Developing a Computer Algorithm for Passive Shim Design

Tim Chiocchio
Mentor: Dr. Bill Brey

Abstract--A passive shim insert is designed for a certain magnet of some measured dimensions, magnetic field, and field inhomogeneity. This means that shims are magnet specific. Quite often there is a need to shim the same magnet operated at different frequencies or field magnitudes depending on the probe inserted. In this case, there needs to be multiple shims for the same magnet. Previously, the design and construction of passive shim inserts have been made either by contracting out to a field mapping and shimming specialist or doing it in house. To develop a shim design algorithm so that the passive shim design and construction could always be done in house would be preferable and is the goal of this research.

The design of a computer algorithm for passive shim design is conceivable with the guidance of the scientific literature and the goal is attainable through the computational aid of MATLAB. The design algorithm centers on the use of dipole modeling for the field contributions of the ferromagnetic shims. The algorithm is designed to work on any magnet of any dimension, field and inhomogeneity with modifications in the necessary parameters. The inputs to the algorithm are the measured field values of a particular spherical harmonic term, which come from the field mapping unit (FMU). The outputs are the necessary magnetic moments of each dipole. Thus, the algorithm gives a map of the various dipole strengths on the shim insert, which is a thin sheet or an unrolled cylinder. The fact that the result of the algorithm is called a map suggests that is not the final product concerning the passive shims. The map must be converted into a realization of the passive shims.

I. Introduction

In magnet science as it relates to nuclear magnetic resonance (NMR) spectroscopy and other magnetic resonance and spectroscopy techniques, there is a push to not only have magnets with higher and higher magnetic fields but also with better and better homogeneity. As an example, The National High Magnet Field Laboratory, NHMFL has plans on building a new hybrid called the series connected hybrid, SCH. The SCH will have higher fields than other magnets with either pure resistive or pure superconducting sections. More interestingly, it is planned to use less power and to have much improved field homogeneity in comparison to its predecessor, the 45T hybrid.

Homogeneity as defined by Sauzade and Kan [1] is "the ratio of the maximum field variation ΔB to the total field B_0 for a given volume". It is usually expressed in ppm (although sometimes as ppb) over a specified spherical region or diameter spherical volume (DSV). The role of the homogeneity of the field in NMR is analogous to the function of the focus and zoom of a camera. If the focus is not functional on a camera, then you will hardly be able to distinguish anything in the picture. Similarly, if the homogeneity is insufficient or the inhomogeneity is too large, then you will not be able to distinguish between distinct resonant frequency peaks. It is also true that the better the zoom on a camera, the more detail you can capture both far and near. Sufficient field homogeneity along with higher fields means then that the researcher can capture more details of more substances under study.

The more mathematical way to understand why NMR requires low inhomogeneity is the Larmor relation where ϖ is the resonant frequency, γ is the gyromagnetic ratio and B_0 is the magnetic field:

$$\varpi = \gamma B_0 \tag{1}$$

The proton value for γ is $2.675 * 10^8 \, rad * T^{-1}$. The Larmor relation shows us that the resonant frequency is directly proportional to the polarizing magnetic field. As an example, the aforementioned 45T hybrid is found to operate at a proton frequency of 1.916GHz using the equation. It is clear that a NMR magnetic field is required to be homogeneous or uniform throughout the sample volume in order to ensure proton resonance at the same frequency.

If homogeneity is essential, then it must be guaranteed whatever the cost. The question, however arises, why not build a magnet with the required inhomogeneity in the field built in. Vadovic [2] states that "to meet this requirement through a complicated design and especially a precise and, therefore, rather expensive manufacturing and setup of the basic field generating system while allowing only negligible tolerances in the prescribed design parameters, is economically ineffective and technically often unrealizable with the given means." The solution lies in field shimming, which he advocates as he goes on to say that "to add a supplementary (correcting) field to the main magnetic field with the aim to obtain the desired shape over the localized region for the sum of both fields is economically more favorable." The technique of field shimming can be further divided into two categories depending on the source of the correcting magnetic field. Passive or ferromagnetic shims refer to a strategic arrangement of a certain ferromagnetic metal or alloy that produces strong magnetic fields in the presence of a magnetizing field [3]. Active shims require current to flow through them, which in turn produces a magnetic field.

