Introduction to GOSIA calculations

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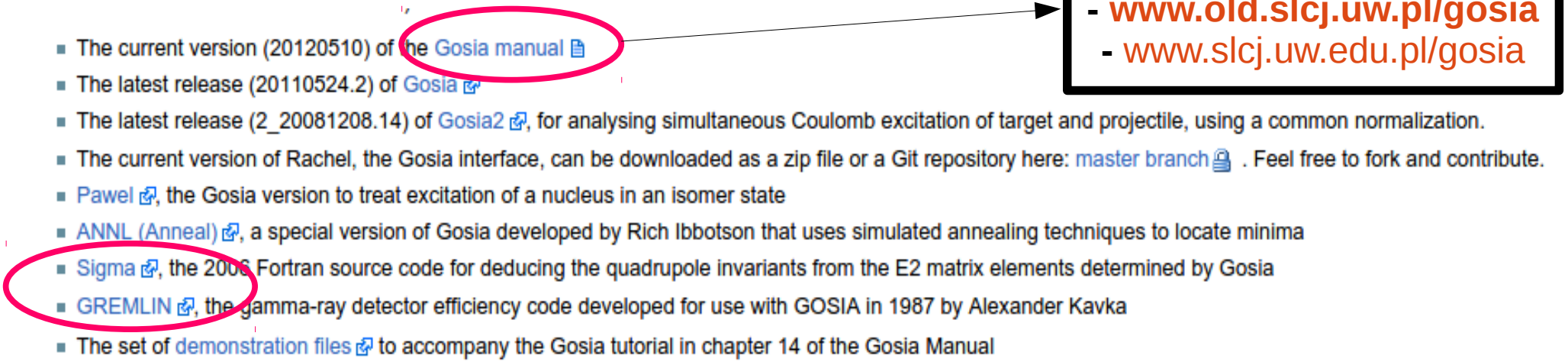
What do you need to start

http://www-user.pas.rochester.edu/~gosia/mediawiki

- GOSIA source code (you need fortran compiler)
- GOSIA manual (pdf file)

More reliable manual:
- **www.old.slcj.uw.pl/gosia**
- www.slcj.uw.edu.pl/gosia



- The current version (20120510) of the Gosia manual
- The latest release (20110524.2) of Gosia
- The latest release (2_20081208.14) of Gosia2, for analysing simultaneous Coulomb excitation of target and projectile, using a common normalization.
- The current version of Rachel, the Gosia interface, can be downloaded as a zip file or a Git repository here: master branch . Feel free to fork and contribute.
- Pawel, the Gosia version to treat excitation of a nucleus in an isomer state
- ANNL (Anneal), a special version of Gosia developed by Rich Ibbotson that uses simulated annealing techniques to locate minima
- Sigma, the 2006 Fortran source code for deducing the quadrupole invariants from the E2 matrix elements determined by Gosia
- GREMLIN, the gamma-ray detector efficiency code developed for use with GOSIA in 1987 by Alexander Kavka
- The set of demonstration files to accompany the Gosia tutorial in chapter 14 of the Gosia Manual

- Example input file
- Some research done before you start

  and
- ...a lot of patience

Some basic facts

- GOSIA is a Rochester – Warsaw **semiclassical coupled-channel Coulomb excitation least-squares search code**, developed 30 years ago by T.Czosnyka, D.Cline, C.Y.Wu and continuously upgraded.

  http://www.pas.rochester.edu/~cline/Gosia/index.html
  www.slcj.uw.edu.pl/gosia

- GOSIA is used for:

  - **analysis** (multidimensional fit of matrix elements to the data)

  - **simulations** (probability of excitation, intensities of the gammas)

- GOSIA - **fortran** code - get used to 'reading it' (*errors will send you to the line number, not to the exact line in your input file)

- GOSIA is a command-line program (*GUI available)

- Input file looks strange and scary..

- **Different files needed** (options: POIN, STAR, INTG/INTI, MINI, ERRO... require separate input files)

