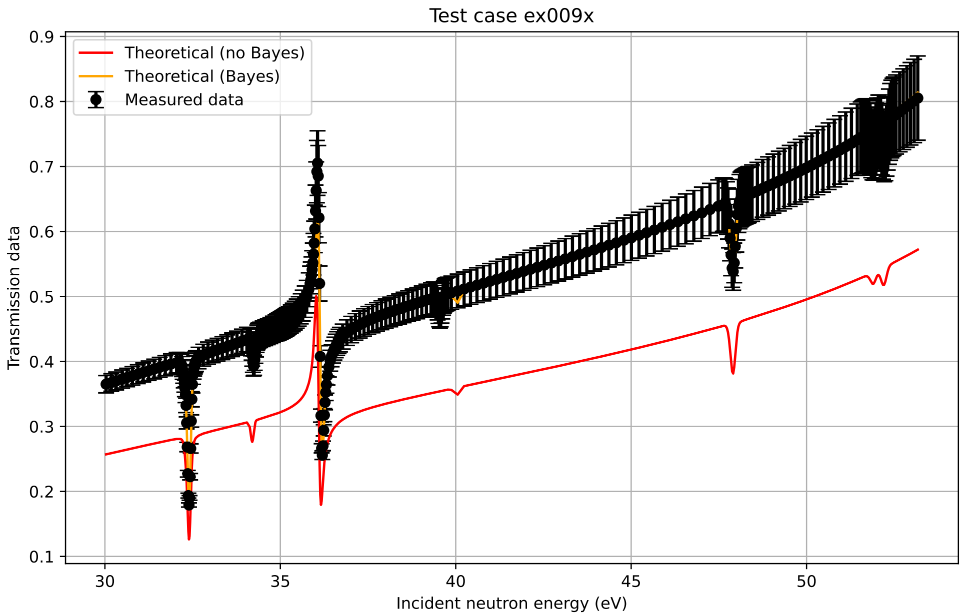
EX008: Resolution broadening (RPI)

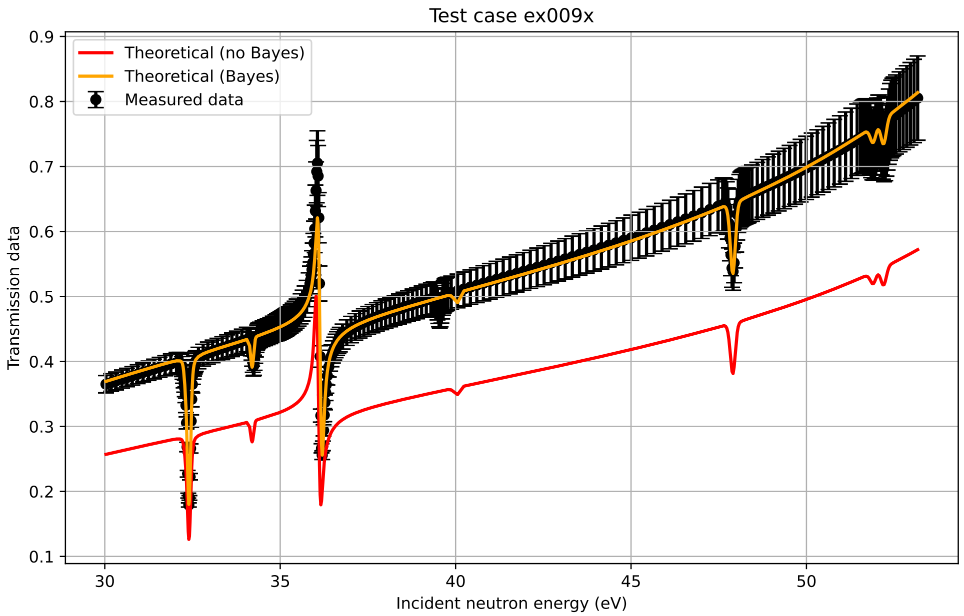
- Input file `ex008x.inp`
- Reaction type: Transmission data on n+^{183}W
- Bayesian with small prior uncertainty on resonance energies



EX009: Normalizations

- Input file `ex009x.inp`
- Reaction type: Transmission data on n+^{58}Ni
- Bayes with background function