If the correction of the inhomogeneity or variation in the field is the goal of shimming, then the characterization or analysis of the field must be an **essential** preliminary step. Hoult and Roméo [4] provide an excellent text on magnet field profiling. They write that in a volume through which no current passes, Laplace's equation is satisfied by the scalar and vector potential as well as by the field itself. The scalar potential is especially useful since it eliminates the initial need to work with Cartesian components. Employing spherical polar coordinates and solving Laplace's equation yields:

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=0}^{n} r^n P_n^m(\cos\theta)[A_n^m \cos m\phi + B_n^m \sin m\phi] \tag{2}$$

Note that the notation is taken from [2] and that the solutions containing r^{-n-1} are excluded since the potential is finite at r = 0. The terms of this series, which form a complete set of eigenfunctions, are commonly called spherical harmonics. The harmonics produced by the m = 0 case are called zonal harmonics. They possess axial symmetry. The rest of the harmonics ($m \neq 0$) are called tessoral harmonics. Their symmetry is less obvious since it depends on the value of n and m. The function of $P_n^m(\cos\theta)$ is called Legendre's associated function where n is the order and m is the degree. The curious reader can learn more about these functions from [4] or from any textbook covering special functions. The usefulness of applying spherical harmonics is not immediately apparent, but it will

be clear later. The magnetic field can be found simply by taking the negative gradient of the potential:

$$\vec{B} = -\nabla\Phi \tag{3}$$

The x and y-components are ignored since one expects them to be much smaller compared to the desired field in the z-direction [5]. In the Operator's Manual for the FMU-BBK Magnetic Field Mapping Unit of Resonance Research Inc (RRI) [6], the magnetic field is found to be the following:

$$B_z = \sum_{n=0}^{\infty}\sum_{m=0}^{n}(n+m+1)r^n P_n^m(\cos\theta)[A_{n+1}^m \cos m\phi + B_{n+1}^m \sin m\phi] \tag{4}$$

The traditional way of expressing this infinite series utilizes Cartesian coordinates and scaled coefficients. The rule for scaling the coefficients is given as:

$$(A_{n+1}^{''m} / A_{n+1}^{m}) = (n+m+1)!/(2^m m!(n-m)!)\text{, and likewise for } B_{n+1}^m \tag{5}$$

Using this rule gives us the familiar series of field gradients where $z2 = z^2 - (1/2)(x^2+y^2)$, c2 = $x^2 - y^2$ and s2 = $2xy$:

$$B_z(x,y,z) = A_1^{''0} + A_2^{''0} z - A_2^{''1} x - B_2^{''1} y + A_3^{''0} z2 - A_3^{''1} zx - B_3^{''1} zy + A_3^{''2} c2 + B_3^{''2} s2 + \ldots \tag{6}$$

Now the advantage of spherical harmonics is clear, as the first term in the series is a homogeneous or uniform field.

The goal of this research is to develop a passive shim design algorithm that will cancel out all the other existing terms or to ensure that only the homogenous field remains. It has been shown by Jesmanowicz et al. that the design of a passive shim insert can be done using dipoles to model the fields due to small patches of ferromagnetic metal (nickel in this case but could be iron, steel, etc) that make up the shim [7]. This approach is taken in the development of the shim design algorithm with the hypothesis that the direct manipulation of spherical harmonics is not required in the design of a passive shim. In other words, one does not have to start with simplified shapes like elementary rings whose field in terms of spherical harmonics can be readily calculated and solve for various parameters of the shapes that lead to only one of the desired spherical harmonic. There is an in depth explanation of this technique in [4] for the interested reader. To avoid confusion, it must be emphasized that the technique advocated here depends on spherical harmonics too since they are essential in profiling or mapping the field of the magnet. Basically, the difference lies in how the correcting gradient or spherical harmonic is derived. The passive shim design algorithm calculates using an error minimization algorithm the dipole strengths of the small patches in order to match a spherical harmonic of specified strength found in the magnet. Thus, the success of the technique rests on dipole modeling and on error minimization and not on the direct use of

spherical harmonics and on the manipulation of the shape parameters to derive the necessary correcting gradient.

