LA-UR-21-22254

DeCE

the ENDF-6 data interface and nuclear data evaluation assist code

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NNSA

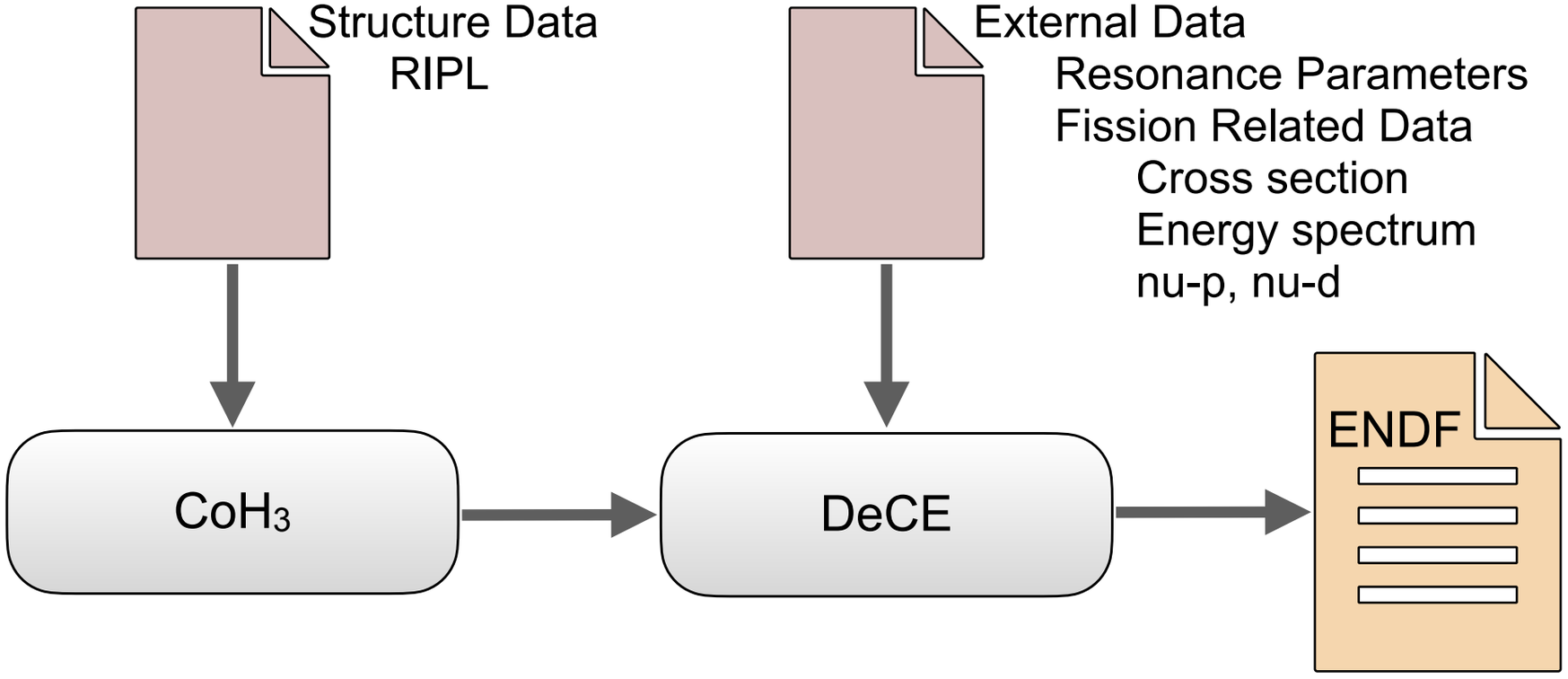
Introduction

Statistical Hauser-Feshbach codes play a central role in producing evaluated nuclear data files

- They provide a complete set of cross sections, energy and angular distributions, including regions where no experimental data are available

Always external data are involved

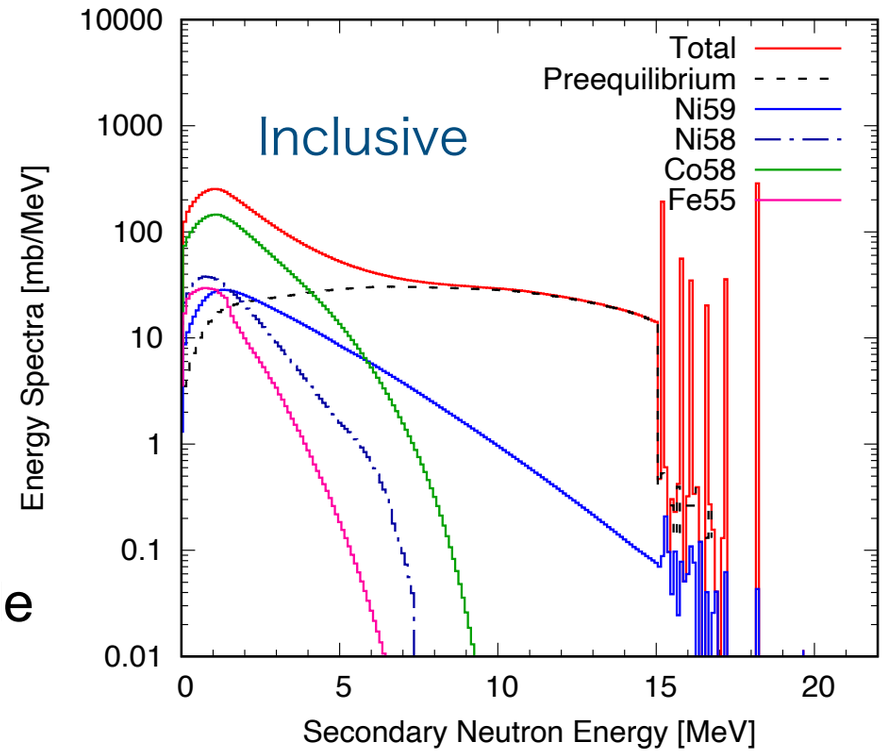
- Model parameter and nuclear structure inputs
- Data evaluated independently

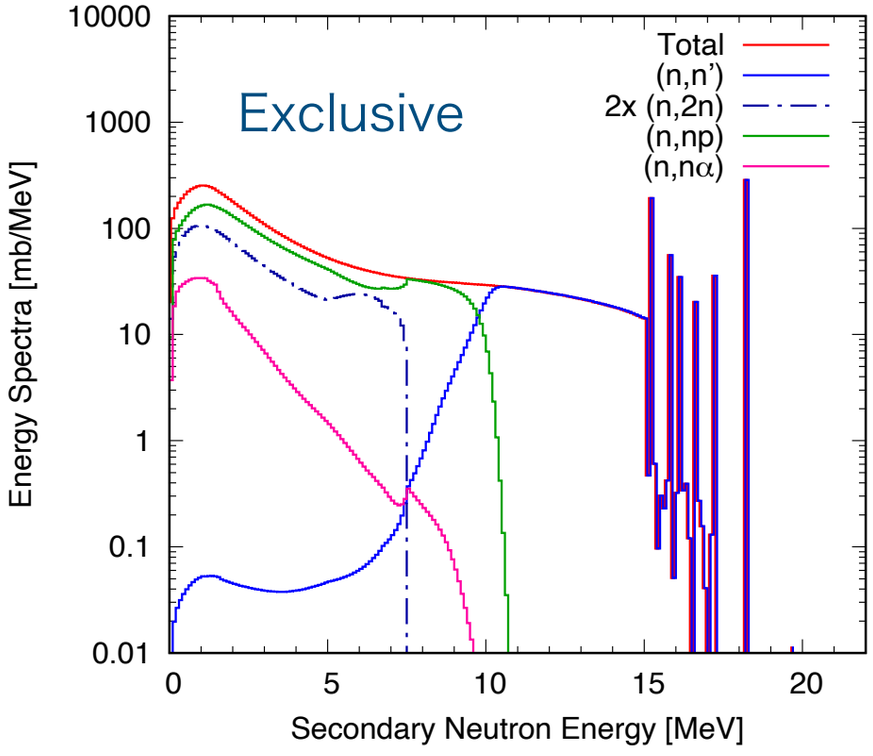


Technical Issues for Making ENDF from HF Codes

Model code outputs, e.g. by the Hauser-Feshbach theory, often need to be reorganized to follow the ENDF-6 protocol

- Exclusive or inclusive reaction representation
  - In the multiple particle emission case, theoretical calculations provide inclusive particle spectra, while ENDF requires exclusive spectra
    - This requires some complicated procedure inside the model codes
  - ENDF often mixes two representations
    - Exclusive below 20 MeV, and inclusive above
- Limited number of discrete levels
  - Cross sections to some levels may need to merge with the continuum
- Boundary between resonance and HF calculated regions
  - The averaged cross section in the resonance region agree with the HF calculation near the boundary





