Implementation of interleaved experiments with Delta Software

Product used : Nuclear Magnetic Resonance (NMR)

Some NMR experiments are combination of two or more individual experiments. Difference experiment of 1D (STD experiment) or 2D type (IPAP experiment) are examples of experiments that consist of two individual experiments. Because the result of combination can still be presented as NMR spectrum, we often refer and treat them as single experiments. There are other cases where rather than combining spectra we combine information and therefore the result of combination cannot be presented as another spectrum. For instance, in order to estimate the value of a variable we may need to feed a mathematical equation with intensity values obtained from different experiments. In all above cases whether we are concerned about the quality of the combined spectrum or the accuracy of the calculated value, it is important that combined experiments are measured under identical conditions. This is particularly true for unstable samples. For this reason, it is strongly recommended that they are conducted in an interleaved way. Delta software implements interleaving at the innermost loop that is the scan loop. Exact form of interleaving (every scan or every second scan etc) is determined by the user through acquisition parameters.

Linear and Interleaved acquisition

In linear mode, experiments are executed linearly that is sequentially, first the first experiment then the second one etc (Fig.1).
In interleaved mode, scans from different experiments are intertwined to the result that all experiments complete simultaneously (Fig.2 and 3). Whether scans from different experiments would be saved separately or not would determine whether the desired spectrum would be obtained directly or after appropriate processing. It is up to the user to decide by setting accordingly related acquisition parameters.

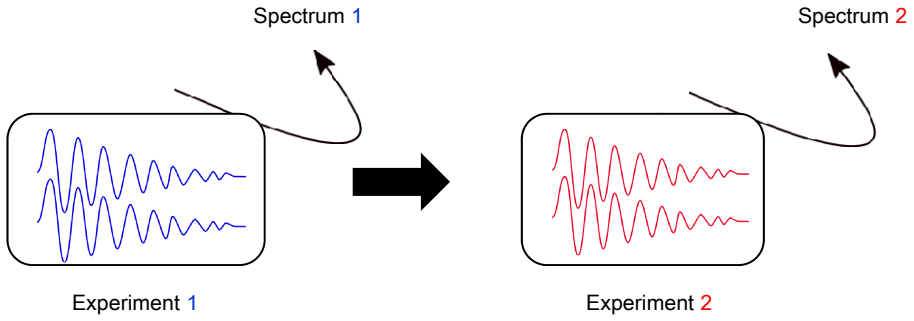

Fig 1: Two 1D experiments executed in linear mode

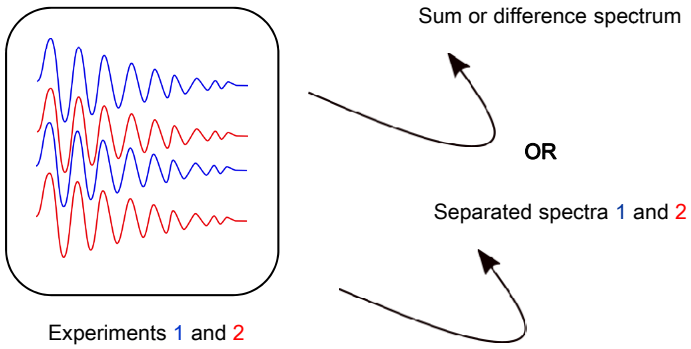

Fig 2: Two 1D experiments executed in interleaved mode

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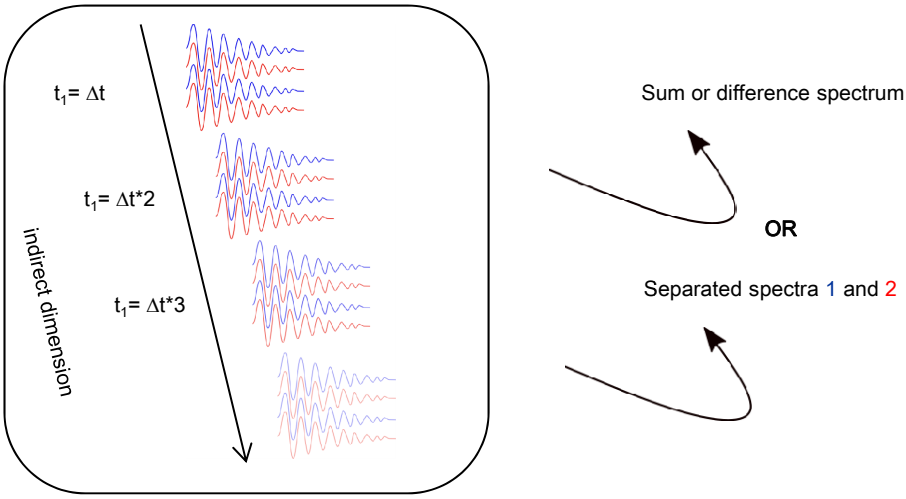

