New developments in TalysLib library

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CONTENTS OF THIS TALK

1. TALYS and TalysLib
2. Sources of experimental and evaluated nuclear data
3. Implementation of the nuclear data access in TalysLib
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TALYS: how it works

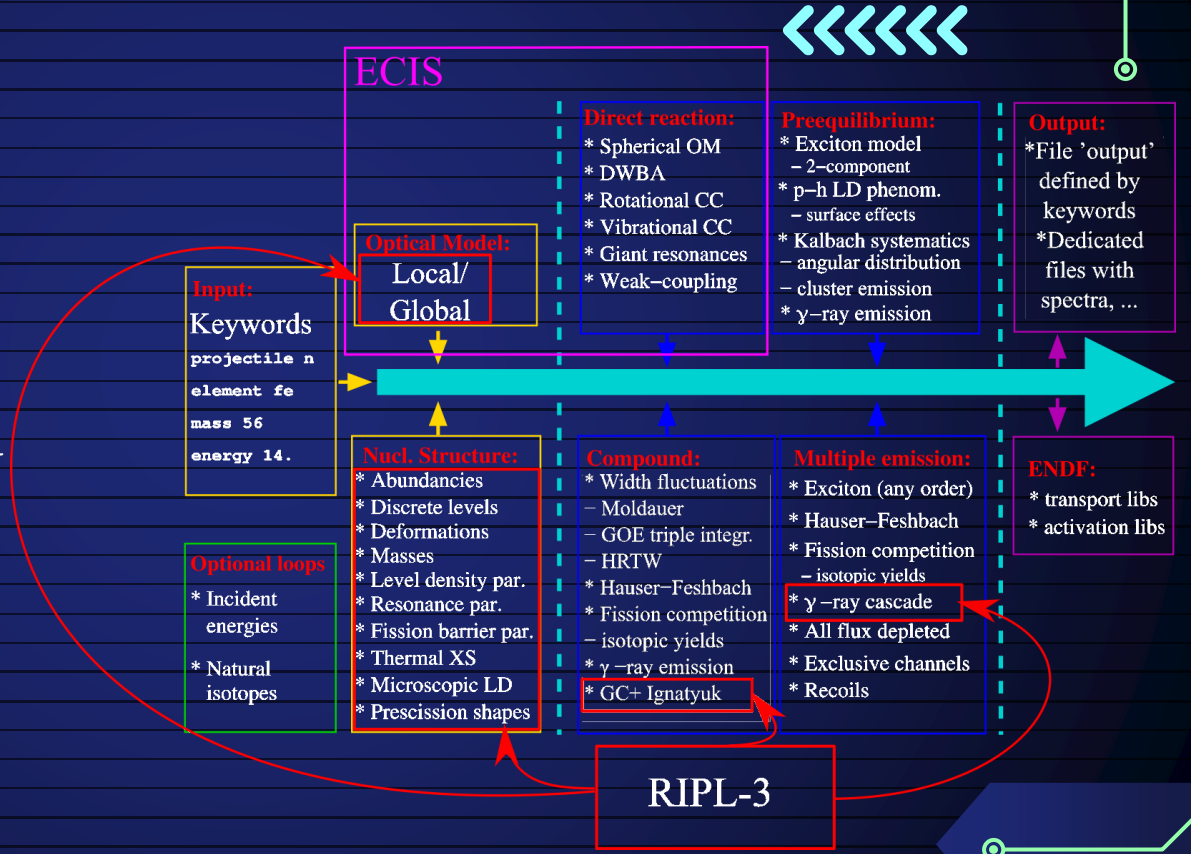
Features:

+ Easy in use
+ Includes large number of theoretical models
+ Application of RIPL-3 library with nuclear structure data, sets of model parameters and nuclear masses
  - It is outdated (2007)
+ Usage of ECIS code for Optical model and coupled channel calculation
+ TALYS is a kind of very progressive interface to ECIS (it is included as subroutine in TALYS)
  - Data transfer using txt files