CoH_3: Coupled-Channels Hauser-Feshbach Code

CoH_3 Overview

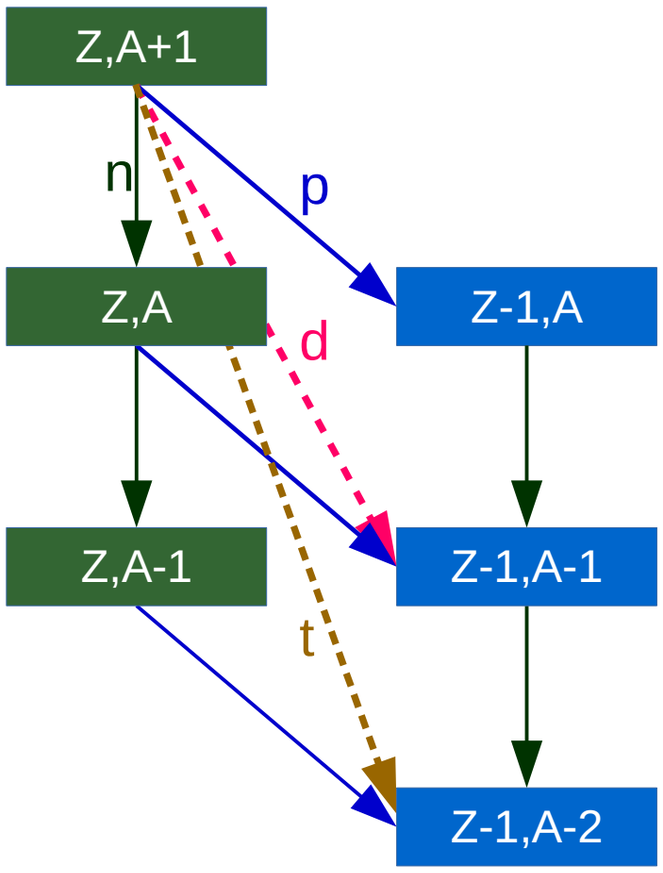
- 45,000 lines C++ code
- Internal optical model / coupled-channels solver
- Compound nucleus decay by deterministic or Monte Carlo

Modules and Models

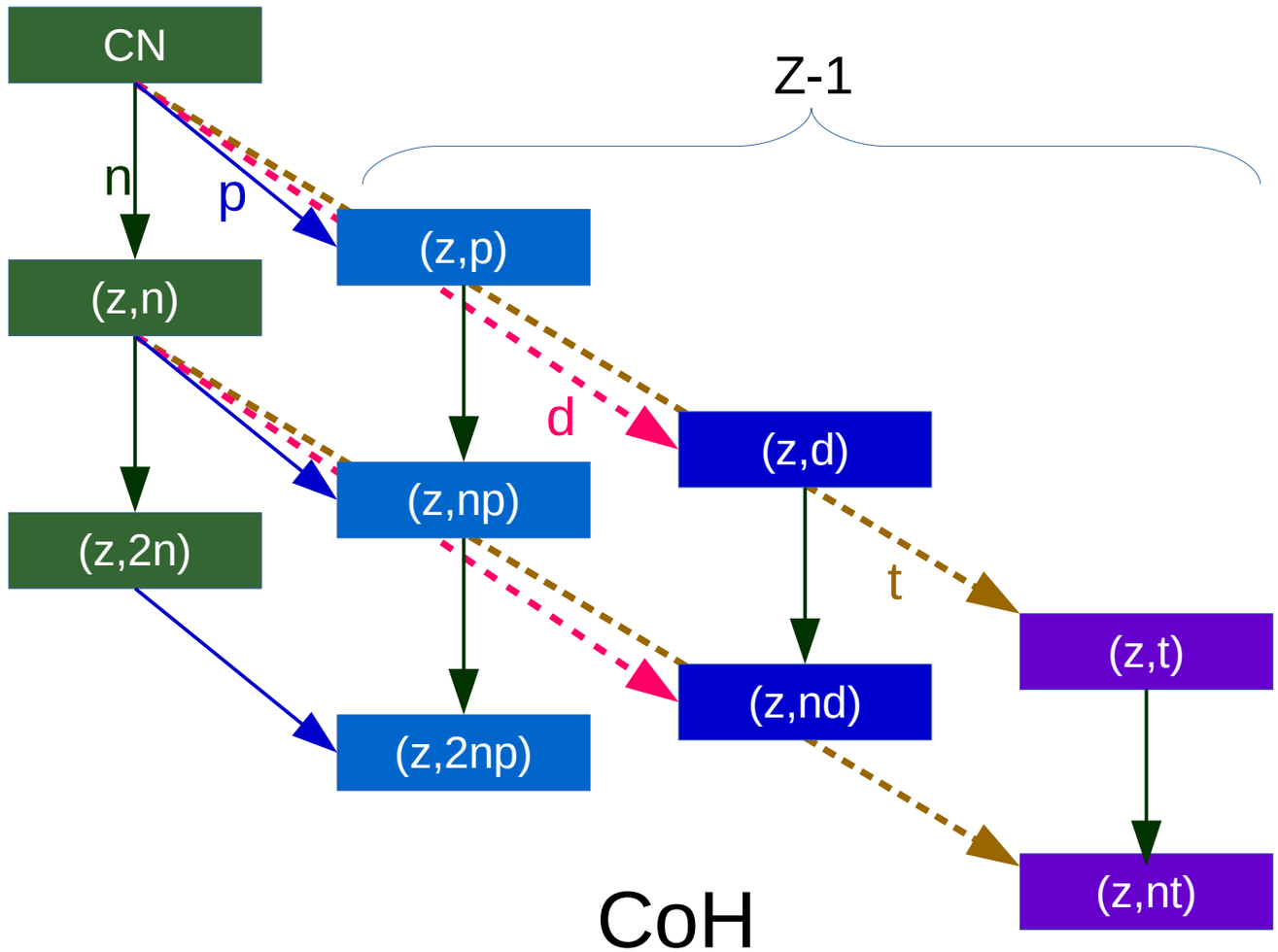
- Optical model
  - spherical and deformed (rotational or vibrational model)
  - DWBA for direct inelastic scattering
- Compound Reaction
  - Moldauer's width fluctuation correction with realistic GOE parameters [NDS 118, 183 (2014)]
  - Engelbrecht-Weidenmueller transformation with direct channels [PRC 94, 014612 (2016)]
  - Gilbert-Cameron level density [JNST 43, 1 (2006)]
  - Gamma-ray strength function
- Pre-Equilibrium Reaction
  - 2-component exciton model, (or FKK MSD/MSC still external code)
- Prompt Fission Neutron Spectrum
  - Advanced Madland-Nix model including pre-fission neutrons
- Direct/Semidirect Capture [PRC 75, 054618 (2007)]
  - Mean-Field Models (FRDM and Hartree-Fock-BCS) [EPJ 146, 12004 (2017)]

Multi-Particle Emission and Exclusive Cross Section

Nucleus object created for all the residual nuclei



General



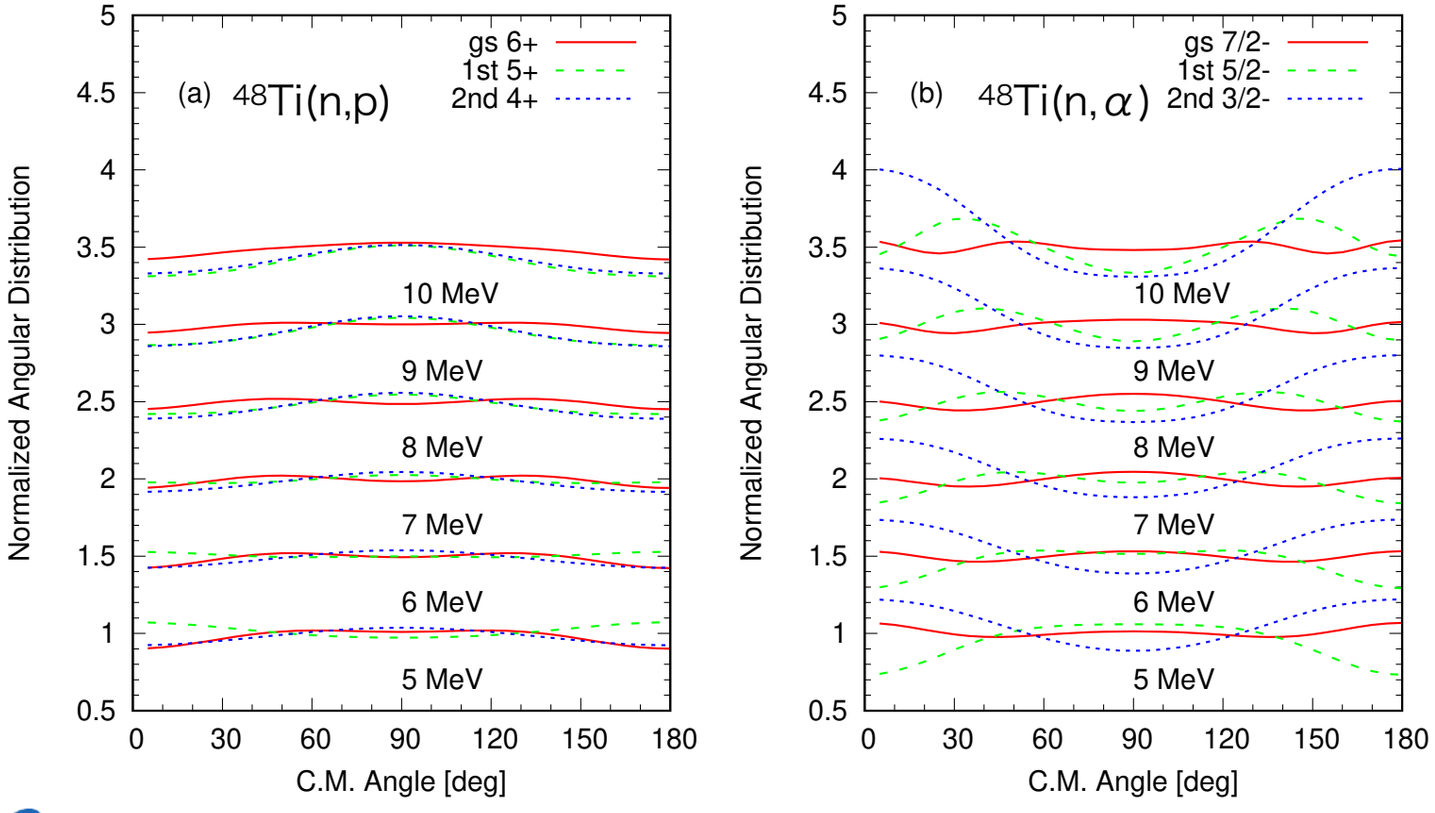
CoH

Nucleus objects for (n,d) and (n,np) channels are different
The current versioin of CoH_3 is slow at high energies, because a large number of CN object emerge

