TalysLib: a ROOT-based toolkit for nuclear data access

N.A. Fedorov, I.D. Dashkov, Y.N. Kopatch, T.Yu. Tretyakova and TANGRA collaboration
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Introduction

Nuclear data represents **measured (or evaluated)** probabilities of various physical interactions involving the nuclei of atoms, as well as nuclear properties. It is needed for:

- Planning of new experiments
- Theoretical models testing
- Reference information in experimental data processing
- Developing of new nuclear facilities

Sources of nuclear data

Evaluated:

- ENDF (characteristics of nuclear reactions)
- ENSDF (nuclear structure)
- AME (nuclear masses)
- RIPL (ENSDF+AME+model parameters)
- **TALYS program**

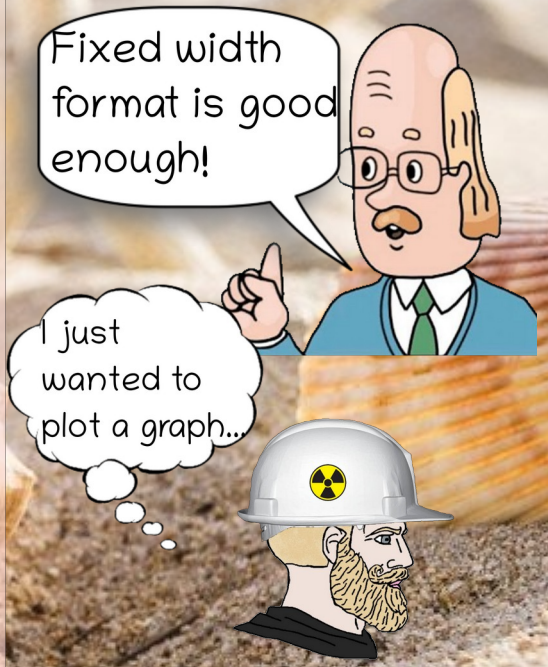
etc...

Measured:

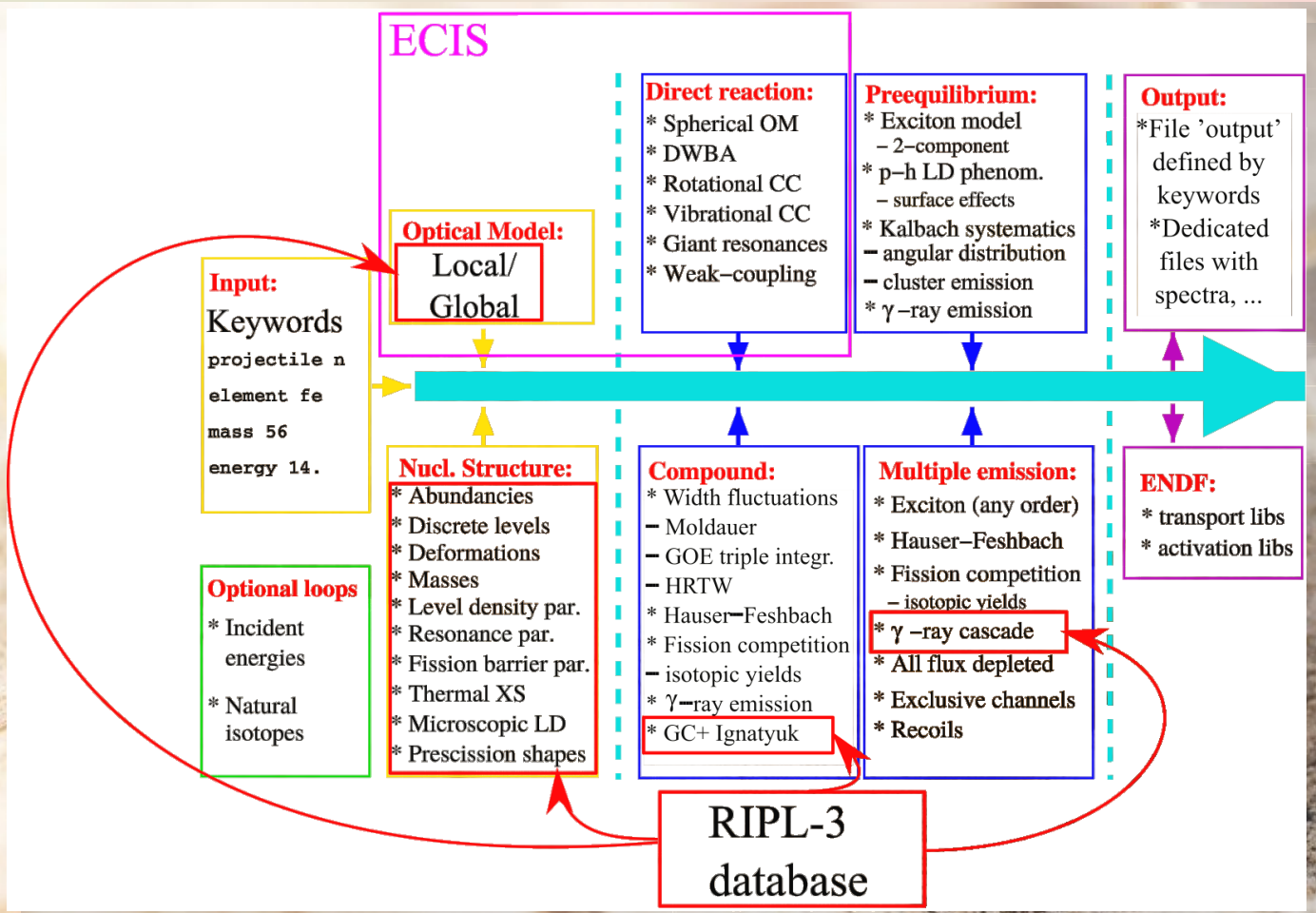
- EXFOR (“Raw experimental data”)
- Pre-processed EXFOR (C4, T4, EXFORTABLES)

Problems

- There is no C++/Python parser for this data
- The EXFOR and ENDF data format is quite complex to read
- One have to perform data search/plotting/processing by hand
- It is interesting to compare your data with other experiments/estimations and calculations. *In automatic mode*