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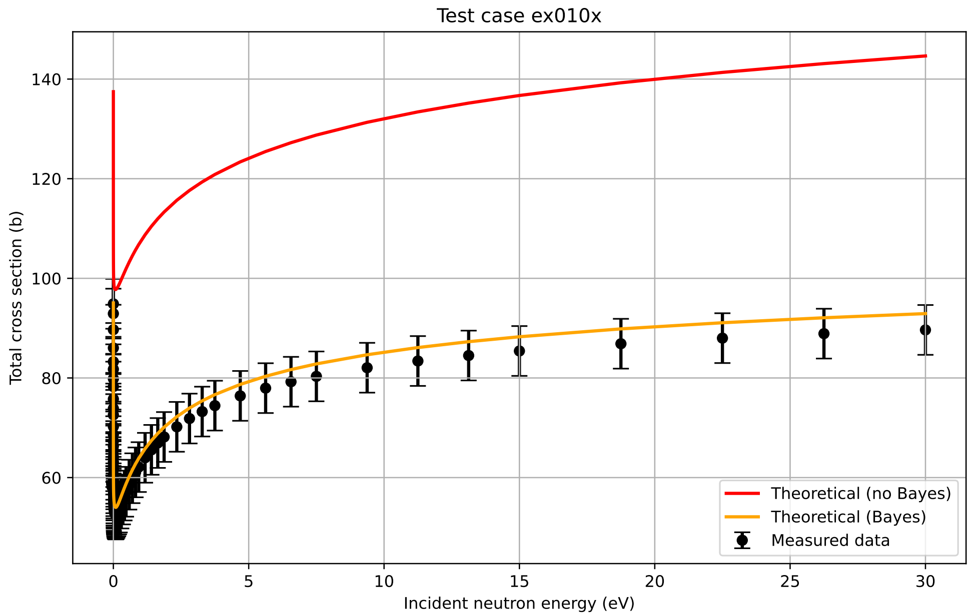
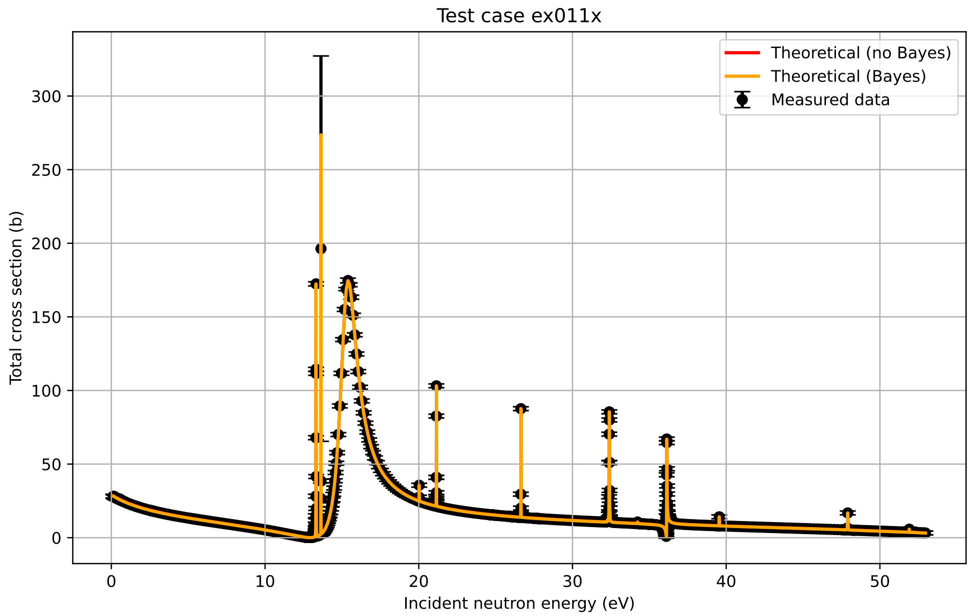
EX010: Normalizations

- Input file `ex0010x.inp`
- Reaction type: Total$\equiv{}^{56}$Fe(n,tot) and ^{58}Ni(n,tot)
- Bayes with background function



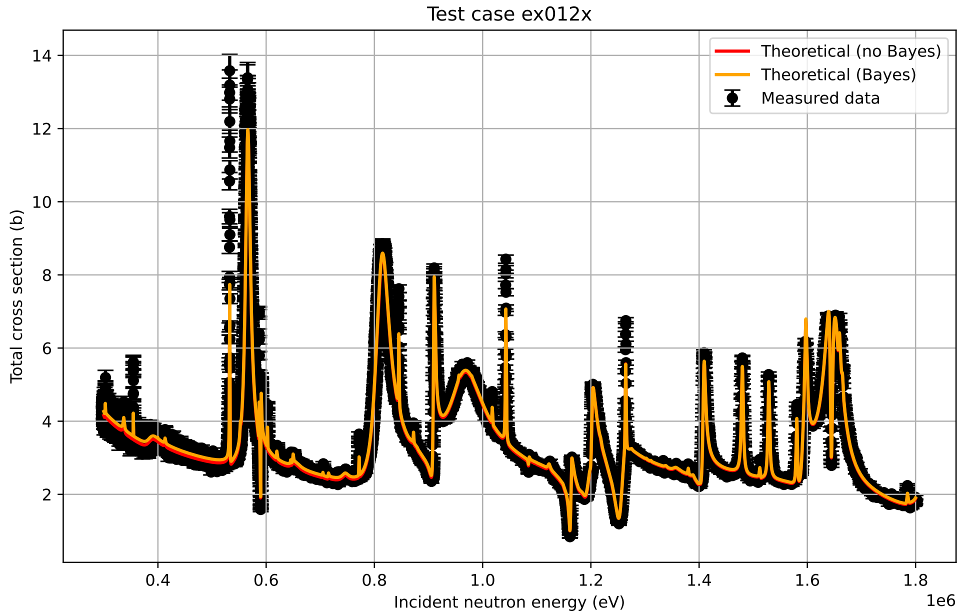
EX011: More than one channel radius

- Input file `ex0011x.inp`
- Reaction type: Total$\equiv^{58}$Ni(n,tot)
- Parameter file with channel radii 6.2 fm (group=1,4,5,6) and 4.2 fm (group=2,3)