- Be critical and use GOSIA with caution

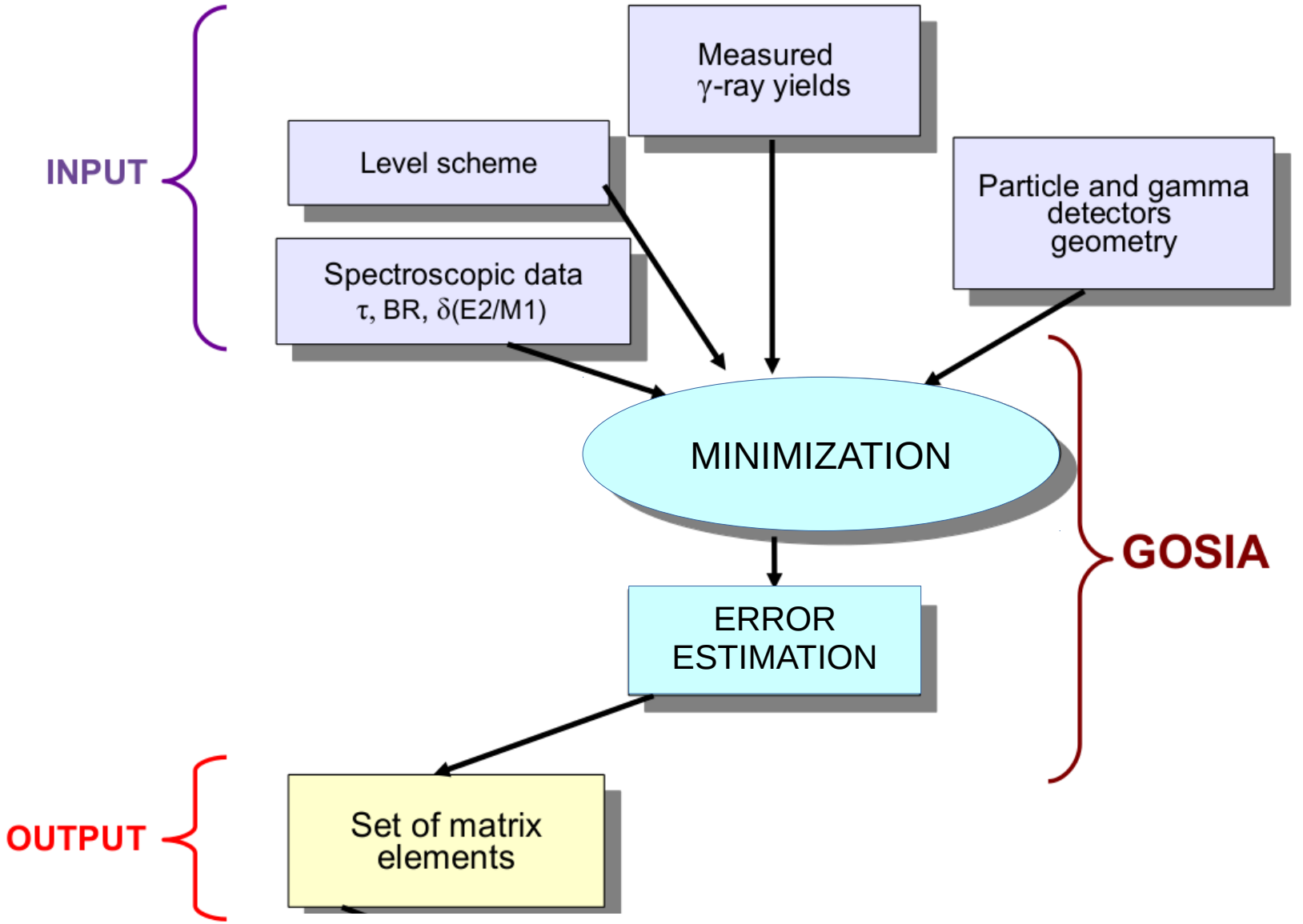
We are here to help you! :)

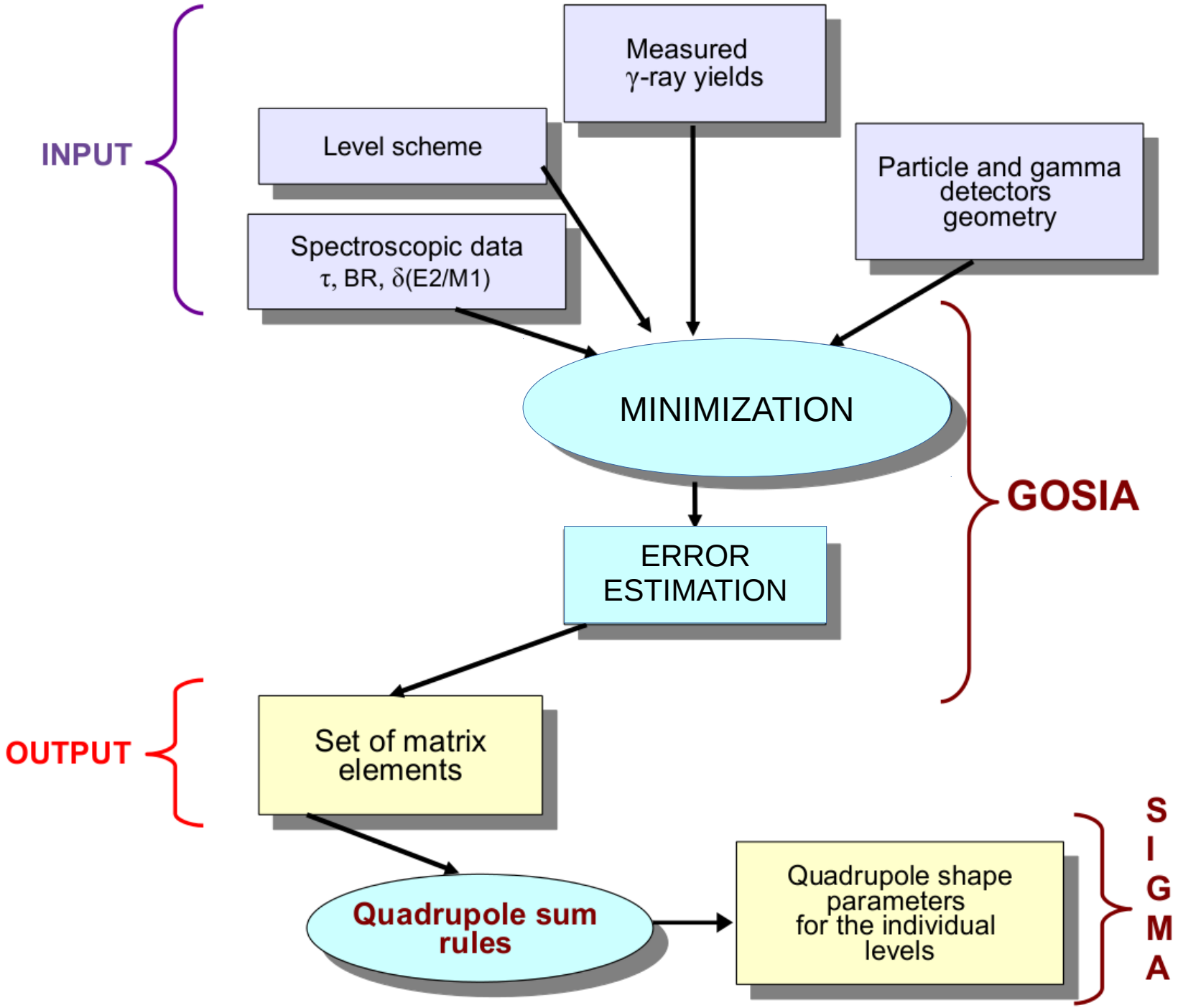
How does it work?