Talys

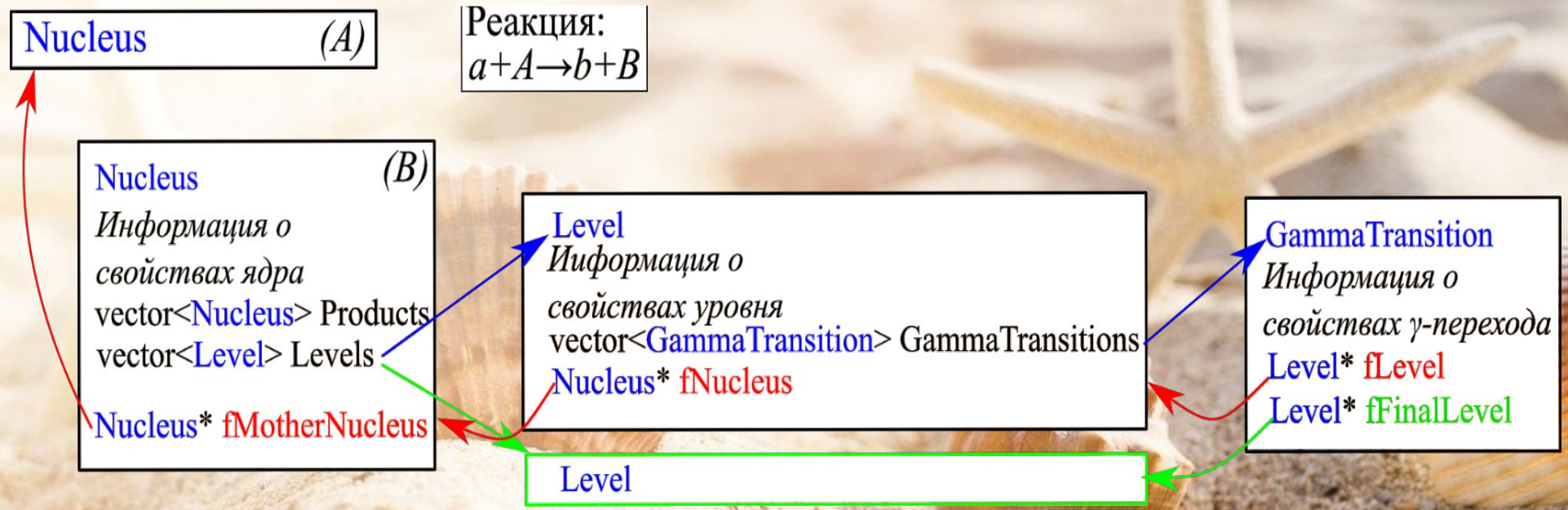

ECIS
Direct reaction:
* Spherical OM
* DWBA
* Rotational CC
* Vibrational CC
* Giant resonances
* Weak–coupling
Preequilibrium:
* Exciton model
– 2–component
* p–h LD phenom.
– surface effects
* Kalbach systematics
– angular distribution
– cluster emission
* γ –ray emission
Output:
*File 'output' defined by keywords
*Dedicated files with spectra, ...
Optical Model:
Local/ Global
Input:
Keywords
projectile n
element fe
mass 56
energy 14.
Nucl. Structure:
* Abundancies
* Discrete levels
* Deformations
* Masses
* Level density par.
* Resonance par.
* Fission barrier par.
* Thermal XS
* Microscopic LD
* Prescission shapes
Compound:
* Width fluctuations
– Moldauer
– GOE triple integr.
– HRTW
* Hauser–Feshbach
* Fission competition
– isotopic yields
* γ–ray emission
* GC+ Ignatyuk
Multiple emission:
* Exciton (any order)
* Hauser–Feshbach
* Fission competition
– isotopic yields
* γ –ray cascade
* All flux depleted
* Exclusive channels
* Recoils
ENDF:
* transport libs
* activation libs
Optional loops
* Incident energies
* Natural isotopes
RIPL-3 database

TalysLib

An object-oriented C++ library for nuclear data access

- TALYS is a powerful nuclear reaction calculation program which uses RIPL-3 database
- ROOT is a data analysis framework used by high energy physics and others
- TalysLib automates work with TALYS and its database
- TalysLib contains parser for ENDF and EXFOR (EXFORTABLES)

TalysLib structure



- The TalysLib structure groups data to related objects.
- Each object has a pointer to parent object.