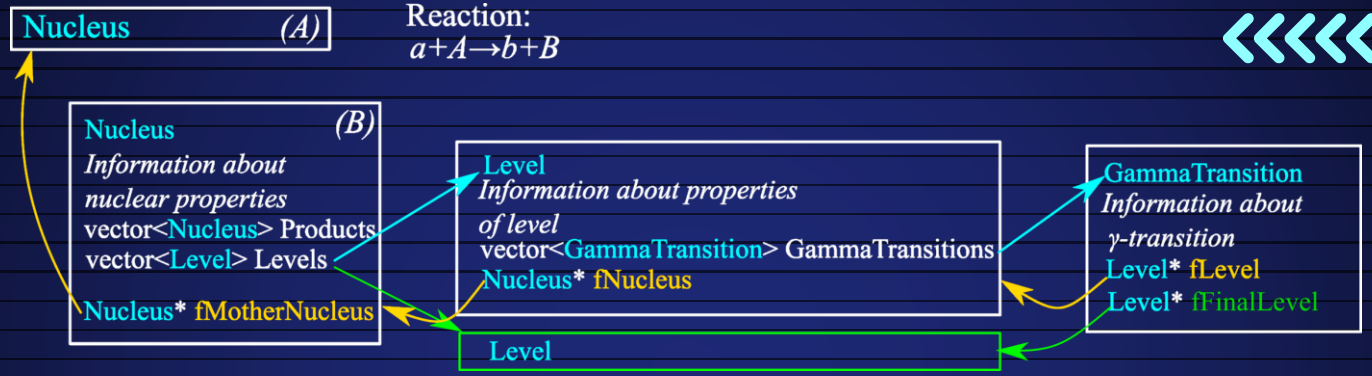
? Fortran77 and Fortan90 language

+ Well documented

- Except ECIS



TalysLib: C++/Python interface to TALYS



We have developed TalysLib for:

- Usage of the RIPL-3 data and TALYS calculation results in the data processing software for TANGRA project:
- γ-spectra interpretation
- Q-value calculations
- Nuclear data processing: search, drawing, transfer to other software using ROOT capabilities
- Model parameters adjustment using MINUIT package (see G.V. Pampushik et al., Online poster session #3 for details)

Sources of experimental and evaluated data: EXFOR, ENDF

EXFOR (Exchange FORmat):

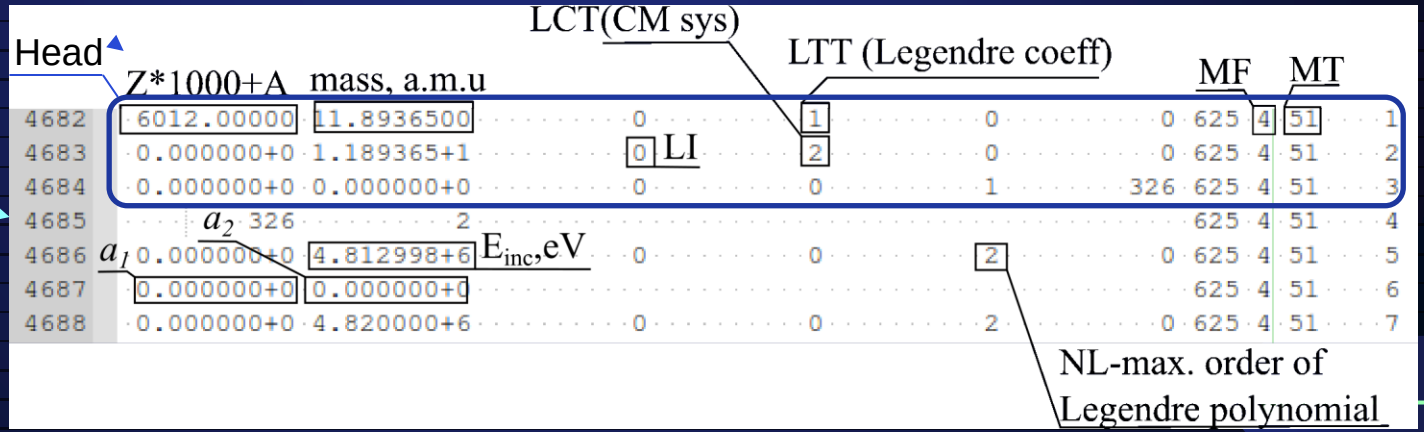
- EXFOR is the library and format for the collection, storage, exchange and retrieval of experimental nuclear reaction data
- The most complete and well-known base of nuclear experiments
- Data format was developed in 1960s and adopted for punch-cards
    - Hard to read with modern programming languages
    - Variable format: same type data could be written differently
    - Files more “human-readable” than “machine-readable”