II. Materials and Methods

The first step to creating the passive shim design algorithm is to study and master the basic building block, the dipole field. In Griffiths [8] the dipole equation is given as:

$$\vec{B} = (\mu_0 m / 4\pi r^3)(2\cos\theta * \hat{r} + \sin\theta * \hat{\theta}) \tag{7}$$

The z-component of the field can be found by converting the spherical unit vectors into their Cartesian unit vectors. After converting coordinates, B_z becomes:

$$B_z(x, y, z) = (\mu_0 m / 4\pi) * (2z^2 - x^2 - y^2) / (x^2 + y^2 + z^2)^{5/2} \tag{8}$$

The result can be verified by plotting the vector field (B_x, B_y and B_z), which give us the expected circular patterns.

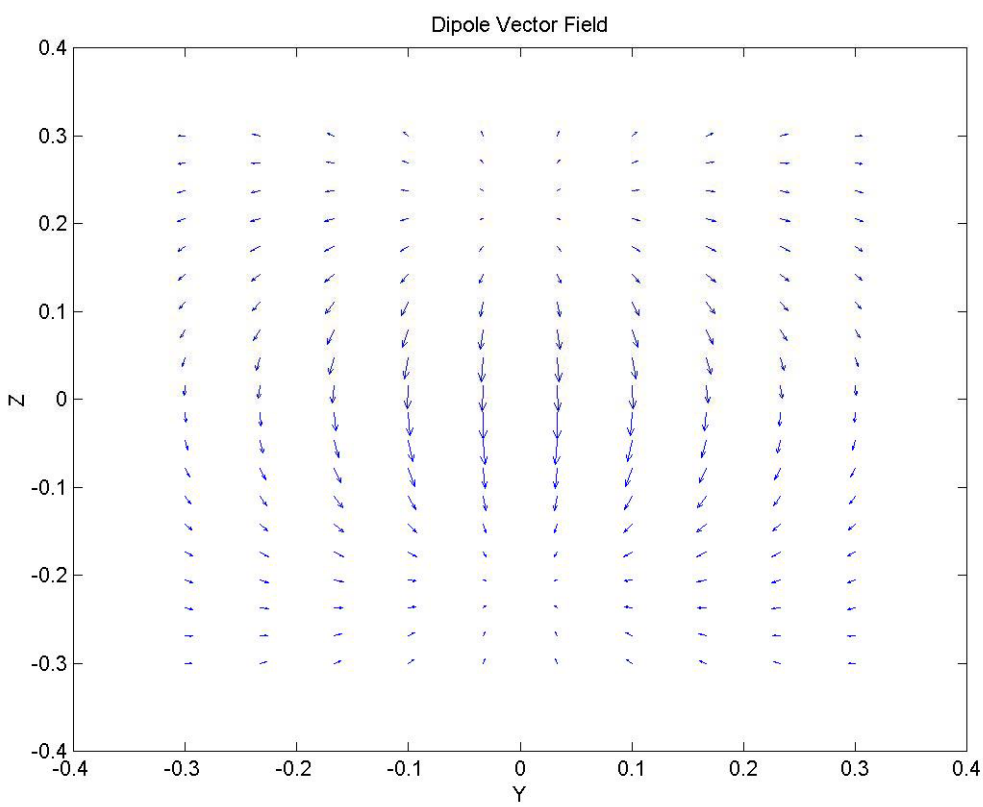

Figure 1-Dipole Field

In [9] the effects of a point dipole are modeled using the equation:

$$B_z = \mu/(4\pi\varepsilon_0 c^2) * (1/R^3 - 3z^2/R^5) \tag{9}$$

This is exactly the same equation ignoring the constant in front and noting that the sign has been reversed.

The next step is to derive the general function for the field $B_z(x, y, z, \rho', \phi', z')$ where (x, y, z) are the coordinates of the field point and (ρ', ϕ', z') are the cylindrical coordinates of the dipole. That equation is expressed as where $x' = \rho' \cos\phi'$ and $y' = \rho' \sin\phi'$:

$$B_z = (\mu_0 m/4\pi) * (2(z-z')^2 - (x-x')^2 - (y-y')^2)/((x-x')^2 + (y-y')^2 + (z-z')^2)^{5/2} \tag{10}$$

The following step is to use the preceding equation to generate the field of a passive shim tube with elements described by a matrix M_{ij}. A matrix M_{ij} for a ZX term is then constructed using the specifications given by RRI for a ZX shim. The RRI design is a good starting place to become more familiar with dipole modeling and to begin developing the passive shim algorithm.

