CoH3 Hauser-Feshbach code, and DeCE ENDF-6 Formatting Code

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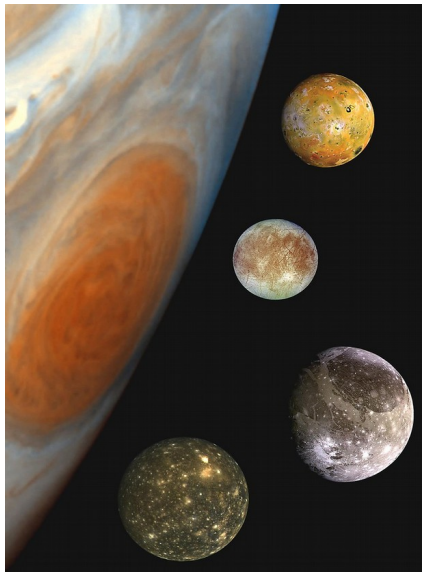
Reaction Modeling and ENDF Evaluation Tools

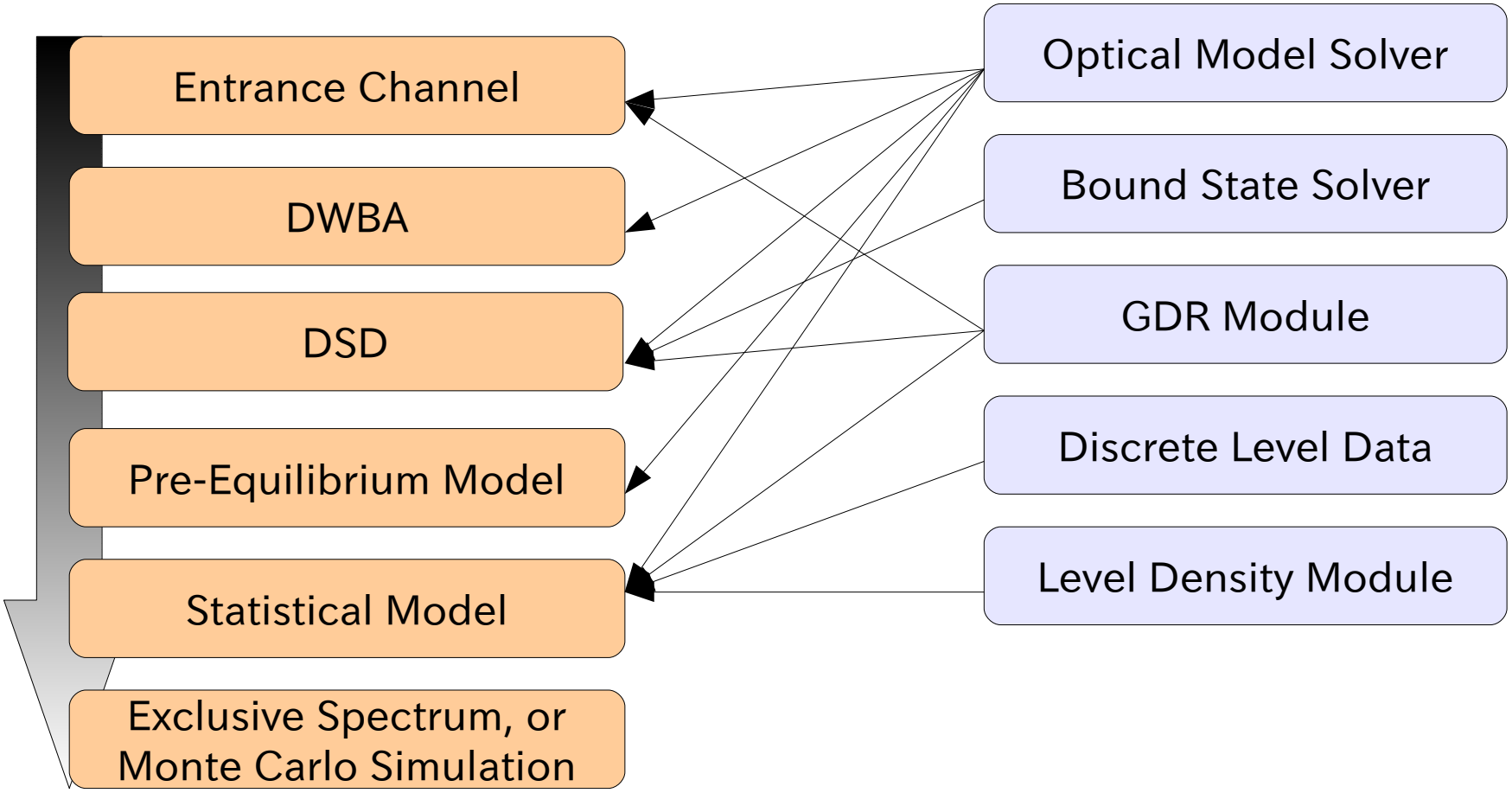
- CoH
  - no acronym
    - was compact optical and Hauser-Feshbach models
    - but no longer “compact”
  - standard Hauser-Feshbach code
- CGM and CGMF (CGM+FFD)
  - Cascading Gamma-ray and Multiplicity
  - Monte Carlo neutron and gamma-ray emission code
  - fission event generator
  - beta-delayed neutron, neutrino, and gamma-ray spectrum
  - not in this talk (see our publications in PRC)
- DeCE
  - Descriptive Correction of ENDF-6 format code
  - ENDF-6 format manipulation code
  - convert CoH results into an ENDF file