- GOSIA solves the set of differential equations, calculates the **excitation probabilities**, gives you the **level populations** and **gamma-ray intensities**

- To get the numbers you **MUST** specify the **experimental conditions** (level scheme, matrix elements, spectroscopic data, gamma and particle detection system)

- Additional effects are considered here: gamma detector size and **efficiency**, internal electron conversion


INPUT
Measured
γ-ray yields
Level scheme
Particle and gamma
detectors
geometry
Spectroscopic data
τ, BR, δ(E2/M1)
MINIMIZATION
GOSIA
ERROR
ESTIMATION
OUTPUT
Set of matrix
elements


INPUT
Measured
γ-ray yields
Level scheme
Particle and gamma
detectors
geometry
Spectroscopic data
τ, BR, δ(E2/M1)
MINIMIZATION
GOSIA
ERROR
ESTIMATION
OUTPUT
Set of matrix
elements
Quadrupole sum
rules
Quadrupole shape
parameters
for the individual
levels
SIGMA

Simulations - before you start

- Do the **research**: data base check, **level scheme**, known **lifetimes**, **branching ratios**, B(E0,E1,E2,E3..), B(M1), **mixing ratios, quadrupole moments**.
- recalculate the transition strengths into matrix elements.
- Read the papers.
- Ask theorists!
- http://bricc.anu.edu.au/ **- electron conversion coefficient** calculator
- Calculate the **SAFE energy** (simulations) for your system
- What is the **beam**? Energy and scattering angles
- What is the **target**? How thick? How complex? Energy loss of the beam in the target material is important (ELO, SRIMM programs)
- **Normalization** method: known target excitation or lifetimes?
- **Detectors**:
  - **Gamma array:** how many? How far from the target? Size? Efficiency?
  - **Particle array:** theta and phi angles, geometry (CD, PIN, MCP...), dead pixels, useful detection range?

GOSIA input structure

1. OP,FILE – header files (TAPEs)

2. OP,TITL

3. OP,GOSI (with fit) - OP,COUL (without fit)

- LEVE

- ME

- EXPT

- CONT

END,

4. OP,YIEL

5. OP,RAW

6. OP,INTG/INTI

7. OP,MINI

8. OP,ERRO

9. OP,POIN

10. OP,STAR

11. OP,THEO

12. OP, MAP

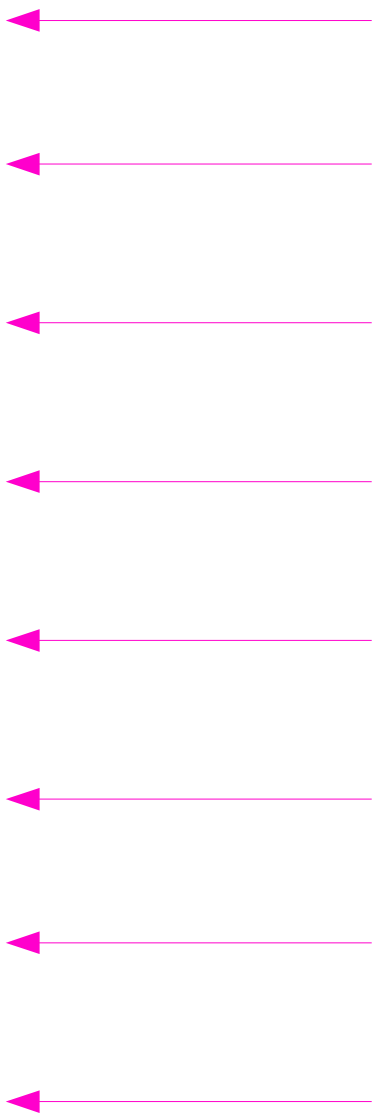
13. OP, REST

14. OP,GDET

15. OP,SIXJ

OP,FILE

```
22 3 1
mini.out
9 3 1
gdet.f9
8 3 1
gdet.f8
12 3 1
matrix.me
3 3 1
yield.f3
4 3 1
corr.f4
7 3 1
map.f7
14 3 1
sixj.14
0 0 0
```



Output file name

OP,GDET output

OP,GDET (if OP,RAW used)

Matrix elements

Gamma yields

Corrected gamma yields (after OP,INTG / INTI)

OP,MAP output

OP,SIXJ output (if this option used)