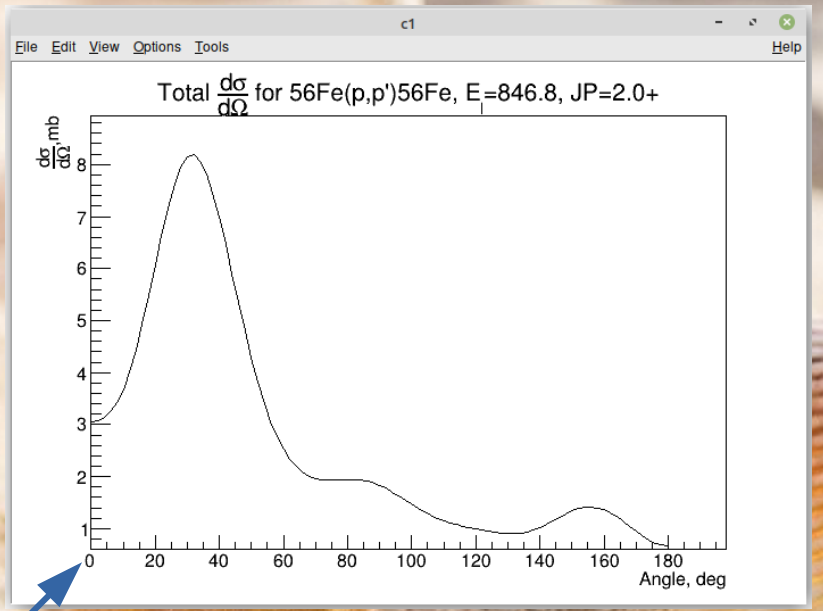
Usage examples

- Calculation of Q value for d(t,n)α reaction

```
user@jinr:~$ root -l
root [0] Nucleus d("2H"), t("3H"), n("n"), a("4He");
root [1] double Q=d.Mass+t.Mass-n.Mass-a.Mass
(double) 17.589895
root [2]
```

- Calculation and plotting 56Fe(p,p'$_1$) angular distribution

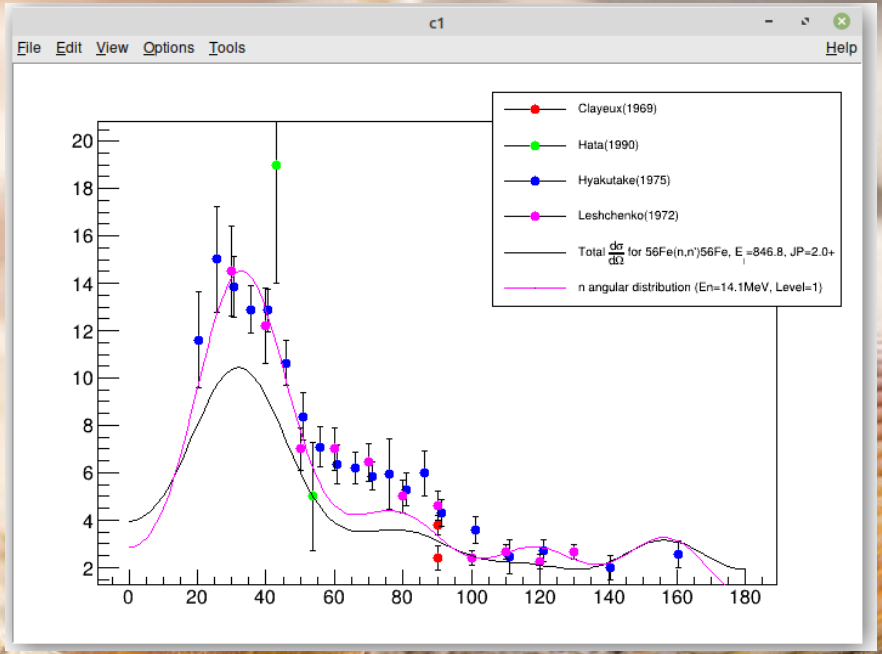
```
user@jinr:~$ root -l
root [0] Nucleus Fe("56Fe");
root [1] Fe.SetProjectileEnergy(20) //In MeV
root [2] Fe.GenerateProducts("p")
root [3] Fe.FindProductsByReaction("(p,p')")-
>Levels[1].GetAngularDistribution()->Draw("al")
```



Usage examples

- Calculation and plotting 56Fe(n,n'$_1$) angular distribution with ENDF and EXFOR