Level productions by Charged Particles

Two ways to store charged particle cross sections in ENDF

- MT 103 - 107 for (n,p), (n,d), etc
  - Level populations not given, discrete gamma-rays stored in MF6
  - Double-differential angular distribution only
- MT 600 - 849 for (n,p_0), (n,p_1), … (n,α_{cont})
  - Level populations given, discrete gamma-rays are in MF12 and 14
  - Angular distribution given in MF6 (or MF4)



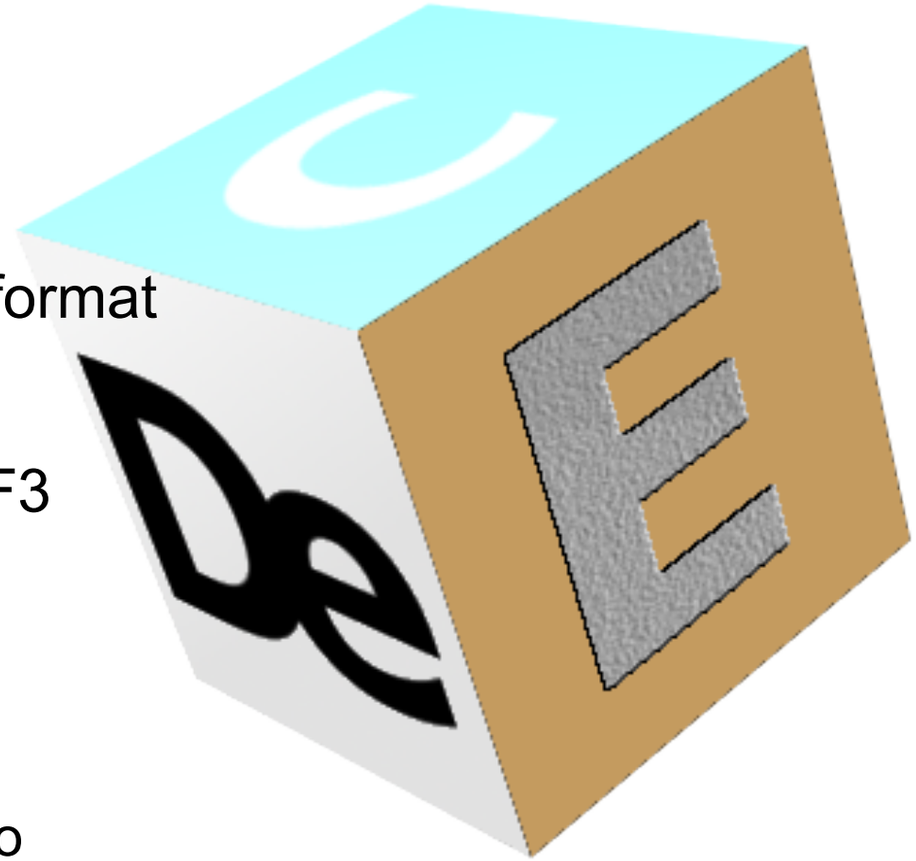
- CoH_3 produces both the data
  - However, users need to tell which option is used prior to calculate energy spectra

HI Kim et al., NIM A **963**, 163699 (2020)

DeCE: ENDF-6 Formatted File Manipulation Code

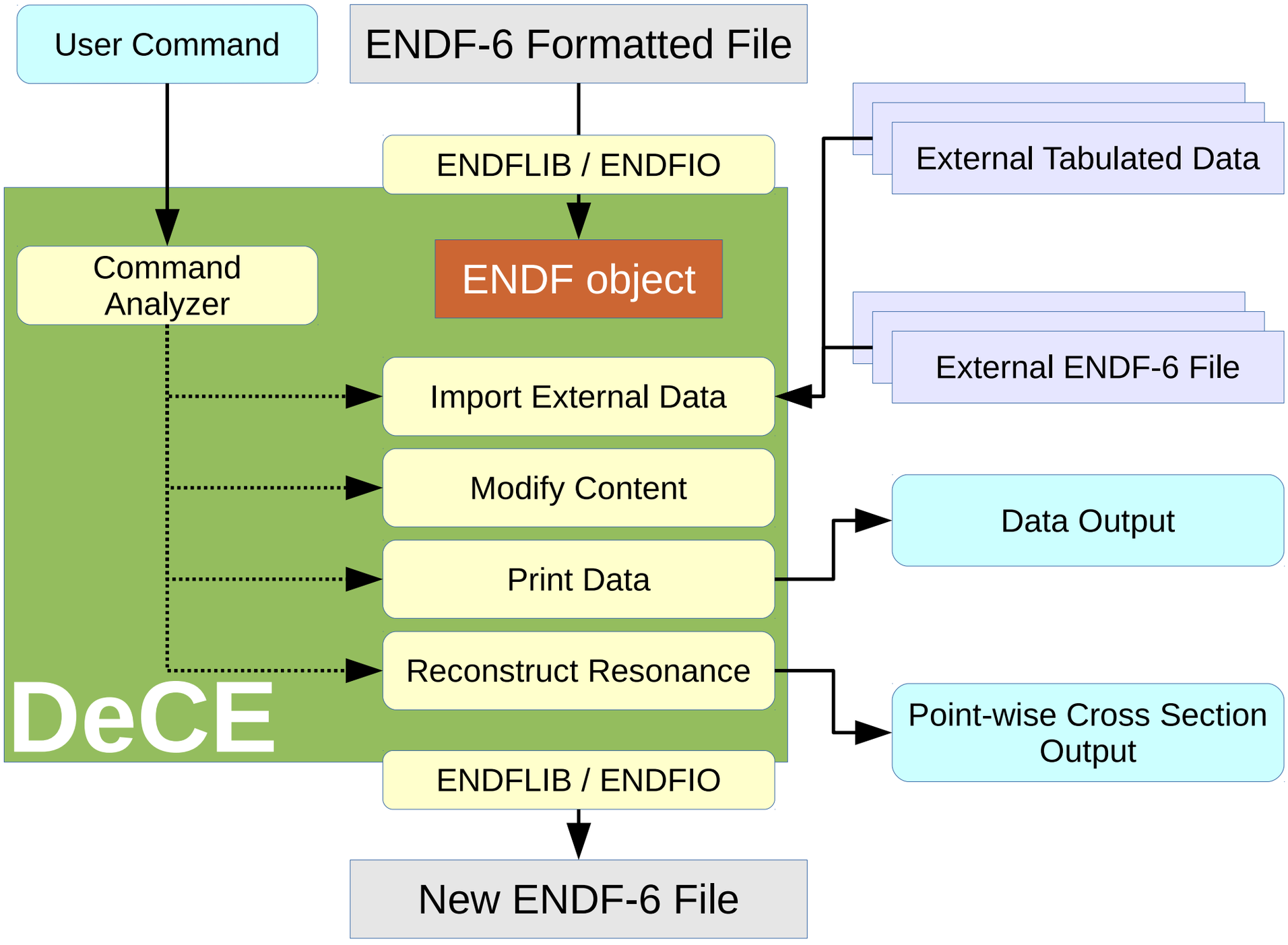
Open source software to assist nuclear data production