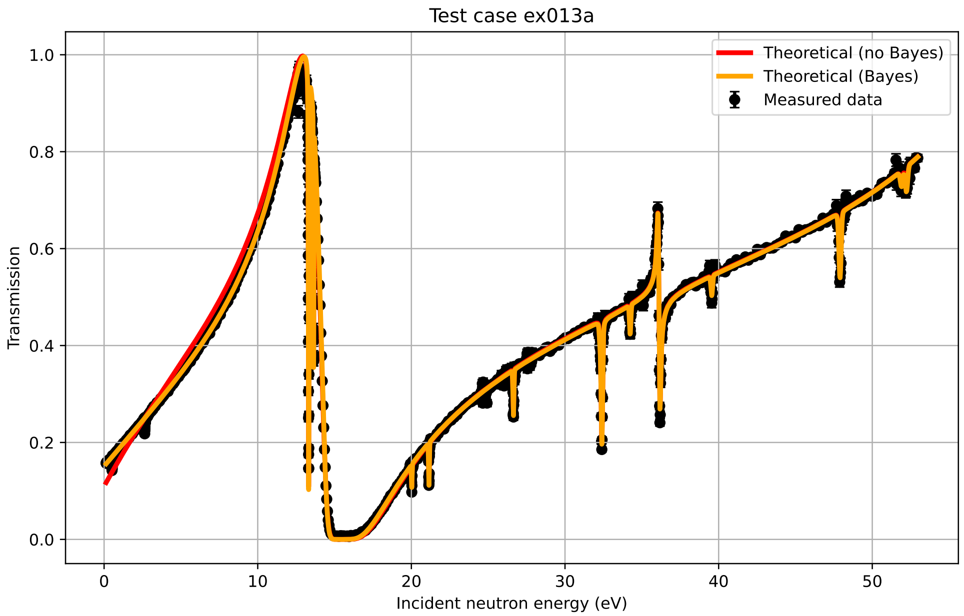
EX012: Multiple nuclides within a single sample

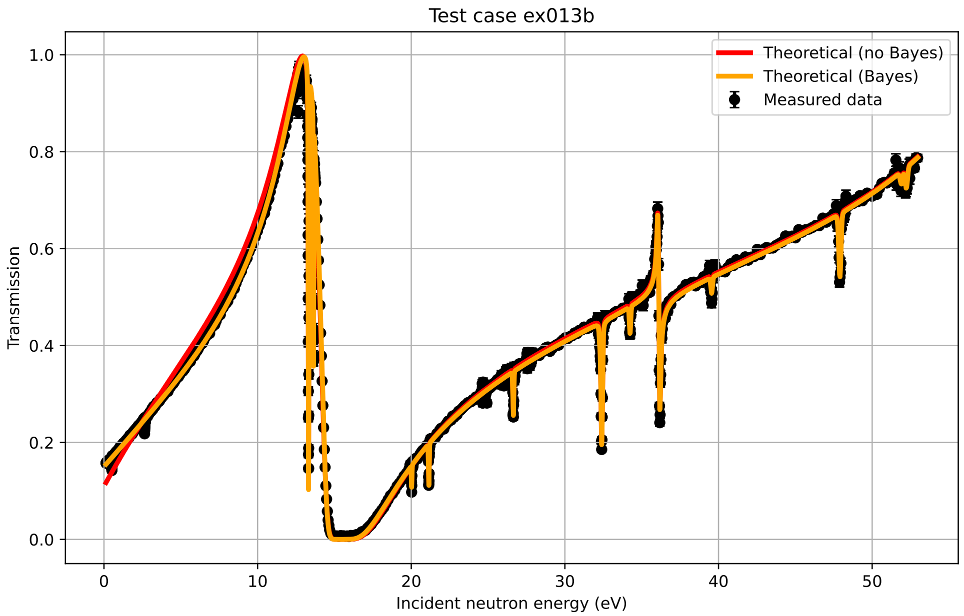
- Input file `ex0012x.inp`
- Reaction type: Transmission on $^{nat}\mathrm{Si}(n,\mathrm{tot})$