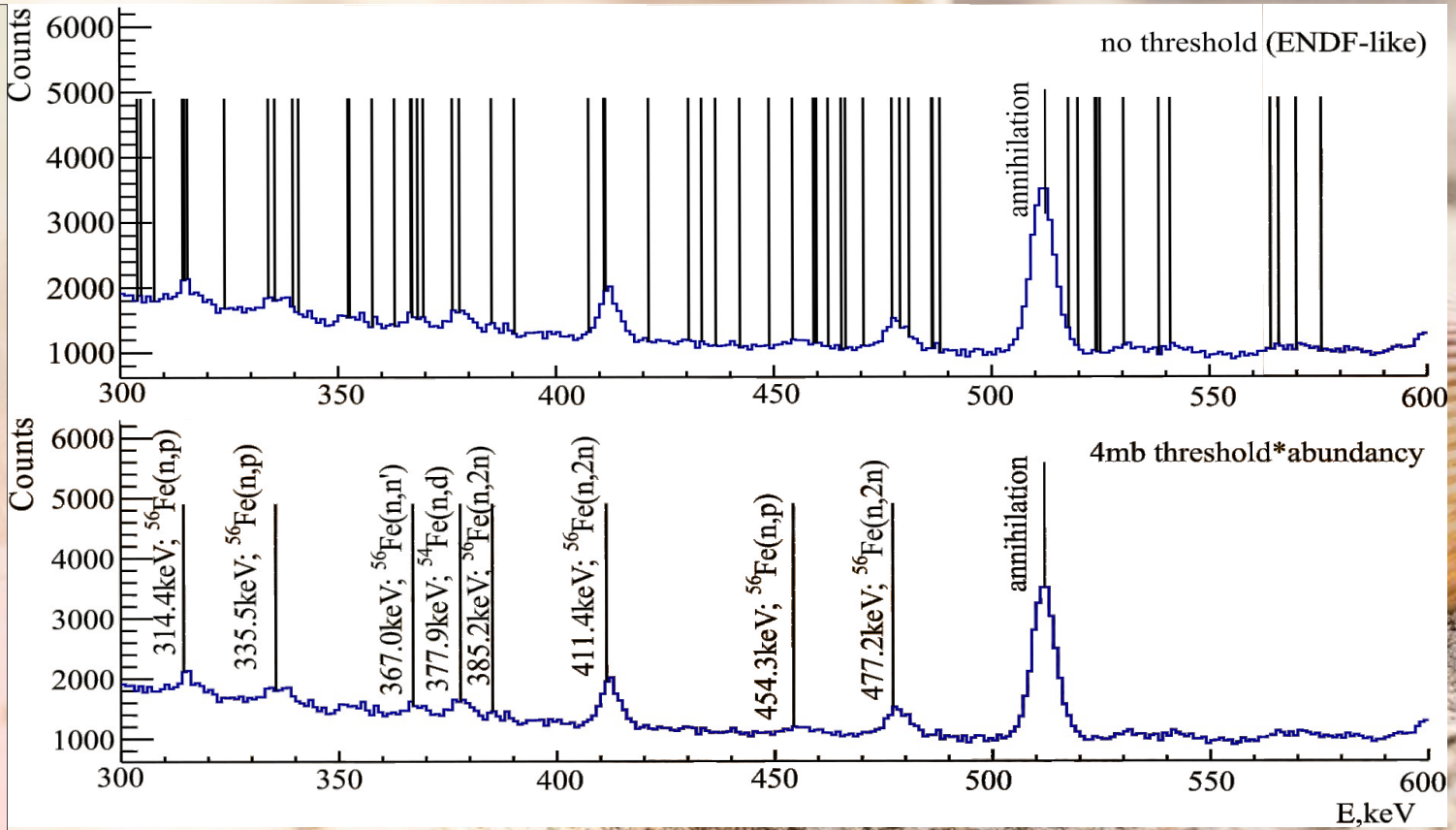
```
user@jinr:~$ root -l
root [0] Nucleus Fe("56Fe");
root [1] Fe.GenerateProducts()//14.1 MeV n by default
root [2] Nucleus* Fe2=Fe.FindProductByReaction("(n,n')")
root [3] g1=Fe2->Levels[1].
GetEXFORTMultiGraphForAngularDistributions(13,15)
//Find data in 13-15 MeV range
root [3]  g2=Fe2->Levels[1].GetAngularDistribution()
root [4] g3=Fe2→Levels[1].
GetAngularDistribution("ENDF")
root [5] g1->Add(g2,"l"); g1->Add(g3,"l");
g1->Draw("ap");
```