- Similar functionality to CRECTJ6
- C++ code to edit ENDF files interactively
  - 25,700 lines
  - class libraries, ENDFLIB and ENDFIO
- Convert ENDF files into human readable X-Y table format
- Read another library or data and merge
- Delete/add/subtract/re-scale each sub-section in MF3
- Automatic generation of index (dictionary)
- Reconstruction of point-wise cross sections from resonance parameters (capability limited)
  - produce angular distributions from resonances too
- Some small utility codes (tools) available



https://github.com/toshihikokawano/DeCE

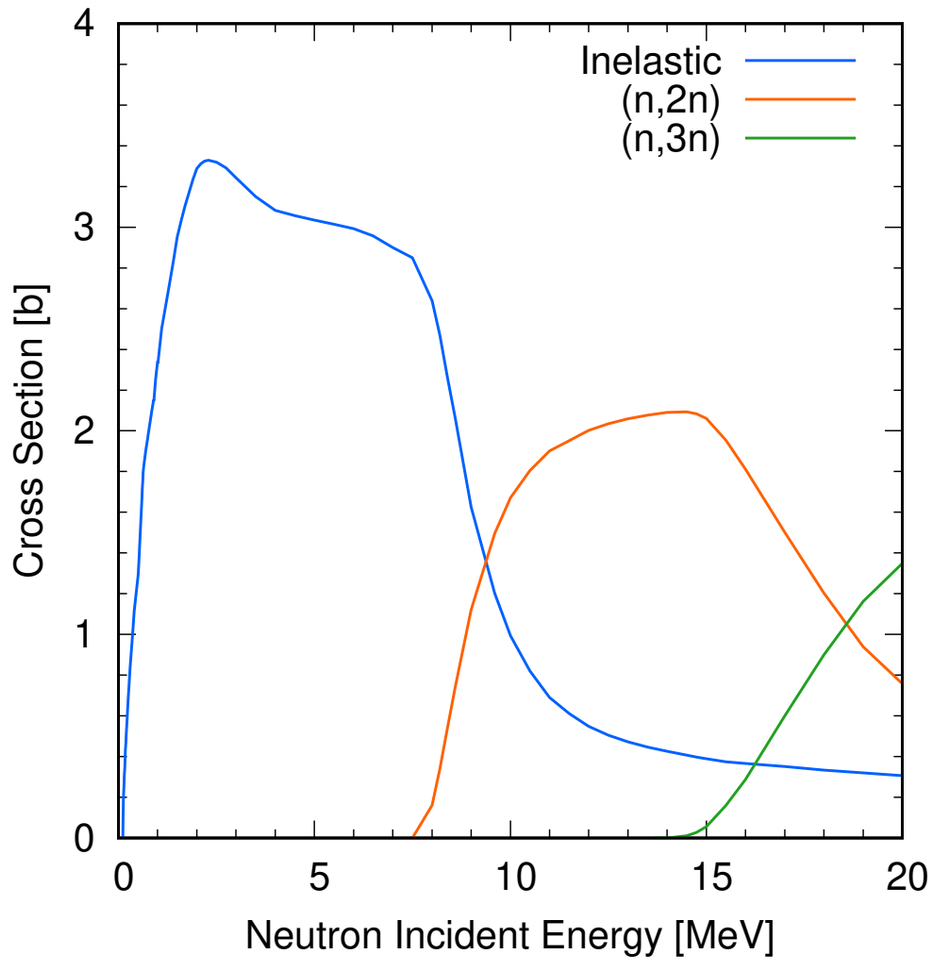
DeCE Package, Main Code and Class Libraries



DeCE Showcase (I) Data Extraction

Command Line Mode

```
% dece -f3 -t4 W184.dat
#    [ 7437 :  3 :   4 ]    74 - 184
# Cross section
#           QM 0.0000000e+00  mass difference Q-value
#           QI -1.112100e+05  reaction Q-value
#           NR             1  number of interpolation range
#           NP            98  lin-lin  interpolation
  1.118200e+05  0.000000e+00
  1.200000e+05  1.180380e-01
  ...
```



Interactive Mode

```
% dece W184.dat
extract 3 4
 7.418400+4 1.823710+2          0          0          0          07437 3   4
 0.000000+0-1.112100+5          0          0          1         987437 3   4
         98          2                                           7437 3   4
 1.118200+5 0.000000+0 1.200000+5 1.180380-1 1.300000+5 1.979930-17437 3   4
 1.400000+5 2.537980-1 1.500000+5         -1 1.600000+5 3.460470-17437 3   4
  ...
```

DeCE Showcase (II) Fixing Header and DICT information

```
                                                                   0 0  0    0
 2.805900+4 5.842807+1          1          0          0          02828 1451    1
 0.000000+0 0.000000+0          0          0          0          62828 1451    2
 1.000000+0 2.000000+7          1          0         10          72828 1451    3
 0.000000+0 0.000000+0          0          0         50          02828 1451    4
 28-Ni- 59 LANL       EVAL-Oct12 T.Kawano,A.Kahler                2828 1451    5
                      DIST-      REV1-                 20121031   2828 1451    6
----ENDF/B-VII.1      MATERIAL 2828         REVISION 1            2828 1451    7
-----INCIDENT NEUTRON DATA                                       2828 1451    8
------ENDF-6 FORMAT                                             2828 1451    9
                                                                 2828 1451   10
**************************************************************** 2828 1451   11
 Test for DeCE
                                    T. Kawano (LANL)
       Text Added                   Nov. 2012

                                                                 2828 1451   53
****************************************  No Dictionary      *** 2828 1451   54
                                                                 2828 1  099999
```

```
                                                                   0 0  0    0
 2.805900+4 5.842807+1          1          0                      28 1451    1
 0.000000+0 0.000000+0          0          0                      28 1451    2
 1.000000+0 2.000000+7          1          0         10           72828 1451    3
 0.000000+0 0.000000+0          0          0         13      186  2828 1451    4
 28-Ni- 59 LANL       EVAL-Oct12 T.Kawano,A.Kahler                2828 1451    5
                      DIST-      REV1-                 20121031   2828 1451    6
----ENDF/B-VII.1      MATERIAL 2828         REVISION 1            2828 1451    7
-----INCIDENT NEUTRON DATA                                       2828 1451    8
------ENDF-6 FORMAT                                             2828 1451    9
                                                                 2828 1451   10
**************************************************************** 2828 1451   11
 Test for DeCE                                                   2828 1451   12
                                    T. Kawano (LANL)             2828 1451   13
                                    Nov. 2012                    2828 1451   14
                                                                 2828 1451   15
                                                                 2828 1451   16
**************************************************************** 2828 1451   17
    1        451        203                                      02828 1451   18
    2        151        103                                      02828 1451   19
    3          1        269                                      02828 1451   20
    3          1         32                                      02828 1451   21
    3          4         39                                      02828 1451   22
```

Text Lengths

New Dictionary

Line Numbers

Line numbers are optional now

just quit

```
% dece -q –o Ni59new.dat Ni59.dat
```

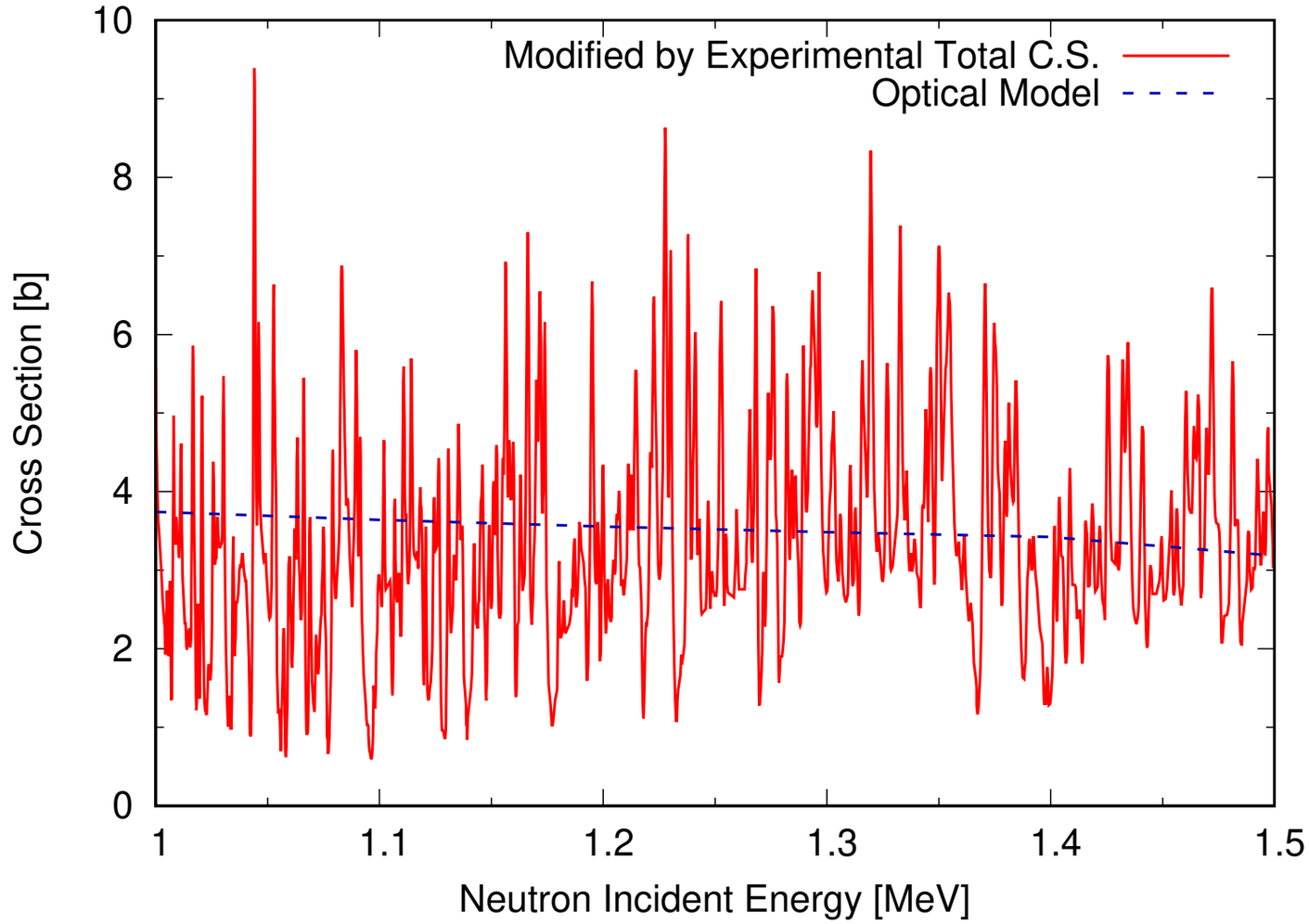
output file

DeCE Showcase (III) Arithmetic Operation

Add, subtract, multiply, and divide a sub-section by another sub-section

- sub-section means one of (MF,MT) segments
- Add partial cross sections (σ(n,n'), σ(n,2n), σ(n,nα), σ(n,γ)) and store it in the non-elastic scattering cross section σ_{nonel}
- Subtract σ_{nonel} from σ_{total} to re-calculate $\sigma_{elastic}$