ENDF (Evaluated Nuclear Data Format):

- Results of nuclear data compilation and evaluation using theoretical models
- Similar problem: outdated data format
- Useful system of MT and MF codes that identify outgoing channel of reaction and data type

ENDF format: main principles

- ENDF file consist evaluations for a number of reaction channels for particular nuclide/material and projectile
- File is splitted to data blocks with particular values of **MT** and **MF** indexes: **MT** determines the outgoing channel, **MF**-type of data. I.e. MT=51 and MF=4 corresponds to $d\sigma/d\Omega$ for a process with emission of 1 neutron and residual nucleus in 1-st excited state
- Standard dimensions are used: barns, barns/steradian, eV, etc.
- Several forms of data representation: tables, Legendre coefficients, probability density. Could be extracted from the head of data block



Interface to ENDF

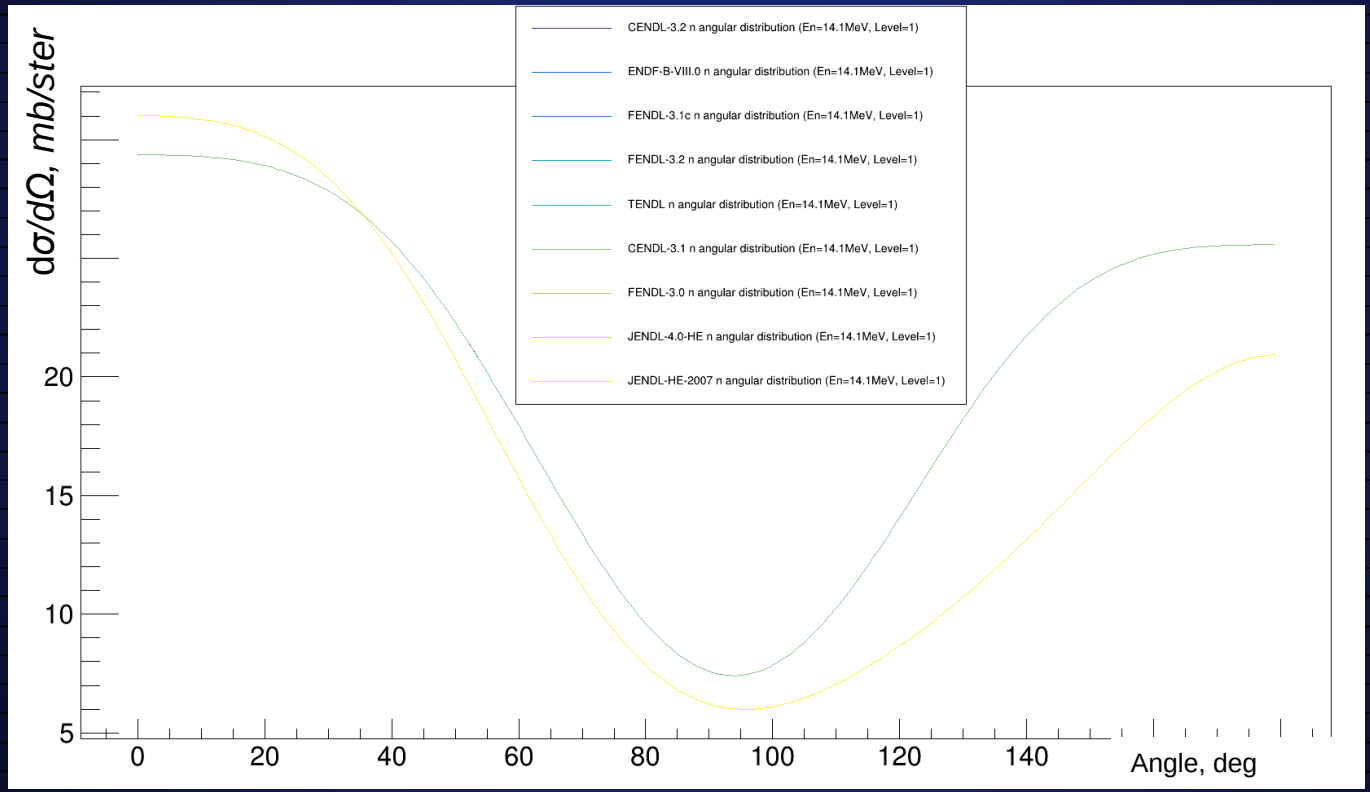
- ENDF format is well documented
- Interface to ENDF is **partially** implemented in TalysLib **(cross-sections and angular distributions with linear interpolation)**. ENDF data could be used from local or remote storage

