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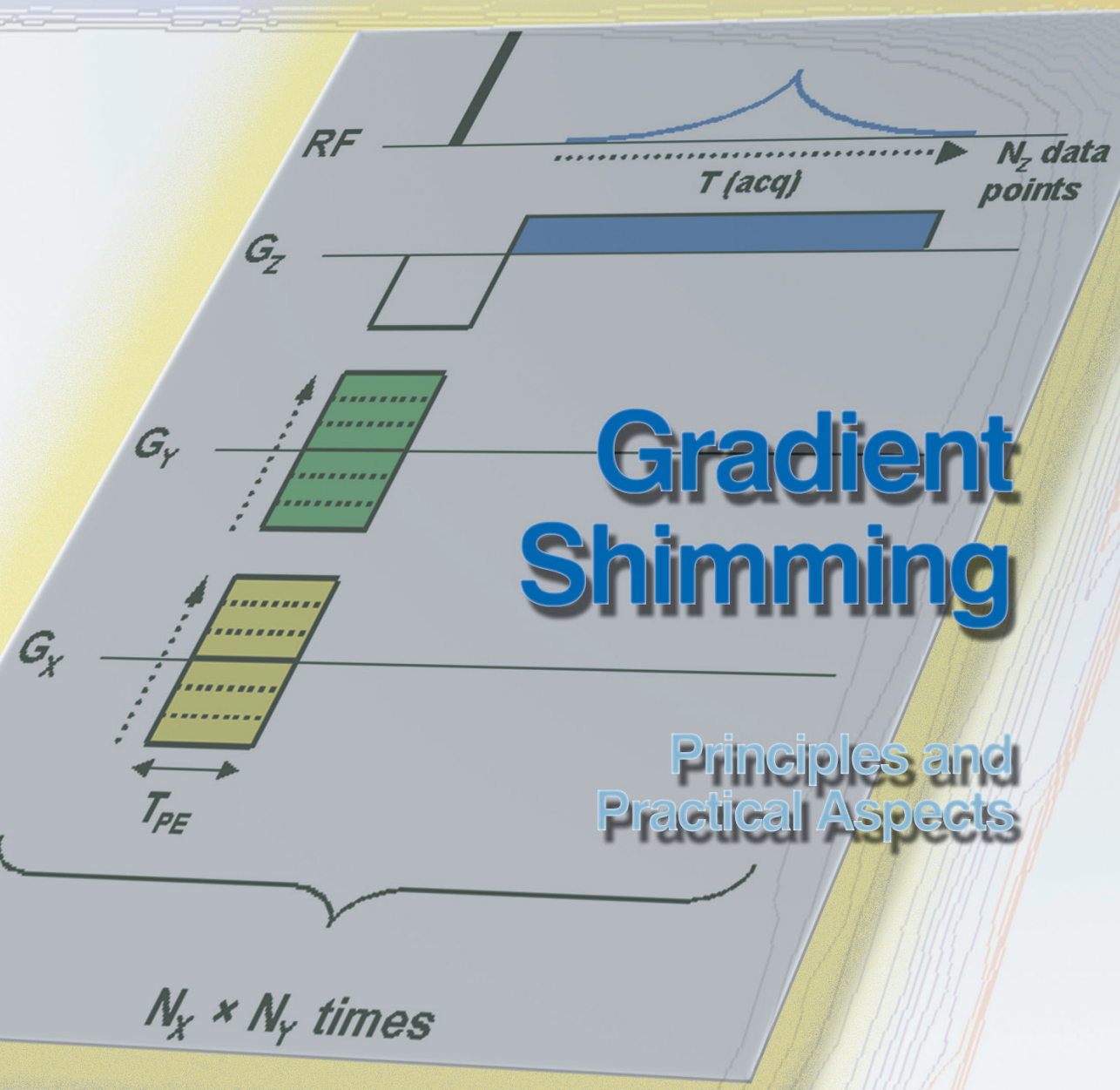

Gradient Shimming

Principles and Practical Aspects

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Gradient Shimming: Principles and Practical Aspects

NMR Tips for Shimming, Part III

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Introduction

Shimming is the process of adjusting the homogeneity of the static magnetic field B_0 by changing the currents through a set of field gradient coils called the shim system. In Parts I and II of this series of articles [*1*,*2*] several aspects of the classical shim hardware and methods and many practical considerations have been discussed. Conventional shimming techniques involve either manual or computerized adjustment (e.g., the *tuning* or *simplex* algorithms described earlier) of appropriate groups of shims and an iterative search for an optimal value of some quality parameter such as the deuterium lock signal amplitude, the ^{1}H FID area, or some lineshape parameter (linewidth, hump). By virtue of the nonlocalized NMR measurement, the detected signal and the derived quality parameter are integrated over the entire detected sample volume and provide only an indirect measure of field homogeneity. Without prior knowledge these methods may require a very large number of iterations, and, particularly when the FID is used as quality parameter, the information feedback loop can require several seconds per iteration. Although proper shimming by conventional methods is not a random process, it can still be quite time-consuming when more than three shims are to be adjusted, and the time required (5 - 20 min or more) can become a significant fraction of the total time needed for routine experiments. Furthermore, the quality of shimming can be highly dependent on the operator's expertise or sample properties, and optimal shim values may not be found in the time allotted for shimming under automation, for example.

Fortunately, the more recent generations of NMR spectrometers provide features such as actively shielded field gradient coils and high-speed gradient current amplifiers which open the door to an entirely new class of shimming methods based on spatial encoding techniques well-known in NMR imaging [*3-5*]. These methods involve the use of gradient echos to actually map the spatial variation of B_0 over the sample and the specific systematic variations caused by each individual shim gradient. Mathematical algorithms can then calculate directly the shim increments needed to minimize B_0 variations, i.e., to maximize homogeneity, essentially in a single or very few iterations. Due to the employment of gradient coils the imaging-based method has become widely known as *gradient shimming*.

In the first part of this article the principles of gradient shimming are described, including a brief introduction to NMR imaging, field mapping, and the shimming procedure itself. The one-dimensional (1D) problem appropriate for optimization of the on-axis Zn shims for probeheads containing a Z-gradient coil is considered first. The technique is then extended to the shimming of off-axis shims for probeheads equipped with a three-axis gradient system. Finally, the specific requirements for a hybrid method of 3D field mapping using a Z-gradient coil in the probehead together with the X and Y shim gradient coils in the shim system are explained.

The second part of this report discusses practical aspects of gradient shimming, translating the theoretical principles into practical execution using Bruker's GradShim software tool, the current implementation for gradient shimming on Bruker spectrometers using XWIN-NMR™ or TopSpin™ software. Hardware requirements, preparation procedures, parameter settings, and step-by-step procedures for GradShim are given.

Principles of Gradient Shimming

NMR Imaging

In the NMR spectroscopy of liquid samples, if the B_0 field is homogeneous across the detected sample volume, signals from equivalent spins I with magnetogyric ratio γ and screening constant σ (responsible for the chemical shift) will have the same Larmor frequency $\omega_0 = -\gamma(1 - \sigma)B_0$ at different locations in the sample, and a single homogeneous resonance line will be observed in the spectrum. In the following we will generally work in the reference frame rotating at the rf carrier frequency $\omega_{rf} = \omega_0$, i.e., the on-resonance condition, and only the relative resonance frequency $\Omega = \omega - \omega_{rf}$ (a function of the applied field gradients and spatial coordinates) will be of interest. As usual, the B_0 field and all other field components are assumed to be oriented along the z-axis.

In contrast to NMR spectroscopy, which requires a homogeneous B_0 field, NMR imaging applies constant field gradients to spatially encode the NMR signal. For example, G_z can be applied so that the total field and the resonance frequency Ω are linear functions of the z coordinate,

$$\begin{aligned}\Omega(z) &= -\gamma\,(1-\sigma)[B_0 + G_z z] - \omega_0 \\ &= -\gamma\,(1-\sigma)\,G_z z \cong -\gamma\,G_z z \end{aligned} \qquad (1)$$

whereby for a given set of spins the chemical shift effect represented by σ in Eq. 1 can be neglected. The position $z = 0$ is defined by the center of the gradient coil (isocenter where $B(z) = B_0$) and is usually closely aligned with the center of the rf coil.

If the so-called *read* gradient G_z is applied *during acquisition* of an FID, then the spatial coordinate z is encoded and *read out* as a frequency component $\Omega(z)$. This situation is depicted in **Fig. 1** and is termed *frequency encoding* of spatial information. Such an experiment can be performed with a high-resolution NMR probehead containing a Z-gradient coil. Fourier transformation of the frequency-encoded FID, followed by magnitude-mode calculation, results in a z-profile or 1D projection image of the sample, where the signal intensity at frequency $\Omega(z)$ represents the integrated signal (spin density) for the corresponding xy-plane perpendicular to the z-axis at the position z.

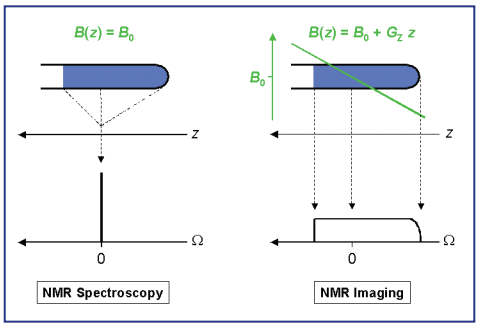

Fig. 1: Frequency encoding of spatial information using a magnetic field gradient. In NMR spectroscopy (left) a homogeneous magnetic field B_0 is applied across the entire sample to give a single resonance line (chemical shift) for each set of equivalent spins in the sample, e.g., protons in water molecules. Here the receiver offset frequency for the rotating reference frame has been placed on-resonance to give $\Omega = 0$ (for definitions, see text). For NMR imaging (right) the B_0 field is given a systematic linear variation along the z-axis by applying a gradient G_z during data acquisition. In this case the resonance frequency Ω varies linearly with the coordinate z. The displayed magnitude-mode spectrum represents a z-profile or 1D projection image of the sample, where signal intensity is proportional to spin density in the xy cross section at each value of z. Note that for spins with positive γ and for positive G_z, increasing z values result in increasing negative frequency in the rotating frame (Eq. 1). Spectrometer software conventions simply treat increasing negative frequencies as increasing positive numbers and display the Ω axis as increasing from right to left.

Depending on the type of pulse sequence used for preparation and acquisition, the signal intensities in the z-profile can be weighted according to properties such as T_1, T_2, T_2*, diffusion coefficient, etc. An important criterion for obtaining a "clean" z-profile is the presence of a single dominant resonance (with on-resonance chemical shift), resulting in an unambiguous correlation between z coordinate and the resonance frequency $\Omega(z)$ according to Eq. 1. This situation applies for ^{1}H NMR of aqueous samples (e.g., 90% H_2O/10% D_2O as solvent), and such samples are ideally suited for gradient shimming on the ^{1}H signal of water. For conventional analytical NMR samples in deuterated solvents with a single ^{2}H signal, gradient shimming on the solvent ^{2}H signal can be performed in the same manner.

If the sample's spectrum contains two or more strong signals and nonselective excitation is used, then multiple overlapping profiles will be generated with intensities and relative shifts in the frequency domain defined by the relative signal intensities and chemical shifts of the signals detected in the normal 1D spectrum. In such cases the use of shaped pulses for selective excitation of a single chosen resonance will be necessary to obtain a clean z-profile.

For the simple magnitude-mode profile discussed above (Fig. 1), the Z-gradient is switched on following the excitation pulse and left on for the duration of the FID. This is sufficient for determining spin density, for example. However, for gradient shimming we are interested in obtaining the full phase information available in the signal since this will be quite sensitive to field inhomogeneities. For this purpose an echo signal is desired and can be conveniently obtained using the *gradient-echo* sequence shown in **Fig. 2**. Following excitation, the transverse magnetization is dephased with the first gradient pulse and rephased with the second gradient pulse, which is left on as the *read* gradient during the data acquisition period T to generate a frequency-encoded echo signal. The degree of dephasing or rephasing depends on the time integral over the gradient pulse, and for rectangular gradient pulses the *maximum* in the echo signal (complete rephasing) occurs at the *echo time* TE when Eq. 2 is satisfied.

$$G_z^{Dephase}\, T^{Dephase} + G_z^{Read}\, T^{Rephase} = 0 \qquad (2)$$

The echo immediately dephases again for $t > TE$ since the gradient remains on. The gradient strength (in G/cm) required during acquisition can be calculated from

$$G_z = N_z / (\gamma\, T\, FOV_z) \qquad (3)$$

where N_z is the number of complex data points sampled during the acquisition time T (in s); γ is the magnetogyric ratio for the nucleus being measured (in Hz/G); FOV_z is the *field-of-view* (cm) along the z-axis and is normally chosen to slightly exceed the detectable z-dimension of the object under study (i.e., the sample length or the effective rf coil length). By analogy with the definition of spectral resolution, the spatial resolution is given as

$$\Delta z = FOV_z / N_z \qquad (4)$$

As a practical example: for ^{1}H imaging with $\gamma = 4258$ Hz/G, $N_z = 256$, $T = 10$ ms, and $FOV_z = 30$ mm, the desired gradient strength would be $G_z = 2.0$ G/cm, and the spatial resolution would be $\Delta z = 0.12$ mm.

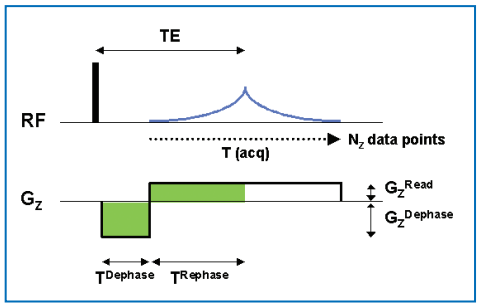

Fig. 2: The simplest gradient-echo imaging sequence for acquiring a *z*-profile. The nonselective rf excitation pulse is followed by a short *dephasing* gradient with sign opposite to that of the weaker rephasing or *read* gradient. Typically, the gradient amplitudes and timings are adjusted according to Eq. 2 to achieve a gradient-echo at time *TE* near the center of the data acquisition time *T*(acq). The echo maximum occurs at the time point when pos. and neg. gradient areas (green) are equal.

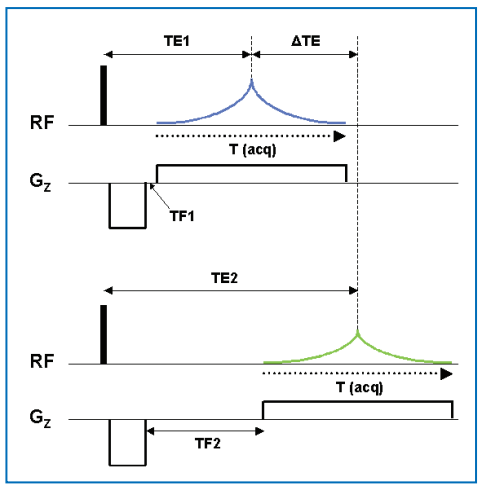

Fig. 3: 1D B_0 field mapping using gradient echos. The sequence shown in Fig. 2 is performed with two different values of *TE* by inserting a variable free-precession delay *TF* between the two gradient pulses. The two frequency-encoded *z*-profiles exhibit differences in phase that are proportional to $\Delta TE = TE2 - TE1 = TF2 - TF1$ and to the deviations (inhomogeneities) $B_i(z)$ in the static field B_0.