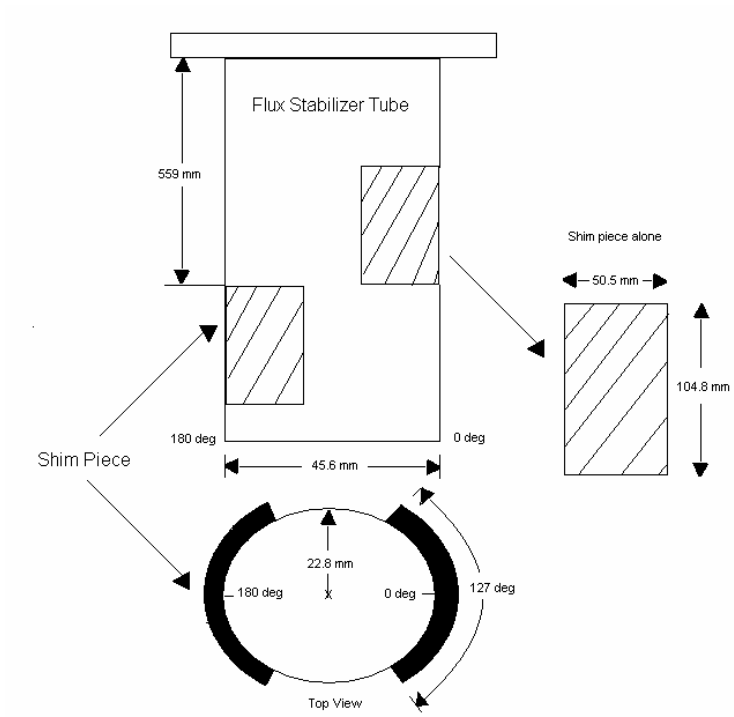

Figure 2-RRI ZX Shim Design

There are a few important things to note about this design. First, the thickness of metal shim piece is exaggerated in the drawing for emphasis and clarity. In all actuality, the gauge is only .001". Second, the sizes of the two shim pieces are identical. Third, the type of spherical harmonic produced depends largely on the orientation of the shim pieces. Referring back to (4) and (6), the index m of the ZX term is found to be 1. Thus,

the 180° separation of the two shim pieces is expected using the formula π / m that [4] derived for the necessary separation to produce tessoral harmonics ($m \neq 0$).

Returning again to the matrix M_{ij}, the field produced by the array of dipoles is plotted in Cartesian coordinates and along a helical path. Let's consider first the plot in Cartesian coordinates, which is a group of 1D plots.