Example of data extraction for $^{12}C(n,n'_1)$ angular distribution:

```
root [1] Nucleus C("12C");
root [2] C.SetProjectileEnergy(14.1);
root [3] C.GenerateProducts("n");
root [4] Level *l=&(C.FindProductByReaction("(n,n')")->Levels[1])
root [5] TMultiGraph* mg=l->GetTMultiGraphForAngularDistributions
("all evaluated");
```

Interface to ENDF

Result of execution:



EXFOR: Alternatives

C4 (Computational format):

- EXFOR data converted to tabulated format using **x4toc4** program
- Standard dimensions are used: barns, barns/steradian, eV, etc.
- MT and MF indexes (not well realized)
- **Information about residual excitation energy is available**

EXFORTABLES (Evaluated Nuclear Data Format):

- Directory-structured database with experimental nuclear reaction data, generated from EXFOR
- Useful system of MT and MF codes that identify outgoing channel of reaction and data type
- No information about **residual excitation energy**

EXFOR_JSON(Evaluated Nuclear Data Format):

- EXFOR entries converted to JSON
- Problem with parsing is solved. **With interpretation is not**.

C4: Format

```
#ENTRY      20559
#AUTHOR1    G.Haouat+
#YEAR       1975
#INSTITUTE  (2FR BRC)
#TITLE      Differential cross sections for carbon neutron
#+          elastic and inelastic scattering from 8.0 to 14.5 MeV
#AUTHOR(S)  G.Haouat, J.Lachkar, J.Sigaud,
#+          Y.Patin, F.Cocu
#REF-CODE   (R,CEA-R-4641,197502)
#REFERENCE  Rept. Centre d`Etudes Nucleaires, Saclay Reports
#+          No.4641, 1975
#DATASETS   3
#
#DATASET    20559008
#DATE       20120704
#REACTION   6-C-12(N,INL)6-C-12,PAR,SIG
#PROJ       1
#TARG       6012
#MF         3
#MT         51
#PRODUCT    6-C-12
#DATA-HDR   DATA
#C4BEGIN    [    1  6012   3  51 C ]
#X4STATUS   [COREL] Data correlated with another data set
#DATA       9
# Prj Targ M MF MT PXC  Energy  dEnergy  Data      dData   Cos/LO   dCos/LO   ELV/HL  dELV/HL I78 Refer (YY)              EntrySubP
#---><----><-><--><--><-------><-------><-------><-------><-------><-------><-------><-------><-><----------------------><---><->
    1  6012   3  51 C  5800000. 200000.0 9.5000-3 0.010000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  6300000. 120000.0 0.186000 0.019000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  6800000. 110000.0 0.133000 0.013000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  7000000. 100000.0 0.177000 0.018000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  7300000. 100000.0 0.206000 0.020000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  7800000. 150000.0 0.302000 0.030000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  8000000. 100000.0 0.383000 0.038000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  8300000. 100000.0 0.200000 0.020000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
    1  6012   3  51 C  8800000. 100000.0 0.309000 0.031000                    4439000.         LVLG.Haouat,ET.AL. (75)     20559  8
#/DATA      9
```

- MT=51 for all channels with one outgoing neutron. This problem could be solved using ELV/HL data (residual excitation energy)

EXFORTABLES

- Problem with identification of data for different excited states: all content of EXFOR subentry attributed to one excited state
- Reason: variety of same data representation in EXFOR
- Cannot be fixed because of absence of excitation energy data

