NMR Tips for Shimming, Part II

Computerized shimming with the Simplex algorithm

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Introduction

In Part I of this series [1] a number of general concepts and recommendations were presented regarding NMR sample preparation and the physics and strategies involved in the optimization of magnetic field homogeneity (shimming) for high-resolution NMR spectroscopy. Beginning with Bruker's AM/AC spectrometer generation with the Aspect 3000 computer, software routines for automatic computer-based shimming were introduced (the *TX* command in DISNMR), namely, the *Tuning* and *Simplex* algorithms. Both of these methods were carried over to later spectrometer generations and are available in the current versions of XWIN-NMR and TopSpin in the form of the *tune* command and the *tunefile* script. The handling of *tunefile* scripts and the details of their command syntax, applicable to both the Tuning and Simplex methods, were covered thoroughly in Part I (knowledge of this material will be assumed in the following). Furthermore, the strategies and internal workings of the Tuning algorithm itself were discussed and script examples presented. In this report, Part II in the series, the more sophisticated *Simplex* algorithm will be presented. Both Tuning and Simplex have the advantage that they can be used with any spectrometer that offers computer control of shim settings. The main disadvantage is the amount of time required to achieve optimal field homogeneity and the "local optimum" problem associated with multidimensional search algorithms (Simplex).

For the latest generations of spectrometer hardware, applications utilizing pulsed field gradients have become readily available. With this technology a new method called *gradient shimming*, based on field-mapping methods derived from NMR imaging, was introduced in the form of the *GradShim* routine. The basic theory and practice of this extremely efficient method will be treated in Part III, which will appear in the next *SpinReport* issue.

The Simplex Algorithm

The Simplex method can be thought of as a multidimensional Tuning procedure with some additional intelligence added. Instead of blindly adjusting one shim after another, the Simplex method changes all shims in a defined group simultaneously and

seeks to optimize *combinations* of shim values via the quality parameter (lock signal amplitude or FID area). The *simplex* can be thought of as an n-dimensional geometrical object (polygon) defined by $n+1$ sets of shim values and the associated quality parameter values. The simplex moves through shim space (**Fig. 1**) by processes called reflection, expansion, and contraction. Expansion increases the volume of the simplex, i.e., the stepsizes for one or more shims; contraction reduces the stepsizes. With each iteration the worst shim set is replaced by a new improved set, if one is found. With time, not only the best shim set improves but all sets which make up the simplex will improve in quality as the (hopefully) global maximum is approached and the volume of the simplex (stepsizes) decreases. The algorithm terminates when a predefined minimum simplex volume (defined by the minimum shim stepsizes *endstep*) has been reached.

Thus, the simplex is like an amoeba, crawling through shim space and looking for maxima in the hypersurface representing the quality parameter. The amoeba moves away from the lowest point, expands when it senses positive improvement in the distance and pulls itself in that direction, or contracts when it senses that it is sitting on a narrow peak or when only negative changes are sensed nearby.

The Simplex method (see text box) contains several decision-making procedures and offers more flexibility in response when compared with the Tuning procedure. By working with complete shim groups and combinations of shim settings, the Simplex method can more readily sniff out complex interactions and dependencies between different shims and is, therefore, much better suited for handling high-order shims in combination with their low-order partners. The only limitation in the method is that, if the starting point is very far from the global optimum, the simplex may seek out a nearby local optimum. Thus, when searching for an optimum for some difficult high-order shims, it is probably best to perform a series of simplex procedures with significantly different starting values for the high-order shims in question. Alternatively, one could set a high-order shim such as Z6 to a series of widely spaced fixed values, shim all the lower-order shims (Z1-Z5) via Simplex at each setting, and compare the overall results.
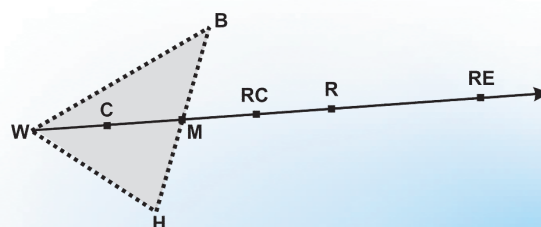

Fig. 1: Graphic representation of a two-dimensional simplex (2 shims) defined by the three vertices *B*, *H*, *W* (best, half, worst; see algorithm). The simplex vector points from *W* towards the midpoint *M*. The distances W-M, M-R, R-RE are equal; the distances C-M and M-RC are half of W-M. The symbols R, E, C refer to the processes *reflect*, *expand*, *contract*. In general, for n shims in a group, the simplex is an n-dim. polygon with $n+1$ vertices.

