Shimming: Theory and Practice

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Necessity for shimming

- For high resolution NMR, the magnetic field must be homogeneous to within 5 parts in 10¹⁰.
- The field from the main magnet is homogeneous to only about one part in 10⁶.
- Any material placed in the bore shim stack, probe, sample – changes the field. A water sample can change the field by parts per million.

Most of the pre-superconducting magnets were made of iron. To render the field more homogeneous, the position of the pole pieces were adjusted by metal shims.

Later, when permanent magnets were developed, it became easier to adjust the homogeneity of the field using small electromagnets that generate magnetic field gradients to compensate for the inhomogeneities of the main magnetic field. The terms 'shims' and 'shimming' were kept.

Mathematical Analysis

<u>Taken from:</u> Concepts in Magnetic Resonance (1990), **2** 131-149

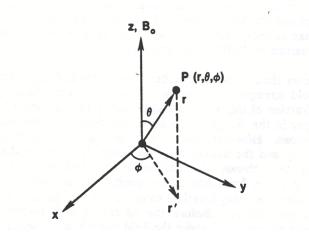
Any steady-state magnetic field in a volume of space in which there are no charges or current obeys the Laplace equation:

$$\left\{\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\right\} B_0 = 0 \quad \text{or} \quad \nabla^2 B_0 = 0$$

The field can be represented as a linear combination of any complete, orthogonal basis set. The *spherical harmonics* are a convenient basis set for this purpose. Thus, B_0 is described by the expansion in spherical harmonics:

$$\mathbf{B}_0 = \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_{nm} \left(\frac{r}{a}\right)^n P_{nm}(\cos\theta) \cos[m(\phi - \psi_{nm})]$$

Where a is the average bore radius, r represents the sample position, and C_{nm} and Ψ_{nm} are constants.



The calculations are easier when performed in spherical polar coordinates.

Since the sample volume is small compared to the bore size, as the order (n) Gets higher, $(r/a)^n$ becomes negligible. Good thing too because the Number of terms in this equation is infinite, and we would need infinitely Many shims!

$$B_0 = \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_{nm} \left(\frac{r}{a}\right)^n P_{nm}(\cos\theta) \cos[m(\phi - \psi_{nm})]$$

The functions $P_{nm}(\cos\theta)$ are polynomials in $\cos\theta$, and when m=0, P_{n0} are the *Legendre Polynomials*.

The first few Legendre Polynomials

 $P_{0}(\sigma) = 1$ $P_{1}(\sigma) = \sigma$ $P_{2}(\sigma) = \frac{1}{2}(3\sigma^{2} - 1)$ $P_{3}(\sigma) = \frac{1}{2}(5\sigma^{3} - 3\sigma)$ $P_{4}(\sigma) = \frac{1}{8}(35\sigma^{4} - 30\sigma^{2} + 3)$ $P_{5}(\sigma) = \frac{1}{8}(63\sigma^{5} - 70\sigma^{3} + 15\sigma)$ $P_{6}(\sigma) = \frac{1}{16}(231\sigma^{6} - 315\sigma^{4} + 105\sigma^{2} - 5)$ where $\sigma = \cos\theta$

Notice that all variation of B_0 with Φ disappears when m=0 because the final cosine term is unity. When m=0 the functions in the equation for B_0 are called *zonal harmonics*, and the zonal field is given by:

$$\underset{zonal}{\mathbf{B}_{0}} = \sum_{n=0}^{\infty} C_{n0} \left(\frac{r}{a}\right)^{n} P_{n}(\cos\theta)$$

You can think of these as the Z components of the field. That is, inhomogeneities that can be canceled by Z shims.

The harmonics for which m is not zero are called the *tesseral harmonics*. note that because of the final cosine term, as we move in a circle around the Z axis (as in a spinning sample), the field oscillates at harmonics of the rotation frequency.

$$\mathbf{B}_0 = \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_{nm} \left(\frac{r}{a}\right)^n P_{nm}(\cos\theta) \cos[m(\phi - \psi_{nm})]$$

When m is not zero, the functions $P_{nm}(\cos\theta)$ are called the Associated Legendre Polynomials:

Some of the Associated Legendre Polynomials

$P_{11}(\sigma)$	=	sinθ	12.13		
$P_{21}(\sigma)$		3sin t cost	$P_{2}(\sigma)$	-	3sin ² 0
$P_{31}(\sigma)$	=	$\frac{3}{2}\sin\theta(5\cos^2\theta - 1)$			$15\sin^2\theta\cos\theta$
$P_{33}(\sigma)$	=	15sin ³ 0			
$P_{41}(\sigma)$		$\frac{5}{2}\sin\theta(7\cos^3\theta - 3\cos\theta)$	$P_{A2}(\sigma)$	=	$\frac{15}{2}\sin^2\theta(7\cos^2\theta - 1)$
$P_{43}(\sigma)$		$105\sin^3\theta\cos\theta$			105sin ⁴ θ
$P_{s1}(\sigma)$	=	$\frac{15}{8}\sin\theta(21\cos^4\theta - 14\cos^2\theta + 1)$			
$P_{s2}(\sigma)$	=	$\frac{105}{2}\sin^2\theta(3\cos^3\theta - \cos\theta)$			
$P_{\mathfrak{S}}(\sigma)$	-	$\frac{105}{2}\sin^3\theta(9\cos^2\theta-1)$	$P_{\rm S4}(\sigma)$	-	$945\sin^4\theta\cos\theta$
$P_{\rm SS}(\sigma)$	-	945 sin ⁵ 0			
		$^{21}/_{\theta}\sin\theta(33\cos^{5}\theta - 30\cos^{3}\theta + 5\cos\theta)$			
		$\frac{105}{8}\sin^2\theta(33\cos^4\theta - 18\cos^2\theta + 1)$			
$P_{\mathfrak{S}}(\sigma)$	-	$\frac{315}{2}\sin^3\theta(11\cos^3\theta - 3\cos\theta)$			
$P_{64}(\sigma)$	=	$\frac{345}{2}\sin^4\theta(11\cos^2\theta-1)$	$P_{65}(\sigma)$	=	$10395\sin^5\theta\cos\theta$
$P_{66}(\sigma)$	=	10395 sin ⁶ 0			
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This separation of harmonics into zonal and tesseral is important when the sample is spinning. The tesseral harmonics are, of course, related to the off-axis shims.

Of all the terms the equation for B_0 , only the one where n=m=0 represents a homogeneous field. For our purposes, all the others are error terms that describe the inhomogeneities of the field.

$$\mathbf{B}_0 = \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_{nm} \left(\frac{r}{a}\right)^n P_{nm}(\cos\theta) \cos[m(\phi - \psi_{nm})]$$

Modern shims are coils that produce extra fields that can cancel the unwanted harmonics in B_0 . The shim coils are designed to produce, when current is passed through them, a single harmonic. Then the current in that shim can be adjusted to exactly cancel that portion of the inhomogeneity described by that particular spherical harmonic.

Shims are usually labeled in Cartesian coordinates. The conversion from spherical coordinates is tedious, but it's just algebra. For example, the 3,1 harmonic shim is:

$$B_{31c} = \alpha_{31c} I_{31c} \frac{3r^3}{2} \sin\theta (5\cos^2\theta - 1) \cos\phi = \alpha_{31c} I_{31c} \frac{3x}{2} (4z^2 - x^2 - y^2)$$

The common name for this shim is xz^2 .

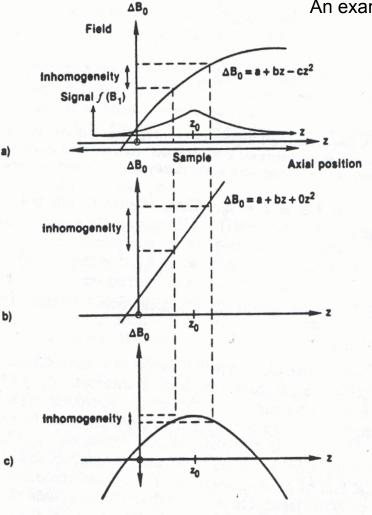
Order n	Degree m	Function	Common Name
1	0	Z	Z
2	0	$2z^2 - (x^2 + y^2)$	z^2
3	0	$z[2z^2-3(x^2+y^2)]$	z ³
4	0	$8z^{2}[z^{2}-3(x^{2}+y^{2})] + 3(x^{2}+y^{2})^{2}$	$ \begin{array}{c} z^2\\ z^3\\ z^4\\ z^5 \end{array} $
5	0	$48z^{3}[z^{2}-5(x^{2}+y^{2})] + 90z(x^{2}+y^{2})^{2}$	z^{s}
1	1	x	x
1	1'	y y	у
2	1	ZX	zx
2	1'	zy	zy
3	1	$x[4z^2 - (x^2 + y^2)]$	zy z^2x
3	1'	$y[4z^2 - (x^2 + y^2)] x^2 - y^2$	$\begin{array}{c}z^2y\\x^2-y^2\end{array}$
2	2	$x^2 - y^2$ is real solution of $x^2 - y^2$	$x^2 - y^2$
2	2'	xy	xy
3	2	$\frac{xy}{z(x^2-y^2)}$	$\begin{array}{c} xy\\ z(x^2-y^2)\end{array}$
3	2'	xyz	zxy
3	3	$x(x^2 - 3y^2)$	x ³
3	3'	$y(3x^2-y^2)$	y^3

Cartesian representation of spherical harmonics:

Because of the phase term (Ψ_{nm}) in the B₀ equation, the phase of the tesseral shims must be adjustable. This could be accomplished by making the shims rotatable. What's done in practice is to make them in pairs. So for each tesseral shim we have separate X (cos) and Y (sin) shims.