EX013: Uncertainties on parameters

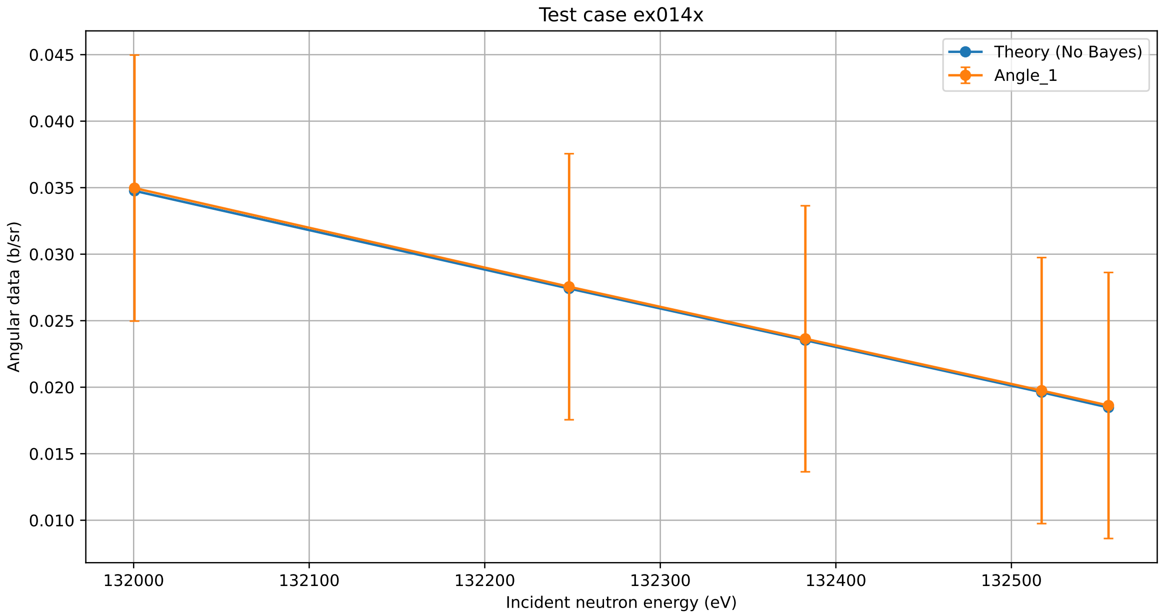
- Input file `ex0013{a,b}.inp`
- Reaction type: Transmission on ^{58}Ni$(n,$tot$)$
- Uncertainty on the resonance energies and explicit parameter uncertainties





EX014: Angular distributions

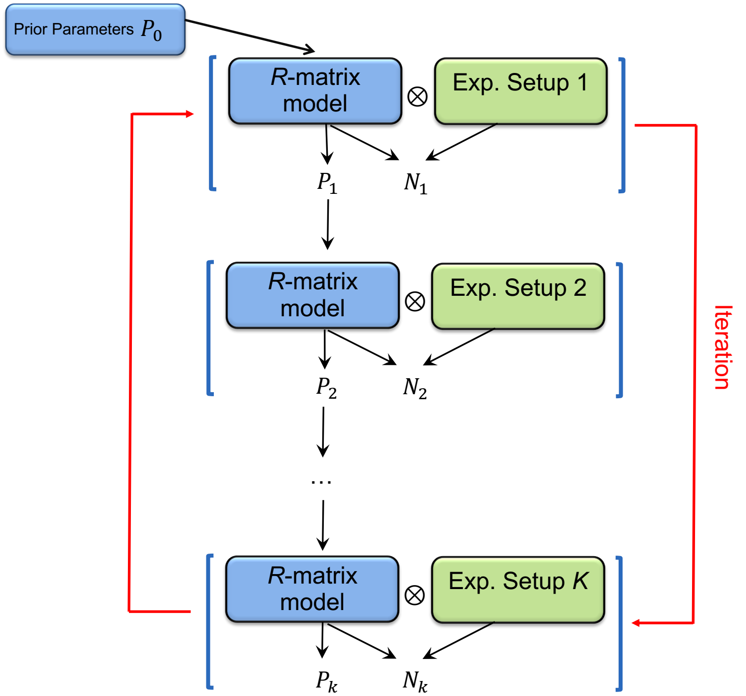
- Input file `ex0014x.inp`
- Reaction type: differential elastic$\equiv d\sigma/d\Omega$ (b/sr) on ^{58}Ni(n, el)
- 19 angles (in degree and laboratory system)
- `ex0014x.xlst` measured data, `ex0014x.lst` calculated data