Field Mapping

The gradient-echo technique discussed above can be used to map field *inhomogeneities* in the *z* direction, $B_i(z)$, i.e., the *deviation* in the static field from its nominal value B_0 as a function of *z*. The local resonance frequency offset $\Omega_i(z)$, which is proportional to $B_i(z)$, is encoded into the phase of the NMR echo signal. The evolution of signal phase caused by field inhomogeneities is additive to and independent of the evolution caused by the imaging gradient G_z itself, whose phase evolution is then "undone" during image reconstruction. However, in order to avoid image distortions due to the inhomogeneities, G_z should be large with respect to the field gradients associated with $B_i(z)$.

The best representation of the phase for the complete echo signal is taken at the echo time, neglecting the duration of the acquisition. Thus, the signal phase at a location *z* for an acquisition with echo time *TE* is given by

$$\varphi(z,TE) = \Omega_i(z)TE + \varphi_0(z) = -\gamma B_i(z)TE + \varphi_0(z) \qquad (5)$$

where $\varphi_0(z)$ is an unknown local phase offset resulting from instrumental conditions, for example, and can be eliminated from the equations by taking the difference in phase for two identical experiments performed with different echo times *TE1* and *TE2* (**Fig. 3**).

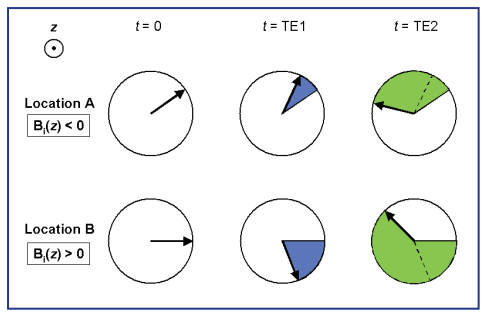

Fig. 4: Phase evolution as a function of position in an inhomogeneous field $B_0 + B_i(z)$. The *z*-axis is perpendicular to the plane of the paper and points toward the viewer. The NMR signal phase can be described as a vector in the *xy* plane of the $\omega_{rf} = \omega_0$ reference frame with an initial phase offset $\varphi_0(z)$ shown at $t = 0$. For positive γ, negative field deviations (location A within the sample) or positive deviations (B) result in counterclockwise or clockwise phase evolution, respectively. The blue and green areas designate the phase accumulated during *TE1* and *TE2*, respectively. The green section between the phase vector and the dashed line represents the phase *difference*, proportional to ΔTE, which is independent of the initial phase and is used to calculate the $B_i(z)$ field inhomogeneity map.

$$\Delta\varphi(z,\Delta TE) = \varphi(z,TE2) - \varphi(z,TE1) = -\gamma B_i(z)\,\Delta TE \qquad (6)$$

The desired field map is then simply

$$B_i(z) = -\Delta\varphi(z,\Delta TE) / [\gamma\,\Delta TE] \qquad (7)$$

Fig. 4 illustrates the behavior of the echo signal phase for two positions in the sample with different *z* coordinates, one with a positive deviation in field and one with a negative deviation.

The results of a typical *z* field mapping procedure are depicted in **Fig. 5** for the case of an NMR sample which is longer than the rf coil. For the sample volume within the coil

a relatively flat signal plateau is observed. At z values corresponding to regions near the upper and lower edges of the rf coil, the signal drops to zero as a result of the decrease in the rf field (flip angle) and the decrease in detection sensitivity that occur at the coil boundaries. Thus, the observed profile represents the rf profile of the coil convoluted with the spin density profile of the sample.

The profile intensity decreases at the longer *TE2*, not only due to T_2 relaxation, but more importantly due to position-dependent dephasing in the *xy* plane (sample cross section) associated with each z value. This dephasing is caused by residual x,y-dependent field inhomogeneities $B_i(x,y)$ and contributes to the so-called T_2* relaxation. The two phase maps shown in Fig. 5 already indicate the form of the field deviations $B_i(z)$, with larger phase changes occurring at the longer echo time *TE2*. Finally, the field map can be calculated from the difference between the two phase maps using Eq. 7. The field map shows the same basic shape as the phase maps but with reversed sign and with the phase offset (linear in z in this case) removed.

Fig. 6 demonstrates some of the difficulties encountered when selecting the echo times *TE1* and *TE2*. The difference ΔTE should be sufficiently large to obtain a reasonable signal-to-noise ratio (S/N) for the phase difference profile $\Delta\varphi(z)$. However, long echo times mean more dephasing due to field variations in the *xy*-plane and loss of absolute signal intensity. Furthermore, at long *TE* values the phase change can exceed π radians, leading to phase wrapping and discontinuities in the phase map. Hence, either the condition

$$-\pi \le -\gamma\, B_i(z)TE + \varphi_0(z) \le \pi \qquad (8)$$

must always be fulfilled or a phase unwrapping algorithm (as employed in the GradShim software) must be applied. In the latter case it is only necessary to satisfy Eq. 8 for phase differences between two neighboring points. For example, for field mapping with $TE = 40$ ms the maximum frequency variation allowed (neglecting differences in the phase offset), either across the entire sample (wrapping not allowed) or from point-to-point (wrapping allowed), is $\pm 0.5/TE$ or ± 12.5 Hz, which corresponds to a field variation of ± 2.94 mG for ^{1}H detection.

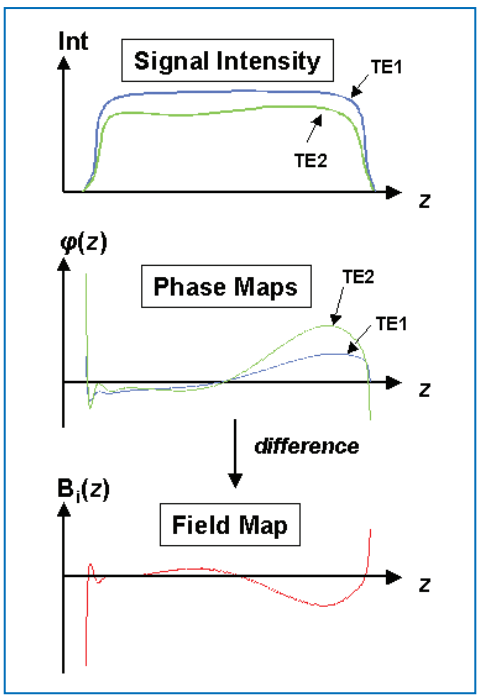

Fig. 5: 1D field inhomogeneity mapping with the sequence of Fig.3 and echo times *TE1* and *TE2*. The z-profile signal intensity (top) decreases at longer *TE* due to T_2* relaxation within the *xy* plane corresponding to each z value. The phase evolution (middle) due to $B_i(z)$ is proportional to *TE*, and the difference $\Delta\varphi(z)$ is used to calculate the inhomogeneity map according to Eqs. 5 - 7.

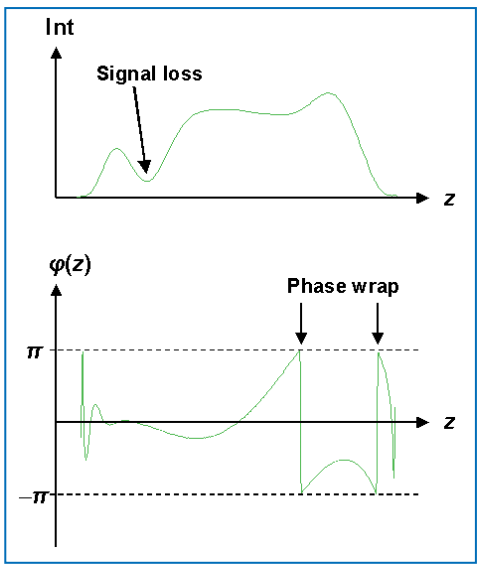

Fig. 6: Signal loss and phase wrapping at long *TE*. A long *TE2* (large ΔTE) improves sensitivity to small field inhomogeneities, but there are limitations due to T_2* -based signal decay and ambiguities due to phase wrapping.

Shim Field Functions

In order to be able to calculate directly the necessary shim currents or increments required to compensate the measured field inhomogeneity $B_i(z)$, the precise spatial distribution of the fields generated by the individual Zj shim coils, on the spectrometer at hand, must be known. Although the ideal field geometries for the various shim gradients are known per definition, for best results it is necessary to use the methods described above to map the *actual* field profiles $B_j(z)$ for each shim j after applying a defined shim current increment U_j. The reference point for this process is the field inhomogeneity map $B_i(z)$ obtained with all shims at near-optimal settings. The desired shim field distribution function per unit shim current, the shim map for shim j, is given by

$$S_j(z) = [B_j(z) - B_i(z)] / U_j \qquad (9)$$

This mapping procedure is carried out for each of the shims to be used subsequently in gradient shimming. Shim mapping need only be executed *once* for a given hardware configuration using the same pulse sequence and acquisition parameters employed in mapping the B_0 inhomogeneities.

Shimming Algorithm

The gradient shimming algorithm aims to compensate the current field inhomogeneities $B_i(z)$ by applying appropriate current increments to a defined set of shims. Mathematically this is equivalent to minimizing the residual field $B_{residual}(z)$ by an optimal choice of the shim coefficients c_j.

$$B_{residual}(z) = B_i(z) - \sum_j c_j S_j(z) = Min \qquad (10)$$

The problem defined by Eq. 10 is uniquely solvable only for the ideal case where the residual field can be brought to zero at all positions z. However, in reality there will always be components of $B_i(z)$ that cannot be fully compensated with the field functions available from the given set of shim coils. The optimization can be executed in a variety of ways, but a common choice is the least-squares method defined in Eq. 11, whereby the sum of squared residuals for N_p data points along the z-axis is minimized.

$$\sum_{k=1}^{N_p} [B_{residual}(z_k)]^2 = Min \qquad (11)$$

Thus, gradient shimming can be thought of as a least-squares fitting of the shim field functions, the basis set $S_j(z)$, to the field inhomogeneity profile $B_i(z)$. The algorithm is illustrated in **Fig. 7** for the case of a shim set comprising the gradients Z1, Z2, Z3, Z4. The top graph shows the initial state of the field inhomogeneity map $B_i(z)$. The middle graph shows the four shim functions multiplied by their "best" coefficients c_j (Eq. 10) and the sum (dashed line) that gives the best approximation to the initial field inhomogeneity map. Application of the shim current increments corresponding to the c_j results in the $B_{residual}(z)$ shown in the bottom graph. The central portion of this plot is flat with near-zero values, but at the highest and lowest z values (corresponding to the edges of the rf coil), high-order curvature of the graph is still evident. It is apparent from Fig. 7 that the edge regions with high-order field deviations cannot be fitted with any combination of Z1, Z2, Z3, and Z4 shim functions. Therefore, for the least-squares evaluation it will be important to select an appropriate value for N_p so that only data points (z values) within the "correctable" zone, corresponding to the

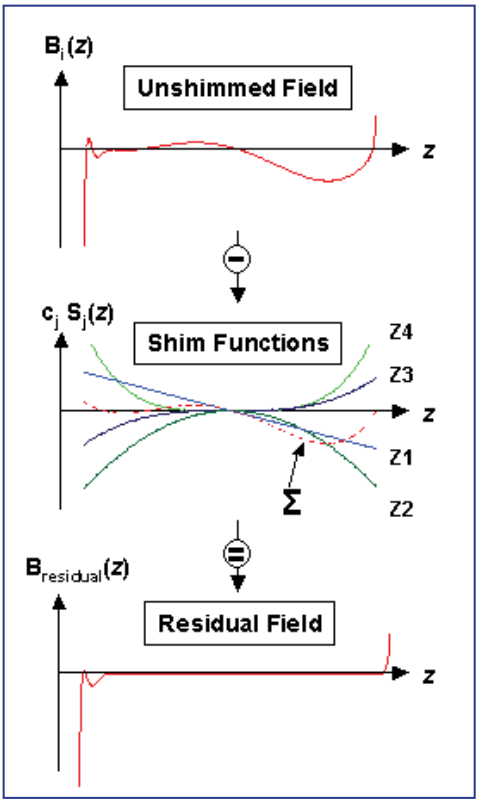

Fig. 7: The 1D gradient shimming algorithm. In a one-time calibration experiment it is necessary to use the method of Fig. 5 to measure the actual field profiles $S_j(z)$ generated by the individual Zj shim coils per unit shim current (Eq. 9). These shim maps must be stored as a library for repeated use. The first step in shimming is to measure the current field inhomogeneity profile $B_i(z)$ (top). An appropriate linear combination (middle, dashed line) of the field profiles for the selected shim functions Z1-Z4 is then computed by least-squares fitting (Eq. 11) to the $B_i(z)$ profile to give the coefficients c_j. The range of z values used for fitting is defined by the number N_p of data points selected. Finally, the shim current increments defined by the c_j are applied according to Eq. 10 to give a residual field with minimum deviation over the range of N_p points.

flat region in the residual field map, are used (see Practical Aspects below).

Ideally, gradient shimming should be a one-step procedure of matching a linear combination of the *measured* shim maps to the *measured* inhomogeneity map. However, a number of practical limitations (measurement accuracy and S/N of the profiles, restricted number of data points along the *z* direction, limited number of shims used in the fitting procedure, nonoptimal settings for shims not used in the fitting procedure) will generally result in small discrepancies between the actual field profile and the profile corresponding to the applied shim corrections. However, as with any least-squares fitting procedure, gradient shimming can be iterated as shown in **Fig. 8**. Iteration will usually improve the results by further reducing residual field inhomogeneities, especially when the initial field was very inhomogeneous. With good S/N and accurate shim maps the convergence of the fitting procedure will be very rapid and typically only two or three iterations will be necessary.

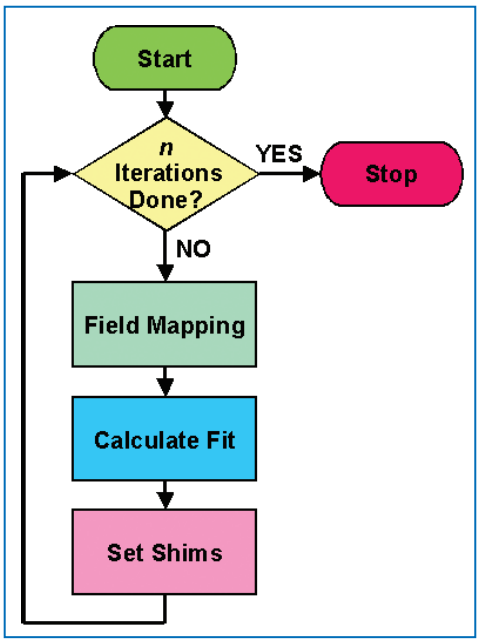

Fig. 8: Iterative shimming procedure using the method of Fig. 7.

3D Field Mapping

In principle, the 1D shimming procedure described above can be readily extended to 3D gradient shimming of on- and off-axis shims by including the coordinates x and y and the gradients G_x and G_y in Eqs. 1-11 above. However, data acquisition must also be extended to all three dimensions, employing X, Y, and Z gradients. This requires a probehead with a three-axis gradient system and an appropriate three-channel gradient current amplifier.