In a perfect world, each shim coil would generate exactly one harmonic. then shimming would be a simple process of going through all the shims one time and maximizing each one.

In reality, due to design compromises and winding errors, each shim coil generates several harmonics and the shims "interact".



An example of how the shims get mixed:

Imagine we had only z and z^2 shims.

In this example the center of the RF coil is above the center of the shim set.

If the initial error in the field is ΔB_0 =a+bz-cz², and the operator first tries increasing z², the field will get worse (b). Decreasing z² reduces the inhomogeneity (c) but the field is clearly not homogeneous so the lineshape will be poor.

In this example, the correct procedure would have been to increase z^2 as in (b), then decrease z until the field was homogeneous.

This illustrates why there are local maxima, and why one often has to move a shim so that the lock level decreases to find a higher maximum.

Since the sample is not centered at z=0, but at z=z₀, z becomes (z + z+₀) and ΔB_0 =cz² becomes:

 $\Delta B_0 = c(z + z_0)2 = c(z^2 + 2zz_0 + z_0^2)$

 Z_0 is a constant, so $2zz_0$ is <u>linear</u>, and the z^2 shim has a z component.

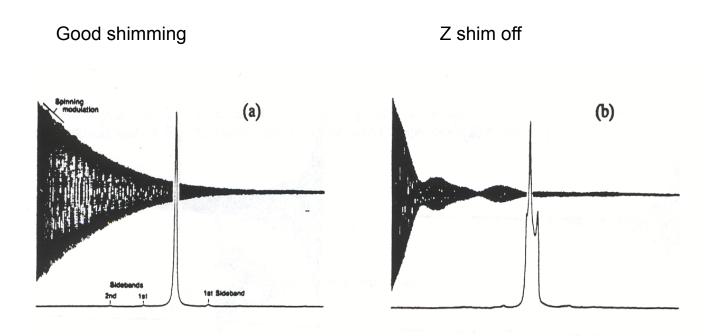
Many other flaws can lead to this sort of thing. Design or manufacturing flaws in the shim coils, shim coils not perfectly positioned, etc, all contribute to mixing of shims. If you extrapolated this example to three dimensions and 28 shims (on our systems), you can see why shimming is so difficult.

Manual Shimming

Once a particular probe in a particular magnet is shimmed, most of the shims don't need adjustment from sample to sample. It's primarily the z shims that change.

Why? The radial extent of our samples is very small and they' re quite radially symmetric. Also there's very little radial change from sample to sample. In contrast, the samples are quite long in the z direction so the shimming is more important (and harder). And there's a lot of variation in length and centering from sample to sample.

Although each shim produces several harmonics, making life miserable for the shimmer, each shim is contaminated by lower order shims of the same parity (z^3 is mostly contaminated by z, and z^4 by z^2 , etc). This makes it easier to find effective shimming strategies. To shim well, one must look at the FID and/or the spectrum, not just the lock level. Getting an idea what these indicators look like when certain shims are off is very helpful. Here are some examples with the z shims:

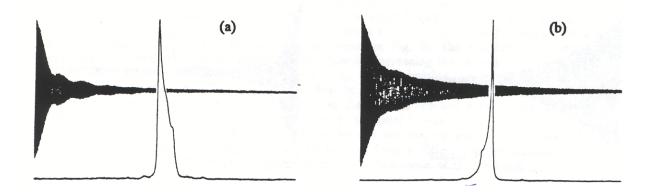


When the z shim is off, the initial decay of the FID is much faster and can have "beats". The spectrum broadens and manifests structure.

Here what look like individual peaks within the single peak are due to B_1 (the field generated by the pulse) inhomogeneities. Local maxima in B_1 close to probe coil conductors cause these 'peaks'.

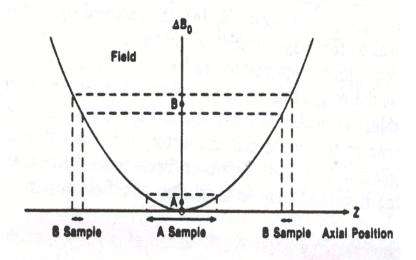
As we misset shims of higher order, the initial fall off of the FID gets faster:

 z^2 shim misset in one direction (a), and in the other (b)



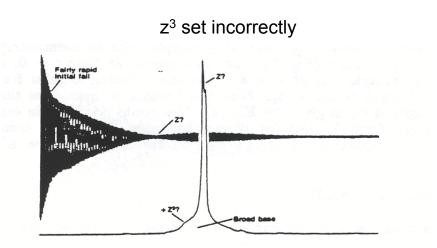
Even orders give a "hump" on one side of the peak. Why?