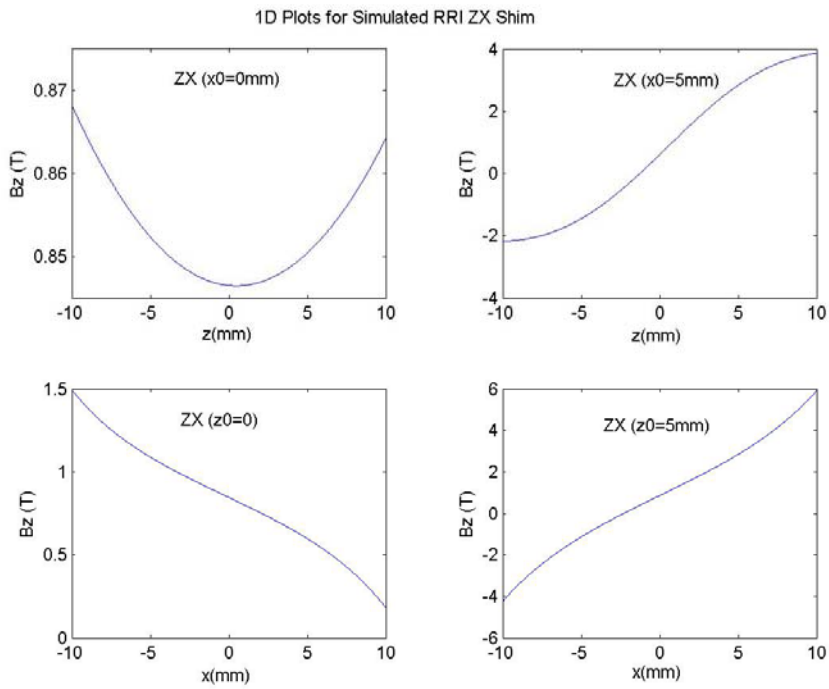

Figure 3-Simulated RRI ZX Shim

The above four plots in figure 3 show the field of the simulated RRI ZX shim as a function of either z or x. The values of the field are arbitrary since all the dipoles have unit magnetic moment. The dipoles are positioned on a cylinder as pictured in figure 2. The dipole dimensions are 1mm x 1mm. There are 210 dipoles in the vertical direction and 143 in the circumferential direction, which makes a total of 30,030 dipoles. Two important observations should be made here. First, the plots demonstrate that the simulated RRI ZX behaves like an ideal ZX near the origin. A ZX shim is expected to be zero along the z-axis and near the origin, which we see in the plot in the upper left corner. If we move off of the axis to say x = 5mm, then we expect the field to increase linearly with z, which the adjacent plot confirms. The plot in the lower left corner is puzzling at first glance. The ZX should be zero along x-axis and clearly it is not. However, the change in the field over the range of x-values is nearly an order smaller than for the case when z = 5mm. Thus, the field in the plot in the lower left corner is relatively zero and the field in the adjacent plot varies linearly with x. Second, all four of the plots have a noticeable field (about .75-.85) with z = 0 or x = 0 where we expect the field to be zero. According to Hoult and Roméo, this result is actually to be expected since not all harmonics of a given parity may be eliminated in a passive shim design. They explain

that this is due to the fact that we do not have the luxury of reversing the permeability, which we can do with currents in an active shim [4].

The second plot is especially important since the FMU measures the field along helical path. This plot shows the field similarly to as it appears in the FMU software. The two plots in figure 4 show an ideal ZX and the simulated RRI ZX along a helical path. The path of the helix is from 10mm below the magnet centerline to 10mm above. The radius of the helix is 7mm and its pitch is 2.5mm, which are typical values used for the FMU. The ZX term has a value of 1ppm over the 20mm range. The two plots look quite similar at first glance. However, the simulated RRI ZX looks like less like a straight-cone, which is typical of a ZX.

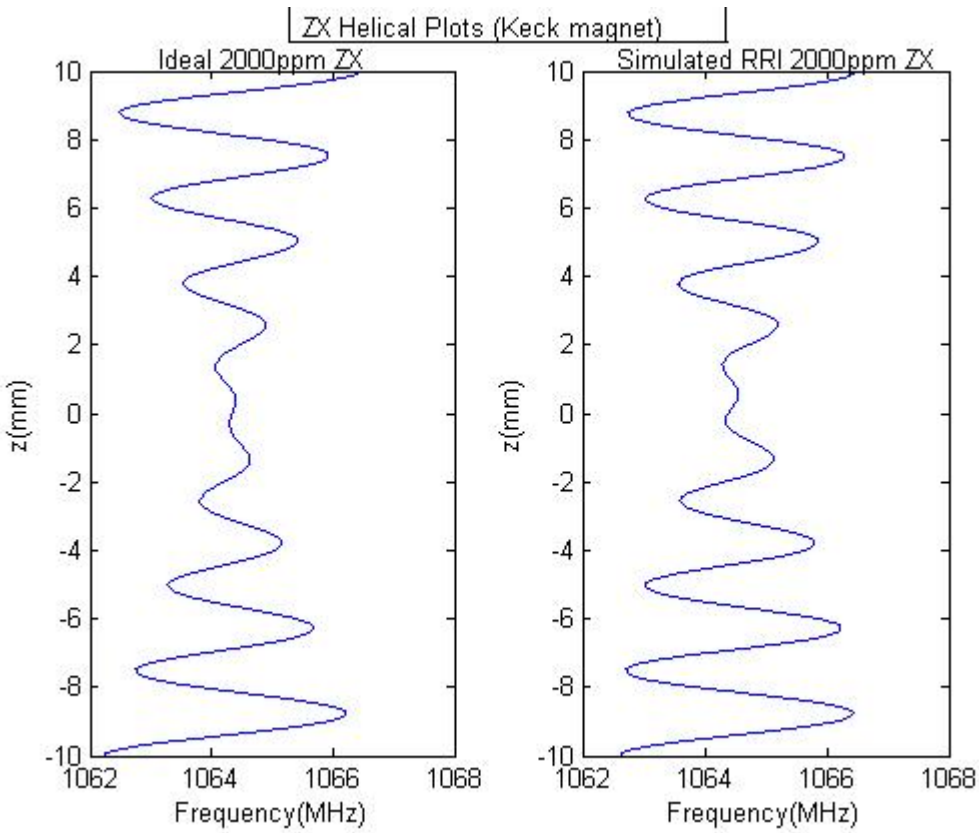

Figure 4-Ideal and Simulated RRI ZX Shim (1ppm)