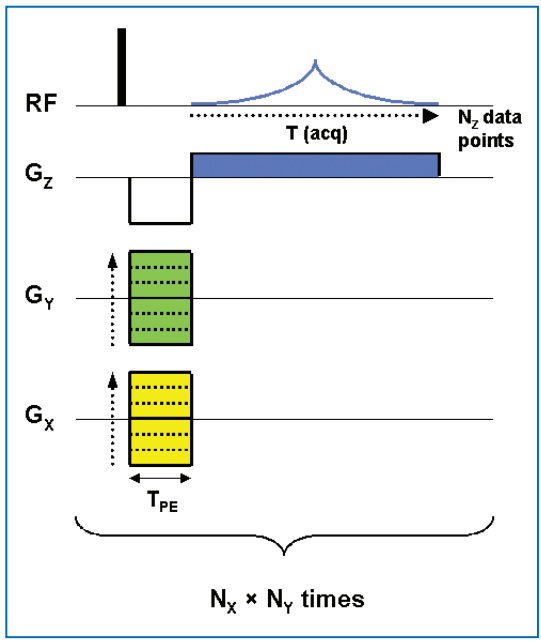

Fig. 9: 3D gradient-echo imaging sequence for a three-axis gradient coil system, employing one frequency-encoding dimension (blue read gradient G_z, N_z data points in acquired echo) and two phase-encoding dimensions with gradient pulses G_y (green), G_x (yellow) of duration T_{PE}. The phase-encoding gradient amplitudes are incremented from $-G_k^{max}$ to $+G_k^{max} - \Delta G_k$, where $\Delta G_k = 2\, G_k^{max} / N_k$ and $k = x$ or y. N_y values for G_y are applied for each of N_x values for G_x, and the total number of data points in the 3D matrix is $N_x \times N_y \times N_z$.

The gradient-echo pulse sequence for 3D imaging shown in **Fig. 9** is based on the 1D sequence of Fig. 2. G_z serves as the frequency-encoding or read gradient, and the additional *phase-encoding* gradient pulses G_y and G_x are applied during the dephasing period prior to acquisition.

Consider for the moment a 2D experiment using only G_y for phase encoding. The pulse sequence is repeated N_y times whereby at each repetition the amplitude of G_y is incremented by a constant amount ΔG_y, beginning, for example, at a

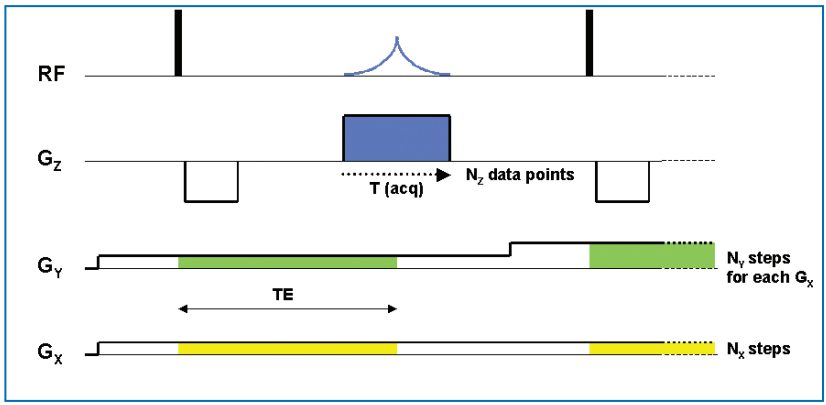

Fig. 10: 3D imaging sequence employing a Z-gradient coil for frequency encoding of the acquired echo (blue) and the Y (green) and X (yellow) shim coils for the application of continuous, ramped phase-encoding gradients using the shim power supply.

maximum negative value $-G_y^{max}$ and ending with $+G_y^{max} - \Delta G_y$. The gradient pulse length T_{PE} remains constant. The incrementing gradient has the same basic function as an incrementing evolution time t_1 in a 2D spectroscopy experiment. The detected gradient-echo signal is frequency-encoded in z and phase-encoded in y. A 2D FT of the resulting $N_y \times N_z$ data matrix generates an image representing a 2D projection of the sample onto the yz plane (the x dimension has not been encoded).

The equivalence of phase and frequency encoding can be understood as follows. Consider acquiring each data point of a 1D gradient-echo in separate experiments. For spectral width sw the first data point is acquired after the first dwell or sampling time $\Delta t = 1/sw$ under the influence of the *constant* frequency-encoding read gradient G_z. The next data point represents the influence of G_z for a time $2\Delta t$, and the last data point is acquired at $N_z\ \Delta t$. The *incremental* effect of the read gradient for *sequential* data points is simply the product $G_z \Delta t$. In the phase-encoding domain the *incremental* effect for *sequential* acquisitions is the product $\Delta G_y T_{PE}$. In one case time is incremented; in the other case the gradient is incremented. When the gradient×time increments are identical, then the two methods and their spatially encoded bandwidths are equivalent.

Consider now the full 3D acquisition sequence of Fig. 9. The X gradient G_x is added as a second phase-encoding scheme. Thus, for each value of G_x with phase-encoding increment $\Delta G_x T_{PE}$ for the x-axis, the value of G_y is stepped through N_y values to give a phase-encoding increment of $\Delta G_y T_{PE}$ for the y-axis. A total of $N_x \times N_y$ echos are acquired with N_z data points each. To improve S/N, NS transients may be acquired for each setting of the gradients. The final 3D data set contains $N_x \times N_y \times N_z$ data points.

The gradient strengths required for 3D applications can be calculated according to Eq. 3 with $T = T_{PE}$. For example, for ^{1}H imaging with $N_x = N_y = 32$, $FOV_x = FOV_y = 1.0$ cm, and $T_{PE} = 3$ ms, the maximum gradient strength would be $G_x = G_y = 2.5$ G/cm. The total duration for a 3D field map with $NS = 1$ for two different echo times and a repetition time of 100 ms would be $2 \times 32 \times 32 \times 100$ ms = 3.4 min.

Using the Shim Gradients for 3D Imaging

The majority of high-resolution NMR probeheads are equipped with only a Z-gradient coil, and the spectrometer may be equipped with only a one-channel gradient current amplifier. For such configurations only the 1D gradient-echo scheme described above can be used for adjusting the Z*n* shims.

In principle it should be possible to use the X and Y coils of the spectrometer's shim system for phase encoding in 3D applications. However, the sequence presented in Fig. 9 requires that not only the Z gradient but also the X,Y gradients be switched on and off very quickly, typically in less than 1 ms, and without distortions caused by eddy currents. With the current generation of NMR spectrometers, the ultrastable shim power supplies are not designed for pulsed operation and cannot rapidly switch shim currents in accurate synchronization with pulse sequences. Furthermore, the shim gradient coils are not shielded so that pulsed gradients would create severe local eddy currents, resulting in unacceptably long settling times.

Fortunately, a modified acquisition technique can be used, whereby the X,Y gradients from the shim system are not pulsed but are *ramped* in a stepwise manner, as depicted in **Fig. 10**. The phase-encoding gradients G_y and G_x are switched on to the required starting values *before* the excitation pulse is applied, with an appropriate delay to allow the shim currents to settle. These gradients remain constant until

the end of the acquisition period, and then the gradients are incremented to their next values. With this technique the relevant duration for phase encoding in the *xy*-plane is the echo time *TE*. When *TE* is increased, the X,Y gradient strengths must be scaled down accordingly.

Two conditions must be fulfilled for this technique to work properly. First, the excitation bandwidth of the rf pulses must be large enough to cover the effective sample profile width generated by the highest phase gradient amplitude. This requirement is easily met for rf pulses of less than 50 μs. Second, the acquisition time T should be relatively short with respect to the echo time minimize overlap of the phase- and frequency-encoding intervals.

Practical Aspects of Gradient Shimming

Shimming based on the gradient-echo technique, as described above, is implemented on Bruker spectrometers with the GradShim tool in XWIN-NMR and TopSpin. GradShim is used in three basic modes or levels of operation.

Level 1: In this setup mode the gradient-echo pulse sequences are executed manually and parameters are optimized to obtain reliable performance for the field strength, probehead, gradient coils, gradient current amplifier, sample type, and NMR signal to be used (e.g. ^{1}H or ^{2}H). The parameters of interest are spectral width, flip angle, repetition time, receiver gain, gradient strengths (profile width and echo position), all delays and especially the free-precession delay between gradient pulses.

Level 2: Once a complete set of acquisition parameters has been defined and optimized for a given GradShim method at Level 1, it is necessary to generate an appropriate library of shim field maps (the shim functions S_j in Fig. 7 and Eqs. 9 & 10) using exactly these parameters.

Level 3: The actual iterative shimming procedure for the current sample is carried out using an appropriate parameter set defined in Level 1 to create maps of the current B_0 field and to compute shim adjustments by fitting the field maps with the corresponding shim maps generated at Level 2.

In general, Levels 1 and 2 need to be performed only once as preliminary experiments for a given hardware configuration, shimming mode and selected test sample. Only the actual shimming procedure at Level 3 will be performed on each of the samples to be studied, using the appropriate parameter set and shim field maps defined at Levels 1 & 2. Whenever changes are made in the acquisition parameters (profile width, echo times, etc.) at Level 1 for application at Level 3, it is *mandatory* that a new set of shim maps be created at Level 2 with these new parameter settings.

System Hardware

The implementation of shimming via field maps based on gradient-echo pulse sequences requires special hardware identical or analogous to that used to generate gradient pulses for gradient-assisted multidimensional NMR, where gradient echos are used for coherence selection rather than spatial encoding. For 1D GradShim optimization of the on-axis (*Zn*) shims, the probe must contain a Z-gradient coil, and the electronics console must include a gradient current amplifier with at least one high-performance channel for pulsed applications. For 3D optimization of on- and off-axis shims two configurations are possible: (a) X,Y,Z gradient coils in the probe and a three-channel pulsed gradient amplifier, or (b) a Z-gradient coil in the probe, a pulsed Z-gradient amplifier, and X,Y shim current amplifiers that can be ramped in a stepwise fashion under continuous operation.

GradShim with ^{1}H signal detection utilizes the ^{1}H channel of the probe, the standard ^{1}H pulse transmitter, and the standard ^{1}H preamplifier. For shimming on the ^{2}H signal of a deuterated solvent, the lock channel of the probe is used in conjunction with the deuterium preamp. The low-power lock channel transmitter is not suitable for GradShim methods; therefore, two possibilities are offered for obtaining moderate- to high-power ^{2}H pulses under pulse program control (see below). The appropriate RF routing changes necessary to deliver these pulses to the probe are handled by special hardware called the *LockSwitch* so that no cables or plug-ins need to be changed to perform ^{2}H shimming.

The hardware configurations and options are summarized for the various GradShim methods in **Table 1**. The LockSwitch is a *required* option for any GradShim method using a deuterium signal, and there are three accessory packages available for AVANCE spectrometers.

(1) **BSMS™ 2H-TX™**: This unit can be installed in the BSMS electronics rack and combines the *LockSwitch* hardware with a *20-W ^{2}H amplifier* and the *RCB controller* for ramping the X,Y shims. This is the most flexible solution since it allows not only ^{2}H GradShim but also complex experiments such as triple-resonance NMR with deuterium decoupling on biomolecules, for example. Adequate power for ^{2}H pulses or decoupling is provided in a compact, independent unit. The RCB controller allows 3D GradShim even on probes which have only a Z-gradient coil (e.g., the CryoProbe).

(2) **2H LockSwitch**: This option contains only the LockSwitch hardware. One of the spectrometer's X-nucleus amplifiers (e.g., BLAX-300) must be used to provide the high-power ^{2}H pulses required for GradShim. This option should be chosen when the 20-W ^{2}H transmitter (2H-TX) in Option 1 is not sufficient to achieve the desired short 90° pulses on the probe's lock channel.

Table 1. Standard Methods and Hardware Requirements for GradShim

Method Name	1D 1H	3D 1H	3D-Ramp 1H	1D 2H	1D sel (shaped pulses)
Nucleus, Signal	^{1}H, solvent	^{1}H, solvent	^{1}H, solvent	^{2}H, solvent	^{1}H / ^{2}H, solvent or sample
Shim Sets Used	on-axis	on-axis, off-axis	on-axis, off-axis	on-axis	on-axis
Gradient Coil	Z	X,Y,Z	Z	Z	Z
Pulsed Gradient Current Ampl.	GAB or GREAT-10	GREAT-10/3 or Acustar [a]	GAB or GREAT-10	GAB or GREAT-10	GAB or GREAT-10
Transmitter	standard ^{1}H	standard ^{1}H	standard ^{1}H	2H-TX (1) or BLAX-300 (2)	standard ^{1}H / 2H-TX (1)or BLAX-300 (2)
X,Y Shim Ramp	No	No	RCB Board (1,3)	No	No
LockSwitch	No	No	No	Yes (1,2)	No / Yes (1,2)
Test Sample for Setup [b]	2 mM Sucrose	2 mM Sucrose	2 mM Sucrose	Lineshape or selected deut. solvent	$CDCl_3$ + TMS; Lineshape or user-defined
Parameter File [c]	gradshim1d1h	gradshimdata	gradshimrcb3d	gradshim1d2h	user-defined
Pulse Program [d]	imgegp1d imgegs1d	imgegp3d imgegs3d	imrcbgegp3d imrcbgegs3d	imgegp1d2h imgegs1d2h	imgegpsp1d / user-def. imgegssp1d / user-def.
Gradient File [e]	Imgegs1d.r	Imgegs3d.r	Imgegs1d.r	Imgegs1d2h.r	Imgegs1d.r / user-def.
AU Program (aunm)	au_zgonly	au_zgonly	rampXY	zg_2Hoffon	au_zgonly / zg_2Hoffon

[a] discontinued option.

[b] Sucrose = 2 mM sucrose in 90% H_2O / 10% D_2O; Lineshape = $CHCl_3$ in acetone-d6.

[c] Path = *home*\exp\stan\nmr\par\ , where *home* = XWIN-NMR root directory, e.g. C:\Bruker\XWIN-NMR\

[d] two forms are in use employing either gradient pulses (gp syntax, XWIN-NMR 3.5, TopSpin) or gradient switching (gs syntax, XWIN-NMR 3.1); Path = *home*\exp\stan\nmr\lists\pp\

[e] required only for pulse programs with gs syntax; Path = *home*\exp\stan\nmr\lists\gp\

(3) **BSMS™ RCB controller**: This option contains the RCB controller only and is required to perform 3D shimming on ^{1}H with probes containing only a Z-gradient coil.

In general, GradShim with ^{2}H will only be performed in the 1D mode since the low inherent S/N for ^{2}H would require a prohibitively long measurement time (*2NS* × 1024 FIDs) for a 3D experiment. Furthermore, a 3D GradShim on ^{2}H using X,Y shim ramps (RCB controller) is not feasible since the shim ramp amplitudes would have to be increased by a factor of 6 to compensate for the lower γ of deuterium.

GradShim Methods and Pulse Programs

The standard methods available for GradShim and their characteristic features are summarized in **Table 1**. Note that the pulse program used by each method exists in two forms. With the newest GCU hardware TopSpin and XWIN-NMR 3.5 use the so-called *gp* syntax whereby a *rectangular* gradient pulse is switched on and off, for example, with the commands *gron1* and *groff*, a delay defines the pulse length, and the amplitude is given by the parameter *gpz1*. **Listing 1** shows the pulse program used for 1D 1H shimming of Z gradients.