Usage examples

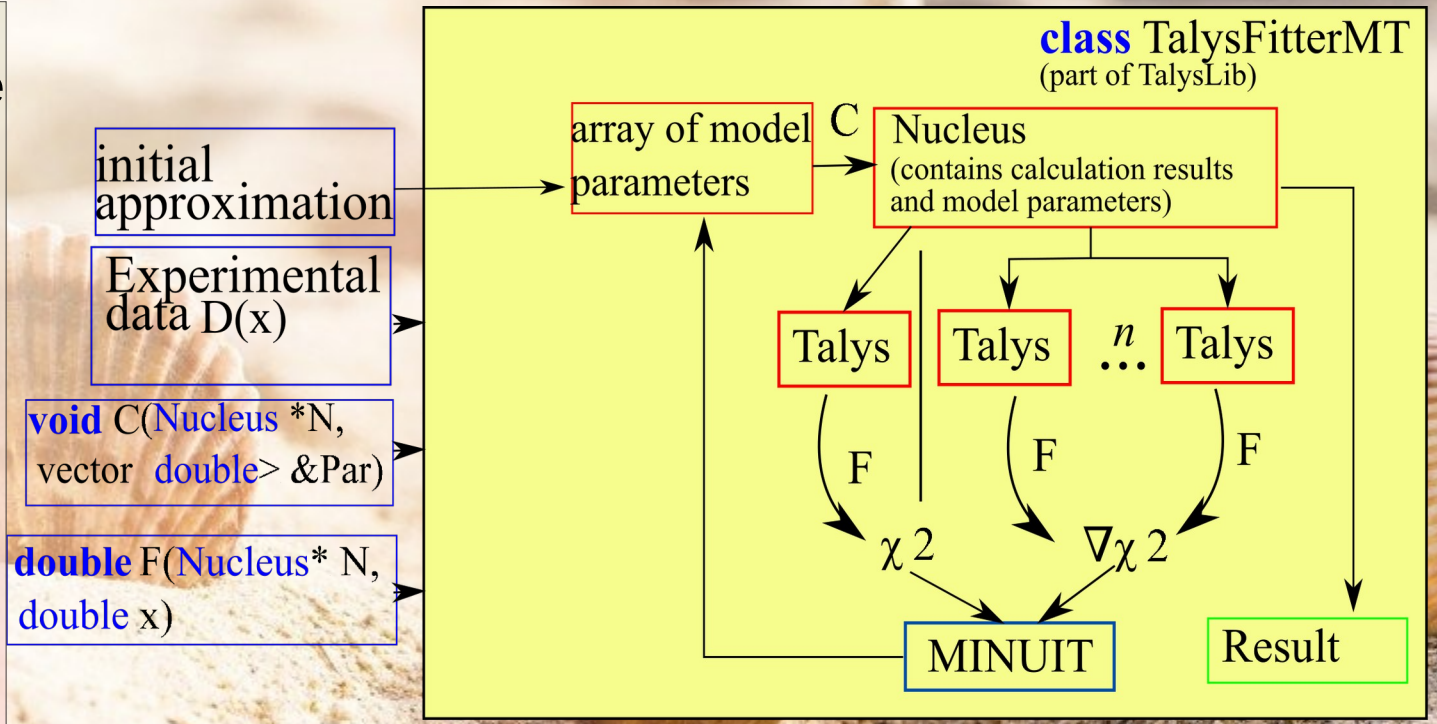
γ-spectrum decoding

- Decoding of the γ-spectrum is a very common task
- γ-transition data from ENDF often cannot be used directly
- Usage of the estimated cross-section data could be useful