EX015: Sequential fitting of data

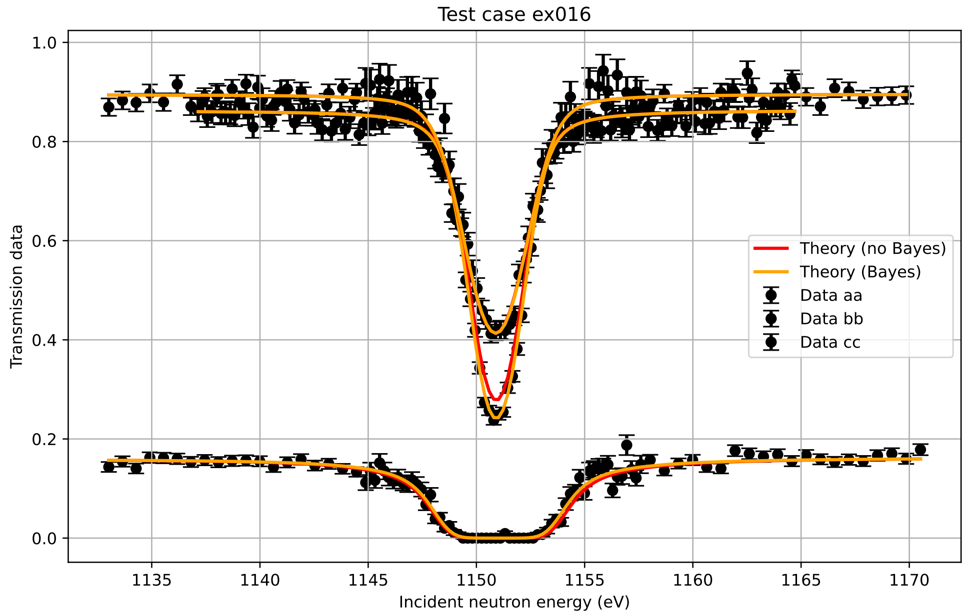
- Input file `ex0015{a,b,c}.inp`
- Reaction type: fission $\equiv {}^{239}\mathrm{Pu}(n, f)$
- 4 energy regions analyzed in four separate SAMMY consecutive runs or in a single run

```
# four energy ranges

ex015a.inp
ex015a.par
ex015a.twenty 10.0,12.1
13.4,18.0
12.1,13.4
08.1,10.0

# one energy range

ex015a.inp
ex015a.par
ex015a.twenty 08.1,18.0
```



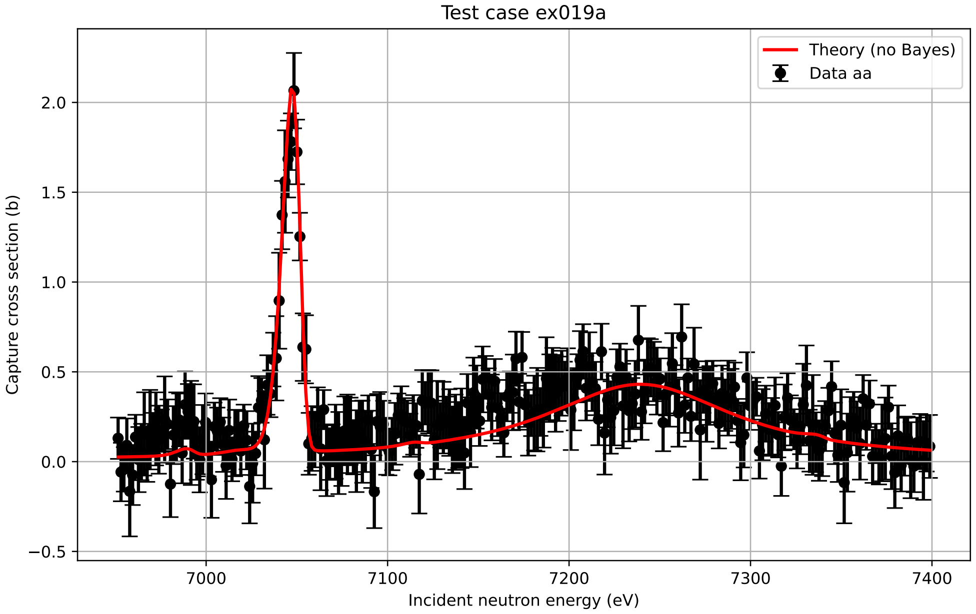
EX016: Fitting 3 data sets sequentially; input covariance matrix

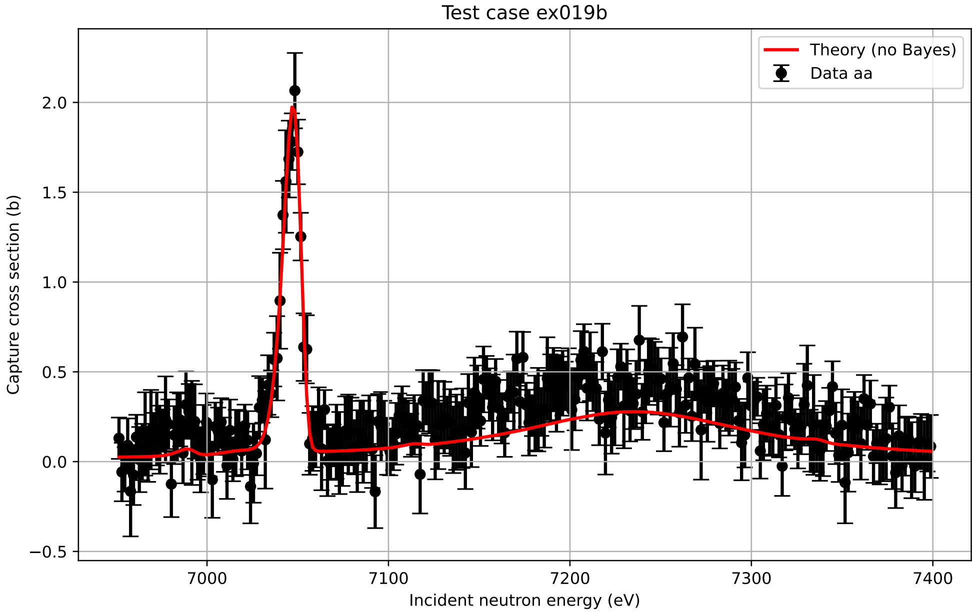
- Input file `ex0016{a,b,c}.inp`
- Reaction type: transmission on n+^{56}Fe
- Sequential fit of three transmission data sets
- Data covariance information in `ex016a.dcv` is in input for `ex0016a.inp`