OP,GDET – gamma detector option

OP,GDET

OP,FILE

22 3 1

gdet.out

9 3 1

gdet.f9

8 3 1

gdet.f8

0 0 0

OP,TITL

Gamma detectors

OP,GDET

-1

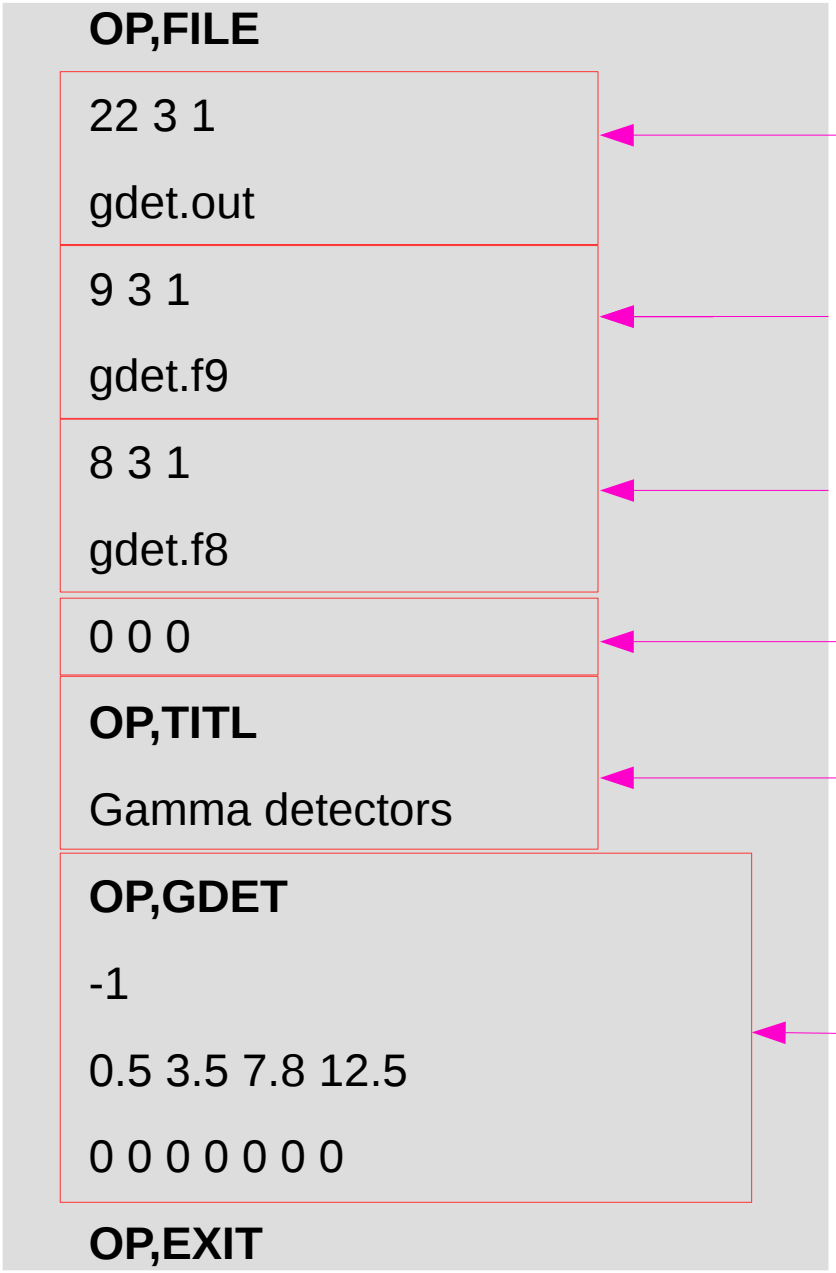
0.5 3.5 7.8 12.5

0 0 0 0 0 0 0

OP,EXIT

This option gives the information about the gamma detectors

OP,GDET



22 – output name

GDET output file – parameters needed to reproduce γ energy dependence on the gamma detector solid angle attenuation coeff. Q_k

GDET output file – absorption coeff. needed to reproduce the detector efficiency, created if NPD is **negative** – related to “raw” spectra defined in OP,RAW

End of OP,FILE

Title

OP,GDET input options

GOSIA

```
OP,FILE
        22 3 1
        star.out
        0 0 0
OP,TITL
        OP,STAR output test
OP,GOSI
        LEVE
                1,1,0,0.0
                2,1,2,1.500
                3,1,4,2.700
                0,0,0,0
        ME
                2 0 0 0 0
                1  2 0.1   1.0  -1.0
                2  2 0.1   1.0  -1.0
                2  3 0.1   1.0  -1.0
                0 0 0 0 0
        EXPT
                1 20 42
                -79 197 100 100  3 1 1 -170 172 0 1
        CONT
                INR,
                INT,1.
                1,1000
                LCK,
                0 0
                WRN,3.
                PRT,
                0 0
END,

OP,STAR
OP,EXIT
```

OP,STAR

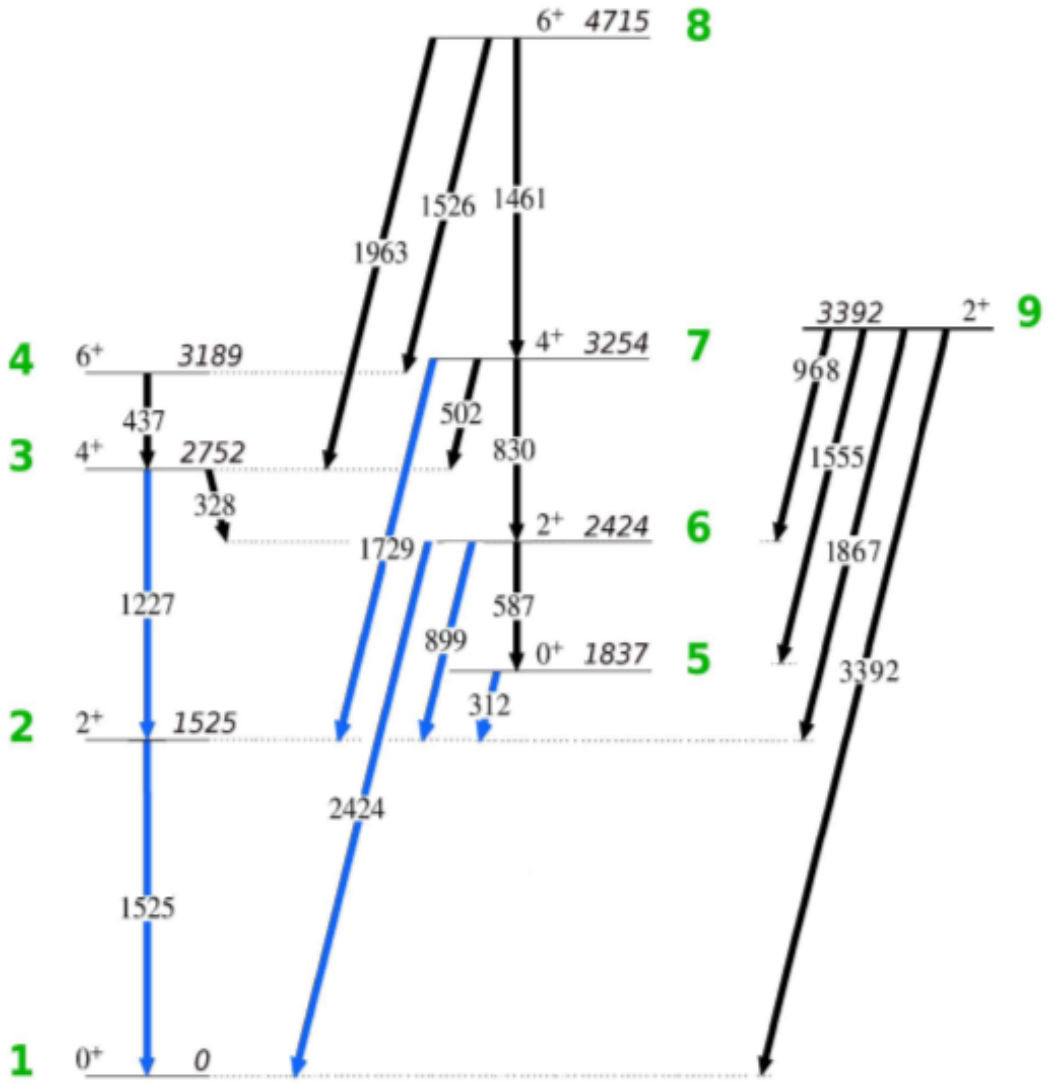
Command to calculate Coulomb excitation amplitudes and probabilities (not the gamma-ray yields)