The last step in creating the passive shim design algorithm is to synthesize the previous work into a functional algorithm or program that designs the shim using error minimization. The algorithm works by solving the following linear algebra equation where A is the dipole matrix of (n x k) dimension with n equal to the number of field points on a helical path and with k equal to the number of dipoles, x is the column vector of unknown magnetic moments needed to match the desired spherical harmonic term and B is the column vector of that term's field values:

$$\vec{A}\vec{x} - \vec{B} = 0 \qquad (11)$$

The unknown magnetic moments are solving using the Moore-Penrose pseudo-inverse, which is the pinv command in MATLAB. The pseudo-inverse calculates using a singular decomposition value algorithm the least squared error values for the unknowns.

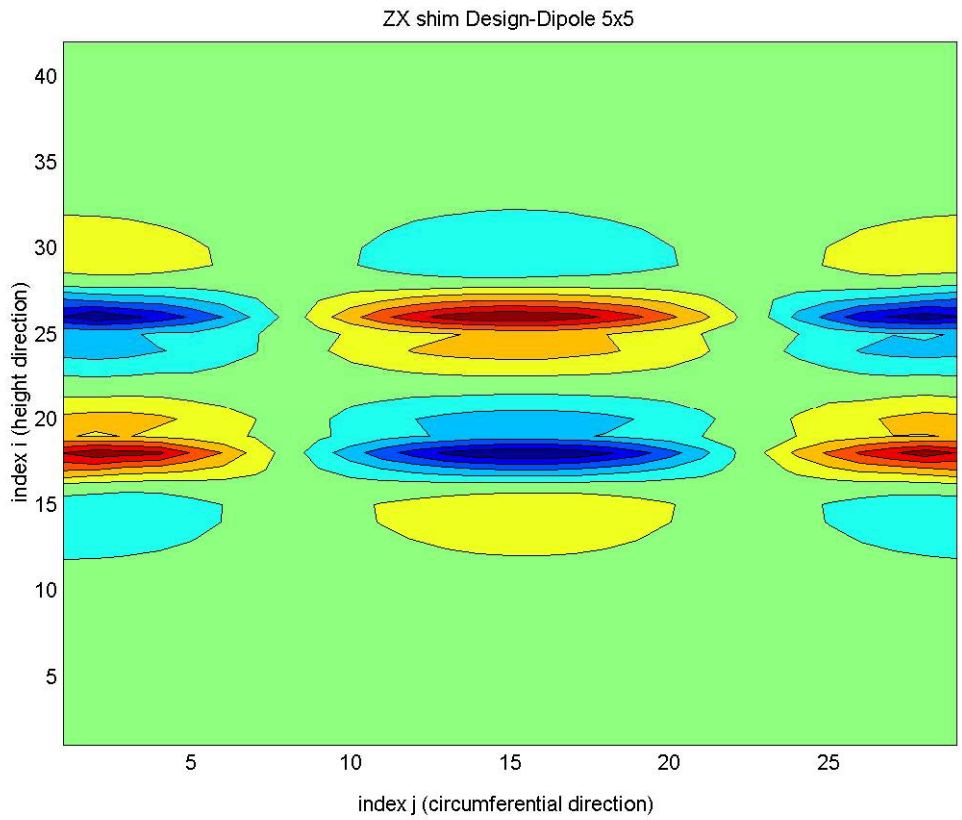

Figure 5-ZX Design Using Error Minimization

Figure 5 displays a passive shim design for a ZX using the design algorithm. The dipoles are made to be 5mm x 5mm. The magnetic moments are adjusted so that no negative value exists. The design has the 180° separation or phase shift between the top and bottom halves like the RRI design. In other words, where the top half is red and at its highest value, the bottom half is blue and at its lowest value.