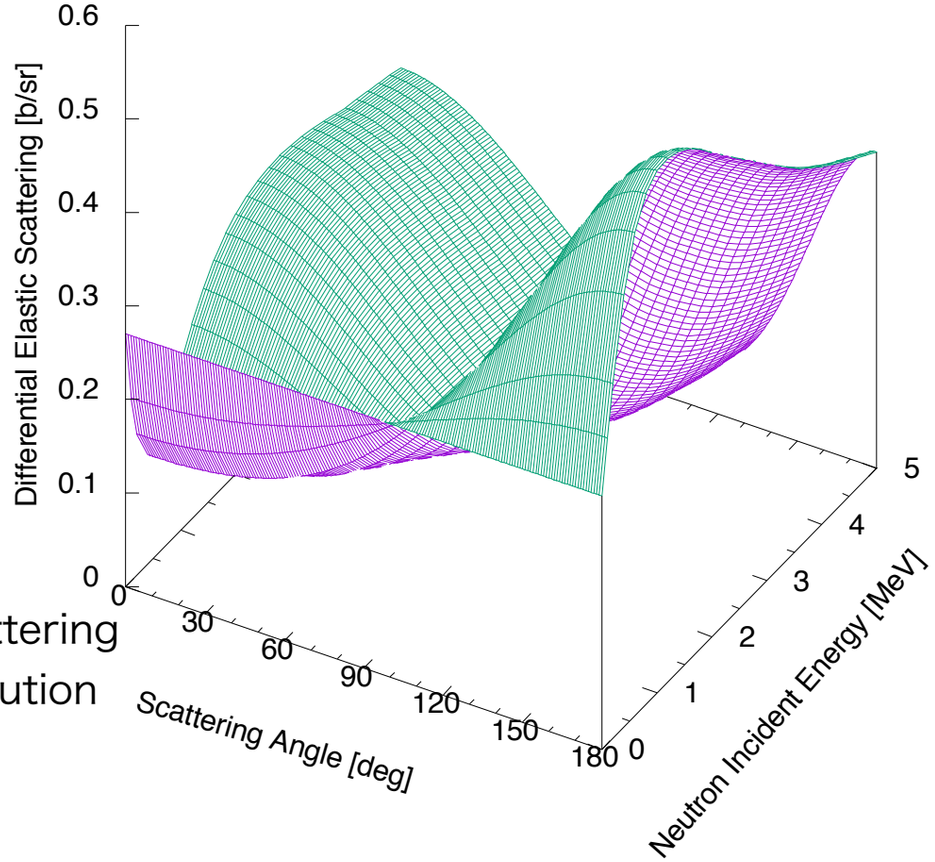
```
% dece -o Ni58new.dat Ni58.dat
calc 3 = 4 + 16
calc 3 = 3 + 22
calc 3 = 3 + 102
calc 2 = 1 - 3
delete 3 3
quit
```



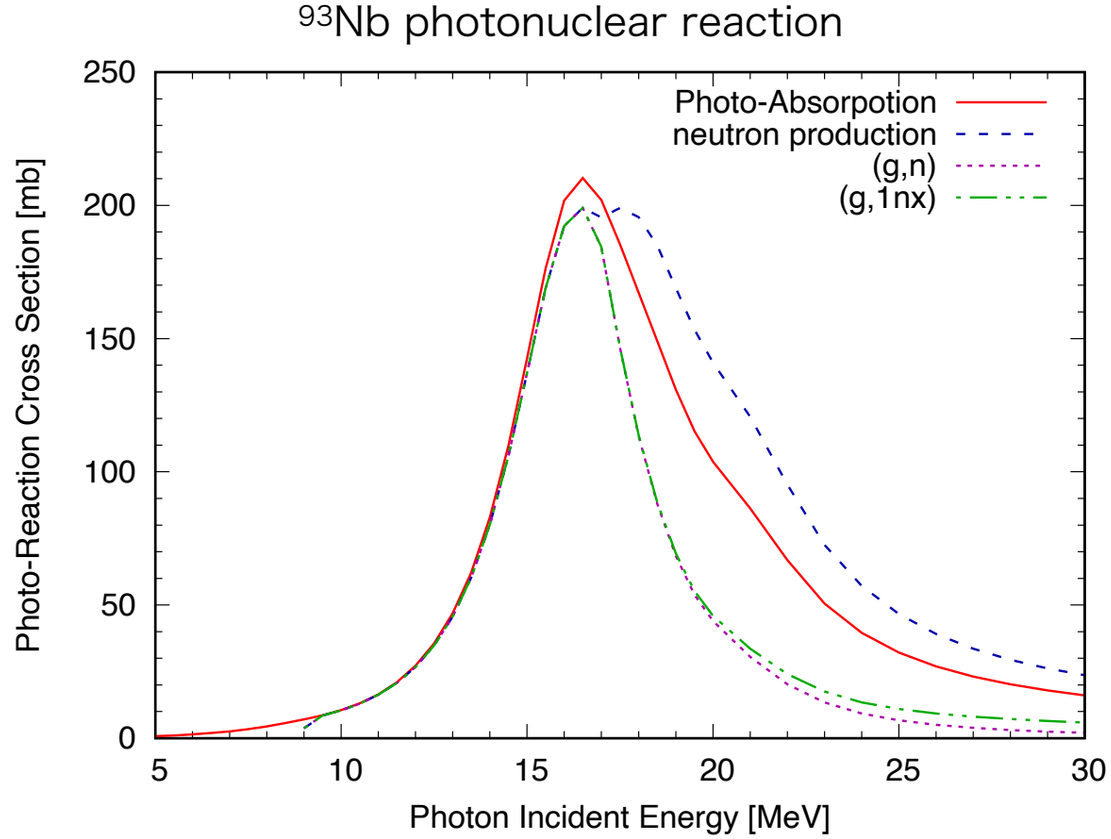
DeCE Showcase (IV) Tools

Tools are external short programs that access ENDF data though ENDFLIB and ENDFIO

- decemf5: convert tabulated energy spectrum data into ENDF-6 format
- decemf6: convert CoH_3 energy-angle spectrum output into ENDF-6
- decemacs: calculate Maxwellian energy average cross section (need PENDF)
- deceangdist: calculate scattering angular distributions from Legendre coefficients
- decephoto: calculate photonuclear reaction cross sections



n+d elastic scattering angular distribution



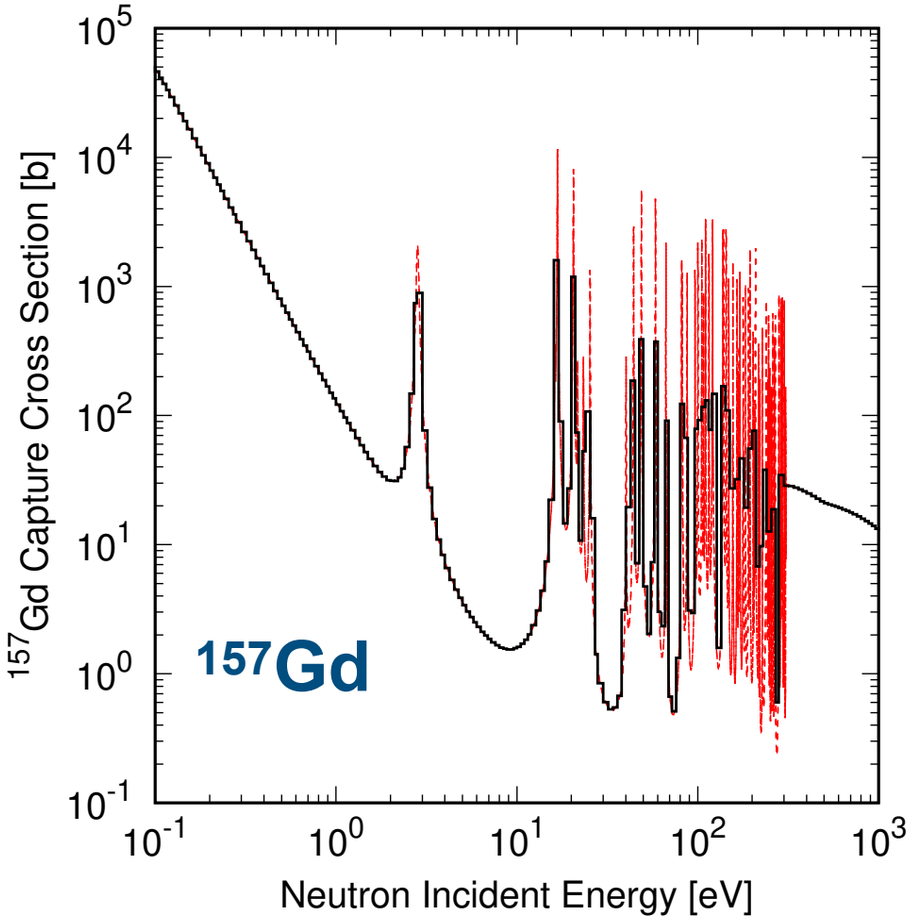
DeCE Showcase (V) Resonance Reconstruction

