For installation, refer to the CONUSS manual. CONUSS can work with both synchrotron Mössbauer spectra (SMS) and conventional Mössbauer spectra (CMS). Current version of CONUSS (2.0.0) executes commands in Linux/Unix terminals. To use CONUSS, it is necessary that you have some idea on what the expected spectra look like for a given set of hyperfine parameters, mainly magnetic hyperfine field, isomer shift and quadrupole splitting. Literature is a great resource for this information.

REFERENCE

1. Sturhahn, W., CONUSS and PHOENIX: evaluation of nuclear resonant scattering data. *Hyperfine Interact.*, 125:149–172, 2000.

CONUSS COMMANDS

1. Command ***conuss rmf*** : simulates a Mössbauer spectrum based on the input parameters (in ex_in, in_kfit, in_kref files; in many cases, ex_in may have been renamed as Fe_in, Fe3C_in, etc.).
2. Command ***conuss rmfx*** : simulates a Mössbauer spectrum based on the input parameters, and plot the simulated spectrum together with the input experimental data.
3. Command ***conuss fit*** : finds the best fitting results for selected parameters (those with a '%' sign in the beginning of a line, see the following example).

   You also need to give the step size of refinement – the number *0.01* in the following example

% (26.1.11) quadrupole splitting / mm/s :: 0.142 *0.01*

   After this command is successfully executed, a file named 'out_kctl' containing the refined parameters will be generated.
4. Command ***conuss mco*** : does a monte carlo search and finds the best fitting results for the selected parameters ('%' sign). A file named 'in_kmco' is required.

   After this command is successfully executed, a few files containing the best parameters will be generated; these files have an extension of '.mco' in the file names.

HOW TO GET HYPERFINE PARAMETERS FROM CONUSS?

1. Find hyperfine parameters that can generate a spectrum closely represent the experimentally measured spectrum. This can be done in two ways:

   Method 1 – manual search:

   a. Initialize hyperfine parameters and other parameters (thickness etc) in the input files (see the following section 'INPUT FILES').

   b. In terminal, run ***conuss rmfx*** to view the simulated spectrum together with the input experimental data.

   c. Repeat step a & b until a reasonable match between the simulated spectrum and the experimental spectrum is reached.

Method 2 – with CONUSS command *conuss mco*:

a. Initialize hyperfine parameters and other parameters (thickness etc) in the input files.
b. In terminal, run ***conuss mco*** to do a monte carlo search for good starting parameters.
c. Repeat step a & b until a reasonable match between the simulated spectrum and the experimental spectrum is reached.

2. Fine tune the selected parameters with command ***conuss fit***.

INPUT FILES

This is where you define hyperfine parameter, thickness, etc. These files can be edited using most text-editing programs, e.g., notepad, wordpad, word, gedit.

- Input files include 'ex_in', 'in_kmco', 'in_kref', 'in_kctl', 'in_kmix', 'in_kfit' files and the experimental data.
- Line (2) in the 'in_kfit' file is where the name of the input experimental data file is defined.
- To covert the raw data collected at beamlines 3-ID-B or 16-ID-D of the APS to 2-column intensity vs. time (in unit of nanosecond) data, you can use a program called 'doget', or you can do the conversion by yourself based on the following information:
  - The one-column raw data represent intensity for each channel.
  - The prompt (generally the channel with the largest count) is the channel of time zero; the channel before the prompt channel is + 0.05 nanosecond.
  - Two channels are separated by 0.05 nanosecond.

INPUT PARAMETERS

Not all of these parameters need to be edited during a fitting. Most of them can take the default values. These parameters are listed in the order that the top ones are the first ones to consider in a fitting, generally speaking.