CoH3 - ver.3.2 Umbriel

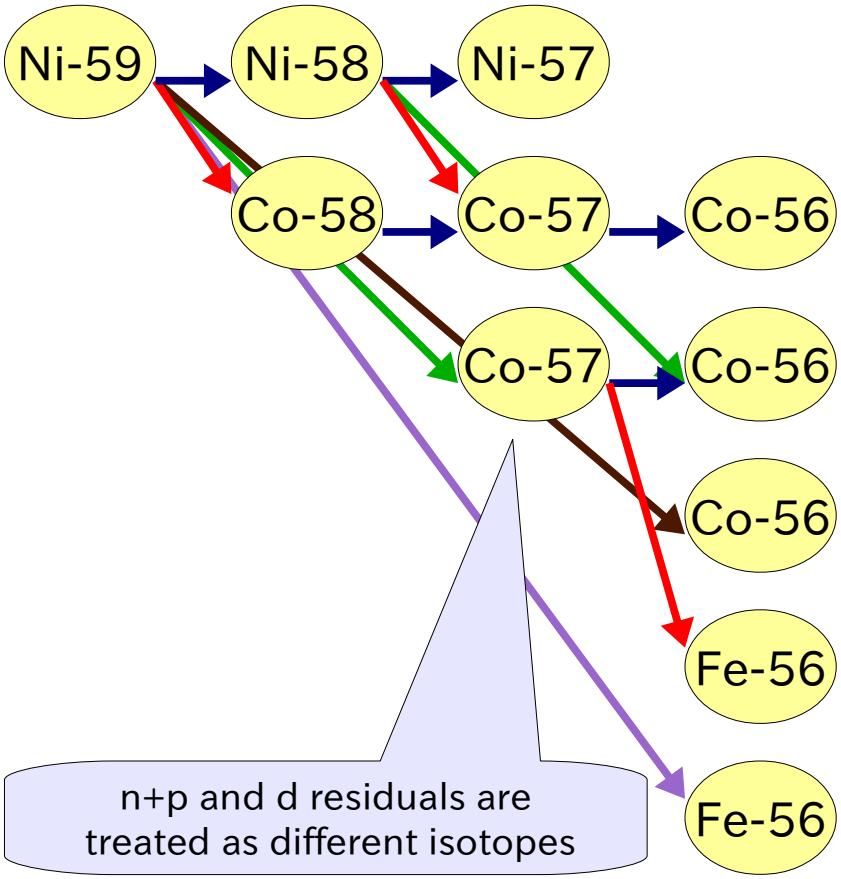
- **Code Structure**
  - Written in C++
    - 64 source files with 35 header files, 25K lines
  - GNU standard package - automake, autoconf
- **History**
  - 1992/5, original C language version, 1.0
    - spherical OM and Hauser-Feshbach-Moldauer for binary reactions
  - 1996/6, all source codes re-written in ANSI-C, ver. 2.0
    - automatic OM parameter search
    - in RIPL web page (ver. 2.1?)
  - 2001/3, ver. 2.3
    - coupled-channels calculation, radiative capture
  - 2009/9, ver. 3.0 Callisto
    - totally re-written in C++
    - multi particle emission, exciton, DSD, DWBA
  - 2010/2, ver. 3.1 Ariel released
    - fission included
  - 2012/10, ver. 3.2 Umbriel released
    - exclusive spectrum calculation combined version