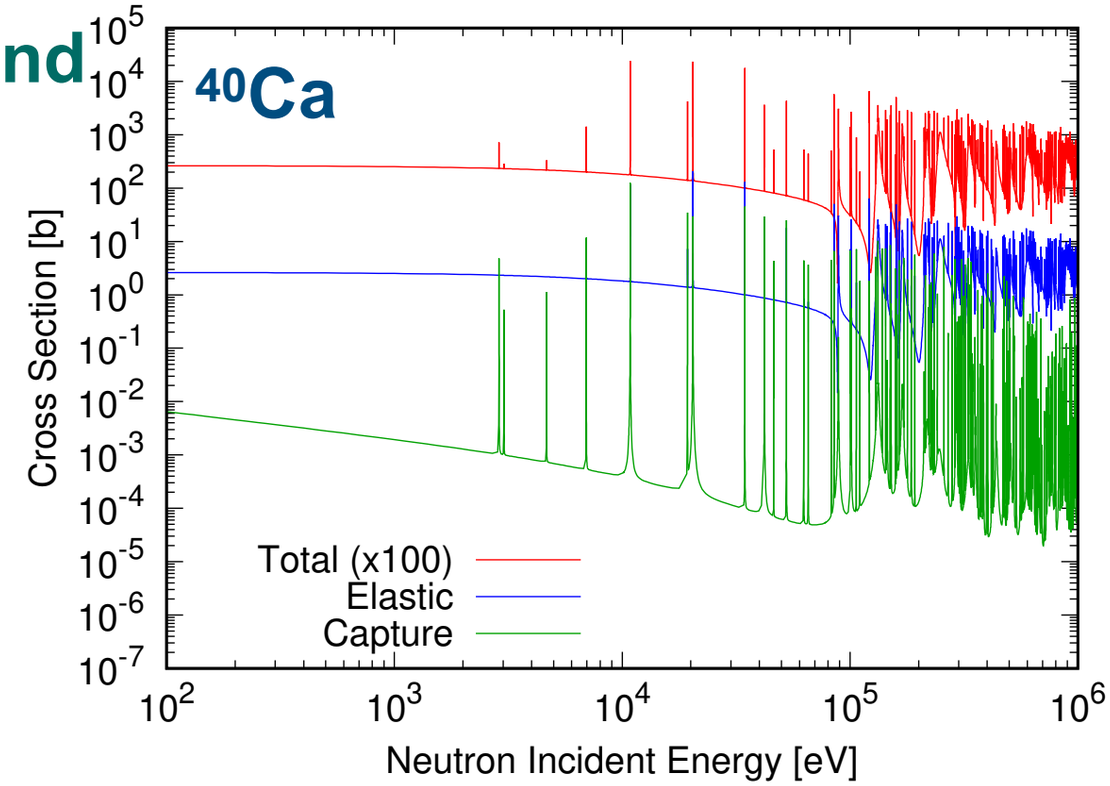
Point-wise cross sections by resolved and unresolved resonance parameters

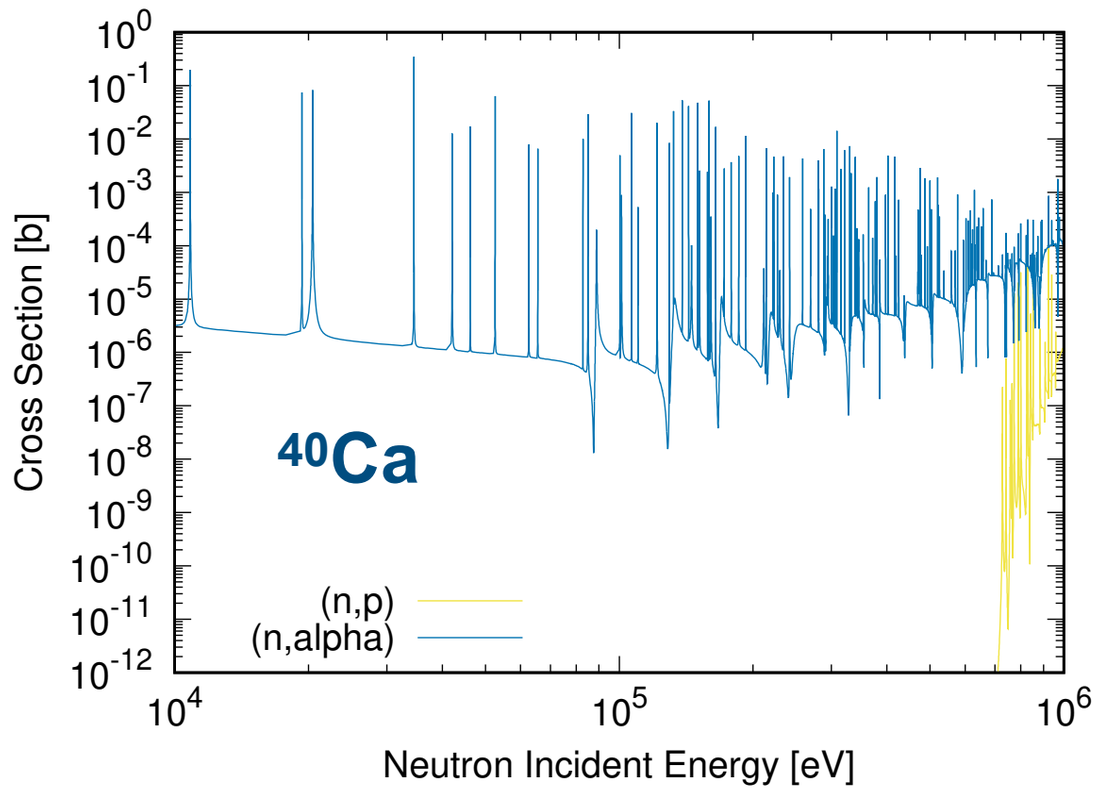
- SLBW, MLBW, Reich-Moore, and RML, including charged particle channels