OP,GOSI – level scheme

```
LEVE
1  1  0  0.0
2  1  2  1.525
3  1  4  2.752
.
.
.
0  0  0  0
```

1 = GROUND STATE

Which nucleus?



OP,GOSI – matrix elements

```
ME
2 0 0 0 0
  1  2 0.20   0.0001  1.5
  2  6 0.08   -1.5     1.5
  .
  .
7 0 0 0 0
  2 6 1.01   -2.      2.
  .
  .
0 0 0 0 0
```

Limits for ME
(R1 and R2)

ME

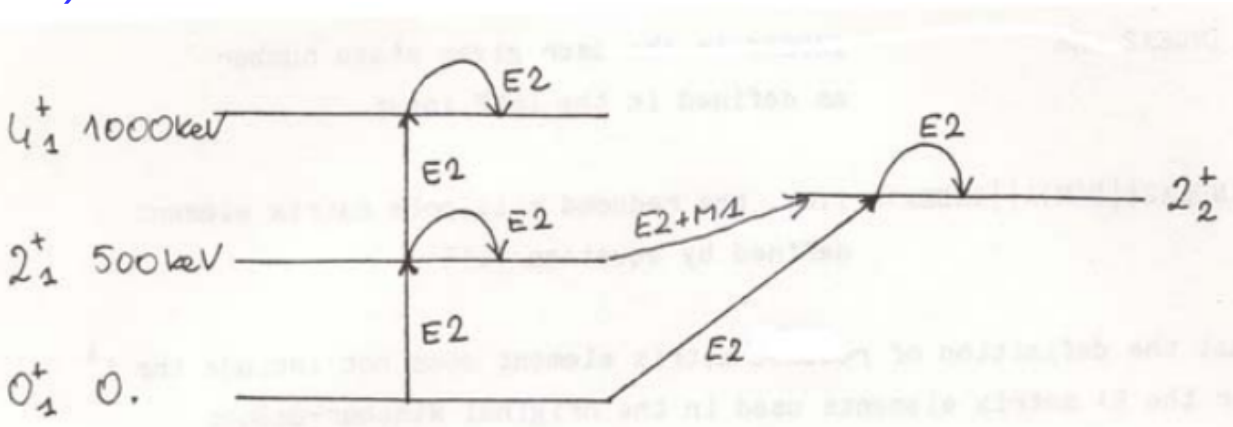
INDEX2

INDEX1

Multipolarity E(M)λ:
1 E1
2 E2
3 E3
..
7 M1
8 M2

< INDEX1 || E(M)λ || INDEX2 >

INDEX1 and INDEX2 are given in increasing order (start with INDEX1)



We need a set of ME to start with

levels.inp

```
1  1  0  0.0
2  1  2  0.413
3  1  4  1.005
4  1  0  0.825
5  1  2  0.881
6  1  4  1.208
0  0  0  0
```

Level E[MeV]

SPIN

Parity

Level number

megen levels.inp

```
1
Create setup for this multipolarity (y/n)
n
2
Create setup for this multipolarity (y/n)
y
Do you want them coupled ?
n
Please give limit value
-1.5 1.5
3
Create setup for this multipolarity (y/n)
n
(...)
7
Create setup for this multipolarity (y/n)
y
Do you want them coupled ?
n
Please give limit value
-1 1
8
Create setup for this multipolarity (y/n)
n
```

E2

M1

We need a set of ME to start with

levels.inp

```
1  1  0  0.0
2  1  2  0.413
3  1  4  1.005
4  1  0  0.825
5  1  2  0.881
6  1  4  1.208
0  0  0  0
```

Level
E[MeV]

SPIN

Parity

Level
number

me.out

```
2 0 0 0 0
  1  2 1    1.5   -1.5
  1  5 1    1.5   -1.5
  2  2 1    1.5   -1.5
  2  3 1    1.5   -1.5
  2  4 1    1.5   -1.5
  2  5 1    1.5   -1.5
  2  6 1    1.5   -1.5
  3  3 1    1.5   -1.5
  3  5 1    1.5   -1.5
initial level | final level | starting value (1) | low limit | high limit
  4  5 1    1.5   -1.5
  5  5 1    1.5   -1.5
  5  6 1    1.5   -1.5
  6  6 1    1.5   -1.5
7 0 0 0 0
  2  2 1    1.0   -1.0
  2  5 1    1.0   -1.0
  3  3 1    1.0   -1.0
  3  6 1    1.0   -1.0
  5  5 1    1.0   -1.0
  6  6 1    1.0   -1.0
0 0 0 0 0
```

E2

M1

OP,THEO

- generates the ME from rotational model
- generates only the matrix specified in the ME input and writes them to the output file
- For **in-band or equal-K** interband transitions only one intrinsic moment for a given multipolarity marked **Q1** is relevant.
- For **non-equal-K** values generally two moments with the projections equal to the **sum and difference of K's** are required (**Q1 and Q2**), (unless one of the K's is zero, when again only Q1 is needed)
- For the **K-forbidden** transitions a three parameter Mikhailov formula is used.