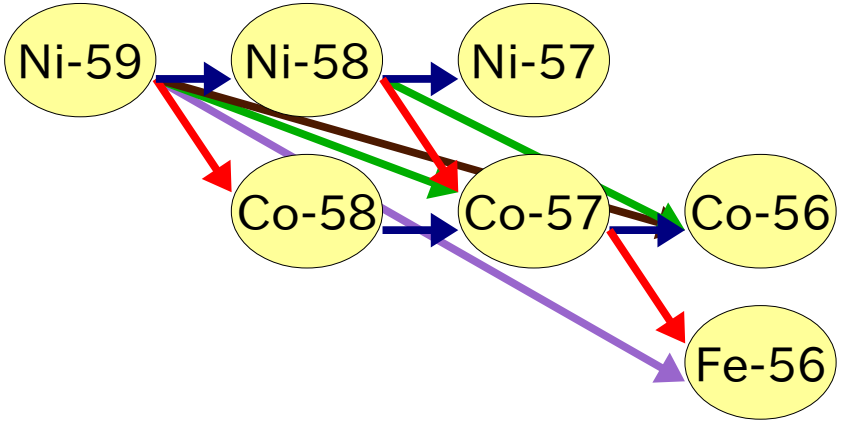
CoH3 Components



Automatic Reaction Chain Set Up

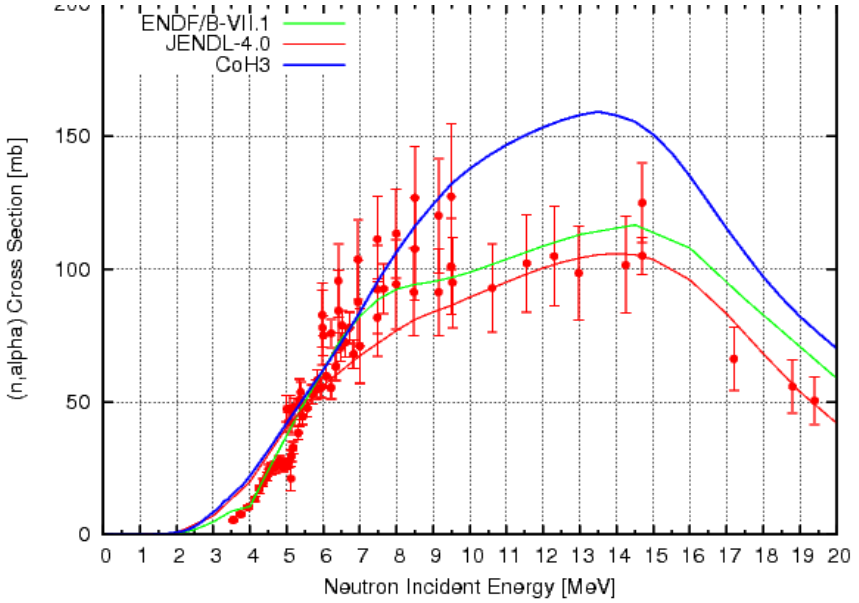


In GNASH,
each isotope appears once



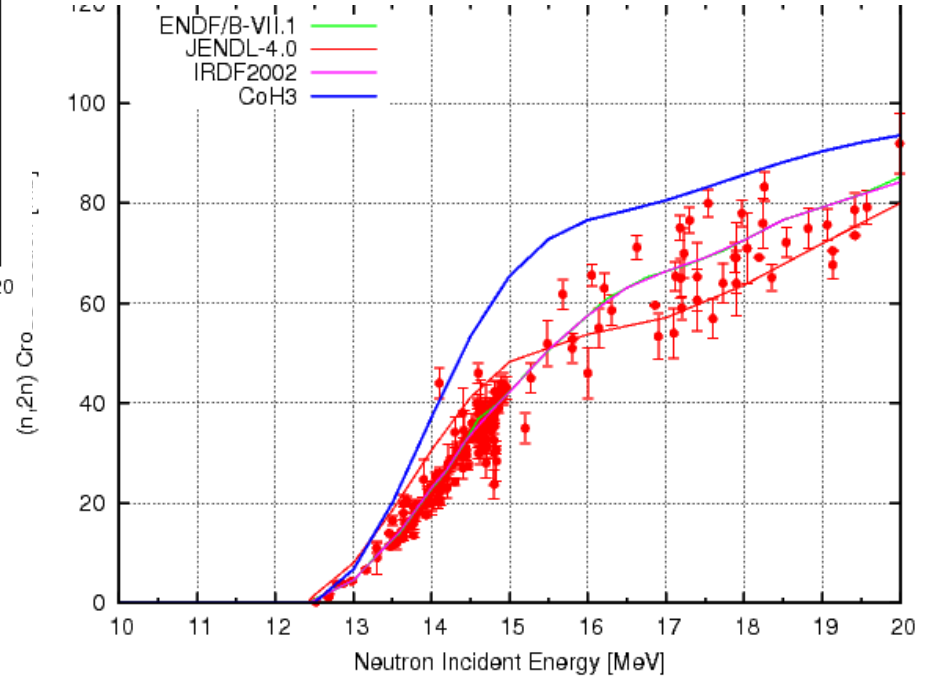
- Chain information in a linked list
- The list is generated automatically
- Easy to distinguish individual reactions
- The # of isotopes explodes quickly
- e.g. 420 compounds at 80 MeV (80 unique)