Z² is an even function:



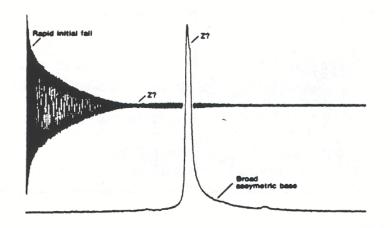
There is much sample volume in the vicinity of field strength A. This gives rise to the main peak. At higher field (like at B) there is some sample (this gives rise to the hump), and there is no field lower than A so there's a sharp cutoff on one side. The hump ends suddenly because the sample tube ends.

For higher orders the hump is lower on the peak but has a longer tail.



In this case, the z^3 shim is contaminated with z and z^2 .

z⁴ set incorrectly



Note that the asymmetric hump is much lower on the peak that It was when z^2 was misset.

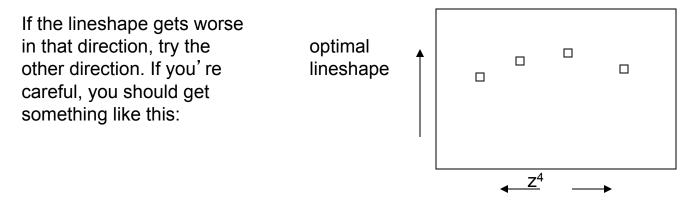
Shimming the higher order z shims:

In order to shim z^4 , you must first optimize $z-z^3$. Then change z^4 in one direction or the other so as to degrade the lock response somewhat. I usually move it 1000 or 2000 units.

**If moving z⁴ initially makes the lock rise, that's probably the right direction.

Then reshim $z-z^3$ and see if the shimming is better than it was with the original value of z^4 .

IMPORTANT! Don't just look at the lock. Carefully examine your spectrum or FID and decide whether it has improved or not. Specifically focus on the effect of misset z^4 (i.e. an asymmetric hump low on the peak). If the hump is coming in, that should be the right direction, even if the lineshape is worse in other ways. If your sample is in water, you must evaluate the shims using a 1D presaturation experiment. Without presaturation, the water line is too broad to see the asymmetries from poor shimming.



After z^4 is optimized, if the lineshape still looks poor, and specifically if it looks like z^5 might be off (symmetric broadening very low on the peak), then you must optimize z^5 in the same way. In principle, every time you change z^5 , you should reoptimize z^4 as above, in practice the process can usually be shortened by paying close attention and getting a feel for which way the shims are moving.

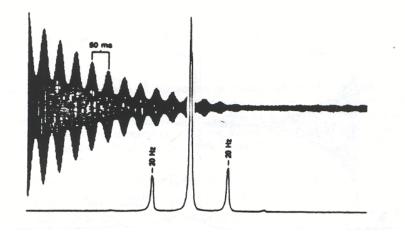
 Z^6 is shimmed the same way. But usually it's not necessary. Usually Z^6 should be left alone. Also – gradient shimming doesn't handle z^6 well, so don't include it in your shim group.

Off-Axis Shimming

As mentioned above, the off-axis, or tesseral, shims don't change too much from sample to sample. Usually it's sufficient to just shim on the lock. I work my way up from low order shims (x, y) to high order shims (xz^4 , yz^4 , xyz^3 , (x^2-y^2) z^3 , x^3z , y^3z) and then back down, working in complementary pairs (*i.e.* xz and yz), and iterating between shims of the same order.

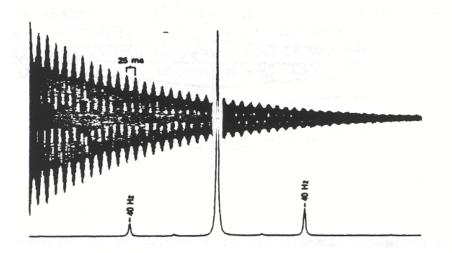
If you need to shim the off axis shims really well, you should spin the sample. If the sample is spun at 20Hz, and a first order tesseral shim is misset, spinning sidebands at +/- 20Hz will appear in the spectrum. This is because each volume element will return to a particular field strength once per revolution.

Effect of incorrect x or y shim with sample spinning at 20 Hz:



Since the modulation is 20Hz, this tells you that the degree of the shim that needs adjusting is 1, but it doesn't tell you which shim(s) is responsible. x, y, xz, yz, xz^2 , etc are all possible.