Fig 3: Two 2D NMR experiments executed in interleaved mode. If we interleave every second scan then for each point in the indirect dimension we collect first the FID of one experiment and then the FID of the other. In other words, we implement interleaving at the level of t_1 loop

An implementation example

To demonstrate the flexibility of Delta software in implementing interleaved experiments, we offer the following example: "CRISIS ghsqcad" experiment can be conducted in three different modes according to the value of acquisition parameter ' multiplicity_edit_mode' .Three different values are provided: 'up_down', 'off', and 'CH_only'. With minor changes in the pulse program file of the above experiment (Fig.4), we executed 'up_down' and 'CH_only' experiments in an interleaved mode.
Because we opted not to save scans from different experiments separately, we obtain directly the difference spectrum that shows only the CH_2 and CH_3 signals distinguishable by their phase sign (Fig.5). By using interleaved mode we ensure that the two experiments are executed under identical conditions. Moreover, by saving the two experiments separately, the user can later combine them in different ways.

```
edit_multiplier   = if multiplicity_edit_mode = "up_down" then 2.0 else
                    if multiplicity_edit_mode = "CH_only" then 1.0 else
                    2.0;
```

```
edit_multiplier   = if multiplicity_edit_mode = "up_down" then 2.0 else
                    if multiplicity_edit_mode = "CH_only" then 1.0 else
                    if multiplicity_edit_mode = "CH2CH3_only" then {2.0,1.0} else
                    2.0;
```

Fig 4: An interleaved experiment was prepared with minor changes in the pulse program file.
Part of the pulse program file of interleaved experiment (right) in comparison with the original one (left).

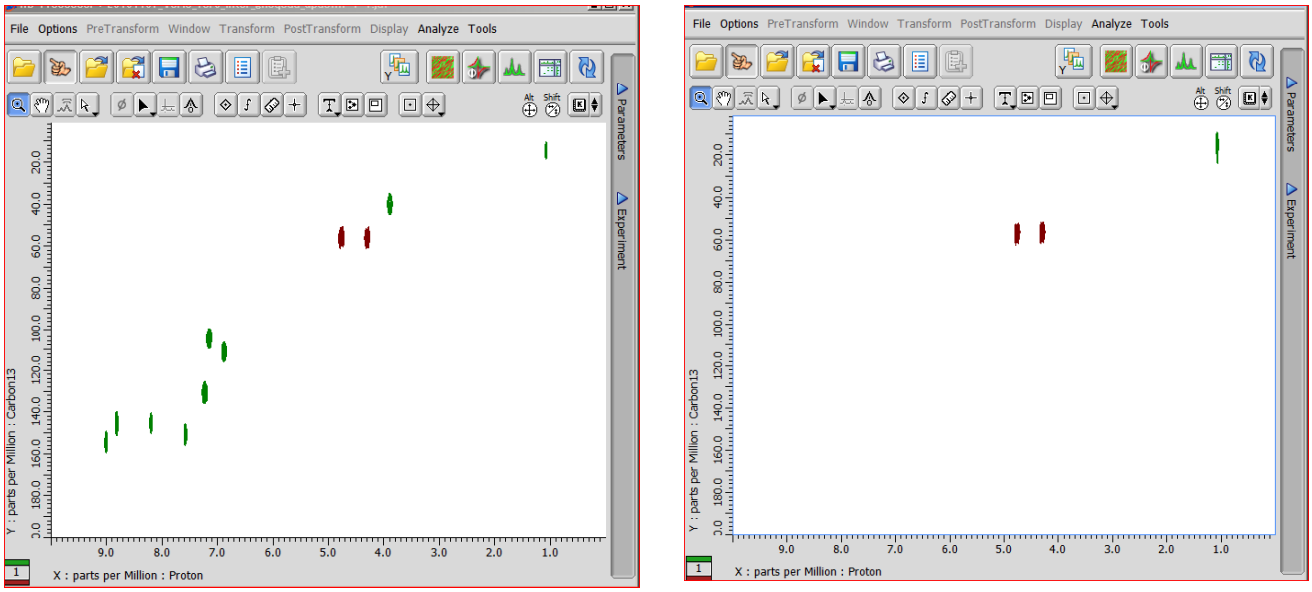

Fig 5: 'up_down' experiment (left) and difference experiment of 'up_down' and 'CH_only' experiment implemented in interleaved mode (right).
Sample: Voriconazole in DMSO-d6

console: JNM-ECZ400S+ROYALPROBE™ HFX

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