CoH3 Default Calculations (Example, Ni-58)

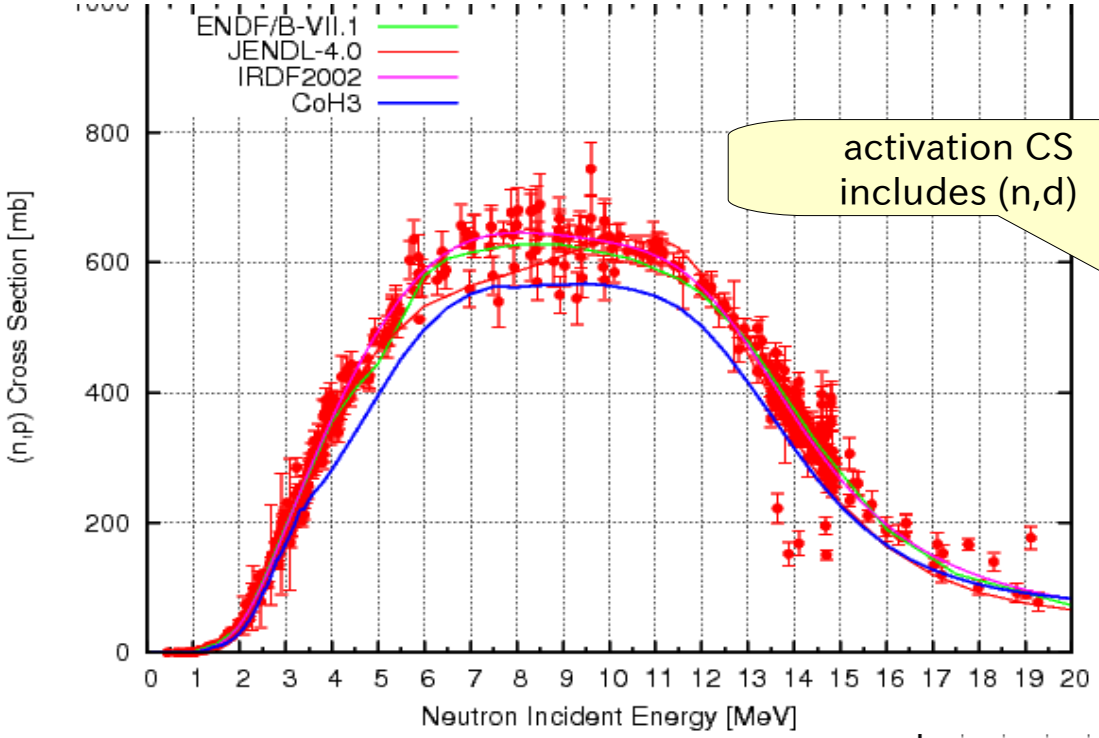


Ni-58(n,alpha) Reaction

Ni-58(n,2n) Reaction



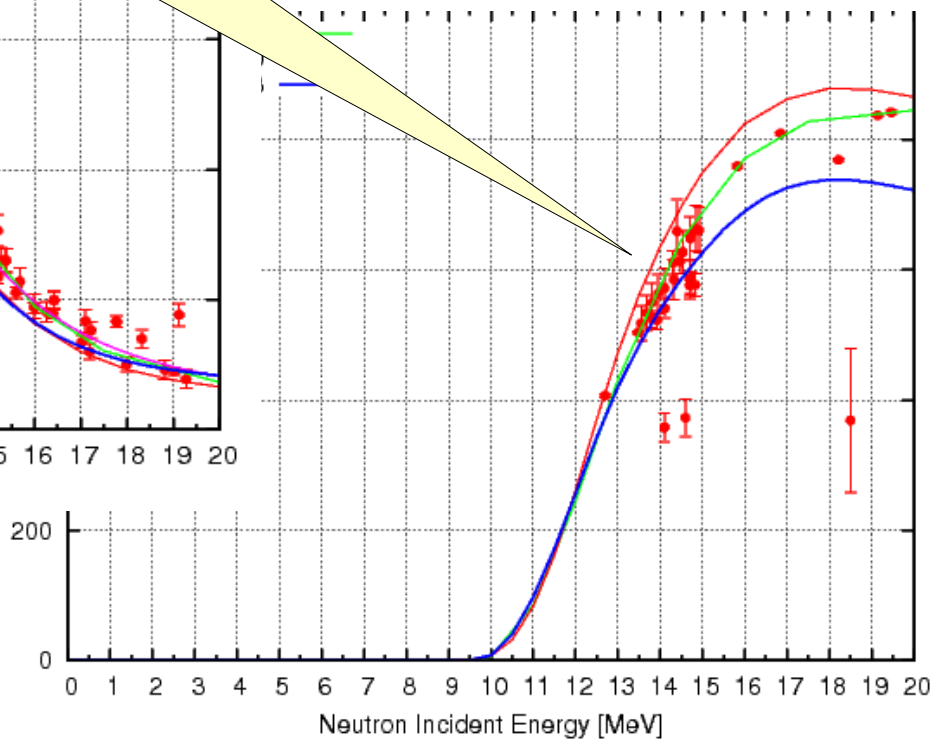
CoH3 Default Calculations (Example, Ni-58)