On older systems XWIN-NMR 3.1 and earlier software use the *gs* syntax (**Listing 2**) whereby gradient amplitudes are simply switched by *ngrad* commands (*next gradient*) followed by appropriate delays to define the pulse lengths. The gradient amplitudes (X,Y,Z) to be set by each successive *ngrad* command are entered as sequential lines of text in a separate gradient program (Table 1) with file extension .r (see first example in **Listing 3**). A line containing zero values is used to turn the gradients off. This technique can also be used for 3D applications by including loop commands for the second and third dimensions and ramp designators which specify how gradient amplitudes are to be incremented during each loop cycle (second example in Listing 3).

For pulse programs using the *gp* syntax, 3D applications such as *imgegp3d* are programmed by inserting *grad* command lines which contain gradient specifications analogous to those used in a gradient program. Additional looping, increment, and reset commands control the gradient ramps for the second (*td1*) and third dimensions (*td2*). Consult the Pulse Program Reference Manual for your software for details.

Note: references to the older *gs* syntax are included here for Bruker users who have not yet upgraded to a *gp*-compatible configuration and can be ignored by users working with the *gp* syntax.

Level 1: Optimization of GradShim Parameters

The key parameters used by the various GradShim programs are summarized in **Table 2**. Default values for all parameters are defined in the parameter files (Table 1) delivered with the NMR software and stored in the standard directory for parameter files. These parameters are adequate for initial experiments. However, the performance of GradShim depends

Listing 1. 1D gradient-echo pulse program for 1H acquisition (gp syntax, XWIN-NMR 3.5 PL6 or TopSpin).

```
;imgegp1d
;avance-version (02/04/11)
;1D Gradient Echo Seq. for GradShim procedure
;with rectangular grad. pulses

; modification WE Hull
;use DS=4 for steady state; NS=2*n for phase-alternating acq.

#include<Avance.incl>      ;hardware commands

#include<Grad.incl>        ;gradient commands
#include<De.incl>          ;ADC definitions & acq. control

"d11=30m"

1 ze                       ;zero data buffer

  d11 UNBLKGRAD            ;activate (unblank) Grad. amp & lock hold
2 d1                       ;relaxation delay
  p0:f1 ph1                ;excitation pulse
  d27 gron1                ;phase-encoding grad. on for time d27
  5u groff                 ;phase-encoding grad. off
  d15                      ;free-precession delay (GradShim variable)
  d21 gron2                ;read grad. on with stabilization delay
  ACQ_START(ph30,ph31)     ;prepare for acquisition
                           ;(define pre-delay DE and use of ph30, ph31)
  aq DWELL_GEN:f1          ;acquire TD points with dwell DW for time AQ
  5u groff                 ;read grad. off
rcyc=2                     ;loop for next acquisition
  400m wr #0               ;store FID
  d11 BLKGRAD              ;blank grad. amp & deactivate lock hold
exit

ph1=0 2                    ;phase-alternating excitation

ph30=0                     ;F1 receiver ref. phase
ph31=0 2                   ;phase-alternating acquisition (ADC add/sub)

;pl1 : f1 pulse power level (typ. 14 dB)
;p0 : f1 pulse for small flip angle [typ. 2-4 usec]
;d1 : relaxation delay
;d11: delay for disk I/O [30 msec]
;d15: variable echo time used by GradShim [typ. 5 and 25 ms]
;d21: read gradient stab. delay [min. 250 us]
;d27: phase-encoding grad. length [typ. 2-3 ms]
;gpz1: phase-encoding grad. amplitude
;gpz2: read grad. amplitude
;NS: 1 or 2*n
;DS: 0 or 4-8
```

Listing 2. Alternative form of 1D gradient-echo pulse program for ^{1}H acquisition (gs syntax, XWIN-NMR 3.1).

```
;imgegs1d
;avance-version (02/07/16)

...
2 d1                        ;relaxation delay
  p0:f1 ph1                 ;excitation pulse
  2u:ngrad                  ;phase-encoding grad. on
  d27                       ;phase-encoding time
  2u:ngrad                  ;phase-encoding grad. off
  d15                       ;free-precession delay (GradShim variable)
  2u:ngrad                  ;read grad. on
  d21                       ;read stabilization delay
  ACQ_START(ph30,ph31)      ;prepare for acquisition
                            ;(define pre-delay DE and use of ph30, ph31)
  aq DWELL_GEN:f1           ;acquire TD points with dwell DW for time AQ
  2u:ngrad                  ;read grad. off
rcyc=2                      ;loop for next acquisition
...


;use gradient program (GRDPROG): Imgegs1d.r  to define grad. amplitudes for
successive ngrad commands.
```

Listing 3. Gradient programs for 1D and 3D acquisition with pulse programs using gs syntax.

Imgegs1d.r [a]

```
{(0) |(0) |(3.112)}
{(0) |(0) |(0)}
{(0) |(0) |(-6.738)}
{(0) |(0) |(0)}
```

Imgegs3d.r [b]

```
loop 32 <3D>
  {
  loop 32 <2D>
    {
       {(0),,r3d(5.057) | (0),r2d(5.057) | (3.112) }
       {(0)             | (0)            | (0)     }
       {(0)             | (0)            | (-6.738)}
       {(0)             | (0)            | (0)     }
    }
  }
```

[a] Each successive text line with format {(X) | (Y) | (Z)} defines the X,Y,Z gradient strengths (in % of max.) set by successive *ngrad* commands in pulse programs using *gs* syntax. For each Z gradient pulse two *ngrad* commands are required [gradient on (value), gradient off (0)], and the gradient pulse length is defined by the time between these two commands.

[b] For the 3D case the Z gradient is switched on and off as in the 1D case to create the gradient echo while the loop commands specify that the Y and X gradient values for phase encoding are stepped through $N_y = N_x = 32$ values each for the second and third dimensions. The inner loop commands r2d(Y_{max}) and loop N_y <2D> specify that, for each X gradient setting, the Y gradient is stepped through N_y values ranging from $-Y_{max}$ to $+Y_{max} - \Delta Y$, with the increment $\Delta Y = 2\,Y_{max} / N_y$ so that $Y = Y_{max}\,[-1 + 2(n-1)/N_y]$ for $n = 1, 2, \ldots N_y$. The gradient reaches zero for $n = (N_y/2) + 1$. The outer loop commands r3d(X_{max}) and loop N_x <3D> define the incrementation of the X gradient in an analogous manner.

explicitly on the quality and information content of the field maps (profiles or images) acquired with the gradient-echo technique. In the following we describe how to optimize the acquisition parameters for the specific hardware configuration and applications at hand. Here, we assume that all experiments will be performed with 5-mm probes and samples. The procedures are the same for other probes and sample diameters, but parameter settings that depend on sample dimensions will be different.

Note: in the Theory section the signs of the dephase/rephase Z-gradients are shown as –/+ in the Figures while in the following sections the Bruker default parameters employ +/– gradients. This difference simply leads to a reversal of the Z-axis direction in the acquired profiles but has no effect on shimming results.

Important: whenever a user-modified parameter set is to be used by GradShim, this set must be stored under a specific and unique name in the parameter directory by using the *wpar* command. Do *not* overwrite the default parameter set. The new parameter set name is required by GradShim for performing shim mapping and iterative shimming with the modified parameters and is used to define the data set name for acquisition.

Note that in the following setup procedures the acquired signal is an echo with its center displaced toward the middle of the time domain. Since the FT will produce a spectrum with a very large phase roll, the profile is most conveniently examined after performing a magnitude calculation *mc*.

Transmitter offset, flip angle, receiver gain

The GradShim methods are designed for on-resonance excitation of a *single* dominant resonance signal. For ^{1}H applications the offset *o1p* has a default value of 4.7 ppm, assuming that solvent water will be used for shimming. If a different solvent is to be used, then this parameter should be modified accordingly in the revised parameter set (see below). For the GradShim methods using the ^{2}H signal from a deuterated solvent, the correct value of *o1p* depends on the solvent. In this case the *au* program *zg_2Hoffon*, which is used by the 1D 2H method, will automatically read the BSMS *Lock Shift* value and store it as *o1p* prior to execution of the pulse sequence.

Table 2. Parameters used in GradShim Setup programs [a]

		Typical or Default Values	
Parameter	**Function**	**^{1}H acquisition**	**^{2}H acquisition**
o1	rf offset	on-resonance for signal of interest	on-resonance
swh	profile field of view in Hz [b]	40 kHz	10000 Hz / 4194 Hz
dw	dwell time = 1/(2 *swh*)	12.5 µs	50 µs / 119 µs
td, *si*	time domain data points (A+B), FT size (real) [c]	512, 256	512, 256
d1	relaxation delay	0.1 - 0.5 s	0.05 s
p0 or p1	excitation pulse	*p0* = 2 - 3 µs	*p0* = 0.15**p1* (*p1* = 90°)
pl1	transmitter power level (atten.)	normal probes: 12 - 16 dB cryoprobes: 24 - 32 dB	BSMS 2HTX: –6 dB Lockswitch & 300-W Transm.: 10-16 dB
d27	fixed phase-encoding time T_{PE} [d]	2 - 3 ms	6 ms
d15	variable free-precession delay for T_2* effects	5 and 25 ms	50 and 110 ms / 5 and 125 ms
d21	read grad. stabilization delay	250 - 500 µs	250 - 500 µs
de	acq. pre-delay	6 µs	50 µs
aq	acquisition time = *TD dw*	6.4 ms	25.6 / 61 ms
rg	receiver gain	16-32	min. 32
ns	number of transients acquired	1 or 2*n	4 (32-128)
ds	number of dummy acquisitions	0 or 4-8	0 (4)
gpz1, *gpz2*	$G_z^{dephase}$, G_z^{read} for *z*-profile (in %) [d]	3.112, –6.738 (%)	6, –10 / 7,–5
	for 3D shimming		
G_x^{max} , G_y^{max}	max. phase-encoding gradient for X,Y [e]	5.057 (%)	
td1, *td2*	number of gradient steps N_x , N_y	32, 32	
nbl = *l1*	no. of blocks, loop counter for 3D = *td1* × *td2*	1024	
d15	variable free-precession delay for T_2* effects	5 and 25 ms (11 and 31 ms[f])	

[a] in all cases AQ_mod = qsim; DIGMOD = digital

[b] The FOV_z in cm depends on *sw* and G_z^{read} and should be sufficiently larger than the *z* dimension of the rf coil so that the magnitude-mode *Z*-profile spectrum fits within *sw* without folding.

[c] Note: these values are used only during manual setup and observation of the Z-profile; for field mapping GradShim uses internally only *td* = 128 and *si* = 64 after data conversion with *convdta* (see text).

[d] Typically $G_z^{dephase}$ (or *d27*) can be adjusted to place the echo maximum at data point n_{max} = ca. 64 in the acq. window, i.e., near the center of the time domain actually used by GradShim after removal of the group delay data points associated with the digital filter (see text).

[e] The *FOV* for the *x,y* dimensions should be 10-20% larger than the sample diameter.

[f] for shimming with RCB controller and BOSS-2 shim system.

As for any NMR experiment where a large solvent signal is present, the combination of flip angle (excitation pulse length) and receiver gain should be carefully adjusted for optimal use of the available dynamic range without exceeding the maximum input voltage that the digitizer can handle. When normal FIDs are acquired for a conventional ^{1}H-NMR spectrum, for example, a small overload of the digitizer due to excessive receiver gain will result in moderate baseline distortion of an otherwise recognizable spectrum. For an echo-based imaging experiment, most of the echo intensity is concentrated within a few time-domain points around the echo maximum, and even a small overload will have a dramatic impact on image quality, as shown for the *z*-profile in **Fig. 11**.

We recommend the following two procedures for adjusting the receiver gain for proton or deuterium detection, respectively.

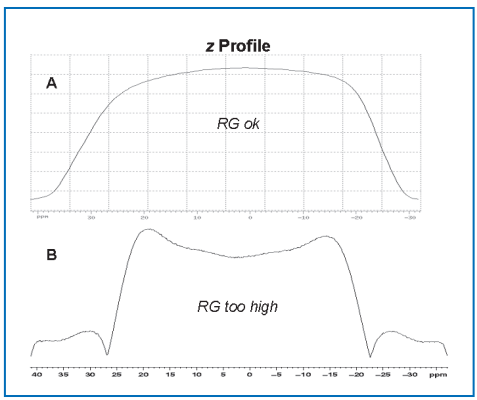

Fig. 11: Comparison of magnitude-mode *z*-profiles obtained with the GradShim acquisition routine when the receiver gain is at a safe level (**A**) or set too high (**B**), resulting in digitizer overload.

GradShim based on the ^{1}H signal from H_2O.

In aqueous solutions containing only a small percentage of D_2O, the ^{1}H signal from H_2O is very strong and has approximately the same intensity for all samples of a given diameter. Thus, the proper flip angle and gain settings will depend mainly on the inherent sensitivity of the probehead (rf coil) and the sample diameter. The optimized parameters for 1D GradShim with Z*n* gradients will also apply when H_2O is used for 3D shimming of X,Y,Z gradients.

- ❑ Insert the water suppression test sample (2 mM sucrose in 90% H_2O/10% D_2O), establish ^{2}H lock, and optimize probe tuning as usual (Wobble routine or automatic tuning).
- ❑ Read in a stored shim settings file that results in good field homogeneity with the current probehead and sample configuration; make fine adjustments manually or, better yet, perform a round of computer-assisted shimming with an appropriate *tunefile* script, as described in Parts I and II of this series of articles [*1*,*2*]. It is important that both on- and off-axis shims be well-adjusted for the following calibration steps. Therefore, optimization of Z gradients at least to 3rd order and X,Y gradients to at least 2nd order is recommended.
- ❑ Open a *new* dataset and read in the default GradShim parameter set (Table 1); e.g., for 1D shimming on ^{1}H, type the command

  rpar gradshim1d1h all

  This parameter set defines the gradient-echo pulse sequence to be used (i.e., *imgegp1d*, shown in Listing 1 or *imgegs1d* in Listing 2) and all appropriate parameters (Table 2) such as the offset frequency *o1p*, the spectral width *sw*, the excitation pulse length *p0*, transmitter power *pl1*, the necessary delays and gradient pulse lengths, as well as the gradient amplitudes to be used (i.e., *gpz1*, *gpz2* or the gradient program *Imgegs1d.r* in Listing 3).
- ❑ For shimming on a solvent signal other than that from water, change *o1p* as needed to place the transmitter offset on-resonance.
- ❑ Switch to the *acquisition window display (acqu)* and activate the Y-axis absolute display mode.
- ❑ Execute *rga* to acquire data and automatically adjust the receiver gain to avoid digitizer overload. Note that for the time domain the initial vertical display limits represent the *maximum* signal intensity that can be digitized without distortion. (For the digital acquisition mode with effective digitizer resolution *dr*, the limits are $\pm 2^{dr-1}$.) Do not alter the display limits with the up/down buttons.
- ❑ Start the gradient-echo acquisition sequence with *zg*. A relatively narrow echo signal should be observed at ca. $t = 2.4$ ms in the time domain (ca. one-third of the acquisition window). The receiver gain set by *rga* should result in a maximum echo intensity of ca. 30% of the vertical display limits (a conservative setting).
- ❑ If the receiver gain *rg* is now in the range 16 to 32, then no further adjustment is necessary, and dynamic range has been optimized.
- ❑ If *rg* is outside the range 16 to 32, then it is necessary to adjust the *flip angle* of the excitation pulse *p0* via the *pulse power* level (attenuation) *pl1*. The pulse length should be kept short (2-3 μs) and constant to ensure uniform excitation over a wide bandwidth. If *rg* is too high (signal too weak), then *pl1* must be reduced to achieve a larger flip angle (a change of –6 dB corresponds to a factor 2 increase in flip angle). If *rg* is too low, then *pl1* must be increased. Make an appropriate change in *pl1* and execute *rga* to optimize receiver gain again. Repeat this procedure as necessary to achieve *rg* = 16 - 32.