EX019: Self-shielding and multiple-scattering corrections

- Input file `ex0019{a,b}.inp`
- Reaction type: neutron capture cross section on n+^{nat}Ba
- Multi isotope for $BaCO_3$ sample (Barium carbonate). No correction (`a`), only self-shielding (`b`)





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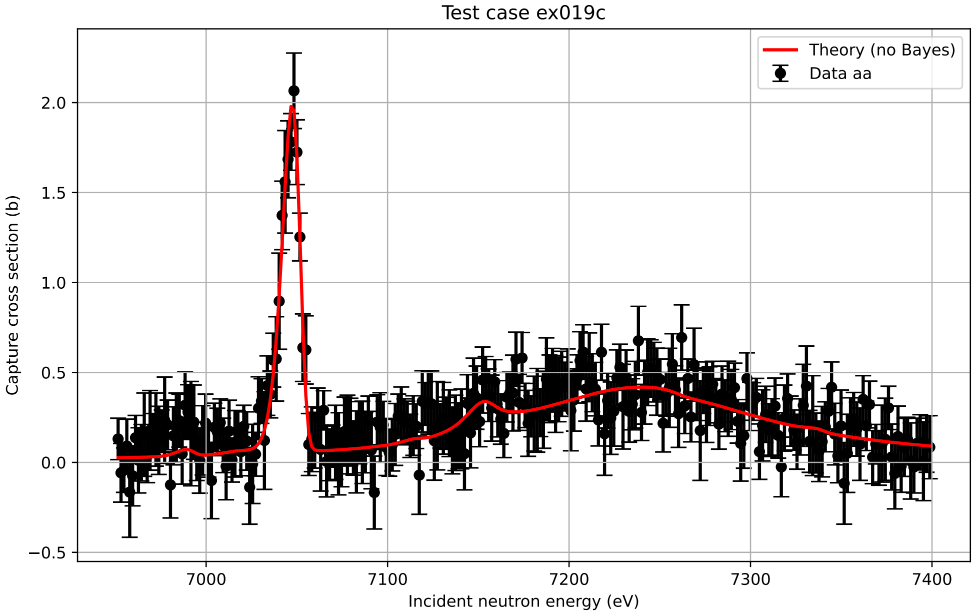
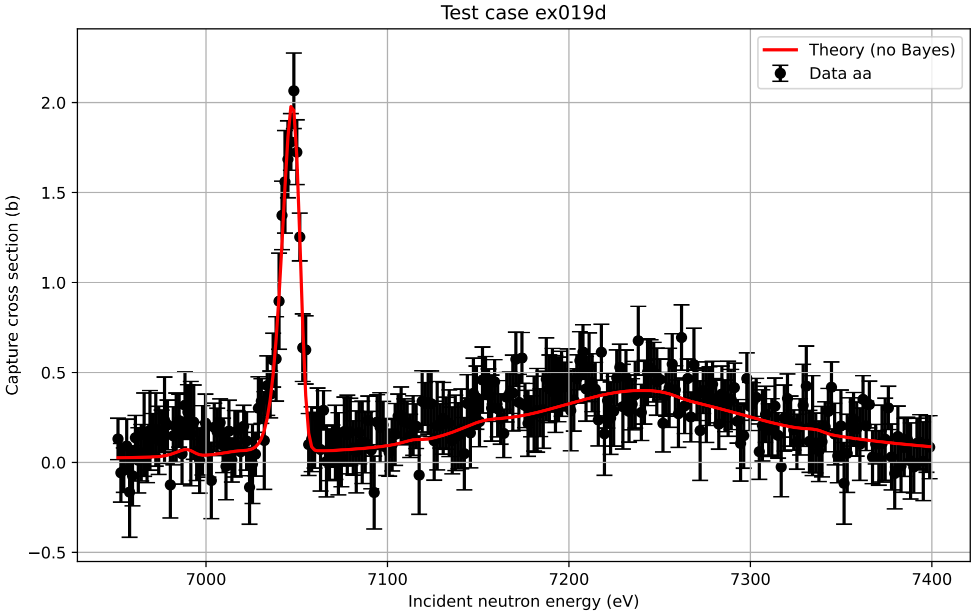
EX019: Self-shielding and multiple-scattering corrections