Ni-58(n,p) Reaction

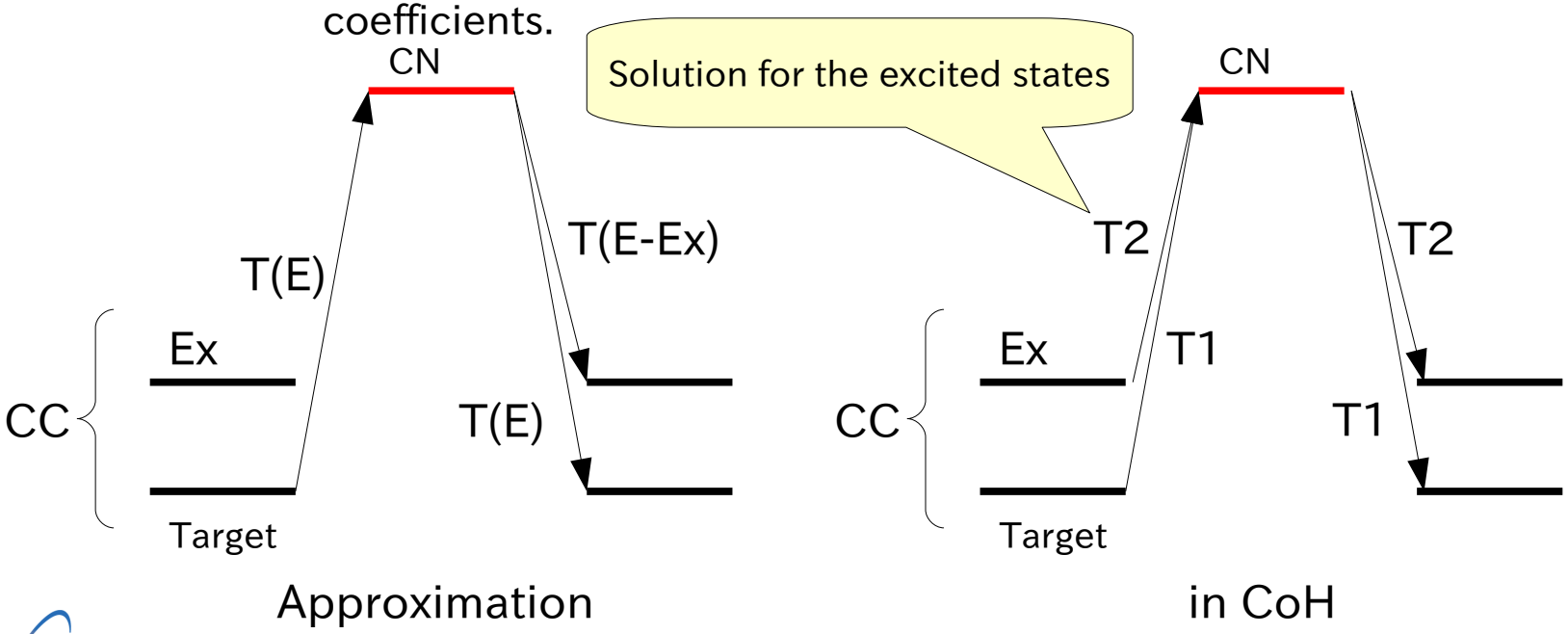
activation CS includes (n,d)

Ni-58(n,n+p) and (n,d)