- ❑ Alternatively, a somewhat better utilization of the available dynamic range may be achieved by setting *rg* to the desired value of 16 - 32 and adjusting *pl1* manually to give an echo maximum of ca. 75% of the vertical display range.
- ❑ When adjustments are complete, store the complete parameter set as a new file with an appropriate name, e.g. *wpar gradshim1d1h.rev1 all*

When shimming on H_2O as solvent, for example, the S/N is so high that a single transient per acquisition is in principle sufficient ($ns = 1$, $ds = 0$). However, for 1D shimming the acquisition time is only a small fraction of the GradShim execution time so that the acquisition of several transients with phase alternation can be advantageous (cancellation of receiver DC offsets, further improvement in S/N and dynamic range). Thus, the program shown in Listing 1 (analogously in Listing 2) has been modified to include phase alternation and is used routinely by one of the authors (WEH) with $d1 = 0.2$ s, $ds = 4$, $ns = 8$.

GradShim based on the ^{2}H signal from a deuterated solvent.

In this case maximal S/N per transient requires a flip angle close to 90°. The required receiver gain will depend on the probe's sensitivity and the deuterium concentration in the solvent. For example, solvents such as D_2O, acetone-d_6, DMSO-d_6, or CD_2Cl_2 give a stronger signal than $CDCl_3$. Since GradShim can be performed with a variety of solvents, it is important to set up the flip angle and gain with the solvent that delivers the *strongest* deuterium signal. These settings will be appropriate for any other solvent since a further increase in the receiver gain for weaker solvent signals will generally not be advantageous in view of the low inherent S/N and limited dynamic range of the ^{2}H signal.

The 90° ^{2}H pulse width will depend on the probe and transmitter being used and must be calibrated first. Note that this procedure differs from the pulse calibration for deuterium decoupling experiments.

1. ^{2}H pulse calibration

- ❑ Insert the lineshape test sample ($CHCl_3$ in acetone-d_6), establish lock, and optimize on- and off-axis shims as described above.
- ❑ Create a *new* dataset and read the default parameter set for 1D GradShim with ^{2}H detection (Table 1):

  rpar gradshim1d2h all
- ❑ Edit the acquisition parameters (*eda*) to set the acquisition sequence to *pulprog = zg2h* instead of the gradient-echo sequence normally used by GradShim (e.g., *imgegp1d2h*).
- ❑ Use *ased* or direct command line entries to define the following parameters:

  $ns = 1$, $ds = 0$, $d1 = 1$ s, $d20 = 1$ s, $o1p = 7.24$ ppm, $sw = 20$ ppm, td and $si = 8$K, $p1 = 50$ µs.
- ❑ The power level *pl1* depends on the transmitter used for the deuterium pulse. Note, that the maximum power allowed on the lock channel for most probes is ca. 20 W. The following settings are recommended:

  a) when using the BSMS 2H-TX unit as pulse transmitter: set $pl1 = -6$ dB (max. power);

  b) when a 300-W X-nucleus transmitter is used with the LockSwitch feature: set $pl1 = 10$-16 dB (ca. 2-8 W).
- ❑ *Set locnuc* = off
- ❑ Using either the BSMS keyboard or *bsmsdisp*, switch *lock* off and *sweep* off.
- ❑ Since the lock transmitter itself can excite deuterium and interfere with the calibration, the lock power should be reduced to –60 dB via the BSMS keyboard or *bsmsdisp*.
- ❑ Change to the acquisition window, switch on the absolute Y-axis scale, and start the acquisition with the command *rga* which will automatically adjust the receiver gain.
- ❑ With this gain setting acquire, process and phase correct the spectrum as usual and save the phase constants.
- ❑ Repeat the experiment (*zg, ft, pk*) with different *p1* values to find the 180° condition (signal null); 90° = half this value (typically 60 - 150 µs, depending on probe type and B_0 field strength).
- ❑ Save the pulse calibration using the *edprosol* routine.

2. Receiver gain adjustment

- ❑ Using the same sample as in (1), make sure that the sample is locked and shims are reasonably well optimized.
- ❑ Create a new dataset and read in the default parameters again with

  rpar gradshim1d2h all.
- ❑ With *eda* check that the acquisition parameter pulprog is now *imgegp1d2h* (or *imgegs1d2h*) and *aunm = zg_2Hoffon*.
- ❑ When using the pulse program *imgegp1d2h* (*gp* syntax), enter the correct value for the 90° deuterium pulse *p1* and the corresponding power level *pl1* determined above, set $ns = 1$ and the relaxation delay $d1 = 1$ s. The actual excitation used will be 15% of *p1*.
- ❑ When using the pulse program imgegs*1d2h* (*gs* syntax), enter ca. 15% of the 90° pulse *p1* as the excitation pulse *p0*, set the power level *pl1* as in (1), set $ns = 1$ and $d1 = 1$ s. Alternatively, an experienced user may choose to modify the pulse program by replacing *p0* with *p1**0.15 so that the excitation is defined via *p1* directly.

- ❑ Change to the acquisition window, switch on the Y-axis absolute scale.
- ❑ Acquisition should now be started with the command *xaua* and not simply *zg*. This ensures that the AU sequence *zg_2Hoffon* first turns off the lock and field sweep before executing *zg* and restores lock when the experiment is finished.
- ❑ As described above for ^{1}H data acquisition, the maximum intensity of the echo signal should not exceed the limits of the acquisition window display as defined by *dr*.
- ❑ Halt acquisition and adjust the receiver gain *rg* as needed to achieve ca. 50% of the display limits and check with *xaua*.
- ❑ Store the current parameters with correct 90° pulse *p1*, power level *pl1*, new *p0* if required, and optimal receiver gain *rg* to a new file, e.g.,

  wpar gradshim1d2h.rev1 all

S/N ratio for ^{2}H shimming

When GradShim is used to shim on a ^{2}H solvent signal via the lock channel of the probe, the S/N with one transient will be relatively low. Therefore, any or all of the following methods are recommended to improve S/N and the quality of the field maps obtained with GradShim.

- ❑ Several transients per experiment may be acquired with phase cycling (included in the 1D 2H pulse programs) and preceded by at least 4 dummy scans to establish a reproducible steady state.
- ❑ If the T_1 of the deuterium solvent is known, then the flip angle β and repetition time *TR* can be optimized to achieve the *Ernst condition* for maximum S/N in a given measurement time (see **Table 3**).
- ❑ The spectral width *swh* can be reduced from the default value of 10 kHz to 5 kHz; the corresponding effective filter bandwidth is automatically reduced with an improvement in S/N.

In XWIN-NMR 3.5 patchlevel 6 the GradShim pulse program *imgegp1d2h* has been modified to use a 0.15**p1* pulse for excitation (13.5° flip), which requires a short repetition time *TR* to obtain optimal S/N per unit measurement time for a large range of T_1 values. With this flip angle the optimal TR/T_1 ratio is 0.029, and values in the range 0.007 - 0.11 will give >80% of the maximum possible S/N. Thus, for shimming on ^{2}H the relaxation delay *d1* can be reduced to 0.05 s (*TR* = 0.1 - 0.2 s, depending on *aq* and *d15*) to give good S/N for T_1 in the range of ca. 1 - 15 s, which should be adequate for most situations. Since 1D shimming needs only two data sets, several transients can be acquired at each *TE* value without a significant increase in the time required for shimming. Thus, with *d1* = 0.05 s, *ns* = 32 - 128 is recommended, depending on solvent and probe sensitivity. From the data in Table 3 we see that 32 transients with 15° flip angle and optimal TR/T_1 will give about the same S/N per unit time as can be obtained with a 90° pulse and $TR/T_1 = 1.27$.

Table 3. Ernst Condition for optimal S/N per unit time.[a]

chosen flip angle	opt. TR / T_1 for max. S/N	TR / T_1 range for S/N > 80% max.
10°	0.016	0.0038 - 0.061
15°	0.035	0.009 - 0.14
20°	0.060	0.02 - 0.2
30°	0.150	0.04 - 0.5
40°	0.270	0.07 - 1.0
50°	0.420	0.12 - 1.5
60°	0.600	0.17 - 2.0
70°	0.830	0.25 - 2.4
80°	1.040	0.36 - 2.6
90°	1.270 [b]	0.55 - 2.7

[a] *TR* = repetition time.

[b] max. S/N = 90% of that obtainable with lowest flip angles in the same measurement time.

A further improvement in S/N can be obtained by reducing the standard spectral width by a factor of two, e.g. from 10 to 5 kHz (default *sw* = 4194 since XWIN-NMR 3.5 PL6). This requires that the profile width in Hz (FOV_z) and the corresponding read gradient also be reduced by the same factor, e.g., in XWIN-NMR 3.5 or TopSpin the gradient amplitude *gpz2* = –5% instead of –10% (in XWIN-NMR 3.1, the analogous Z gradient value in the gradient program *imgegs1d2h.r* should be reduced). According to Eq. 2, if the dephasing gradient *gpz1* is left unchanged (6 - 7%), then the time for rephasing will increase by the same factor by which the read gradient is decreased, and the echo maximum will remain at about the same relative position (data point) within the acquisition window.

Remember: all changes in parameters that are to be subsequently used by GradShim must be saved in a revised parameter file using the *wpar* command.

Profile Width

If the echo maximum appears at a cursor position corresponding to ca. 40% of *td*, as in **Fig. 12A**, then one can proceed with optimization of the *z*-profile width (Fig. 11). If the echo position is severely displaced (e.g. Fig. 12B), then it should first be adjusted as described in the next section.

The field of view, corresponding to the defined spectral width, and the read gradient are related by

$$FOV_z\,[\mathrm{cm}] = swh\,[\mathrm{Hz}] / \{\gamma\,[\mathrm{Hz/G}] \times C_z\,[\mathrm{G/cm\ \%}] \times G_z^{read}\,[\%]\} \qquad [12]$$

$$G_z^{read}\,[\%] = swh\,[\mathrm{Hz}] / \{\gamma\,[\mathrm{Hz/G}] \times C_z\,[\mathrm{G/cm\ \%}] \times FOV_z\,[\mathrm{cm}]\} \quad [13]$$

where units are shown in square brackets, C_z is the calibrated gradient strength at 100% divided by 100 (if 100% = 50 G/cm, then $C_z = 0.5$), and $\gamma = 4258$ Hz/G for ^{1}H and 653.6 Hz/G for ^{2}H.

Thus, for $G_z = 50$ G/cm at 100%, *swh* = 40 kHz, and $G_z^{read} = -6.738$, the calculated $FOV_z = 27.9$ mm, which is sufficiently larger than the length of a 5-mm rf coil so that the *z*-profile should fit within *sw*.

For maximum information and details in the *z*-profile and field maps, it is important to adjust the profile to just fit within *sw* with minimum extent of zero baseline at both edges while avoiding folding or truncation. The profile should be reasonably symmetric and centered when the offset *o1* is on-resonance. The profile width within the spectral window can be adjusted by varying either *sw* or G_z^{read}. Any parameter changes made here will influence the echo position within *aq*, which can be checked and corrected as described below.

Echo position

The position of the gradient-echo maximum within the acquisition time is defined to a good approximation by the following formulas (see Table 2).

$$d27\,G_z^{dephase} + G_z^{read}\,[d21 + de + (n_{max}\,dw)] = 0 \quad [14]$$

$$G_z^{dephase} = -G_z^{read}\,[d21 + de + (n_{max}\,dw)] / d27 \quad [15]$$

$$n_{max} = [-d27\,(G_z^{dephase} / G_z^{read}) - (d21 + de)] / dw \quad [16]$$

where $aq = TD\,dw = TD / (2\,swh)$ and n_{max} is the cursor point where the echo maximum occurs at the time $n_{max}\,dw$.

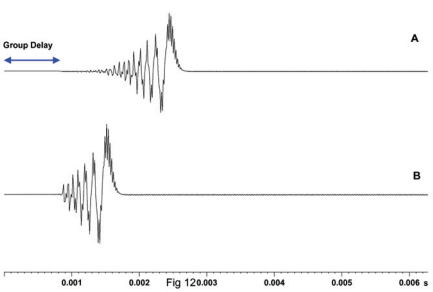

Fig. 12: Opimally positioned echo (**A**) appears at about one-third of the displayed time domain (shuffled FID display). The initial portion of the FID represents the group delay associated with the oversampling and digital filtering mode of data acquisition. The command *convdta* can be used to remove the group delay data points and display the actual time domain used by GradShim for subsequent processing. When the phase-encoding gradient amplitude $G_z^{dephase}$ (*gpz1*) is too low, the echo occurs too early (**B**), and the initial portion of the echo is distorted or clipped. The echo position can be optimized by setting $G_z^{dephase}$ according to Eq. 15.

These formulas apply when the field homogeneity is relatively good. When strong residual field gradients are present, they will contribute to the effective values of $G_z^{dephase}$ and G_z^{read}, resulting in a shift of the echo position.

A further complication has to do with the use of oversampling and digital filtering (DIGMOD = *digital*). The initial portion of the time domain viewed in the standard FID display mode *sh* (shuffled) represents the so-called *group delay* and does not contain useful data (Fig. 12A). The effective *aq* for which the above equations apply begins *after* the group delay, which for *gradshim1d1h* and its default parameters can be ca. 1.7 ms or ca. 135 data points. Thus, under these conditions the echo maximum as viewed in the display will occur at ca. 2.4 ms (cursor point 190) or ca. 0.7 ms after the end of the group delay, corresponding to $n_{max} = 55$ within the true *aq* time frame.

The *td* and *si* values of 512 and 256 are used for viewing profiles during GradShim setup. When GradShim is running on its own to create field maps, the acquired time domain data are first converted internally from the digital mode to the analog mode via the routine *convdta*, and the initial data points corresponding to the group delay are removed. GradShim then sets internally *td* and *si* to 128 and 64 points for subsequent processing, i.e., only the initial 128 points of the effective signal time domain are used. Therefore, for symmetry and optimal echo acquisition, the echo maximum should occur close to data point $n_{max} = 64$ (after the group delay). *Note:* the original *td* of 512 should be maintained in the acquisition parameters to allow for the sizable group delay and to facilitate visualization and positioning of the echo.

While setting up parameters, the user can execute the command *convdta* manually. The digitally filtered FID is converted to a quasi-analog FID with the group delay data points removed and written to a new file with user-defined *expno*. In the display mode *calibrate* one can now view the cursor point number at the end of the time domain; *td* (512) minus this value gives the number of points in the group delay. The cursor position of the echo maximum (n_{max}) can also be read out directly, and the goal is to shift the echo as needed to achieve n_{max} = ca. 64, the center of the time domain actually used by GradShim. Once the number of points in the group delay for a given *sw* has been determined using *convdta*, this value can be subtracted from the cursor positions read out from the original (digital mode) time domain display. In the TopSpin software the acquisition status parameter *grpdly* indicates directly the number of complex pairs of data points that make up the group delay.