When the sample is spun, the zonal and tesseral inhomogeneities are separated out. The tesseral inhomogeneity determines the depth of the modulation and the size of the sidebands, while the zonal inhomogeneity controls the overall shape and duration of the FID and the lineshape. Effect of '2,2' (xy or x^2-y^2) inhomogeneity with sample spinning at 20 Hz:



Now the spinning sidebands are at +/- 40Hz because each volume element will pass through a given field strength twice per revolution.

This is quite useful in shimming because it narrows down the shims that need adjusting. Of course there are problems with this as well:

- Less than 20% modulation of the FID gives mostly mth degree spinning sidebands, but more than this (if a shim is really far off) gives sidebands at integer multiples of the spinning frequency. So it can be confusing. You best bet is to work on lowest degree (in x and y) shims first, then move to higher degree shims.
- Even in a perfectly homogeneous B₀ field, B₁ inhomogeneity can produce spinning sidebands

A Shimming Procedure

Before you start shimming there are a few things you should always do.

- Make sure your sample is at the right depth centered if it's a short sample or in a Shigemi tube, 21mm otherwise (depending on the probe).
- Start from good shims. Read in a previously saved shim file and make sure it's from the same probe you are using.
- Always lock it with "lock D₂O/H₂O". This sets the loop gain, loop filter, and loop time and the lock power. After you do this once you can lock and unlock it manually.
- Unlock the spectrometer and adjust the lock phase. You should also check this sometimes during the shimming process because changes in the shims can change the lock phase.
- Carefully adjust the lock power so it's as high as it can be without saturating. -17 for water and -25 should be close.

Shim z, z^2 , and z^3 first, carefully and iteratively. Often you can pull a lot more out of these than you would think.

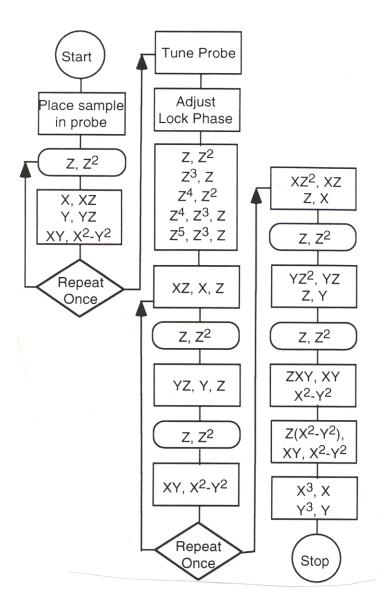
Shim the lower order off axis shims from lowest to highest and back. For Example, shim $(x, y) (xz, yz, (x^2-y^2), xy)$ and $(xz^2, yz^2, (x^2-y^2)z, xyz)$. Then $(xz, yz, (x^2-y^2), xy)$ and (x, y). Iterate between all the ones in parentheses. In particular remember that if a higher order shim changes (e.g. xz^2), you must reshim the lower orders of the degree (xz and x, and also yz and y).

Reshim z, z^2 , and z^3 . If there are changes, you might check the low order off axis shims again, then reshim z, z2, and z3. Up until now, all the shimming has been on the lock.

Now look at the spectrum and evaluate the shimming (remember that you must use a presaturation experiment for water samples). If necessary, shim z4 and z5 as described above. If the z shims change significantly, redo the off axis shims and $z - z^3$.

In most cases this is all you need to do to get a good shim. If all of this doesn't yield a decent lineshape, go to the higher order off axis shims. Keep trying! A lot of good shimming is attitude.

Of course it's possible there's a real problem. One of the cryoshims might have quenched. Is there a large piece of metal hanging from the bottom of the magnet? Is the magnet tilted?



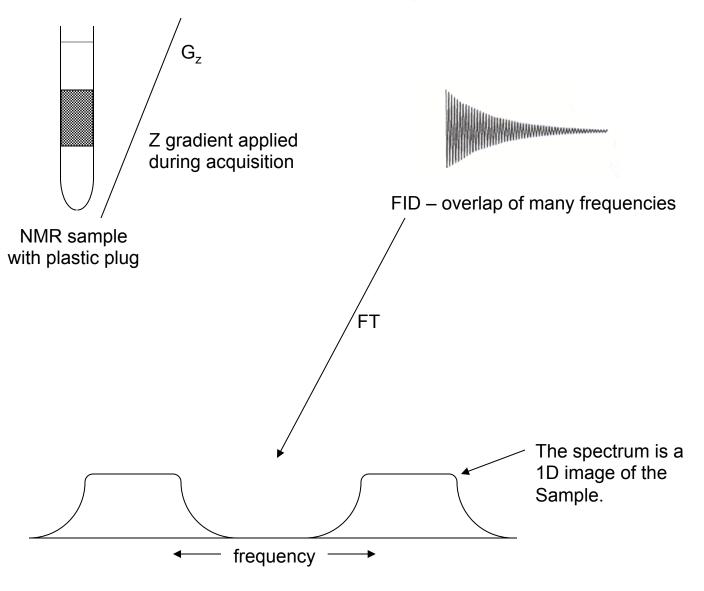
There's no "right" way to shim. No two people do it exactly the same way. Here's another shimming procedure from the **Protein NMR Spectroscopy** book.