OP,THEO for ^{188}Hg (example)

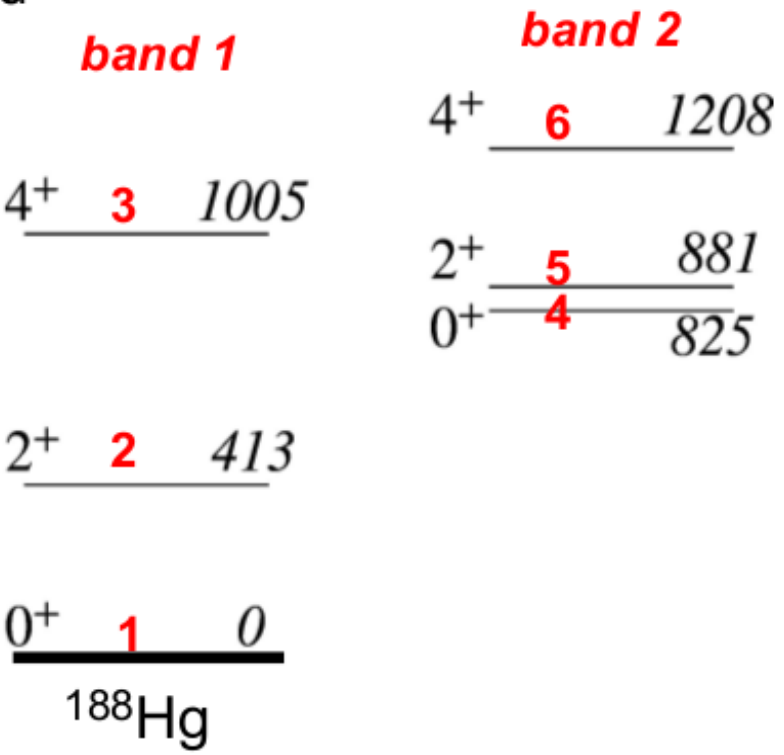
$$\left\langle KI_f \left\| \hat{M}(E2) \right\| KI_i \right\rangle = \sqrt{(2I_i+1)} \left\langle I_i, K, 2, 0 \mid I_f K \right\rangle \sqrt{\frac{5}{16\pi}} eQ_0$$

```
OP,THEO
2
0,3
1,2,3
0,3
4,5,6
2
1,1
Q1,0,0
1,2
Q1,0,0
2,2
Q1,0,0
0,0
0
```

number of bands (2)
First band, K and number of states
band member indices
Second band, K and number of states
Multipolarity E2
Bands 1 and 1 (in-band)
Moment Q1 of the rotational band

end of multipolarities loop

end of band-band input



Courtesy: K. Wrzosek-Lipska

OP,GOSI: EXPT

Here we declare the most important details about the experiment:

Energy, angles, Z+A target and projectile

EXPT

NEXP Z1 A1

+/-Z2 A2 Ep +/-θ_{proj} Mc Ma IAX φ1 φ2 IKIN LN

EXPT

2 20 42

-79 197 167 122 3 1 1 -170 172 0 1

-82 208 167 122 3 1 1 -170 172 0 2

^{42}Ca beam on
^{197}Au and ^{208}Pb targets

OP,YIEL

```
OP,YIEL
0
5 2
0.1 0.3 0.5 1.0 1.5
1
0.000829  2.41E-5  5.60E-6  1.143E-6  0.000269
2
0.01175   0.0001328  2.06E-5  2.59E-6  8.94E-5
5  5
1  2  3  4  5
25  55  85   130  172
40  75  270 325  59
1  2  3  4  5
25  55  85   130  172
40  75  270 325  59
2 1
1                                   !EXP1
0.0001
1
1                                   !EXP2
0.0001
1
3
```

Here we put Information about:
- electron conversion coefficients
- gamma detection geometry
- normalization transition
- type of our analysis

OP,YIEL

```
2    1.0
     4 5 4 2   0.007  0.003
     5 1 5 2   0.34   0.02
2    1.0
     2    1.19  0.04
     3    4.45  0.10
1    1.0
     6 2  -0.18     0.02
1    1.0
     2  2  2    -0.25  0.051
```

Here we put Information about the spectroscopic data:
- lifetimes,
- branching ratios,
- mixing ratios,
- known transition probabilities

```
0 0
0 0      in case nothing is known
0 0      about the investigated nucleus
0 0
```

YIELD definition

POINT

- **One** energy (E)
- **One** angle (Θ)

  as defined in EXPT

  use **OP,POIN**

INTEGRATED

- Energy **range**

  (E_{min}-E_{max})
- Angular **range**

  (Θ_{min},φ_{min})–(Θ_{max},φ_{max})

  as defined in **OP,INTG / INTI**

Matrix elements values, excitation probability

OP,POIN

- This option evaluates the point gamma yield in the laboratory frame for the $I_i \rightarrow I_f$ transition for **one energy** and **one particle scattering angle** given in **EXPT**

$$Y^{Point}(I \rightarrow I_f) = \sin(\theta_p) \int_{\phi_p} \frac{d^2\sigma(I \rightarrow I_f)}{d\Omega_\gamma d\Omega_p} d\phi_p$$