The formulas given above allow the user to accurately place the echo maximum without trial and error. Once the value of G_z^{read} (*gpz2*) has been optimized to give the desired *z*-profile width within *sw* (e.g. Fig. 11A), the value of $G_z^{dephase}$ (*gpz1*) required to place the echo at $n_{max} = 64$ can be calculated directly from

Eq. 15. One can also shift the echo by varying *d27*, but this alternative is less desirable since it alters the pulse sequence timing. A reasonably good centering of the echo within the time domain used by GradShim (*td* = 128) is important to avoid any strong truncation effects (Fig. 12B) which would distort the profiles and field maps to be acquired. Note that any changes in *sw*, G_z^{read}, or any of the other parameters in the Eqs. 14-16 will require readjustment of $G_z^{dephase}$ to optimize echo position.

Acq. pre-delay de

When using GradShim with deuterium detection, it is recommended to increase the prescan delay *de* to a value of 20 to 50 μs. When *de* is too short, the *z*-profile for ^{2}H may exhibit some baseline distortion due to a spike at the beginning of the FID or the end of the group delay of the digital filter **(Fig. 13)**.

Free-precession delay d15 and echo times

As described in the theory section above, GradShim records for each field or shim map *two* profiles with different total echo times by setting the free-precession delay *d15* to the value *TE1* for the first acquisition and *TE2* for the second data set. These delays are defined via the *Shim Map Parameter Editor* when the *Create Shim Map* procedure is started (Level 2 in GradShim, see below). *Note:* these two values for *d15* actually correspond to the delays labeled *TF1* and *TF2* in Fig. 3 (and not the total echo times). For GradShim it is the time *difference* $\Delta TE = TE2–TE1$ that is of key importance since it determines the spatially encoded *difference* in phase evolution of the spins between the two measurements, which in turn depends only on the inhomogeneity of B_0 (the function $B_i(z)$ in Eqs. 5-7) and not on the applied gradients.

Case 1: good B_0 homogeneity

For normal day-to-day shimming with typical samples, the basic B_0 field will be in good shape and good initial shim settings will be known (stored). Therefore, only fine shimming of sample-dependent field distortions will be necessary.

The value of *d15* for the first measurement (*TE1*), a reference profile with minimal ΔB_0 effects, can be as short as a typical gradient recovery delay (0.3 ms) but is usually set to 5 ms for shimming on ^{1}H, for example. The default value of *TE2* for the second measurement is 25 ms for ^{1}H, and ΔTE determines the phase modulation due to ΔB_0 and the precision of the resulting shim map.

For ^{2}H GradShim methods the default values for *TE1* and *TE2* were previously 50 ms and 110 ms, respectively, but have been changed to 5 and 125 ms since XWIN-NMR 3.5 PL6. Under good S/N conditions the precision of the shim maps is improved with the larger ΔTE. **Fig. 14** presents an example of 1D 2H shim maps which have an undesirable amount of noise because *TE2* and ΔTE were too small.

In the setup mode described above, after all other parameters have been optimized, a suitable value for *TE2* can be found by performing trial measurements of the *z*-profile with different values of the delay *d15*. First, record a reference profile with a very short echo time, i.e., *d15* = 1 ms. Then increase *d15* in steps of 5 ms for ^{1}H experiments or 20 ms for ^{2}H, for example, and monitor the changes in the profile relative to the reference. The largest acceptable value for *d15* is when the intensity of the profile decreases in a relatively uniform manner without large, local variations.

For shimming on ^{2}H one must keep in mind that the phase evolution is proportional to γ. Therefore, ΔTE should be about 6.7 times larger for ^{2}H compared to ^{1}H in order to obtain the same degree of evolution. However, the largest *TE2* that can be used in practice may be limited by T_2* for ^{2}H.

The default delays are appropriate for typical solvents at room

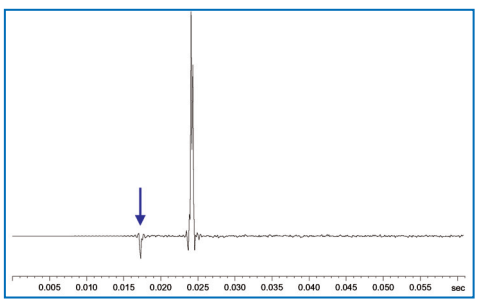

Fig. 13: When the pre-scan delay *de* for ^{2}H GradShim is too short, a spike may appear at the beginning of the FID (arrow) and cause distortions in the profile after FT. In such cases, *de* should be increased to at least 20 μs to eliminate the spike.

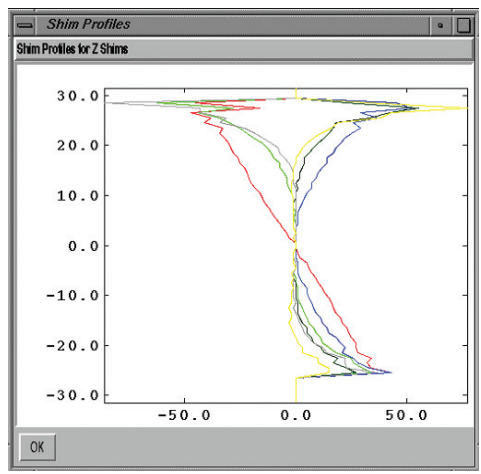

Fig. 14: Shim maps for deuterium gradient shimming show excessive noise because the echo time *TE2* was too short. The traces for Z^1 to Z^6 shims are in red, blue, green, black, gray, yellow, respectively.

temperature under conditions of relatively good B_0 homogeneity. Under non-optimal conditions (viscous samples with short solvent T_2, short T_2* due to large B_0 inhomogeneities), it may be necessary to modify *TE2* (see below). Note that when a new set of *TE1*, *TE2* values has been chosen by experimenting with *d15*, these values can only be entered into GradShim by creating a new set of shim maps (Level 2 procedures).

Case 2: poor B_0 homogeneity

A large variation of B_0 across the sample will generally result in distorted or asymmetric field profiles (e.g., initial shimming of a new magnet or a new probe for which no good starting shim values are available). The *z*-profile recorded under such conditions may have a strong drop of intensity in the center or to one side (Fig. 6 and **Fig. 15**). As a result, the field map may be too distorted or narrow on one or both sides, which makes proper shimming of the higher-order shims quite difficult.

When confronted with non-routine conditions, the user should check the basic homogeneity before using GradShim for either 1D or 3D shimming. For the 1D case, acquire a profile as described above, change *si* to 512 points (zero-filling) and perform FT and magnitude calculation with the command *fmc* (Fig. 15). If there are obvious problems, then it will be necessary to improve the basic homogeneity either by manual shimming or, preferrably, by using the Tuning and Simplex routines described previously [*1*,*2*].

Alternatively, one can create a new set of shim maps using a shorter value for the echo time *TE2* in GradShim to compensate for the short T_2* caused by the large inhomogeneities. The precision of the shim maps may be reduced (smaller ΔTE), but they should nevertheless provide sufficient data for calculating improved shim settings which will then allow a new set of shim maps to be generated with the original echo times and better precision. An appropriate value for *TE2* can be found by incrementing the delay *d15* in trial experiments as described above.

It is commonly thought that off-axis shims need not be well-adjusted when creating shim maps for the on-axis shims. This is incorrect because dephasing caused by gradients in the XY plane at each *z* coordinate will alter the *z*-profile intensity which represents a sum over all *x*,*y* positions for each *z* position. Furthermore, poorly adjusted mixed shims such as XZ or YZ[2] will certainly contribute to the *z*-profile. Sample rotation is not a solution for this problem and may even aggravate the situation. The read gradient produces a gradient echo by reversing only that component of phase evolution caused by the dephasing gradient. Local B_0 gradients cause dephasing throughout the echo time, and their effects can be modulated by sample rotation but not reversed, unless by chance a given voxel spends equal amounts of time in a positive and negative local gradient.

For ^{1}H GradShim routines the default values for *TE1* and *TE2* are 5 ms and 25 ms, respectively (11 and 31 ms for *gradshimrcb3d* and the BOSS-2 shim system). When B_0 homogeneity is initially very poor, these delays should be changed to 0.5 ms and 10 ms. When homogeneity has been significantly improved, one can return to the default values or possibly even longer values for *TE2*.

For ^{2}H GradShim, when B_0 homogeneity is very poor, it may be advisable to first create shim maps with delays of 1 ms and 50 ms, for example, and then to create new maps with increased *TE2* when conditions have been improved.

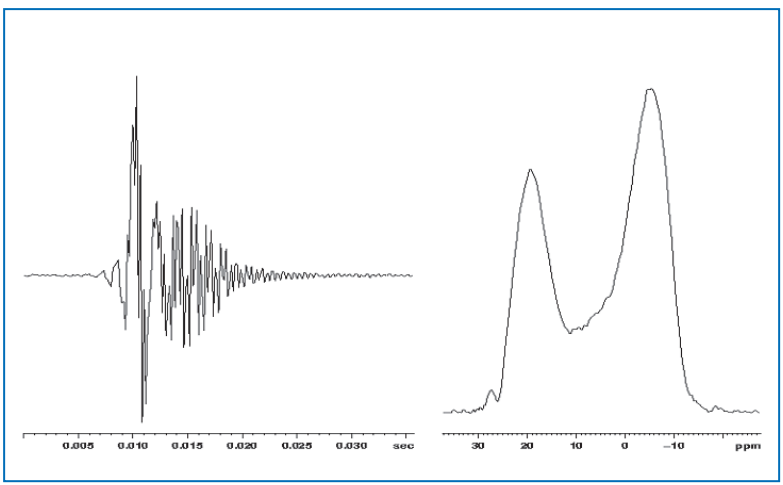

Fig. 15: The effects of strong B_0 inhomogeneity are shown for the acquired echo and the resulting z-profile (with a "hole" in the middle).

Prior to 3D shimming, one can check profile quality in all three directions (X,Y,Z). First acquire a 3D data set with default or modified parameters using the appropriate pulse sequence (Table 1). Following a 3D transform the data displayed in the 3D box should show a well-defined cylindrical form with somewhat rounded ends in the Z direction. The cylinder should fill out the box without touching the sides (see below). One can also analyze the data in the 2D mode by applying *xfb* to the *13* (YZ) or *23* (XZ) dimensions of the dataset. Select a central plane in the X or Y direction and check that the two-dimensional profile does not have "holes" or other large distortions (see **Fig. 16**).

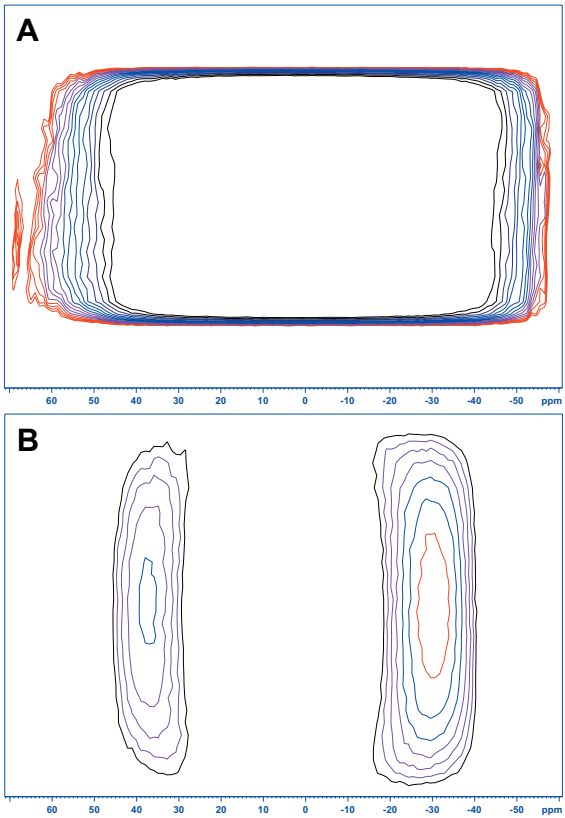

Fig. 16: A 3D ^{1}H field map was generated using a probe with Z-gradient coil and the RCB controller to ramp the X and Y shims. A 2D FT was performed in the X and Z dimensions, and the central plane (number 16) is shown for Case 1 (**A**, good B_0 homogeneity) and for Case 2 (**B**, poor B_0 homogeneity). In Case 1 the field map nicely fills out the 2D plane with relatively uniform intensity. In Case 2 the profile exhibits a gap in the middle and lengthened and distorted contours in the X dimension due to strong B_0 gradients.

Fine tuning of shim step sizes

During the shim mapping procedure, the current for each individual shim *j* is incremented by a specific step size U_j (Eq. 9) to create a reference field profile. The amount of phase evolution $\Delta\varphi$ produced for each coordinate position in the shim map is proportional to ΔTE and the step size U_j. Since ΔTE is the same for all shim maps, it is necessary to choose appropriate step sizes U_j according to each shim's sensitivity (ΔB per unit current). For optimal mapping it is desirable that the maximum $\Delta\varphi$ achieved at the edges of the profile be approximately the same for each shim. The GradShim routine accesses a set of reference parameter files for shim mapping (*ref.par* and *refparxx.nn* in *home*/conf/instr/autoshim/refmaps). Since the shim sensitivities depend strongly on the shim geometry, the type of shim system, current ranges defined for the BSMS, and the magnet bore diameter, it may prove useful to optimize the step sizes for the hardware configuration at hand. The master file *ref.par* is generated the first time *gradshim* is started and contains default parameters for all available shims. When shim mapping is executed with a specific method and probe, the current parameters are stored in the file *refparxx.nn*, where *xx* reflects the method (e.g., 1D or 3D) and *nn* represents the id number for the current probe. The *refpar* file for 1D shimming has the format shown in Listing 4.

Listing 4. Example of a *refpar1D.nn* parameters file used by GradShim.

```
64 1 1
5 25
34
1
z 1500 1
z2 1000 1
z3 2000 1
z4 5000 1
z5 10000 1
z6 50000 0
x 4000 0
xz 6000 0
xz2 10000 0
...
y3z 50000 0
```

The first line of the *refpar* file contains the *si* parameter or number of points used for the profile calculation in the *z y x* dimensions, i.e., the entries 64 1 1 represent a 1D experiment with 64 points along the *z* axis while 64 32 32 defines a 3D mapping procedure. The second line of parameters specifies the echo delays *TE1* and *TE2*, as selected by the user when setting up the mapping routine. The third line specifies the total number of shims available, in this case 34 for a BOSS-2 shim system. In each of the following lines that begins with a shim name (the list must be identical to the list of shims displayed

by the *vsh GSHIM* command, for example) the corresponding step size U_j is given (in the units used by the BSMS controller), followed by the digit 0 (shim not mapped) or 1 (shim mapped). *Note:* the data in any specific *refparxx.nn* file correspond to the current set of shim map profiles and *must not* be altered manually by the user.

A set of near optimum shim map profiles for Z^1-Z^6 is presented in **Fig. 17**. The maximum phase evolution $\Delta\varphi$ achieved at the positive and negative limits of the *z*-profile is close to ±360° for all shims. The relative values of the shim step sizes have been adjusted to give similar values for $\Delta\varphi_{max}$ at the edges of the profiles. The absolute values of $\Delta\varphi_{max}$ for all shims will then be scaled by the ΔTE used for mapping. To ensure that the phase unwrapping algorithm performs correctly, $\Delta\varphi_{max}$ should generally not significantly exceed ±360°.