This is a "complete" shimming procedure, but they' re only using 17 shims while our systems have 28. You can extrapolate to the higher order shims and use this procedure to shim on our systems.

NMR Imaging and Gradient Shimming

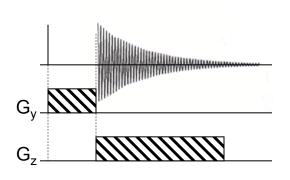
A short description of NMR imaging

Applying a gradient across a sample during an NMR experiment translates spatial information into frequency information:

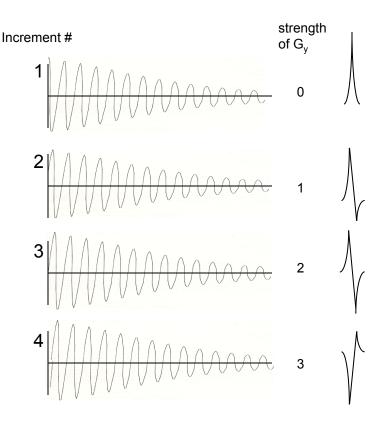


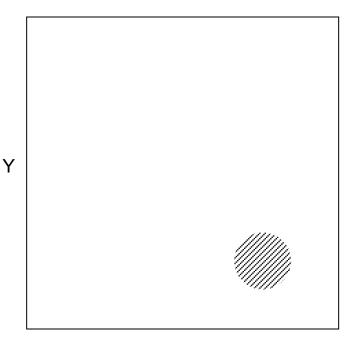
Lauterbur, P.C. Nature 242 (1973) 190-191

Fourier Imaging



2D imaging – YZ plane Several experiments are done. G_y strength is incremented.





Frequency during acquisition determines position along z-axis.

Change in phase with incremental change in G_y determines position along y-axis.

Kumar, Welti, and Ernst JMR 18 (1975) 69-83

Gradient Shimming

from:

J. Magn. Reson. A (1994), **111**, 203-207

A *phase image* of the sample reflects the evolution of the magnetization.

When the carrier is on resonance, the phase difference $\Delta \phi(r)$ obtained at a certain position in the sample from images taken at two echo times (TE) is determined by the field inhomogeneity $\gamma \Delta B(r)$:

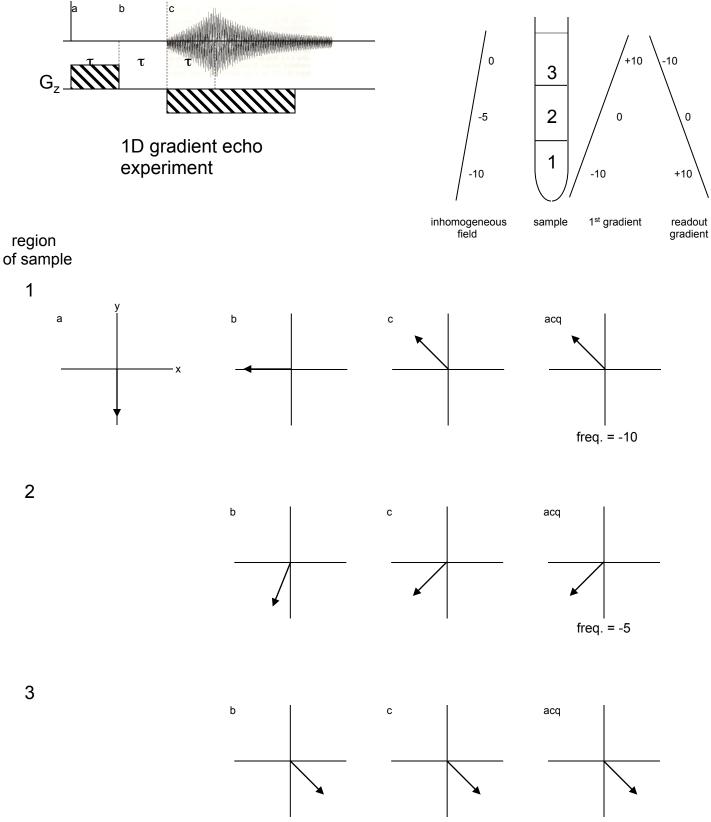
$$\Delta \phi(\mathbf{r}) = \gamma \Delta \mathbf{B}(\mathbf{r}) [\mathsf{TE}_1 - \mathsf{TE}_2]$$