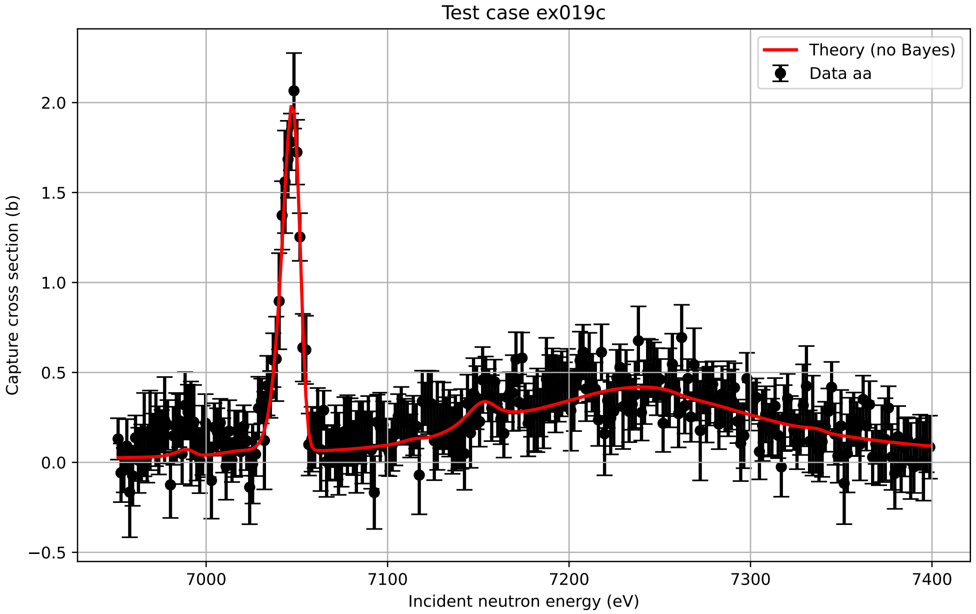
- Input file `ex0019{c,d}.inp`
- Reaction type: neutron capture cross section on n+^{nat}Ba
- Single/infinite slab (`c`), Single (`d`)

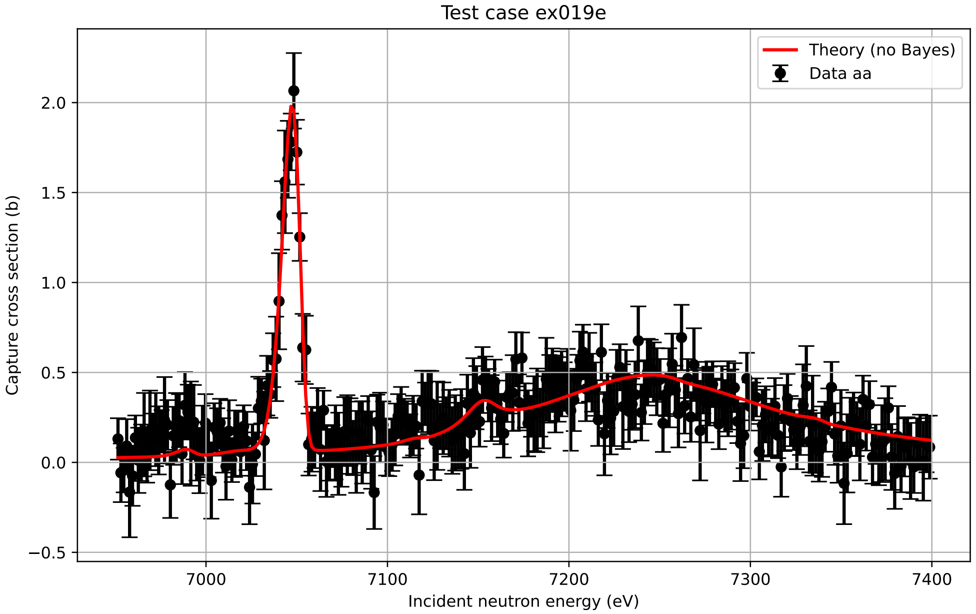




EX019: Self-shielding and multiple-scattering corrections

- Input file `ex0019{c,e}.inp`
- Reaction type: neutron capture cross section on n+^{nat}Ba
- Single/infinite slab (`c`), Double/infinite slab (`e`)





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EX020: Integral quantities[1]

- Input file `ex0020{a,b,c}.inp`
- one “real” resonance plus two dummies, non-fissile “experimental” grid is arbitrary, with `NXTRA=9`
- fissile, using a few resonances from ^{235}U ”experimental” grid is arbitrary, with `NXTRA=9`
- just like #2 but with expl-data-correlations
- ntg file