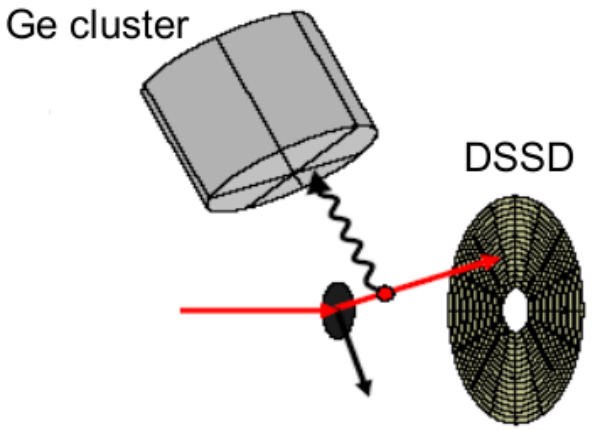
- includes the **Rutherford cross section**, the sin(Θ) term, integration over the projectile φ scattering angle, the deorientation effect and gamma-detector attenuation coefficients (from OP,GDET)
- Calculates the yield for one system – defined as one **θ-E** point
- We use OP,POIN after OP,YIEL

  But..
- In real life we use REAL detectors with continuous dimensions

Why integration?

- REAL conditions - GOSIA calculates **yields** from ME to get **realistic comparison** with experimental data
- integration over **solid angle** of the particle detectors, **energy loss in the target,** full correction for the velocity of the deexciting nucleus and the **deorientation effect** is included
- the Rutherford scattering is integrated over the particle detectors and energy loss in the target – an absolute normalization.
- the '**GOSIA yield**' may be understood as a mean differential cross section multiplied by a target thickness (in mg/cm^2)

  [Y] = [mb/sr] × [mg/cm^2]



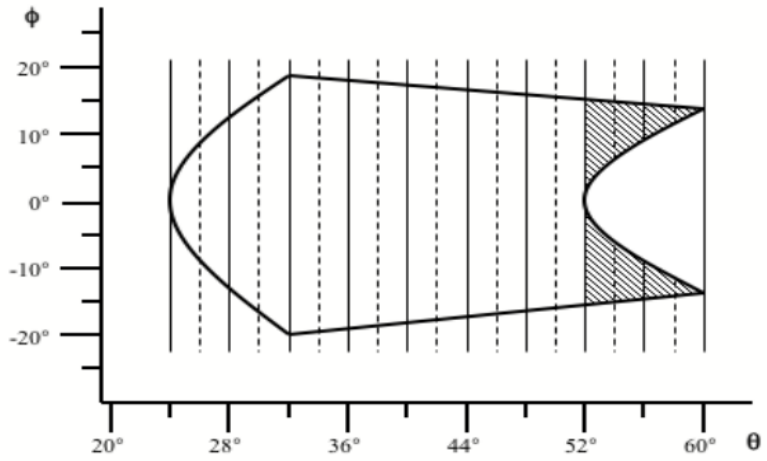
OP,INTG

2 stages:
- γ yields integrated over azimuthal angle **φ** for each energy **E** and center-of-mass scattering angle **θ** meshpoint. The calculation of the meshpoint yields is repeated for each experiment (**as declared in EXPT**) – point yields

- integration over bombarding energy **E** and the range of scattering angles **θ** of the particle detectors which is performed by **<u>interpolating</u>** between the yields calculated at each **E-θ** meshpoint

(*circular detectors option recommended)

OP,INTG
NE +/-NT E_{min} E_{max} θ_{min} θ_{max}
E_1 E_2 ... E_{NE}
$+/-\theta_1$ $+/-\theta_2$ ... $+/-\theta_{NE}$
NFI
φ_1 φ_2 ...
NP
E_1 E_2 ... E_{NP}
$(dE/dx)_1$ $(dE/dx)_2$ … $(dE/dx)_{NP}$
NI_1 NI_2

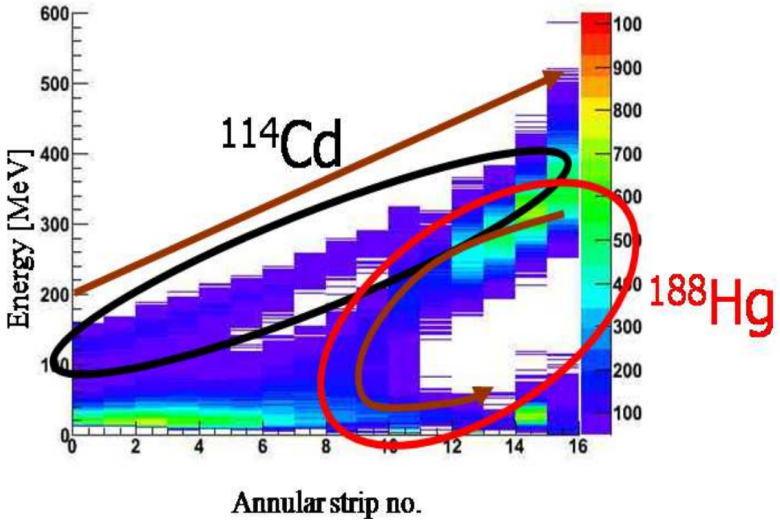


OP,INTI

- integration of systems involving inverse kinematics - when the **recoiling target nucleus is detected** (→ 2 kinematic solution).

For each beam E and each angle the special subroutine INVKIN calculates the appropriate value of kinematic flag and set it **automatically**

Θ angles correspond to laboratory scattering angles of the **detected particle**
- the angle of the scattered projectile if it is detected
- the angle of the recoiling target nucleus if it is detected.