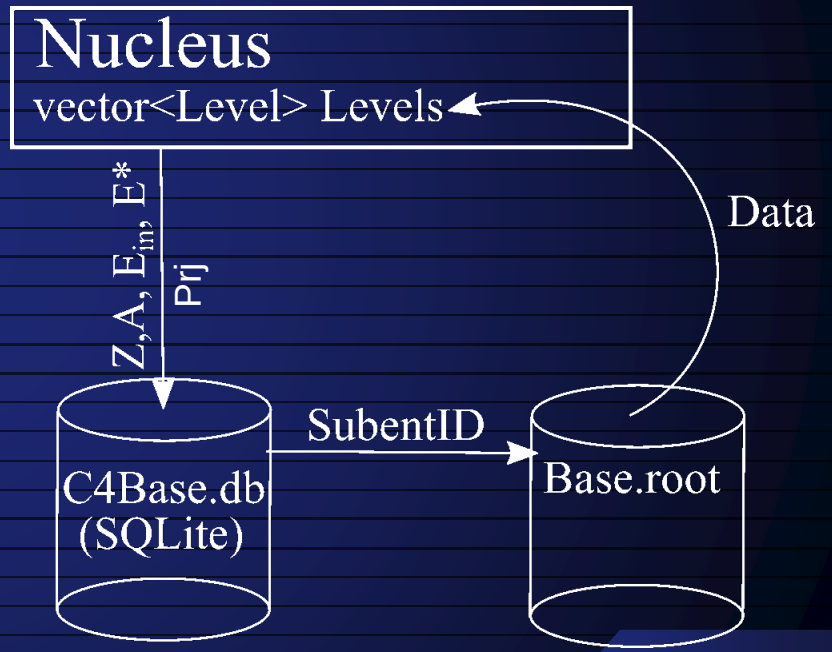
```
# Target Z    :   6
# Target A    :  12
# Target state:
# Projectile  : n
# Reaction    : Inelastic scattering
# E-inc       :   14.760 MeV
# E-exc       : 10.84400 MeV (EXFOR: 10.80000)
# Quantity    : Angular distribution
# Frame       : C
# MF          :    4
# MT          :   55
# X4 ID       : 20223003
# X4 code     : 6-C-12(N,INL)6-C-12,PAR,DA
# Author      : Kuijper
# Year        : 1972
# Data points :     19
#  Angle(deg)    xs(mb/sr)   dxs(mb/sr)  dAngle(deg)
  4.04000E+01  1.50000E+00  8.00000E-01 MT=55
  6.99001E+01  7.50000E+00  1.70000E+00
  6.43001E+01  6.80000E+00  1.40000E+00
  6.00001E+01  6.50000E+00  8.00000E-01
  4.89001E+01  7.80000E+00  1.40000E+00
  3.99000E+01  8.60000E+00  1.30000E+00
  2.63001E+01  6.30000E+00  1.90000E+00
  6.85001E+01  1.10000E+00  4.00000E-01
  6.30001E+01  4.00000E-01  5.00000E-01
  5.88001E+01  1.30000E+00  5.00000E-01
  4.79000E+01  1.30000E+00  4.00000E-01
  3.91000E+01  1.40000E+00  4.00000E-01
  2.58000E+01  4.00000E+00  1.50000E+00
```

MT=53
E=9.6 MeV

MT=52
E=7.6 MeV

Implementation of experimental data access in TalysLib

- Methods for work both with EXFORTABLES and C4 are implemented.
- Due to unfixable issues in EXFORTABLES usage of C4 is more prospective
- C4 files are quite long and their processing is time consuming → we converted them into C4Entry objects and stored in .root file for further access by SubentID
- All files were parsed to extract projectile energies Ein, excitation energies E*, data types MF, reaction codes MT and a corresponding SQLite database was built for data search