The effect of the shims can be similarly mapped by measuring the phase difference between images at two different shim settings:

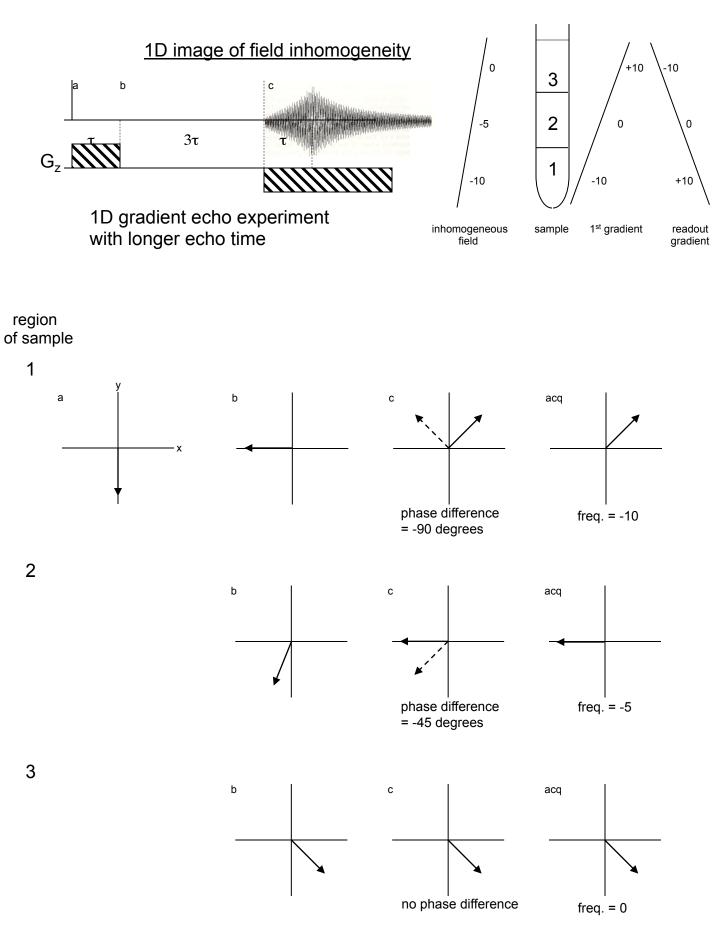
 $\gamma[\Delta B(r)_{shimset 1} - \gamma[\Delta B(r)_{shimset 2}] = [\Delta \phi_{shimset 1}(r) - \Delta \phi_{shimset 1}(r)] / [TE_1 - TE_2]$

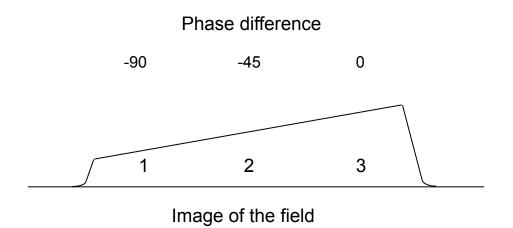
Optimum shim settings can then be calculated using the measured field inhomogeneity, and the known effects of each shim.

1D image of field inhomogeneity



freq. = 0





When the carrier is on resonance, the phase difference $\Delta \phi(r)$ obtained at a certain position in the sample from images taken at two echo times is determined by the field inhomogeneity $\Delta B(r)$.

 $\Delta \phi(\mathbf{r}) = \gamma \Delta B(\mathbf{r})[TE_1 - TE_2]$

An image of the field is made by plotting the phase difference divided by the echo time difference against frequency. (remember that because of the acquisition gradient, frequency corresponds to position in the sample)

Field Mapping

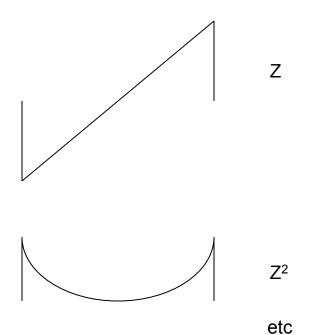
The field correction provided by the shims for a given change in shim current can be mapped similarly.