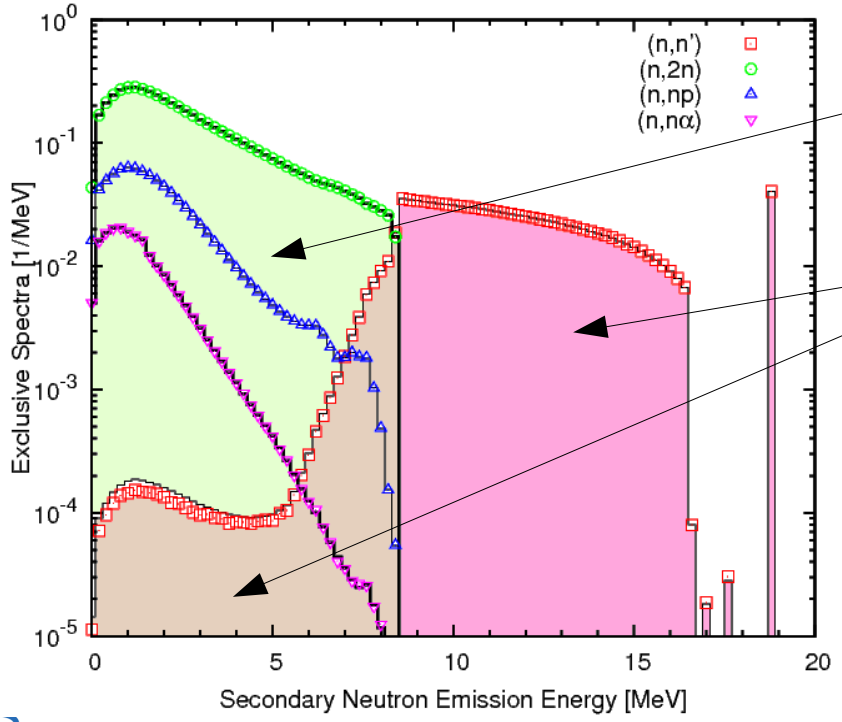
Coupled-Channels Hauser-Feshbach (Detailed Balance)

- **Transmission Coefficients to Excited State from CC Calculations**
  - The coupled-channels equations are solved internally
  - Gives correct Transmissions for the inverse reactions
  - Width fluctuation corrections applied to these transmission coefficients.



Exclusive Particle Energy Spectra and Energy Balance

- **New Algorithm Developed for Exclusive Energy Spectra**
  - truncation of gamma-ray emission at each intermediate stage optimized
  - calculated results confirmed by the Monte Carlo calculations



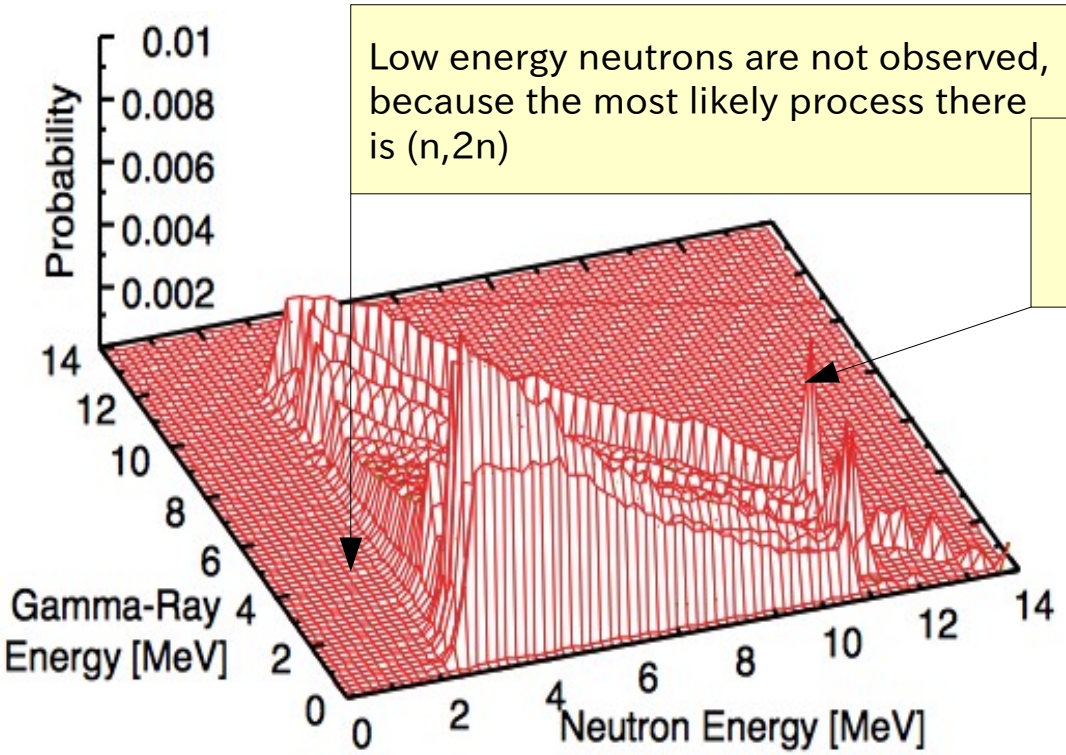
(n,2n) reaction

inelastic scattering

DeCE converts the outputs (particle and gamma-ray) into ENDF-6 format, MF=6
Energy balance checked with NJOY HEATR