Simplex Algorithm (see Fig. 1)

1. Define a set of shims that are to be adjusted; define for each shim an *initstep* and an *endstep*.

2. Evaluate the quality parameter (*QP*) for the current set of shim values.

3. Add *initstep* to each of the *n* shims, one at a time, to create an initial *simplex*, which is equivalent to an *n*-dimensional polygon with $n+1$ vertices; each vertex represents one combination of shim values at which *QP* is evaluated.

4. Define simplex. The current list of *QP* values and their associated shim settings can be ordered from bottom to top (pos. 1 to $n+1$) as worst *W* to best *B*. The shim set at or just below the midpoint in the list (depending on whether $n+1$ is odd or even) is labeled *H*.

5. Create a simplex vector pointing from the "worst" vertex (lowest quality parameter) through the "midpoint" *M* of the (*n*-1)-dim. "surface" containing the other vertices.

6. Reflect the worst vertex *W* through *M* to create a new combination of shim values *R* and evaluate the result.

7. If $R > B$ in quality, i.e., $QP(R) > QP(B)$, then evaluate the expanded reflection *RE*.

8a. If $RE > R$ in quality, *replace* the shim set *W* in the list with *RE* (*RE* rep. *W*; reflect and expand simplex). Go to (16).

8b. If $RE <= R$, then *R* rep. *W* (reflect simplex). Go to (16).

9. If $R <= B$ and

    a) If $R > H$ (upper half of quality range), then *R* rep. *W* (reflection). Go to (16)

    b) If $R <= H$, (lower half) go to (10)

10. Evaluate point *RC* halfway between *M* and *R* (reflect and contract simplex).

11a. If $RC > R$ and

    1) If $RC >= W$, then *RC* rep. *W*. Go to (16).

    2) If $RC < W$, then go to (12).

11b. If $RC <= R$ and

    1) If $R >= W$, then *R* rep. *W*. Go to (16).

    2) If $R < W$, then go to (12)

12. Evaluate point *C* halfway between *W* and *M* (contract simplex).

13a. If $C > W$, then *C* rep. *W*. Go to (16).

13b. If $C <= W$, then no improvement above *W* was found. Go to (14).

14. Rotate direction of simplex vector. Use next higher quality shim set as vertex for constructing simplex vector via step (5). If still no improvement is found, perform this rotation procedure up to *n*-1 successive times. If still no improvement above *W* can be found, then go to (15).

15. Create new simplex starting from current best shim set *B* using current increments; continue with step (5).

16. Check for convergence. If shim increments have been reduced by contraction to < *endstep* for all shims (simplex volume has reach the desired minimum), terminate shimming; otherwise continue at (4).

Simplex Setup

The Simplex method requires basically the same setup in the *tunefile* script as for the Tuning method. The commands ROTATION, TIMEOUT, USE_LOCKLEVEL, USE_FIDAREA are used to define basic conditions and the quality parameter to be used. Specifically for Simplex, however, the definitions of the initial step size and final step size for *each* shim to be used must be made in preparatory SET statements (see Part I, Table 2) before shimming begins.

    SET *shim_name initstep endstep*

The required values for *initstep* can be based on the set of increments determined as described in Part I for the Tuning method (i.e., *initstep* should cause 5 - 15% change in the quality parameter). With larger *initstep* values a larger initial simplex is generated in shim space, covering a larger range of shim value combinations but taking a longer time to contract and converge on the maximum. With smaller *initstep* values the smaller initial simplex will converge faster but may end up on a local rather than the global optimum. In general, *initstep* should increase with shim order, e.g., from small values of 20 - 50 for the X,Y,Z shims to values of 1000 - 10000 for third- or higher-order shims. The shimming procedure is initiated by the script command SIMPLEX followed by a list of names of the shims (separated by spaces) to be adjusted simultaneously.