Group average cross section

- SAND-IIa, LANL70, VITAMIN-J



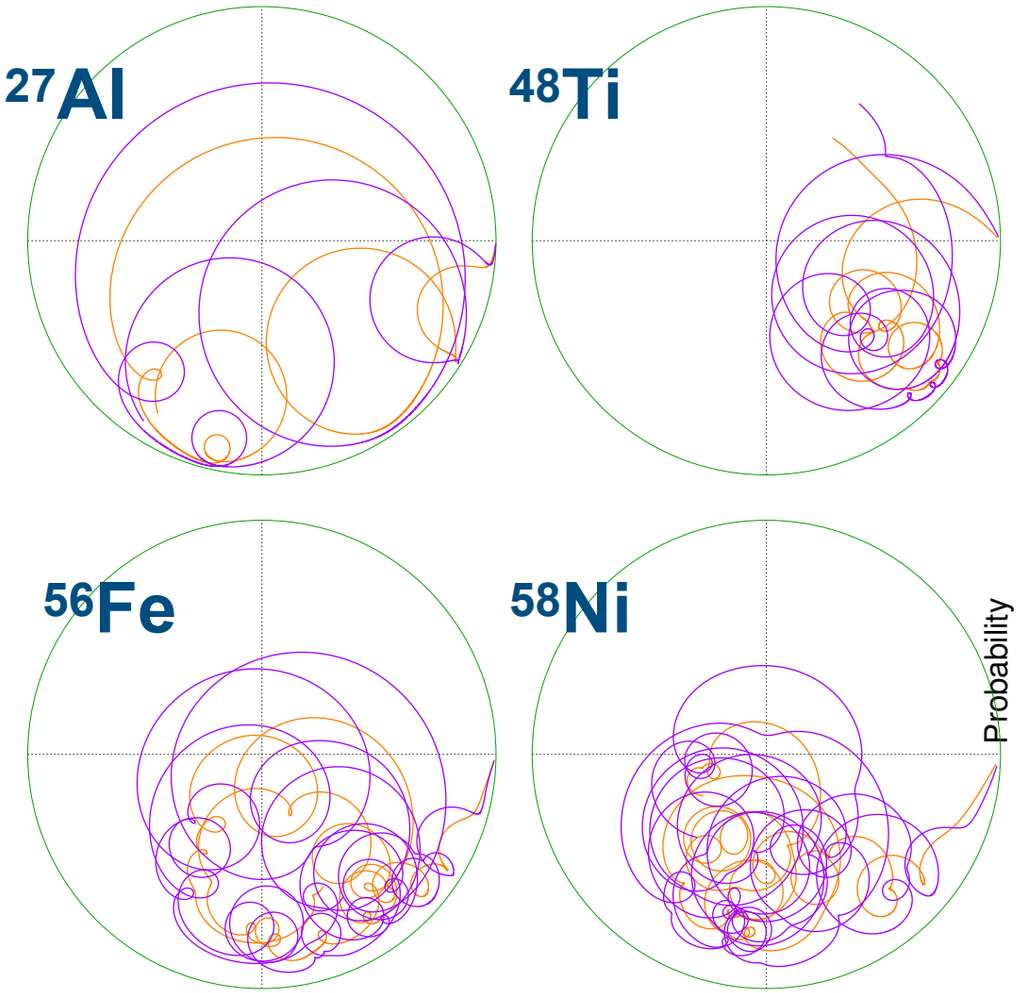


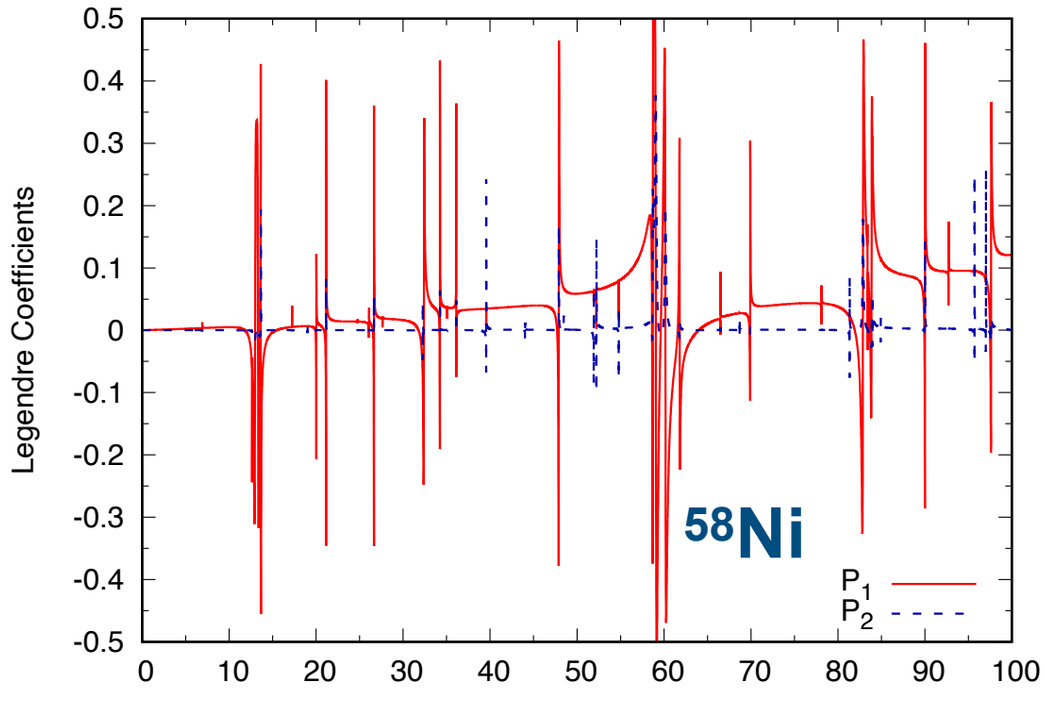


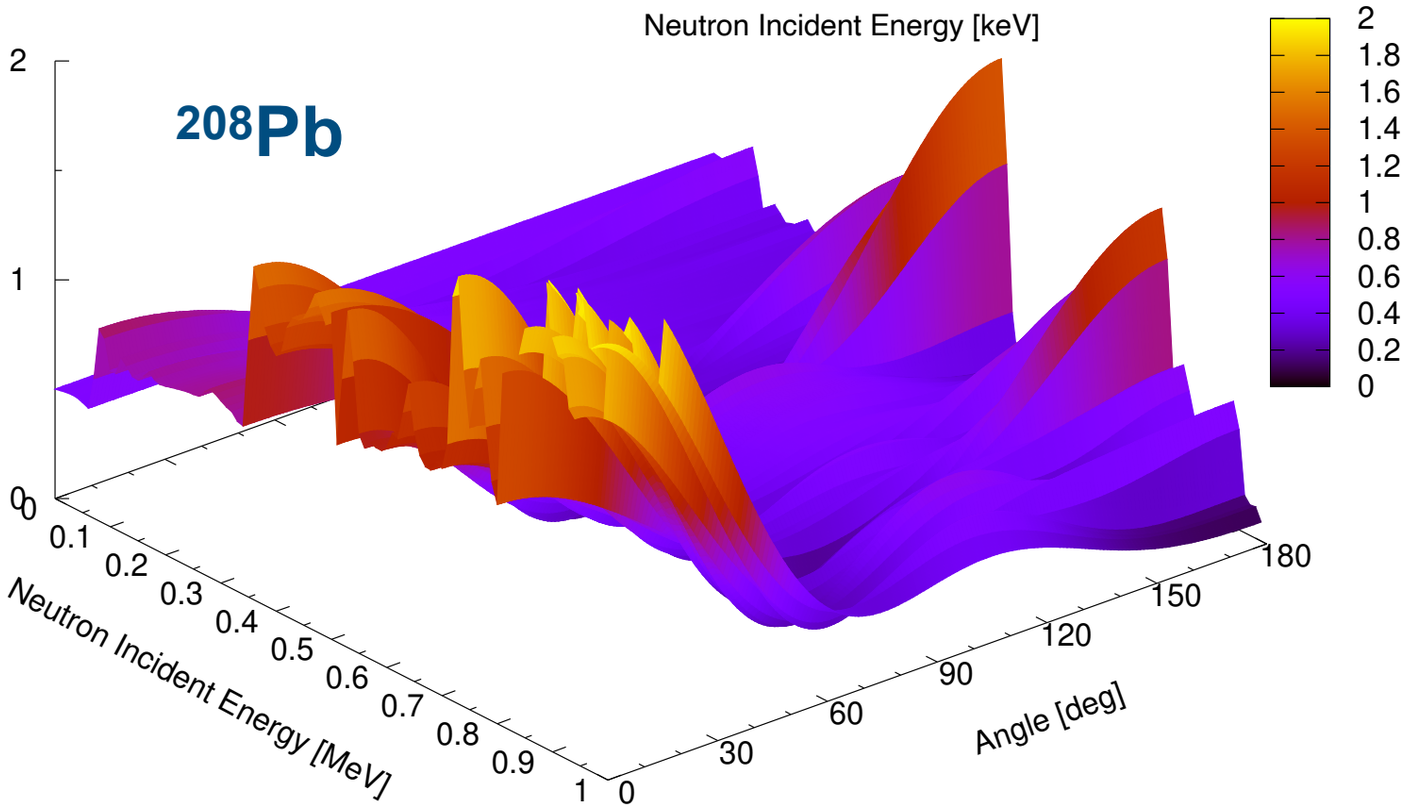
DeCE Showcase (VI) Angular Distribution in RRR

Blatt-Biedenharn formalism for elastic angular distributions

- S-matrix calculated from resonance R-matrix







DeCE Showcase (VII) Covariance Data

```
% dece -f32 n-092_U_233.endf
#    [ 9222 : 32 : 151 ]    92 - 233
# Resonance Parameter Covariance Matrix
#          NER              1  number of energy ranges

#   Subsection              0
#         Emin 1.0000000e-05
#         Emax 3.0000000e+02
#          LRU              1
#          LRF              3
#        LCOMP              2  compatible flag 0:ENDF/B-V, 1:general case, 2:compact format
#          ISR              0  0: no scattering radius uncertainty, 1: data given
#         NRSA            404  total number of resonances
#        NDIGT              5  number of digits
#          NNN           2020  total number of resonance parameters
#           NM         223624  number of INTG data lines
#         MPAR              5  number of parameters per resonance (ER, GN, GG, ...)
#     Parameter     Uncertainty   Correlation
    0 -1.060000e+03 1.9443396e-03 1000
    1 1.5240000e+00 9.5345341e-01   -1 1000
    2 4.0000000e-02 9.9999775e-01    0    0 1000
    3 2.3700000e-01 9.9671308e-01    0   -9    0 1000
    4 -8.000000e+02 2.3649988e-03    0   -6    0    0 1000
    5 1.3150000e+00 9.6446160e-01    0    0    0    0    0 1000
    6 4.0000000e-02 9.9999675e-01    0  -61    0   -2    1   -1 1000
    7 -2.250000e-01 9.9634044e-01    0    0    0    0    0    0    0 1000
    8 -5.750000e+02 2.3354765e-03    0    3    0    0    0    0   -7    0 1000
    9 8.0790000e-01 9.4186001e-01    0   -1    0    0    0    0    7    0    0 1000
…
```

DeCE Commands (selected)

Command	Operation
calc	calculate sum etc. of two sections in MF3
make4	create MF3,MT4 from MF51 - 91
duplicate / copy	copy section into another MT
read / multiread	read cross section data in an external file (X-Y table)
libread / multilibread	import a section or multiple sections from another ENDF-6 file
angdist / mutiangdist	read angular distribution data or Legendre coefficients
table	print internal data in a tabulated format
extract	extract a specified section and print as is
addpoint / delpoint	insert / delete one data point in a section in MF3
reconstruct	calculate cross sections from resonance parameters
index	print stored section index
set / unset	set / unset global options, such as energy unit, line number