Monte Carlo with CoH, N-G Correlation in (n,n') Reaction

Joint probability of neutron and gamma energies for V-51+ n at 14 MeV (n,n') reaction



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DeCE: ENDF Format Utility, ver. 1.1.2 (Turquoise)

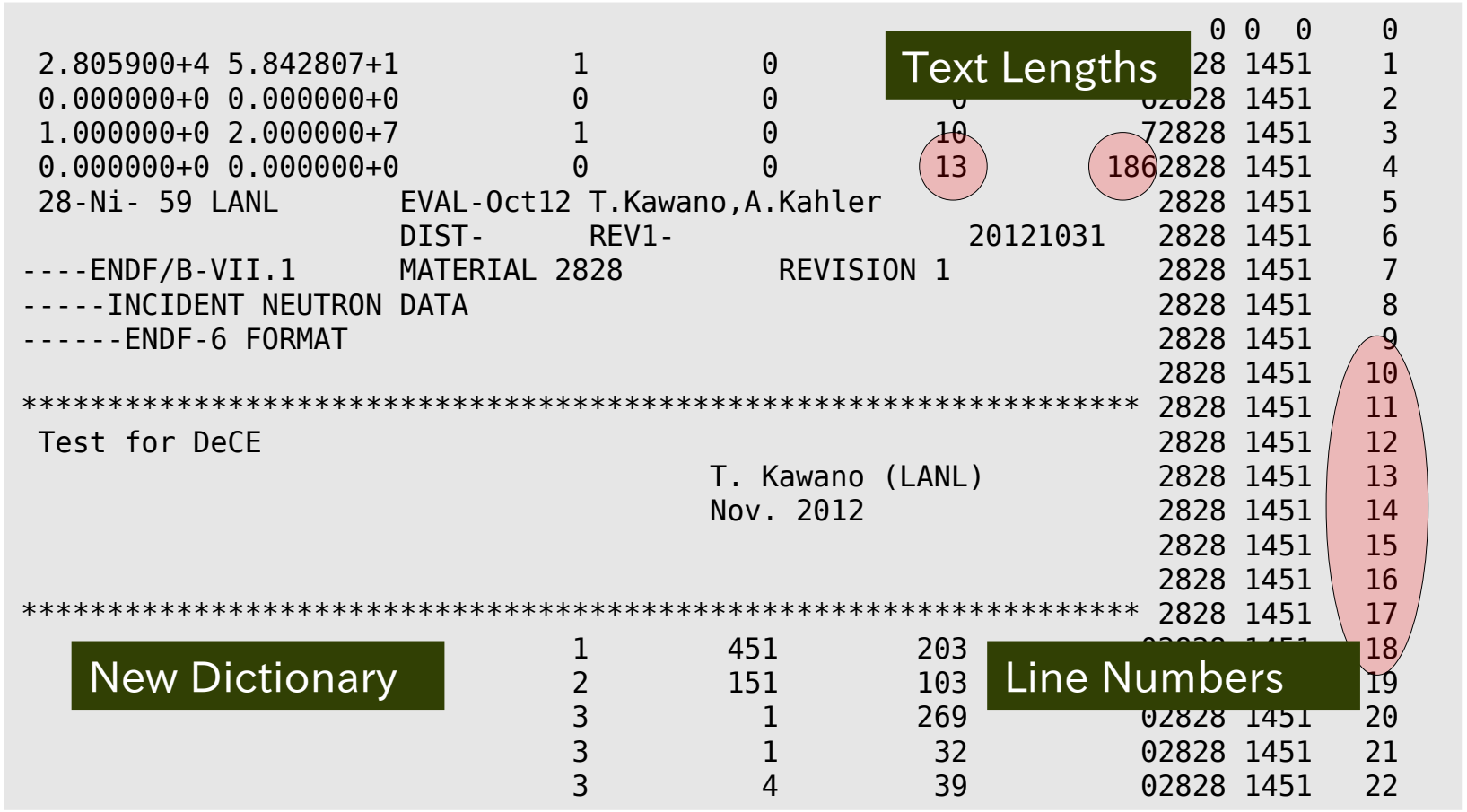
- **What Does DeCE Do?**
  - facilitates ENDF-6 data file manipulations
    - add two sections, renormalize data, add/delete points, etc
  - converts model calculation results into ENDF-6 format
  - re-constructs pointwise cross sections from resolved resonances
  - converts ENDF-6 formatted data into more human friendly form
    - X-Y data table that includes "E", XML
- **C++ Objective-Oriented Code**
  - each section (MF/MT) is an object
  - class ENDF includes
    - MAT/MF/MT
    - HEAD record
    - CONT records
    - integer and floating point data arrays
    - pointers to each data section