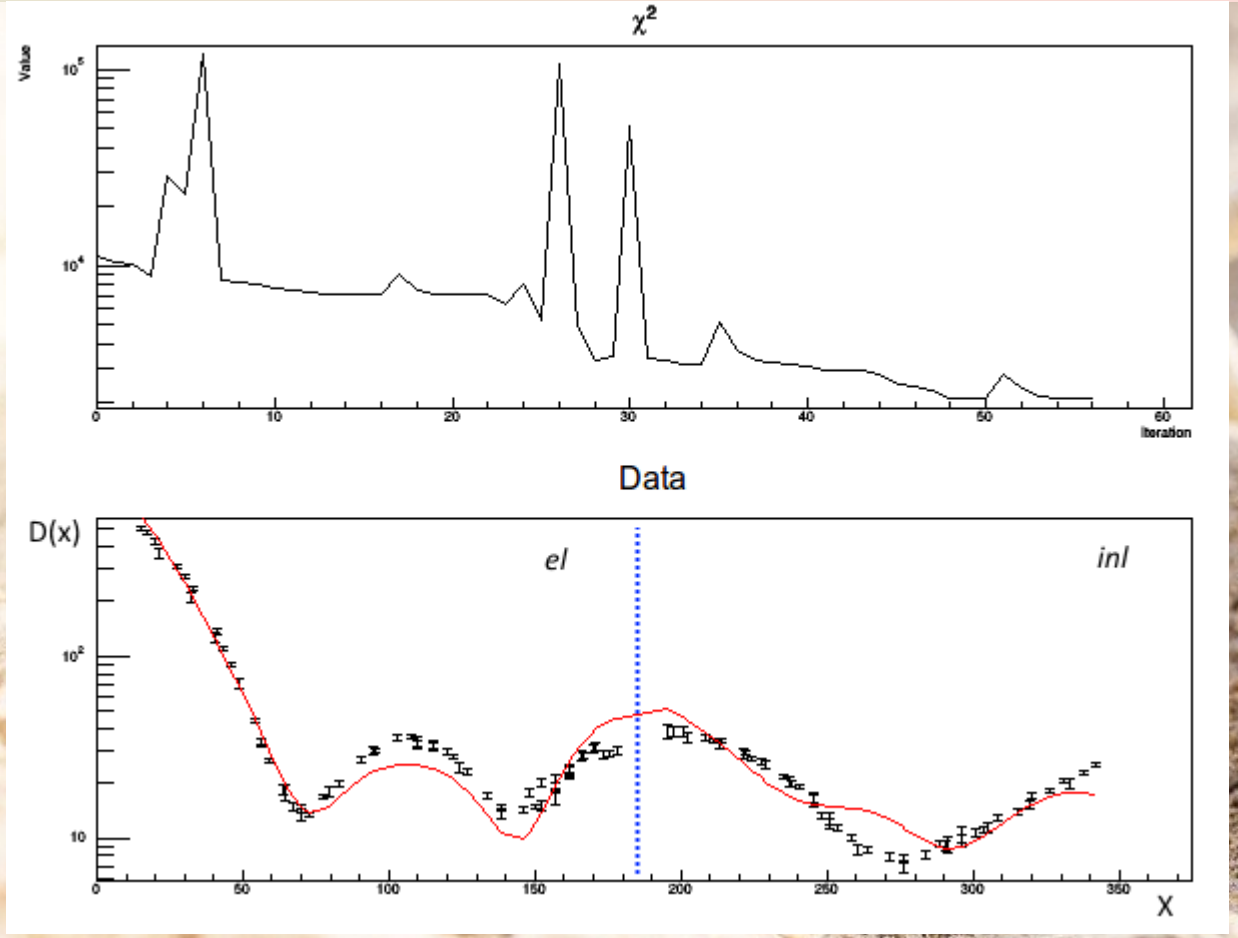


Model parameters adjustment

- The MINUIT package is used to minimize the χ^2
- The experimental data is presented as D(x) function
- Function C connects the model parameters and minimization parameters
- F returns calculation results in the same representation as D(x)