EX026: Create ENDF File 2

- Input file `ex0026{a,b,c}.inp`
- sequential fit of transmission and capture data
- `SAMMY.PAR,COV` formatted in evaluated nuclear data format (ENDF)
- Check `SAMMY.{ENDF,ENDFX}`

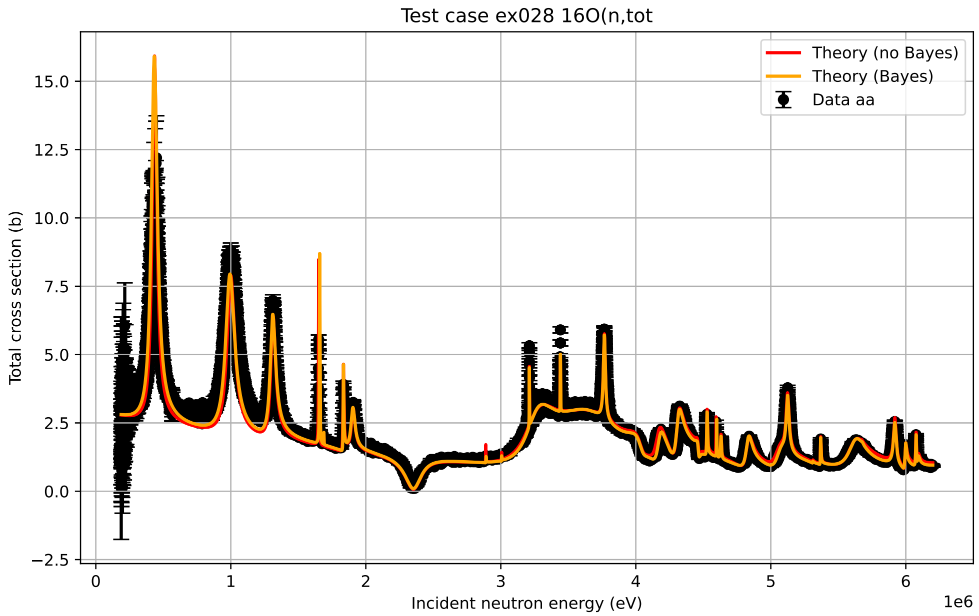
[1]Maxwellian capture, thermal capture, resonance integral,…

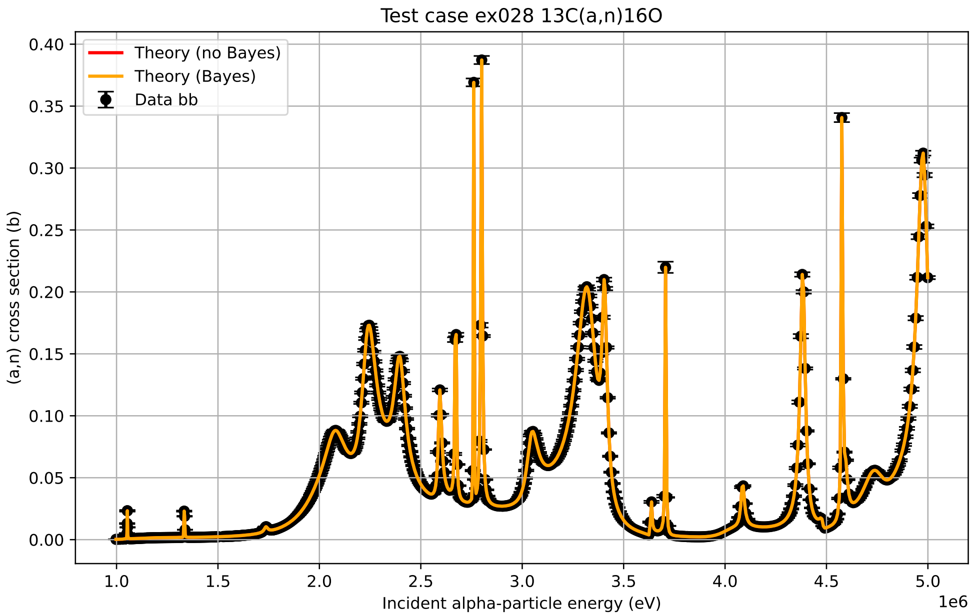
EX027: Running SAMMY with ENDF file for input

- Input file `ex0027{a,b}.inp`
- `ex0027a.inp` reads ENDF file as input
- `ex0027b.inp` starts fitting from retrieved resonance parameters
- Reaction type: ^{238}U(n, γ)

EX028: Fitting two datasets with inverse channel option

- Input file `ex0028{a,b}.inp`
- Reaction type: $^{16}O(n,tot)$ and $^{13}C(\alpha,n)^{16}O$
- Inverse channel option





EX029: Fitting two datasets with inverse channel option plus normalizations

- Input file `ex0028{a,b}.inp`
- Reaction type: $^{16}O(n,tot)$ and $^{13}C(\alpha,n)^{16}O$
- Inverse channel option plus normalization for each dataset