***File storage:***

The output files from using internal\_correlation\_function, complete\_relaxation\_rate\_program, and noe\_curve can be deleted almost entirely. This reduces the file storage from >200 GB for a protein with 16 sparse residues to a couple of MB.

*Internal correlation and complete relaxation rate calculations*

For a given magnetic field, the required files to reproduce the noe build-up curves are

complete\_relaxation\_rate\_matrix\_...\_.. (1)

for each sparse residue. In the example crrm directory this is complete\_relaxation\_rate\_matrix\_14\_21. The noe\_curve program will parse these files in creating the build-up curves. The same name is used for this header file in the complete relaxation rate matrix directory for each residue. For N sparse residues, there will be N required files in order to reproduce the noe build-up curves. All other files in the internal correlation function and complete relaxation rate directories can be deleted.

If more than one magnetic field, i.e. different spectrometer such as 900 or 600 MHz, is used, then it is recommended to run the complete\_relaxation\_rate\_program for both before the file deletion. Store the different magnetic field results in different directories for each magnetic field. Then delete all files from the fist 2 programs except for (1) in each directory.

*Noe curve program*

This program takes several minutes to run for each sparse residue. To minimize the file memory use all of the output files should be deleted. The program should be run and after the excel sheet with all of the 1-D curves are created, then the output files should be deleted.

The software is designed to be modular – that is, minimize the inputs at each step of the calculation to the set of 1-D spectral curves. All of the calculations of the noe build-up curves and the resulting spectra can be reproduced if these files are not deleted:

1. complete\_relaxation\_rate\_...\_...
2. predicted chemical shift files

In this way the initial/final spins of the protons can be changed and used to recalculate the noe build-up curves and spectral curves.

All of the files could be deleted except for those mentioned. After doing this, however, the magnetic field can not be changed. That is the reason for calculating all of these files for the different desired magnetic field before deletion.

The amount of memory used should be on the order of a couple of MB. If the files are not deleted then the memory used could be hundreds of GB.