- Hyperfine filed strength (in unit of Tesla): 'ex_in' (26.1.6)
- Quadrupole splitting (in unit of mm/s): 'ex_in' (26.1.11)
- Isomer shift (in unit of mm/s): 'ex_in' (26.1.5)
- Thickness (in unit of micron):
  - 'in_kref' (18) - if you don't apply thickness distribution
  - If you apply thickness distribution, see thickness distribution in the later part of this section for details.
- Number of sites: 'ex_in' (24)
  - If the sample contains 2 sites (different sites have different hyperfine parameters), change this number to 2, copy the block of code from line (26.1.1) to (26.1.20) and paste it underneath this block. So now you have two blocks of hyperfine parameters. CONUSS will read the file and

assign the 1st block to site #1, and the 2nd block to site #2.

- Texture coefficient / %: 'ex_in' (26.1.18)
  - 100 -- single crystal or all crystals aligned along the same direction
  - 0 – no preferred orientation in sample
- Distribution of a parameter - to apply distribution,
  - Replace the line

    (26.1.17) name of the distribution input file ::

    in 'ex_in' file with the following 4 lines

    (26.1.17) name of the distribution input file ::<!
    Target *isomer shift*
    Make *Gaussian 80 @&distr*
    !

    - Text in red *isomer shift* can be replaced by *hyperfine field* or *efg* depending on your need. efg – electric field gradient; here it refers to quadrupole splitting
    - *Gaussian* can be replaced by *Laurentian*
    - *80*: create 80 points
  - Define the parameter *&distr* by adding a line at the beginning of the 'ex_in' file:

    @ &distr := 3 0.01

    - The distribution for hyperfine filed strength or quadrupole splitting is in fraction; for isomer shift, the distribution is an absolute number in unit of mm/s. For example, for quadrupole splitting of 1.2 mm/s, 0.1 distribution means a full width at half maximum (FWHM) of 1.2× 0.1 mm/s.
    - '3' – distribution; '0.01' – refinement step size
- Angles
  - (26.2.13) euler angle alpha for efg=>xtal /deg
  - (26.2.15) euler angle gamma for efg=>xtal /deg
  - These two numbers are only meaningful when there is texture is the sample (see Texture coefficient).
- Thickness distribution
  - Line (18) of 'in_kref' file: defines the unit thickness
  - Lines (19) – (21) of 'in_kref' file: create a database of simulated results with each thickness in the given range
  - Lines (13) & (15) in 'in_kfit' file: define the thickness and thickness distribution.
  - Only the combination of these three sets of parameters (above) is a meaningful set.

➢ All other parameters in input files

NOTATIONS AND ADDITIONAL TIPS

A notation is placed in the very beginning of a line.

- *: comment line
- %: this parameter will be fitted when you run ***conuss fit*** or ***conuss mco***.
- %w for parameter 1, and %ws for parameter 2: the sum of parameters 1 & 2 is fixed during fitting. %w for parameter 1, and %w for parameter 2: parameters 2 has the same value as parameter 1 during fitting.

  '%', '%w' or '%ws' should be separated from the rest of the line by at least one space, e.g.,

```
* defining MB site #1
…
%w (26.1.4) weight of the sublattice                    ::    0.15 0.01
…
* defining MB site #2
…
%ws (26.1.4) weight of the sublattice                   ::    0.85
```

- Parameters can be defined in the beginning of a file. For examples, in file 'ex_in', one can define the isomer shift for site 1 in the beginning of the file as following:

```
@ &isosite1 := 0.14      0.01
```

  Correspondingly, line (26.1.5) can call this variable as following:

```
(26.1.5) isomer shift      / mm/s        :: @&isosite1
```

BETWEEN SMS AND CMS

To switch between SMS and CMS, only this parameter needs to be modified:

- In 'in_kmix' file, line (3)

  For SMS

```
(3) mode :: time
```

  For CMS

```
(3) mode :: energy
```

If this does not work, also check the following parameters.

- In 'in_kfit' file, lines (6) and (7) should be the following for both SMS and CMS.

```
(6) begin energy/time    range / gamma/ns       :: -999
(7) end ..                                      :: 150
```

- In 'in_kmix' file, line (5) should be the following for both SMS and CMS.

```
(5) separation of the SR pulses / ns                :: 153
```