If a standard shim mapping procedure with the default parameters given by the *ref.par* file indicates a substantial deviation from optimal scaling for any particular shim, then the following procedure can be used to adjust the shim step sizes.

- ❑ Perform shim mapping (for details, see below) with the current optimized GradShim parameter set.
- ❑ Examine the profiles and estimate the percentage change in step size needed to achieve a uniform $\Delta\varphi_{max}$ for each shim.
- ❑ Exit from the GradShim routine, closing all associated windows.
- ❑ Delete the current *refparxx.nn* file corresponding to the shim mapping just performed.
- ❑ Make a backup copy of the *ref.par* master file; open *ref.par* with an editor and make the necessary changes in the step sizes for the shims of interest.
- ❑ Save the edited *ref.par* file.
- ❑ Restart GradShim, open the *Setup - Shim Mapping* menu, and check that the parameter set, *TE* values, and shim group are defined as desired.
- ❑ In the Shim Mapping window open the menu *Misc* and click on *Save as Mapping Parameters* to create a new *refparxx.nn* file, which can be examined with a text editor to check that the desired changes have been incorporated.
- ❑ Execute Shim Mapping with the new shim increments and check the results in the Shim Profiles.

Note: only when GradShim is restarted and shim mapping is performed, will the edited *ref.par* master file be used to recreate the deleted *refparxx.nn* file and incorporate the step size changes made. If the defined step sizes result in $\Delta\varphi_{max}$ close to ±360° for the chosen *TE1* and *TE2* (also stored in the *refparxx.nn* file), then ΔTE cannot be increased much further without possible problems with phase wrapping. Therefore, for ^{1}H applications requiring a large increase in ΔTE, it may be necessary to make a proportional decrease in the step sizes for all shims involved. The optimal step sizes determined for ^{1}H shimming should be applicable for ^{2}H shimming as long as $\Delta TE(^2H)$ does not significantly exceed 6.7 times $\Delta TE(^1H)$.

Multiple solvent signals

Bruker's GradShim methods assume that the acquired shim or field maps result from the phase evolution of a *single*, dominant resonance, such as that from solvent water or an appropriate deuterated solvent. GradShim will not function correctly when two or more strong signals are excited (e.g., methanol or solvent mixtures). In such cases it will be necessary to employ selective excitation of the resonance of interest by using Gauss or Sinc pulses, for example. For shimming on a proton signal (e.g., TMS in samples without a strong solvent signal or the CH_3 signal from methanol), the pulse program *imgegpsp1d* (or *imgegsspld*, see Table 1) is provided and differs from the standard *...1d1h* program (Listing 1) in one command line where a selective shaped pulse *p11* is used instead of a hard pulse.

```
p11:sp1:f1 ph1
```

For deuterium shimming there is currently no standard pulse program provided for selective excitation, but one can be easily prepared from the *...1d2h* program by copying the standard program to a new file called *imgegpsp2h*, for example, and changing the excitation pulse command line.

```
(p11:sp1 ph1):D
```

Note: there is no default parameter set supplied for selective excitation applications. The user must prepare one based on an optimized parameter set for hard-pulse applications. All parameters such as delays and gradients as well as flip angle and repetition time criteria remain unchanged; only the excitation pulse (shape, duration, amplitude) needs to be appropriately defined for selective excitation.

In general a 5-ms Sinc.1000 waveform is recommended for the selective pulse *sp1*. The power level for a 90° pulse must be calibrated in separate experiments or calculated via *edprosol* (if a *cortab* transmitter calibration is available). Since the excitation must be applied on-resonance for the signal of interest, the parameter *spoffs1* must be 0, and the correct transmitter offset should be entered as *o1p* or *o1*.

More general use of the 1D selective shimming method is facilitated by the AU program *gssel_setup*, which automatically acquires a ^{1}H spectrum using the standard parameter set *PROTON* and the pulse/power parameters defined in *edprosol*. The biggest peak in the spectrum is picked and *o1* is set to this value. This new offset can then be used for the subsequent measurement of field profiles with selective excitation and echo delays *TE1* and *TE2*. To automatically perform this offset adjustment during the gradient shimming procedure,

the processing parameter *AUNMP* in the current *gradshim* parameter set must be set to *gssel_setup*. Furthermore, the gradient shimming resource file for the current user (*userhome*/.xwinnmr-<computername>/autoshim/resources or *userhome*/.topspin-<computername>/autoshim/resources) must be modified by changing the line

```
##.do.xaup=no
```

to

```
##.do.xaup=yes
```

This change ensures that when *gradshim* is executed the program *gssel_setup* specified by *AUNMP* will use expno 599 to determine *o1* for the biggest peak in the ^{1}H spectrum of every sample prior to shimming with selective excitation. Since all of the standard parameter sets for the various GradShim acquisition schemes have *AUNMP* set to *proc_no*, normal nonselective shimming sequences will execute as usual, even after the *xaup* option has been enabled.

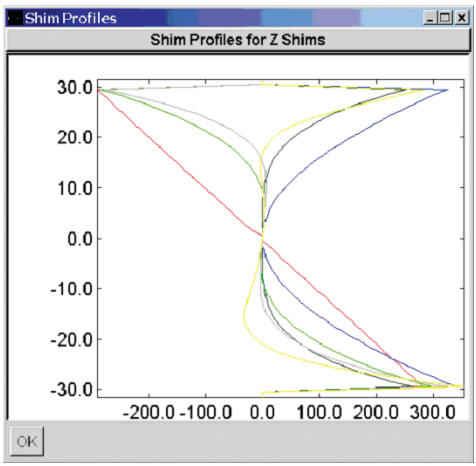

Fig. 17: Shim mapping profiles for the Z^1 to Z^6 shims (red, blue, green, black, grey, yellow) showing the *z* coordinate (±32 data points) on the vertical axis and the phase evolution (in deg) on the horizontal axis. For maximal profile sensitivity $\Delta\varphi$ should be on the order of ±360° for each shim. The step size for Z (red line) was increased from 1000 to 1500 units to achieve a max. $\Delta\varphi$ of ca. ±300°. The step sizes for the other shims are nearly optimal, except for Z^4 where an increase of ca. 15% could be employed.

Due to the limited digital resolution used to acquire the profiles, selective shimming can be performed using a strong doublet or multiplet as well as a singlet signal. The main limitation with selective shimming is the S/N achieved by the selective excitation. For 1D shimming S/N can be significantly improved by an appropriate choice of *ns*.

Note: after the parameter set for selective shimming with *imgegpsp1d* has been defined and tested by examination of the profile, the current parameter set must be stored with an appropriate name, e.g.,

wpar gradshim1d1hsel.

If the parameter set for selective shimming is based on a nonselective parameter set with no changes in *sw*, gradient strengths, dephasing and rephasing times, and echo delays, then the shim maps already created for the nonselective application (with high S/N) can be used directly for selective applications. Simply copy the appropriate fieldmap file *fieldmap1D.nn* (in *home*/conf/instr/autoshim/refmaps, where *nn* is the probe id) to a new file *fieldmap1DSEL.nn*. This file can be then linked to the selective shimming parameter set as follows.

- ❑ Open the GradShim *Shim Mapping* window and select the method *1DSel*.
- ❑ Enter the correct file name for the stored parameter set for selective shimming and the appropriate disk and user information.
- ❑ Enter the same echo times and shim group as used for nonselective 1D shim mapping.
- ❑ Open the drop-down menu *Misc* and select *Save as Mapping Parameters*.

The 1DSel shimming procedure can now be executed with the parameters so defined and the shim maps stored in *fieldmap1DSEL.nn*.

3D Shimming

The extension of GradShim methods to the 3D case requires appropriate hardware for applying gradients along the X,Y,Z axes and the appropriate pulse sequence in which phase encoding in the X and Y dimensions is employed together with frequency encoding in the Z dimension. The possibilities are summarized in Table 1.

Since a 3D field map is acquired with 32×32=1024 phase-encoding steps for each of two echo times, a short repetition time with optimal flip angle and *ns* = 1 will be desired (given sufficient S/N). It is not feasible to use dummy scans to establish a steady state in this case because the pulse programs are so written that *ds* scans would be executed for *each* phase-encoding step. A steady state will be established through the repetitive pulsing accompanying the phase-encoding ramps. The low flip angle conditions used for 1D ^{1}H shimming on solvent and *d1* = 0.05-0.1 s should provide efficient data acquisition.

Important: the *FOVs* in the X,Y directions are defined by 32 data points (±16 points from the origin). In the 3D GradShim fitting procedure a *fixed* range of ±9 data points will be used (while the Z range can be defined as shown below). Thus, it is critical that the *FOVs* for X,Y be sufficiently small that the profile widths extend over at least ±10 data points, resolution), and the (measured) gradient calibration factor C_x specifies the gradient strength in G/cm at 100%, divided by 100. With these equations one can calculate the gradient *increment* required to achieve a specified FOV, or vice versa. Note that the gradient increment determines the spatial width in the phase-encoding dimension just as the dwell time (*aq*

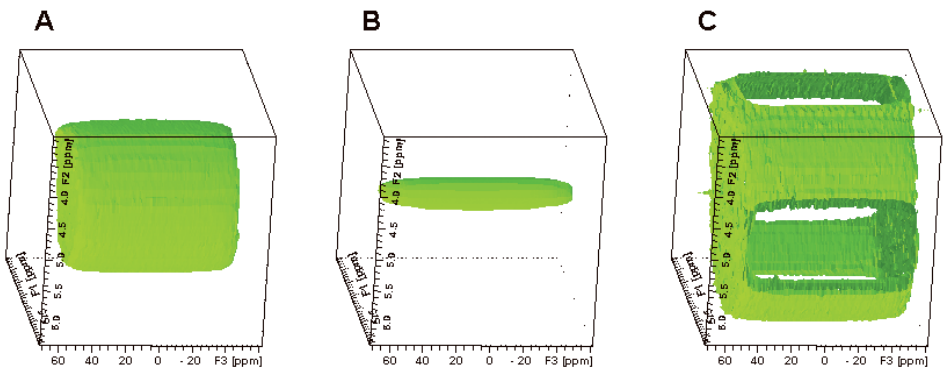

Fig. 18: 3D field maps obtained with the RCB controller and a Z-gradient probe. A: optimal X,Y shim ramp increment and phase-encoding period T_{PE}(RCB) (see Eq. 22) result in a cylindrical profile which optimally fills the X,Y *FOV*. B: *FOV* is too large. C: *FOV* is too small. The Z-axis is horizontal.

i.e., the *FOV* should be in the range 1.1 - 1.5 times the sample inner diameter.

Probe with X,Y,Z gradient coils

For applications with probes equipped with X,Y,Z gradient coils, the phase-encoding situation for pulsed gradients can be defined by the following equations, by analogy with Eqs. 12-13.

$$FOV_x\,[\mathrm{cm}] = 1 / \{\gamma\,[\mathrm{Hz/G}] \times C_x\,[\mathrm{G/cm\ \%}] \times \Delta G_x\,[\%] \times T_{PE}\,[\mathrm{s}]\} \quad [17]$$

$$\Delta G_x\,[\%] = 1 / [\gamma\, G_x\, FOV_x\, T_{PE}] \quad [18]$$

$$G_x^{init} = -N_x \Delta G_x / 2 \ \text{ and } \ \Delta G_x = -2\, G_x^{init} / N_x \quad [19]$$

$$FOV_x\,[\mathrm{cm}] = N_x / [\gamma\, G_x\, 2\, |G_x^{init}|\, T_{PE}] \quad [20]$$

Analogous equations apply for the Y gradient. Here, we define a positive gradient increment for phase encoding since it should have the opposite sign compared to the read gradient, which is negative in the default parameters. The term T_{PE} represents the phase-encoding time (*d27* in the pulse programs), N_x is the number of phase-encoding steps employed (digital increment) determines the spectral width in the frequency encoding dimension. The initial value of the gradient ramp G_x^{init} is defined by Eq. 19 to give a nearly symmetric ramp starting with a maximum negative value and reaching zero at step number $(N_x/2) + 1$. As an example, Listing 3 shows the default gradient program for 3D shimming, where the initial value for X and Y gradients is defined as (–)5.057% (the ramp multipliers r2d and r3d begin with the value –1). For 32 phase-encoding steps we have $\Delta G = 0.316\%$, and for $C_x = 0.5$ (100% = 50 G/cm) and $d27 = 2.0$ ms, the calculated *FOV* is 7.4 mm for the X and Y dimensions and is somewhat too large for an inner sample diameter of ca. 4.7 mm. An *FOV* of 6 mm would be more appropriate.

Probe with Z-gradient only

The situation is more complicated for the 3D GradShim method that uses a Z-gradient probe and the BSMS RCB controller to ramp the X,Y shims for phase encoding. The corresponding pulse program (e.g., *imrcbgegp3d*) uses the same method and values for the pulsed Z-gradient as in the 1D case. However, the X,Y gradients are not executed as pulses but are applied continuously (Fig. 10) via the X,Y *shim* coils and their corresponding current supplies in the BSMS unit.

Thus, there are severe restrictions on the *maximum* shim currents that can be applied, and this must be taken into account by GradShim when computing the ramp function.

The maximum allowed shim current depends on the type of the shim system being used. For a BOSS-1 shim system each off-axis shim gradient is produced by a single current supply feeding a single shim coil of the appropriate geometry. In contrast, the BOSS-2 shim system features a so-called matrix design for the off-axis shims, whereby several individual coil elements and their specific current supplies may be used to generate one particular shim gradient. Therefore, one current supply may participate in the generation of several different shim gradients. Depending on the off-axis shim settings that are currently being used, a given current supply may be required to deliver substantial current just for the shims and may reach its current limit when it is also employed in the generation of an X or Y ramp. Therefore, the maximum ramp value allowed for BOSS-2 shim systems is automatically reduced by about a factor of 4 compared to the BOSS-1 case.

The standard echo times *TE1* and *TE2* used for 3D shimming with the RCB controller also depend on the shim system being used and settling times for shim settings (BOSS-1: 5 and 25 ms; BOSS-2: 11 and 31 ms).

The pulse program used for 3D shimming via the RCB controller must be started via an *xaua* command since the AU program defined by AUNM = *rampXY* must be executed first to automatically calculate and load the X,Y ramp values into the RCB controller. The software asks the BSMS which shim system is present and sets a ramp scaling factor called *fact* to the proper value (*fact* = 2.0 for BOSS-1, 0.45 for BOSS-2). The initial ramp values (X,Y shim offsets) are simply

$$G_x^{init} = G_y^{init} = fact*50000 \text{ (in shim units)} \qquad [21]$$

The ramp increments ΔG are calculated using Eq. 19 with $N_x = N_y = 32$, and the complete set of 32 ramp values for X and Y shims are loaded into the RCB controller.

In contrast to phase encoding with pulsed gradients for a constant time $T_{PE} = d27$, phase encoding with shim ramps is applied for the entire duration of the pulse sequence, which varies according to the variable echo delay *d15* = *TE1* or *TE2*. Therefore, *rampXY* uses the following definitions.

$$T_{PE}(\text{RCB}) = t_{rcb} + d15$$

$$t_{rcb} = d27 + d21 + t_{echo} \qquad [22]$$

where the constant $t_{echo} = 0.70$ ms is the assumed time of the echo maximum within *aq* for standard ^{1}H applications.