DeCE Example I: Edit Comment Section (before)

```
                                                                      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
                                                                  2828 0  0    0
 2.805900+4 5.842807+1          0          0          1          02828 2151    1
 2.805900+4 1.000000+0          0          0          2          02828 2151    2
 1.000000-5 1.000000+4          1          2          0          02828 2151    3
```

DeCE Example I: Edit Comment Section (after)




```
                                                                0 0  0     0
 2.805900+4 5.842807+1          1          0                   28 1451     1
 0.000000+0 0.000000+0          0          0                   02828 1451     2
 1.000000+0 2.000000+7          1          0                   72828 1451     3
 0.000000+0 0.000000+0          0          0                   2828 1451     4
 28-Ni- 59 LANL       EVAL-Oct12 T.Kawano,A.Kahler             2828 1451     5
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**************************************************************** 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
```

DeCE Example II: Interactive Mode

- **Step by Step Modification to ENDF-6 Formatted File**

Print (n,2n) Section

```
% dece n-028_Ni_059.endf
extract 3 16
 2.805900+4 5.842807+1          0          0          0          02828 3 16    1
-8.999398+6-8.999398+6          0          0          1         232828 3 16    2
         23          2                                           2828 3 16    3
 9.153423+6 0.000000+0 9.500000+6 8.847654-3 1.000000+7 4.231216-22828 3 16    4
...
 1.650000+7 3.667532-1 1.700000+7 3.617123-1 1.750000+7 3.558410-12828 3 16    9
 1.800000+7 3.494444-1 1.850000+7 3.434382-1 1.900000+7 3.377164-12828 3 16   10
 1.950000+7 3.320694-1 2.000000+7 3.282886-1                     2828 3 16   11
                                                                 2828 3  099999
calc 100 = 16+22
extract 3 100
 2.805900+4 5.842807+1          0          0
-6.100396+6-6.100396+6          0          0
         27          2
 6.204805+6 0.000000+0 8.000000+6 7.31688-16 8.5000
...
 1.750000+7 4.358034-1 1.800000+7 4.398236-1 1.8500
 1.900000+7 4.472759-1 1.950000+7 4.495027-1 2.000000+7 4.521536-12828 3100   12
                                                                 2828 3  099999
quit
```

Make a new MT=100 section, as the sum of (n,2n) and (n,n alpha)

DeCE Commands (part)

Command	Operation	Example
read	read external file	read 3 102 “capture.dat”
libread	replace section by another library	libread 2 151 “ENDF.DAT”
table	tabulate data	table 3 18
extract	print data in ENDF-6 format	extract 3 18
delete	delete one section	delete 15 102
factor	scale data by a given factor	factor 3 102 1.2
calc	arithmetic operation for MF=3	calc 1=2+3
make4	make MF3/MT4 from 51 - 91	
reconstruct	cross section from resonances	reconstruct 1e+3 8e+8 1e+3

ENDF Class Library

- Abstraction of ENDF-6 Formatted

```
class Record{
 public:
    double    c1;
    double    c2;
    int       l1;
    int       l2;
    int       n1;
    int       n2;
    Record(){
      c1 = 0.0; c2 = 0.0;  l1 = 0;  l2 = 0;  n1 = 0;
    }
    void setRecord(double a, double b, int c, int d, i
      c1 = a  ; c2 = b  ;  l1 = c;  l2 = d;  n1 = e;  n2 = f;
    }
};
```

```
class ENDF{
 private:
  int       mat;
  int       mf;
  int       mt;
  Record    head;
  DataSize  size;
 public:
  int       *idata;
  double    *xdata;
  int       **iptr;
  double    **xptr;
  Record    *rdata;
};
```

```
void ReadMF3(ifstream *fp, int mf, int mt)
{
  ENDF lib(M);
  ENDFReadMF(fp,&lib,mf,mt);
  ENDFWriteMF(&lib)
}
```

Remarks

- **Statistical Model Code Development**
  - CoH Hauser-Feshbach code for ENDF evaluation
  - CGM and CGMF Monte Carlo neutron and gamma-ray emission (not in this talk)
- **ENDF-6 Format Utility**
  - DeCE
    - convert CoH results into ENDF
    - can reduce human mistakes
- **CoH Future Plans**
  - Better fission modeling
  - Sensitivity calculation (on going)
  - High energy extension (alpha cluster model)
  - etc.