ENDFLIB Class Library Example I: Print MF/MT

```
#include “endflib.h"

int main(int argc, char *argv[])
{
  ifstream fpin;
  ENDF lib;

  fpin.open(argv[1]);
  ENDFReadMF(&fpin,&lib,3,1);
  fpin.close();

  ENDFPrint1Dim(&lib,0);

  ENDFWrite(&lib);

  return 0;
}
```

instance object

read MF3 MT1 data

print X-Y table

print ENDF-6 data

ENDFLIB Class Library Example II: Read/Print Entire File

```
ENDFDict dict;
ENDFScanLibrary((string)argv[1],&dict);
ENDFWriteTPID(&dict);
ENDFExtract(&fpin,1,451);
for(int mf=1 ; mf <= 40 ; mf++){
  bool mfexist = false;
  for(int i=0 ; i<dict.getSEC() ; i++){
    if(dict.mf[i] == mf){
      ENDF lib;
      ENDFRead(&fpin,&lib,mf,dict.mt[i]);
      ENDFWrite(&lib);
      mfexist = true;
    }
  }
  if(mfexist) ENDFWriteFEND(dict.getMAT());
}
ENDFWriteFEND(0);
ENDFWriteFEND(-1);
```

scan contents

print MT451

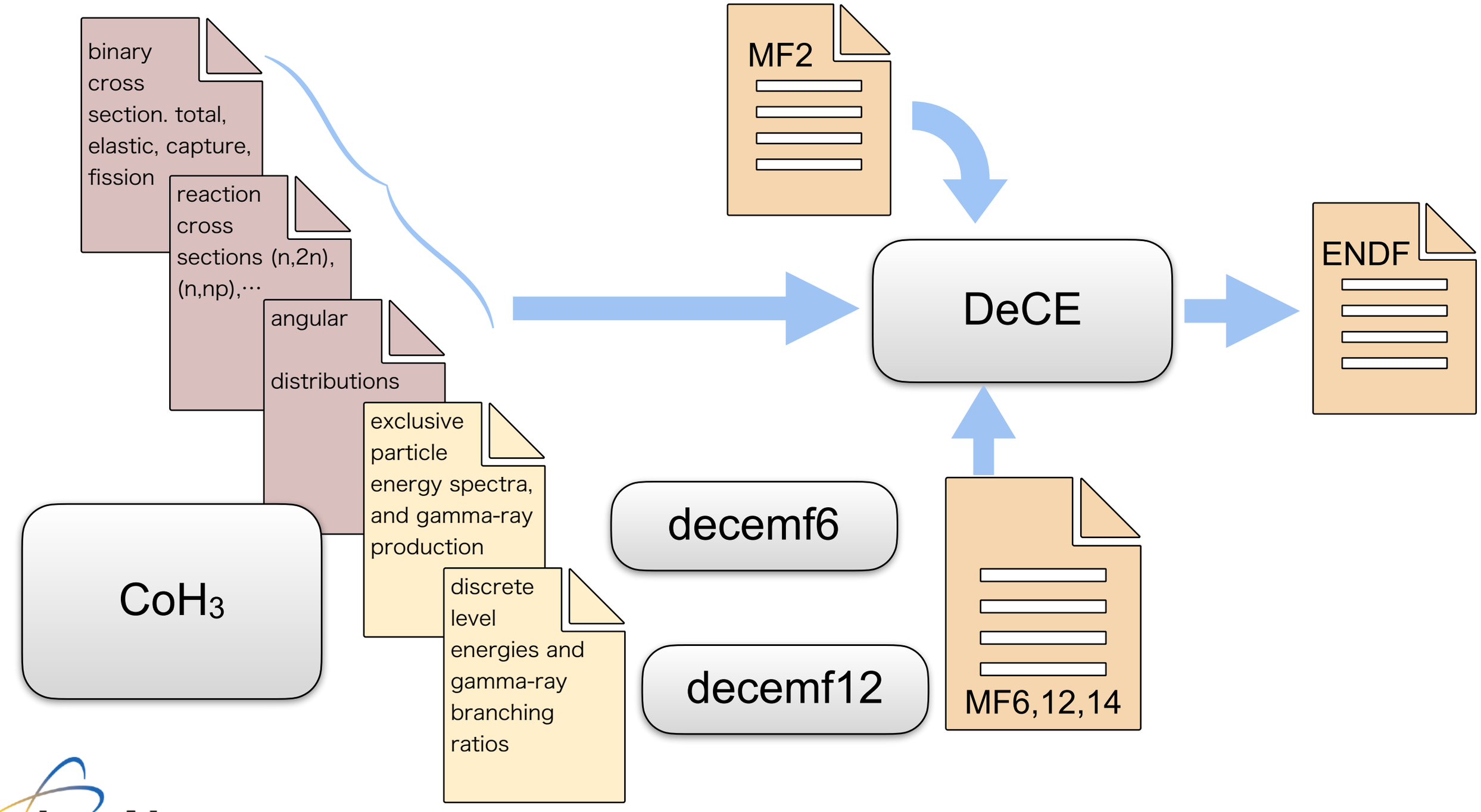
print all given sections

print MF delimiters

Connecting CoH_3 and DeCE to Create ENDF

CoH_3 produces some interim data files, and DeCE processes them

- However, DeCE is designed to accept any data files (X-Y table)



User Community (yet small …)

Feedback

- Bugs occasionally reported by users
  - Sep. 2020, MF3 MT50 was missing for charged-particle reactions
  - The most recent one was Mar. 2021 by IAEA
  - See ChangeLog for all changes

Recent requests

- Responded
  - Scaling factor applied to P_1 Legendre coefficients
  - Some special cases for charged-particle reactions
  - Print-out redirect by “set Output” command

- Users’ pull-request
  - Handling very large/small numbers, like 10^{123}, 10^{-123}
  - SAND-IIa 725 group extension
- Not resolved yet (or not considered)
  - Windows version
  - Data visualization package

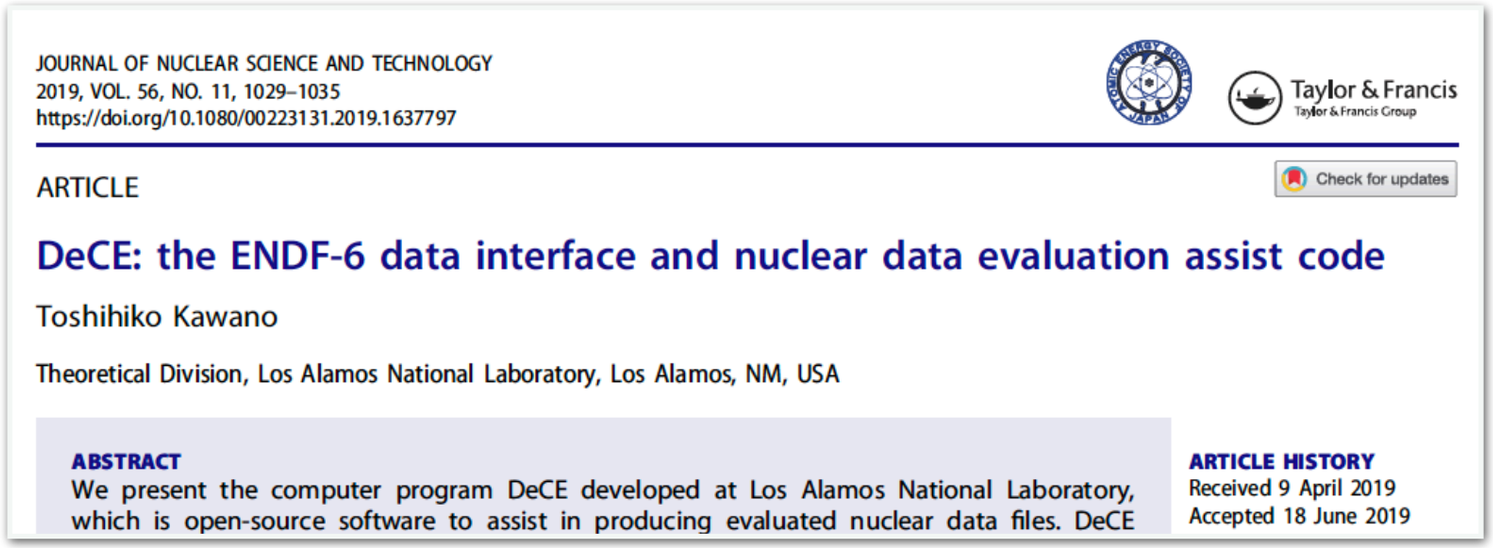
Concluding Remarks

CoH_3 Coupled-Channels Hauser-Feshbach code

- The statistical Hauser-Feshbach code provides a complete nuclear data above the resonance range
- CoH_3 produces several interim files - cross section, angular and energy distributions, etc. - for creating a new ENDF file by DeCE

DeCE ENDF data manipulation code

- DeCE facilitates ENDF data file manipulation and production
- Essential tool for producing new ENDF files at LANL
- Document and source code available at:
  - https://doi.org/10.1080/00223131.2019.1637797
  - https://github.com/toshihikokawano/DeCE



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2019, VOL. 56, NO. 11, 1029–1035
https://doi.org/10.1080/00223131.2019.1637797

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ARTICLE

Check for updates

DeCE: the ENDF-6 data interface and nuclear data evaluation assist code

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ABSTRACT

We present the computer program DeCE developed at Los Alamos National Laboratory, which is open-source software to assist in producing evaluated nuclear data files. DeCE

ARTICLE HISTORY
Received 9 April 2019
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