Since the X,Y phase-encoding increments are proportional to $\Delta G\, T_{PE}(\text{RCB})$, the shim ramp for the second acquisition with *d15* = *TE2* is recalculated and appropriately scaled by the ratio of the phase encoding times.

$$G_x^{init} = G_y^{init} = fact*50000\ (t_{rcb} + TE1)/(t_{rcb} + TE2) \qquad [23]$$

In general, it is not intended for the user to alter the initial offset or increment for the X,Y gradients; therefore, these parameters cannot be varied to define the *FOV* in the X,Y dimensions, as was illustrated above for the pulsed gradient case. A special case is when ramping of X,Y shims causes the BSMS to exceed its current limits, either for the total current or, more likely, for a specific shim power supply, e.g., when relatively high off-axis shim currents with a BOSS-2 shim system are required for good homogeneity. This situation may result in a BSMS error, truncation of the G_x and/or G_y ramp, and a 3D field profile that is no longer a cylinder but rather flattened in the X or Y dimension.

There are several possible remedies for this situation. The total maximum current limit for the BSMS can be adjusted using the BSMS service tool, but this will not be useful if the current limit for a specific shim current supply is being exceeded. In such a case it will be necessary to edit the *rampXY* ascii code and *reduce* the numerical value used to define the scaling factor *fact* for BOSS-2 (the *if* statement immediately preceding the statement `STOREPAR("CNST 30", fact);`). Unfortunately, a reduction in *fact* would result in a proportional reduction in ΔG, an increase in $FOV_{x,y}$ (see Eq. 17) and an *xy*-profile that is too small.

The internal GradShim routines assume that the *xy*-profile extends for at least ±9 data points along the *x* and *y* axes, and it may be necessary to adjust the *FOV* appropriately. For example, a reduction in the profile width caused by a reduction in the parameter *fact* can be compensated by increasing both echo times *TE1*, *TE2* at constant ΔTE (this increases T_{PE}(RCB) in Eq. 22). Alternatively, one could adjust T_{PE}(RCB) via the delay *d27*. However, this delay defines the dephasing time for the gradient echo according to $G_z^{dephase}$, which must then be adjusted inversely to maintain a constant product $d27\ G_z^{dephase}$ and constant echo position within *aq*. The reduction in *FOV* that can be achieved by an increase in phase-encoding time has practical limits governed by the loss of signal due to T_2* decay.

Note: once a 3D profile has been obtained, the *xy*-profile width (in data points) and the sample's inner diameter (cm) can be used to calculate the scale factor cm/pt and the *FOV* (cm). The phase-encoding time T_{PE}(RCB) is known, and the gradient increment C ΔG (G/cm) can be calculated using Eqs. 17 & 18. With this *calibration* of the shim ramp, one can calculate the required delays for any desired *FOV*.

Examples of 3D field maps obtained with the RCB controller and a Z-gradient probe are shown in **Fig. 18**.

After the GradShim methods of interest have been tested manually at Level 1 and all parameters defined and optimized as needed, these parameter sets must be stored (*wpar*) with unique filenames for later use.

Level 2: Creating Shim Maps

A key requirement for the GradShim methods of shimming via field maps is a set of shim maps that must be acquired for each probe under the same conditions (pulse sequence parameters) used for shimming (see Eq. 10). Thus, whenever parameters are modified as described above, for example, it will be necessary to create a new set of shim maps. This applies strictly for changes in spectral width, gradient amplitudes and pulse lengths, echo position, and delays, i.e., all parameters that influence field profile width and shape. Furthermore, shim maps created with relatively poor B_0 homogeneity will be less than ideal and should be replaced with new maps after B_0 has been significantly improved. For minor changes in flip angle or repetition time, it will usually not be necessary to generate new shim maps. The applicability of the current shim maps is reflected in the rate and degree of convergence in the iterative shimming process. Good maps result in very rapid convergence (2-3 iterations) to a stable solution with very small variations in shim values for subsequent iterations.

Start the GradShim routine and select the method to be used (1D, 3D, etc.). The identifying name of the current probe will be displayed, along with a statement whether or not a shim map exists. Under *Data Set* the current root or home directory and user name will be shown. In a multi-user environment it is advantageous to have a special, common "user" just for shimming, e.g., with the user name *gradshim* and the *home* directory c:\bruker\xwin-nmr\ , for example. Thus, all acquired data sets for shimming will be stored with a filename derived from the parameter set name using the path:

home\data\gradshim\nmr\...

and the standard and user-defined parameters sets for shimming will be found in

home\exp\stan\nmr\par\...

From the drop-down menu *Setup*, select *Shim Mapping*. A shim mapping window will open, displaying information similar to that in the GradShim window (Method, Current Probe, and Data Set). Additional elements are Parameter Set, Echo Times, and Shim Group for Mapping. For the 1D 1H shim method, for example, the last used parameter set filename might be *gradshim1d1h* (default set) or some user-defined parameter set that was generated and stored as described under Level 1 procedures (e.g., *gradshim1d1h.rev1*). If a different parameter set is to be used, then its name must be entered in the filename field (the only position where the parameter set name for GradShim can be defined by the user). The Data Set disk (*home* directory) and user (e.g., *gradshim*) should be defined as desired. The acquisition data set filename will be identical to the parameter set filename.

Note: for each GradShim method and probe configuration only *one* set of shim maps is stored in

home\conf\instr\autoshim\refmaps\...

with the filename *fieldmapxx.nn*, where *xx* is the method code and *nn* is the probe ID number. When a different parameter set is used to generate a new set of shim maps, *the previous maps will be overwritten*.

The key variables for shim mapping are the Echo Times (i.e., the free precession delays) *TE1* and *TE2* which represent the values to be used for the delay *d15* in the two measurements required for mapping. In these two data fields (and only here), the user can enter new echo times chosen on the basis of trial measurements or experience. When shim mapping is completed, the specified delays, the number of data points in each dimension, and the offsets applied to each shim will be stored in *refparxx.nn* in the directory where the *fieldmap* files are stored.

Finally, the group of shims to be mapped must be defined in the group name field. The current default and user-defined groups can be examined and edited via the *Edit - Shim Groups* menu. For 1D methods a group containing all available Z^n shims should be selected. For 3D methods a group containing all possible on- and off-axis shims is appropriate (e.g. *shim34* for BOSS-2 shim systems). Important is that the shim group defined for mapping *must* contain *all* shims that will be used (perhaps in various subgroups) for subsequent iterative shimming.

For 3D shim trials with a new method, parameter set, or echo times, it may be useful to first create maps for a limited subset of shims (e.g., all Z^n shims plus X, Y, XY, X^2–Y^2 and their combinations with Z and Z^2) to save time. Trial shimming can then be performed only with the defined subset of shims. When the method parameters have been optimized, then a complete set of shim maps can be created for later use.

Before starting the shim mapping procedure, one should store the current shim settings in the temporary file used by GradShim (*wsh GSHIM*); mapping is started by clicking the *Start Shim Mapping* button. Gradient-echo measurements are first performed with the current parameter set for the delays *TE1* and *TE2* at the current shim settings. Then, one after the other, the shims to be mapped are incremented by an offset defined in the *refpar* file for the current method, measurements with *TE1* and *TE2* are carried out (total of $2n+2$ measurements for n shims), and the shim maps are calculated. This is a reasonably quick procedure for the 1D case. However, for 3D applications with $ns = 1$ and a repetition time *TR*,

the total measurement time is $1024(2n+2)TR$ for n shims. Once the maps have been acquired, the current parameter set and any combination of the shims included in the mapping procedure can be used in the GradShim routine.

The actual shim maps (profiles) for the 1D case can be visualized graphically as shown in Fig. 17. In the 3D case only a single graph is presented with z projections. The horizontal axis is a phase axis, and the maximum phase evolution achieved for each shim should approach but not exceed ±360° (see above). The vertical axis represents a data point number in the spatial domain with a value zero corresponding to the gradient system isocenter and limits of $\pm si/2$ (FT size) defining the *FOV*. The default values of *si* used by GradShim for the Z, X, Y axes are 64, 32, 32, respectively.

Level 3: Iterative Shimming

After a set of shim maps has been generated for a given method and parameter set, iterative shimming with GradShim can be performed according to definitions made in the Iteration Control File, whose current name appears in the filename field in the GradShim window. The contents of this file are shown as a list of Iteration Steps. The user can select any of the predefined control files via the menu button in the filename field and can edit these files or create new ones via the GradShim menu *Edit - Iteration Control*.

Iteration Control File

The complete set of defined control files can be viewed and edited in the Shim Iteration Editor window using the buttons *New* (create new file with specified name), *Open* (open existing file from list), and *Save* (save current file). Each control file can contain one or more steps, and each step is defined by two entries: the *shim group name* for the shims to be adjusted at a given step and a *size* parameter, which specifies the maximum value of the spatial coordinate (number of data points, positive or negative) defining the extent or width of the field profile to be used for shim optimization (fitting).

For the selected control file the iteration steps are listed in the display. The last step can be deleted with the *Delete Step* button (also repeatedly), and additional steps can be added with the *New Step* button. A set of default control files are provided in the *autoshim* directory where the shim maps are stored. Control files created by the user are stored in a *user-specific* data area (e.g., c:\WINNT\Profiles\...). The individual steps in a control file can be used to shim the same group several times or different groups of shims in succession with different *size* parameters, if desired.

Shim Groups

The desired shim group must be defined for each step in an iteration control file. The list of predefined groups is presented in the upper part of the Iteration Editor window, and these groups can be created and edited via the Shim Group Editor. All of the shims in a selected (sub)group must be members of the group that was defined for shim mapping, i.e., a map must exist for each shim that is now to be optimized by GradShim. Furthermore, the groups must be chosen in a logical and practical manner. For 1D shimming on H_2O at high field, it should generally be possible to shim a group comprising Z^1 to Z^5. Whether or not Z^6 can also be successfully adjusted will have to be determined by trial and will depend on the S/N available in the field profile and the *size* parameter described below. At low fields, when a deuterium solvent signal is used with X-nucleus probes such as the BBO, QNP, or DUL versions, the limited S/N available may not be sufficient for shimming Z^5 or Z^6 or the higher-order off-axis shims.

The size parameter

The shim map diagram for the Z^n shims in ^{1}H applications should be similar to that of Fig. 17; for ^{2}H applications the S/N will be somewhat lower but should be better than the poor example shown in Fig. 14. In Fig. 17 the interval over which the shim maps are well-behaved ranges from spatial coordinate –28 to +28 (vertical axis), i.e., somewhat less than the *FOV* defined by the data points –32 to +32. The usable range is primarily determined by the ratio of the profile width, defined by G_z^{read}, to the spectral width *sw*. At the edges of the profile width, the shim profiles break down.

Thus, it is necessary to restrict the fitting procedure, which calculates new shim settings from the measured field profile (Eqs. 9-11), to the limited region over which the shim maps are correct, taking any asymmetry into account. Thus, the *size* parameter in the iteration control file defines the profile range (data points from –*size* to +*size*) that will be used for calculating the shim corrections. In the case of Fig. 14 or 17 the maximal usable value for *size* would be 23 or 28, respectively, and this limiting value or a smaller one should be entered along with the chosen shim group name in the iteration control file.

Note that the value of *size* must be as small as necessary to remain within the usable profile width but as large as possible to provide a sufficient number of data points for calculating high-order shims. In Fig. 17 one can see that the curvature of the Z^6 profile (yellow) lies in the regions with data point numbers >19, i.e., at the top and bottom of the sample region where the lineshape hump originates. In general, the higher the shim order, the larger the *size* required for determining the shim correction needed. However, the *size* parameter should not exceed the smaller of the two limiting values (positive or negative) where the shim profile becomes too noisy or reverses direction.

For the example of Fig. 17, it would be useful to define control files for the shim group Z^1 to Z^6 with *size* = 25, 26, or 27 and a similar set for the group Z^1 to Z^5. Shimming trials can then be performed with the various control files, and the

resulting lineshape or quality of water suppression can be examined to check performance and dependability.

If the sample height is reduced to be close to or smaller than that of the rf coil, e.g., through the use of Shigemi or other susceptibility-matched NMR tubes, then it may be necessary to reduce the *size* parameter since the profile width may be less than the maximum suggested by the shim map profiles obtained with longer samples. The situation can be checked by clicking the command button *Show Current Field Profiles* at the bottom of the GradShim window. A field profile measurement with the current parameter set and echo times will be carried out (without shim adjustments), and the result will be displayed in the *Shim Results* window. The turning points of the profile can then be used to redefine the *size* parameter if necessary.

Note: in the above discussion the *size* parameter refers to the Z dimension exclusively. For 3D shimming applications GradShim automatically assumes a *fixed* range of ±9 data points for the X,Y dimensions. Thus, it is important that the *FOV* for X,Y be properly defined so that the corresponding profile widths cover at least ±9 data points from the center.

Gradient Shimming

When appropriate shim maps have been generated and an iteration control file defined, the user can start the shimming procedure by clicking the button *Start Gradient Shimming*. Acquisitions are carried out for the two delays *TE1* and *TE2*, the current field map is calculated and displayed in the *Results* window (**Fig. 19**), and the shim corrections required to minimize the rms field deviation are calculated and set using the BSMS. The text window below the profile display can be scrolled to view information such as the profile data point ranges used for shim calculation, the measured rms field deviation *before* shim correction, the predicted rms after shim correction, and the shim corrections applied. The profile in the display is highlighted in a different color for the data points included within the specified *size*. If further interations are specified, the procedure continues by measuring the current profile, which is added to the graphic display in a different color, and calculating new shim corrections. Note that the *last* profile displayed represents the situation *before* the final shim corrections were applied. To measure and view the *final* field profile *after* shimming, click on the *Show Current Field Profiles* button.

The frequency scale of the profile display will be defined by the first measurement where the field deviation is largest. Subsequent profiles for a given set of iterations will appear on the same scale and will overlap strongly when the deviation becomes small. To optimally view the final field profile or a new set of iterations, simply close the Results window (*OK* button) before starting the next profile measurement.

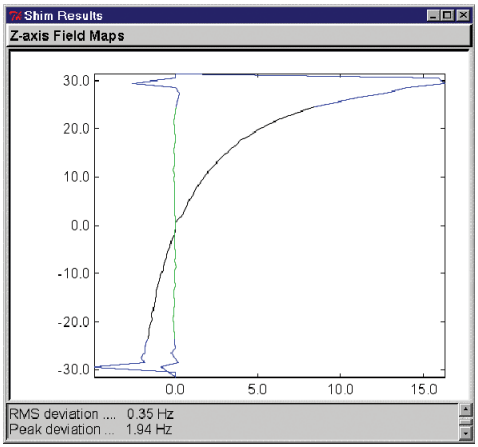

Fig. 19: Example of 1D 1H shimming on an AVANCE 600 with 5-mm TBI probe. The magnet was previously shimmed on H_2O with a short aqueous sample (length ca. 35 mm). The long water-suppression test sample was inserted and *gradshim1d1h* was started for the shim group Z^1 to Z^6 and *size* 25. The curved field profile with the black inner region represents the initial state (rms dev. 23 Hz); the profile with the green inner region defined by *size* represents the result of *one* shim iteration (rms = 0.35 Hz; the shim increments applied were 726, –381, 324, –1020, 3037, –6788 for Z^1 to Z^6.

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