    SIMPLEX *shim_1 shim_2 ... shim_n*

As the simplex contracts during shimming, the shim stepsizes will decrease, and the procedure will terminate when all stepsizes are below the values *endstep*. These values should be roughly *proportional* to *initstep* (e.g., 10% of *initstep*) and should represent increments that still cause barely detectable changes (e.g., 0.5 - 1%) in the quality parameter. If the *endstep* are (a) too large, the routine may terminate before a maximum is accurately found, (b) too small, the simplex will waste time by crawling around the maximum for a long time after it has been found. Thus, some experience on the spectrometer at hand will be needed in order to find an efficient set of parameters.

Simplex Execution

An example of a *tunefile* script for Simplex shimming is shown in the colored box. Simplex commands can be alternated with Tuning commands, can be placed in loops, or can be performed in succession using "coarse" and "fine" stepsizes. In principle, a Simplex group could contain any number of shims, but in practice it is probably better to work with a maximum of 6 - 8 shims at a time to keep the iteration time reasonable (5 - 20 min per group). The Z*n* shims form one natural group and can be shimmed with or without sample rotation. The X,Y shims come in pairs which should be taken together and shimmed

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```
# tunefile script for SIMPLEX

# set initial and end step sizes

SET Z 20 4

SET Z2 30 4

SET Z3 100 10

SET Z4 300 30

SET Z5 600 60

SET X 30 5

SET Y 30 5

SET XZ 200 20

SET YZ 200 20

SET XZ2 800 80

SET YZ2 800 80

SET XY 500 50

SET X2Y2 500 50

SET XYZ 2000 200

SET X2Y2Z 2000 200

SET X3 5000 500

SET Y3 5000 500

# turn on sample rotation

ROTATION ON WAIT

# use lock level

USE_LOCKLEVEL

# initial on-axis shimming

SIMPLEX Z Z2 Z3

ROTATION OFF WAIT

# off-axis shimming up to third order

SIMPLEX Z X Y XZ YZ XZ2 YZ2

SIMPLEX XY X2Y2 XYZ X2Y2Z X3 Y3

SIMPLEX Z X Y XZ YZ

ROTATION ON WAIT

USE_FIDAREA

# final shimming on-axis using FID

SIMPLEX Z Z2 Z3 Z4 Z5
```

While the Tuning method can be used effectively only for shims to second or perhaps third order, the Simplex method can be used to adjust *all* available shims in a stepwise manner using logical groups of shims. Thus, Simplex can be used to perform a thorough first-time shimming of a new probehead, for example. There are obviously many ways to combine the off-axis and $3D$ shims, e.g., constant X,Y components with various Zn or a constant Zn component with various orders of X,Y. When extensive off-axis shimming is required, it is probably best to proceed in an up-down cycle, beginning with groups of low-order shims, progressing to higher-order groups, and then returning successively to the lower orders. The last round of shimming should always include the first-order shims X,Y,Z. Off-axis shimming will usually only be necessary once a day or even less frequently. Tuning of $Z1$-$Z3$ or Simplex shimming of $Z1$-$Z4$ should be sufficient to handle sample-to-sample variations in routine work. Changes in solvent, temperature, or volume may require Simplex shimming up to $Z6$.

Although shimming with the lock signal as quality parameter is significantly faster than use of the FID, it is also significantly less sensitive (see Part I). One strategy would be to use the lock for off-axis shimming and the FID for Zn shims. However, one should keep in mind that for typical applications at very high field strengths with data acquisition *without* rotation, both the on- and off-axis shims will influence lineshape and hump.

Simplex in DISNMR

In the Aspect 3000 software module *TAXIS* (*TX*) the Simplex routine operates as described above with minor differences. The routine performs automatic adjustment of *initstep* in a preliminary setup round to give at least 6% change in QP; the user can only set an upper limit for *initstep* with a single parameter *J0*. Only a single *endstep* value can be set with the parameter *R9*. Termination of iterations occurs (a) when at least half the shim increments are less than *R9* (convergence) or (b) after $(n+1)^2$ iterations without improvement.

without rotation, e.g., X, Y, XZ, YZ, XZ2, YZ2. It is also useful to include Z in an off-axis shim group to adjust for changes in Z that may occur with and without sample rotation (vortex formation in short samples).

References

Hull WE, Bruker SpinReport 152/153 (2003) 53-61.