III. Discussion

There are a few problems associated with the development of a passive shim design algorithm. First, an appropriate size for the dipole must be selected when using dipole modeling. The general reason for this is that a magnetized material is in fact made up of many dipoles, which are nothing more than tiny current loops. Each atom has its own magnetic moment and group of atoms with the same magnetic moment make up magnetic domains. It is clear then that increasing the dipole size means that the approximation is greater and that there will be potentially greater error. In the simulation of the RRI ZX shim design, there is always a bit of error in trying to reproduce the exact

dimensions of RRI ZX design. It is possible that this error is what causes the simulated ZX to look slightly uneven. The field behaves quite similarly to an ideal ZX with a dipole size of 1mm x 1mm, at least this was the case near the origin. If the dipole size is increased beyond this, the field begins to behave less and less like a ZX. In the passive shim design algorithm, the result was less sensitive to the dipole size. That is to say that the dipole size could be increased up to 5mm x 5mm and the algorithm will give a map with the corresponding ZX symmetry. A possible reason for the algorithm to be less sensitive to dipole size is in the power of the error minimization of the pseudo-inverse. The pseudo-inverse has problems minimizes the error if the dipole size is increased past 7.5mm x 7.5mm. At this size, however, the ZX shim map lacks any obvious ZX symmetry.

The second problem also relates to dipoles. The dipole field in the z-direction can be derived using (7), which results in (8). When (8) is used in simulating the RRI ZX, the plot is inverted as if multiplied by negative one. If (9) used the plot is inverted back to the expected orientation. It is unclear at the moment why this is so. Nevertheless, the sign is chosen so that the fields are oriented similarly.

The third problem is to decide on over-determining or under-determining the system of linear equations for solving for the unknown magnetic moments. Over-determining means that there are more points along the helical path than dipoles. In other words, there are more equations than unknowns. Under-determining, therefore, means more unknowns than equations. The motto taught in school is to have the same number of equations as unknowns. Unbelievably, both conditions can be used to match the helical plot of an ideal ZX. However, the over-determined system produces maps with smoother curves and better symmetry. In the design algorithm, the system is made optimally over-determined by having 10x as many points as dipoles. Smaller factors seem to lessen the smoothness and symmetry, whereas larger ones seem to make portions of the map disappear.

The fourth problem is that performing the pseudo-inverse on large matrices is very computational. The computer made available initially is a Dell with only 256 MB of RAM and a 1.7GHz processor speed. The computer performs the pseudo inverse only with a dipole size of 10mm x 10mm, which means a matrix size of 2940 x 294. After many attempts to solve the problem at smaller dipole sizes, it was clear that a computer with more memory is required. The next computer, also a Dell, has 3GB of RAM and a 3.1GHz processor speed. This computer performs the pseudo-inverse at a dipole size of 5mm x 5mm, which means a matrix size of 12180 x 1218, in about five minutes.

IV. Conclusion

Based on a symmetry analysis, the shim design algorithm seems to be working. The pseudo-inverse is a powerful tool, but it requires enormous amount of memory at dipole sizes of 5mm x 5mm and smaller. There is room improvement in the algorithm. It would be preferable if the solution could be found without having to compensate for the negative magnetic moments. What is done in the algorithm is the quick and easy solution. This entails adding a homogenous field to the positive dipoles, which is the first solution that [7] proposed. The second is to use a linear programming algorithm to solve for the magnetic moments needed to shim several field gradients with the constraint that

the magnetic moments must be positive. The algorithm is not useful and not truly complete until one finds a method of realization. There is a method in mind but there was not enough time to develop it. The method uses circular holes of varying diameter to represent the dipoles, but it is not clear at the moment if this technique will work with dipole sizes of 5mm x 5mm.

V. Acknowledgements

There are quite a few people to whom I owe a great deal of thanks for the success of this research. I want to express my thanks first to my mentor Dr. Brey and his group. They believed in me and also guided, corrected, encouraged, tolerated and congratulated me gracefully the whole way through. I want to especially thank Eduard and Kiran for helping me to find a computer more up to the task. I owe so much to the staff of the NHMFL's Center of Integrated Research and Learning (CIRL). I am very grateful for their work to ensure the success of the REU program. I am also greatly indebted to the NHMFL and NSF to have had the opportunity to participate in a REU program. I hope to make you all proud.

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