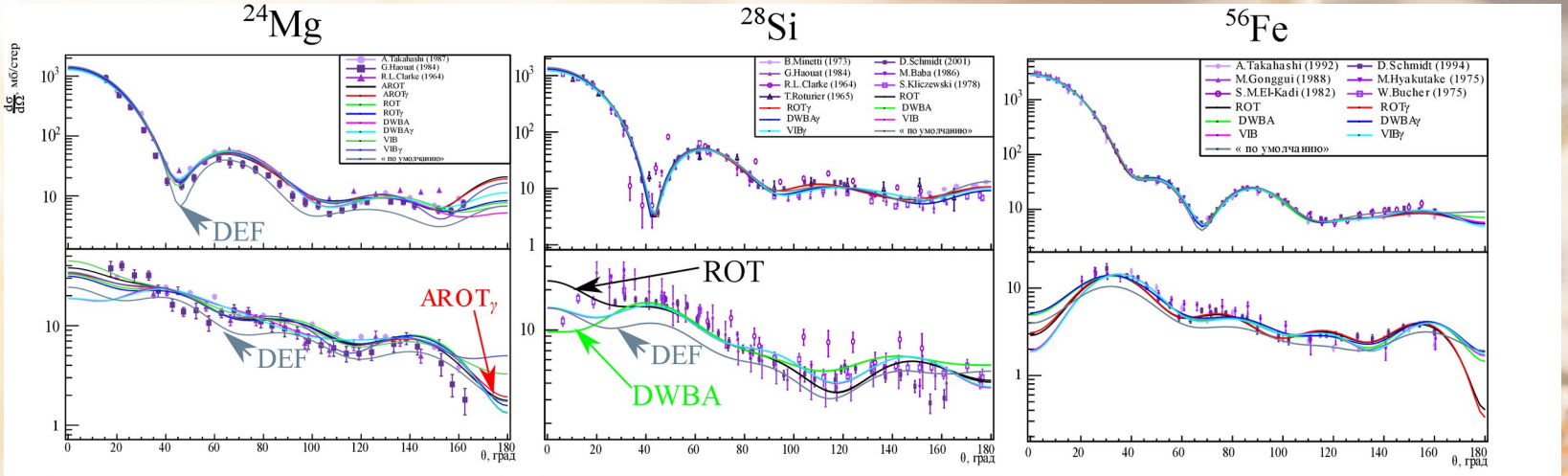


Model parameters adjustment



Usage examples

Optical model fit



	AROT	AROT$_\gamma$	DEF(AROT)
χ^2/N	8,37	8,35	26,51
χ^2_n/N	7,16	7,19	28,52
χ^2_γ/N	17,47	17,11	11,39

DWBA	DWBA$_\gamma$	ROT	DEF(ROT)
8,975	9,028	9,436	18,017
8,818	8,873	9,276	18,229
13,553	13,531	14,080	11,845

ROT	ROT$_\gamma$	VIB	VIB$_\gamma$	DEF(DWBA)
6,13	6,08	6,10	6,29	10,05
5,20	5,15	5,18	5,40	8,89
13,62	13,52	13,49	13,50	19,32

AROT – асимметричный ротатор
ROT – ротатор
DWBA – Борновское приближение искаженных волн
VIB – осциллятор
DEF(...) – параметры "по умолчанию"
Индекс γ показывает, что в выборку включены γ-выходы

$$\chi^2/N = \frac{1}{N}\sum_{i=1}^{N}\frac{(x_i^{exp}-x_i^{th})^2}{(\sigma_i^{exp})^2},$$

χ^2/N – отклонение для всей выборки
χ^2_n/N – для ***нейтронной*** части
χ^2_γ/N – для ***γ-выходов***

Conclusion

- There is a new *automated* way to get nuclear data
- There are a lot of bugs, but it works
- If somebody asks, we will add new features

  https://github.com/terawatt93/TalysLib