The phase difference between images at two different shim settings is measured:

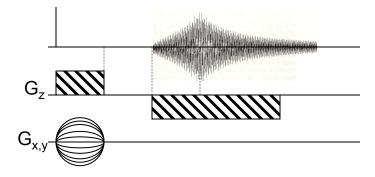
 $\gamma[\Delta B(r)_{\text{shimset 1}} - \Delta B(r)_{\text{shimset 2}}] = [\Delta \phi_{\text{shimset 1}}(r) - \Delta \phi_{\text{shimset 2}}(r)]/[TE_1 - TE_2]$

Therefore to map the shims, an image of the field is generated once with reasonable shims. Then a shim is moved significantly and another image is taken. This shim is returned to its original value. This is done with each shim in turn.

The 1D field maps generated by missetting individual shims look something like this:



3D images and field mapping



3D images can be done by performing many 1D scans, incrementing the strength (or length) of the X and Y gradients in a nested fashion.

Each 3D experiment takes almost 2 minutes, so each 3D image takes almost 4 minutes to acquire (2 experiments are necessary, using two different echo times).

You can see that 3D field mapping takes awhile. To map all 28 shims, 58 experiments must be run (2 + 2[28]).

The field maps are empirical maps of the real effects of the shims.

Gradient Shimming

When gradshim is executed, an image (1D or 3D) is taken of the field using two echo delays (TE₁ and TE₂) as before.

The image is compared to the field maps, and the computer calculates how best the change the shims to make the field homogeneous.;

Here's how the calculation is done:

Optimal shim settings are calculated by solving the following least-squares problem using singular value decomposition:

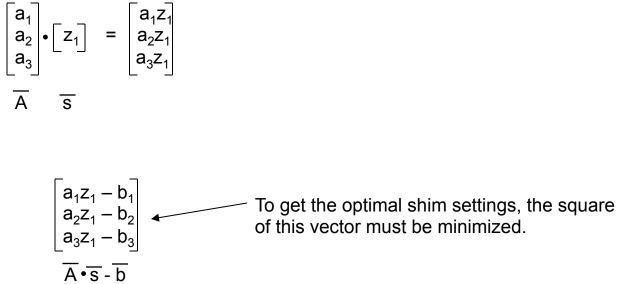
$$\overline{S}_{opt} = arg. min. (||\overline{A} \cdot \overline{S} - \overline{b}||^2)$$

where

- \overline{A} = matrix of n column vectors, each one a vector of field changes per unit shim change for m spatial positions. n is the number of shims.
- \overline{b} = vector of current field values for m spatial elements
- \overline{s} = vector of n starting shim settings

 \overline{S}_{opt} = optimal shim settings

Here's a simple example: 1 shim (z), 3 spatial positions



Bruker uses 128x32x32 points (that is: 32 increments in each of the G_x and G_v dimensions, and 128 points in the acquisition) with a field of view of 28x6.4x6.4 mm.

So there are 131,072 'voxels', roughly 35,000 of which are contained in the sample.

Each of these volume elements is 8.8 x 10⁻⁹ liters.

<u>Topshim</u>

Topshim is essentially gradient shimming using a better algorithm. In principle it achieves a better shim than gradshim, and it does it faster.

The main difference is that everything is automatic. The program decides which shims to use, determines the best length of sample, and iterates until the shimming is optimized. It even comes with built-in field maps.

Basic usage:

	topshim:	automatically	performs 1	1D gradient	shimming
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topshim 3d: automatically performs 3D gradient shimming.

- topshim gui: opens the graphical user interface. From the gui you can start topshim with many different options.
- There are dozens of parameters and options. Their use is covered in the Topshim manual (available under the help menu in Topspin). All are accessible from the GUI or the command line.

To successful shimming with Topshim, always do these two things first:

- 1) Open the data set of the planned NMR experiment.
- Lock the sample for the correct solvent using the *lock* command. Topshim optimizes things differently for each lock solvent. Note in particular that the *shimming methods for D2O and H2O+D2O are different.*

Spectrum Optimization

Topshim performs an optimization of some criterion for the quality of the spectral line. There are four options:

ls	lineshape with narrow width	(default for D2O)	
lshump	lineshape with narrow hump		
SS	solvent suppression	(default for H2O+D2O)	
optoff	no optimization, use standard spatial weighting		

These can be invoked from the command line or from the GUI. Example: *topshim 3d Ishump*

Tune

Sometimes it's helpful to remove residual shim gradients after gradient shimming. This can be done using the *tune* option in Topshim. It just maximizes the lock level using a subset of the shims. It can also be done just before gradient shimming. This can be useful, for example, to prepare the best off-axis shims before running 1D gradient shimming.

For example:

topshim tunebxyz tuneaz: this tunes Z, X, and Y before and after 1D gradient shimming.

topshim tune tunea: this tunes Z, X, Y, XZ, and YZ and does no gradient shimming at all.