Implementation of experimental data access in TalysLib

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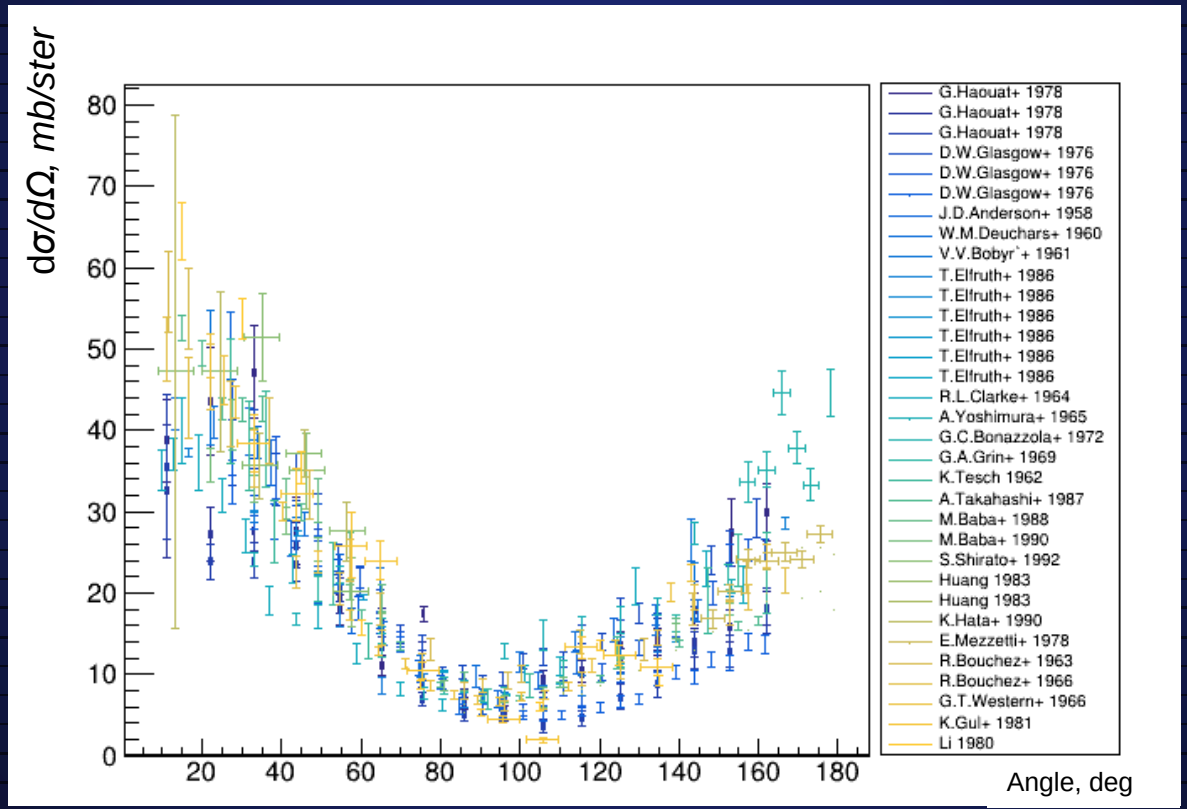
root [4] Level *l=&(C.FindProductByReaction("(n,n')")->Levels[1])
root [5] TMultiGraph* mg=l->
GetEXFORTMultiGraphForAngularDistributions(13,15)
```

Implementation of experimental data access in TalysLib



TODO

- Documentation
- Implementation of ENDF interpolation schemes
- More data types (i.e. resonance parameters)
- Some important (for us) data is absent in C4. Parsing of raw EXFOR data cannot be completely avoided
- Fix of C4 data: sometimes relative errors interpreted incorrectly
- Actualization of references to source publications: DOI is presented not for all papers in database.
- Web interface development

Conclusion

- Methods for work with nuclear data were implemented in TalysLib. They are more or less working
- Available tabulated interpretations of EXFOR were analyzed, it was established that C4 format is most useful for automatic processing nowadays
- There a lot of work should be done in future to make TalysLib more useful and comfortable for users. But now it significantly simplify work with nuclear data in TANGRA project.
- Community support will be very welcome

References:

- TalysLib: https://github.com/terawatt93/TalysLib
- TALYS: https://www-nds.iaea.org/talys/
- C4: Included in EMPIRE package (EMPIRE-3.2.3/EXFOR). Could be found at https://www-nds.iaea.org/cdroms/
- EXFORTABLES: https://www-nds.iaea.org/talys/codes/exfortables.tar
- ROOT: https://root.cern.ch/

Analogues:

- PyNE: https://pyne.io/
- EMPIRE

Thank you!