N. Bree, PhD thesis, KULeuven,

OP,INTI
NE +/-NT E_{min} E_{max} θ_{min} θ_{max}
E_1 E_2 ... E_{NE}
θ_1 θ_2 ... θ_{NE}
NFI
φ_1 φ_2 ...
NP
E_1 E_2 ... E_{NP}
$(dE/dx)_1$ $(dE/dx)_2$ ... $(dE/dx)_{NP}$
NI_1 NI_2

```
OP,INTI                          !for axial sym. and circ. det.
8 9 226 240 133 168
226 228 230 232 234 236 238 240
133 135 140 145 150 155 160 165 168
8
226 228 230 232 234 236 238 240
12.2 12.17 12.13 12.10 12.05 12.00 11.90 11.80
20,20
```

OP,INTG / INTI – yield correction

- Minimization of is usually performed using **corrected** yields
- Correction depends on the set of ME: GOSIA calculates the **point** yield ($\mathbf{Y_p}$) and the **integrated** yield ($\mathbf{Y_I}$) from the ME and gives the **correction factors CF** for each experimental yield (**OP,CORR** needed):

$$\mathbf{CF} = \frac{Y_P}{Y_I} \longrightarrow \mathbf{Y}^{\mathbf{c}}_{\mathbf{exp}} = \mathbf{Y}_{\mathbf{exp}} \cdot \mathbf{CF}$$

  After minimization the correction procedure should be repeated with a new set of ME (better fit, different correction) → until the solution is converged

- CF are calculated for **each** experimental yield

^{42}Ca on ^{197}Au

E_{av} = 167 MeV

Θ_{av} = 122°

EXPERIMENT 2 DETECTOR 1

NI	NF	YEXP	YCOR	COR.F
3	2	.112E+00	.113E+00	.101E+01
6	1	.380E-01	.374E-01	.984E+00
6	2	.106E+00	.102E+00	.966E+00
5	2	.854E+00	.822E+00	.962E+00
2	1	.124E+02	.120E+02	.969E+00

GOSIA AS A SIMULATION TOOL: YIELD ⇒ COUNT RATE

$$Counts = 10^{-27} \cdot \left[\frac{Q}{\hat{q}\,e}\right] \cdot \left[\frac{N_A}{A}\right] \cdot [\rho\, dx] \cdot Y^{INTG}(I \rightarrow I_f) \cdot \Delta\theta_p \cdot \varepsilon_p \cdot \varepsilon_\gamma \cdot \Delta\Omega_\gamma$$

Where:

Q – integrated beam charge [C]

q – the average charges state of the beam

e – the proton charge [1.602 x 10^{-19} C]

N_A – Avogadro number [6.022 x 10^{23} atoms/mol]

A – target mass number [g/mol]

ρdx – areal target thickness [g/cm^2]

Y^{INTG} (I → I_f) OP,INTG or OP,INTI output in [mb/sr/rad]

$\Delta\theta_p$ – projectile scattering angle range [rad]

ε_p – particle detection efficiency per unit solid angle

ε_γ – gamma detection efficiency excluding the geometrical solid angle

$\Delta\Omega_\gamma$ – geometrical solid angle of the gamma-ray detector. Note that usually one only knows the product $\varepsilon_\gamma * \Delta\Omega_\gamma$

$$\textbf{Count Rate} = \frac{7.6\times10^{-6} \times yield \times current[pps] \times eff}{A_{target}}$$

OP,RAW

- This option needs energy-dependent efficiency calibration for each individual gamma detector (GREMLIN, EFFIT..)
- the first entry of OP,GDET should be **negative** to produce the **TAPE8**
- Need to declare which efficiency parametrization you need!
- **Do not use if all gamma intensities are efficiency-corrected**

```
OP,RAW
IEXP
A1 A2 A3 A4 A5 A6 A7 A8
A1 A2 A3 A4 A5 A6 A7 A8
…
...
A1 A2 A3 A4 A5 A6 A7 A8
NC
ID1
I1 I2 … I(ID1)
ID2
I1 I2 … I(ID2)
...
…
0
```

OP,MINI
χ^2 function minimization

$$\chi^2 = \frac{1}{p}\left\{ \sum_{i=1}^{N\exp} \sum_{j=1}^{N\det} \sum_{k=1}^{N\gamma} \left[\left(\frac{C_{ij} Y_k^{(T)} - Y_k^{(E)}}{\Delta Y_k^{(E)}} \right)^2 \right. \right.$$

$$\left. \left. + \sum_{i=1}^{Ns.d.} \left(\frac{d_i^{(T)} - d_i^{(E)}}{\Delta d_i^{(E)}} \right)^2 \right\} \right.$$

experimental yield

calculated yield

normalisation factor

spectroscopic data point

calculated magnitude

The fitting procedure is continued, until the convergence of the χ^2 is achieved and the set of matrix elements optimally reproduce the experimental data.

Remember to run **OP,MAP** before **OP,MINI**, each time you change something in ME (insert OP,MAP command directly after OP,YIEL). This option stores the **q-parameters** important for **reorientation effect** (effective strength, related to the magnetic sub-states coupling) on **TAPE7**

OP,ERRO

- for estimating the error bars to be assigned to the set of matrix elements corresponding to the minimum value of χ^2

Mode flag:
0 – diagonal
1 – correlated

OP,ERRO
IDF MS MEND IREP IFC RMAX

- **two separate stages:**

1. the **“diagonal“,or uncorrelated errors** (calculated individually for each matrix element) and write them on TAPE15

0 MS MEND 0 0 RMAX

2. the **“overall“, or correlated errors** (the total errors which are the widths of projections on each matrix element’s axis of the minimum at the $\chi^2 = \chi^2 + 1$ level).

1 MS MEND 1 1 RMAX

What else is there?

- There are **other options**, which can or should be used depending on the analysis needs (OP,STAR; OP,SIXJ; OP,RAND; OP,TROU; OP,BRIC..)
- **GOSIA2** for the radioactive beam experiments →target normalization tool
- **RACHEL** (GUI gosia)
- **SIGMA** – quadrupole sum rules code → shape invariants → deformation parameters