Quick Acquisition of 2D Spectra using Non-Uniform Sampling (NUS)
Basic Concept of Non-Uniform Sampling

• Generally, multi-dimensional NMR data is acquired linearly in uniform time increments and is then processed using a FTT algorithm.

• The data points acquired in the indirect dimension(s) form a grid where the distance between the points on the grid is given by the sweep width and the number of points by the TD for each dimension respectively.

• The key principle of NUS is to acquire only a subset of data points in a random manner while still using the same grid.

• As seen in the figure to the right, only 25% of the data points are collected. With the reduced acquisition time in the direct dimension, the overall experimental time will be much lower.
NUS Setup in Topspin

- Bruker has made NUS acquisition standard in TOPSPIN 3.0. **For now, this is only available on the UTL300 and UTL400 spectrometers.**
- **Steps:**
  1. Read in the desired 2D sequence that you would like to acquire.
  2. Under the *AcquPars* tab in the *Experiment* section, set *FnTYPE* to “non-uniform_sampling”
NUS Setup in Topspin

3. On the left list, click on NUS to get to the NUS parameter section
NUS Setup in Topspin

- Acquisition parameters:
  - **NusAMOUNT[%]** - percentage amount of sparse sampling, default is 25
  - **NusPOINTS** - number of complex data points to be recorded, for nD experiment it is \([(td_1 \times td_2 \times \ldots \times td_n) \times \text{amount} / 100] / 2^{(n-1)}\)
    - Note: As a rule of thumb the number of hypercomplex points should be at least the same as the number of frequencies (signals in the spectrum).
  - **Jsp [Hz]** - J coupling, default is 0. In the case of J evolution in an indirect dimension the points acquired can be matched to the maxima of such a FID by setting this coupling constant.
  - **T2 [s]** - T2 relaxation time, default is 1. For indirect dimensions with so called real time evolution the FID in the indirect dimension will decay according to the T2 relaxation time of the spins evolving in this dimension. By setting the T2 parameter according to the relaxation time, parts of the FID with more intensity will be strengthened (exponential weighting of sampling scheme)
    - Note: If an evolution period is implemented as constant time in the pulse program, exponential weighting must not be used!
  - **seed** - random number generator seed, responsible for the different distribution of data points, default is 54321
  - **Calculate** - allows to calculate and then view the distribution of points without starting the experiment.
NUS Processing

• Processing can be done using:
  – Topspin 3.0 or higher with the additional NUS processing license (JHU does not have this specific license).
  – Mestrenova 9.0 or higher.
    • With MNOVA this is standard and is available for all license types. It is available on the 45 day trial version of the full version, however, MNOVA Lite does not support NUS processing.

• Processing with either software is straight forward:
  – Read/open the data set and process as you normally would
  – The software looks for specific files, which are generated with NUS data, and read in the proper parameters for data extrapolation / calculation.