



B₀ Detoxification through Magnetic Field Shimming

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Abstract

MR imaging (MRI) and spectroscopy (MRS) allow unrivaled noninvasive access to *in vivo* anatomy, microstructure and physiology, but suffer from methodological limitations. Especially, imperfections of the B_0 magnetic fields can easily render MRI/MRS investigations useless. Varying B_0 conditions lead to line broadening in MRS, and spatial distortions and signal dropout in MRI. The experimental homogenization of B_0 conditions in a process called B_0 shimming is therefore mandatory for every MR investigation and high quality B_0 shimming is arguably one of the most important ingredients for successful MRI and MRS.

The BODETOX ("*beau-detox*") software has been tailored to provide efficient and reliable processing solutions for B_0 shimming. The BODETOX software includes basic and state-of-the-art techniques for B_0 shimming in a one-stop-shop solution and stands out by its comprehensiveness, user-friendliness, possibility of automation, and high optimization level of the achieved solution. The software stands out by its potential for automation and its user-friendly work flow. All parameters of the software are automatically maintained in protocol files that can be loaded to restore parameter settings to previously selected values. Besides convenience, functionalities like this ensure reliable and consistent processing throughout multi-scan studies. BODETOX has been developed for biomedical research and is specifically tailored to its needs. Scientists and clinicians in both academia and industry aiming for optimal experimental B_0 conditions and MRI/MRS outcome will find this software useful. Give it a try!

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Introduction

MR imaging (MRI) enables the non-invasive mapping of brain characteristics as different anatomy, microstructure or function. MR spectroscopy (MRS) allows the chemical analysis of physiological processes *in vivo* and together these methods provide powerful tools in the natural sciences, the life sciences and for clinical diagnostics.

Excellent spatial homogeneity of the main magnetic field B_0 , i.e. the static magnetic field, is essential for meaningful results. In an ideal scenario, the B_0 field over the regarded region-of-interest (ROI) is perfectly homogenous, i.e. it exhibits no spatial variation. In reality, however, spatial variations of the B_0 field e.g. over the human brain are the rule rather than the exception. In MRI, the presence of magnetic field inhomogeneity can lead to image distortion and signal loss, whereas spatial field variations in MRS cause loss of sensitivity and spectral resolution. Although manufacturing imperfections such as minute variations in magnet coil windings exist, the majority of magnetic field imperfections are sample-induced. Materials differ in their permeability to magnetic fields, an effect governed by the material's magnetic susceptibility [1]. Materials of different magnetic susceptibility therefore express different interior magnetic fields when placed in a magnetic field along with a transition zone at their boundary. The largest differences in magnetic susceptibility occur between brain tissue and air in the nasal and auditory passages and lead to strong magnetic field distortions in the frontal cortex and temporal lobes, respectively.

Basics of B_0 Magnetic Field Shimming

Magnetic fields obey the superposition principle and, therefore the effective magnetic field present during an MR experiment can be manipulated by addition of correction fields in a process called magnetic field shimming. To do so, the magnetic field distribution in the considered region-of-interest (ROI) is measured and the best correction field is determined. The ideal shim field exactly resembles the distortion at hand, however, at reversed polarity such that its application removes all inhomogeneity. The standard approach to minimize magnetic field variations is to superimpose magnetic fields with a spatial variation governed by spherical harmonic (SH) functions [2]. SH functions are 3-dimensional shapes that become more complex and spatially specific the higher the order. For instance, the (single) zero-order term describes an offset, the (three) first-order terms resemble linear gradients identical to the ones used for spatial encoding and the (five) second-order terms provide parabolic shapes. In reality, shim methods are limited by the ability of the field-generating technique to reproduce the distortion at hand and differences of the applied shim field from the magnetic field imperfection to be minimized manifest themselves as residual inhomogeneity after the correction process. The application of more shapes in the shimming process through inclusion of higher SH orders improves the modeling of the field distortion and, therefore the expected outcome of the shimming procedure.

We recently demonstrated that a set of simple circular coils can be converted to a powerful magnetic field modeling system when the electrical coils are driven individually [3]. The superposition of these multi-coil (MC) basis fields allows the synthesis of magnetic field shapes

that can be considerably more complex than those realizable with conventional SH coil systems. We applied MC-based magnetic field modeling to the long-standing shimming problems in the mouse [4], rat [5] and human [6] brain and showed that shimming with MC-generated correction fields outperforms SH techniques including state-of-the-art dynamic shimming with all zero to third order SH terms [7].

BODETOX Software

The BODETOX software provides algorithms to decompose a 3-dimensional B_0 distribution, e.g. measured from phantoms or human/animal subjects, in sets of spherical harmonic or multi-coil basis shapes. For any SH or MC B_0 shim system for which the performance has been properly characterized, shim hardware settings corresponding to the determined optimized correction fields can be derived.

Overall Structure and Application Pages

Overall, the software is organized in application pages resembling the work flow chronology of the optimization of B_0 shim fields and, when possible, organized from top to bottom and from left to right. For instance, B_0 field maps are first read on the *Data* page (left), before the ROI to be optimized is selected on the *ROI* page (center) and the SH or MC shim analysis is performed on the *SH-Shim* or *MC-Shim* pages, respectively (right). Similarly, data selection and processing options are typically located in the upper part of each page, followed by analysis and visualization options at the bottom of the pages.

Note that the data processing is streamlined and intermediate calculations are done automatically when needed. For instance, the data file and the ROI selection criteria do not need to be redefined after software restart, and the analysis of optimized shim fields can be reduced to a single button push on the later shim analysis pages *MC-Shim* and *SH-Shim*.

1) The *Data* page

Loading of experimentally acquired B_0 field maps. The 3-dimensional MR images are reconstructed and the B_0 field information is extracted and kept in memory for further processing.

2) The region-of-interest (*ROI*) page

A series of image- and B_0 field-based selection criteria and quality measures are available and can be combined with a Boolean AND operation to define the ROI at hand.

3) B_0 shimming with spherical harmonics (*SH-Shim*)

Conventional B_0 shimming is achieved with basis fields that resemble the shapes of low order spherical harmonic functions. This page allows the optimization of spherical harmonic-based correction fields for both static and slice-wise dynamic shimming in an ROI-specific fashion.

4) B_0 shimming with the multi-coil technique (*MC-Shim*)

A set of generic localized coils can be converted to a powerful magnetic field modeling system when each of the electrical coils is driven individually. This multi-coil concept allows for the synthesis of both simple and complex magnetic fields in a flexible and accurate fashion via the superposition of generic non-orthogonal basis fields. The multi-coil page provides algorithms for multi-coil B_0 shimming, both statically and dynamically (dynamic multi-coil technique or DYNAMITE).

Protocol Files

All BODETOX parameter settings are saved to file when the software is closed properly via the *Exit* button and automatically reloaded when the software is restarted. This functionality allows users to close the software at any time and to return to the exact same situation easily at a later time. Notably, this also includes the BODETOX page selection, e.g., *Data* or *MC-Shim*. In addition, the full set of BODETOX parameters can be saved to a user-specified protocol file (see the *Data* page for details).

Units

All spatial dimensions are given in millimeters, and angles are expressed in degrees. B_0 fields are consistently expressed in Hertz (Hz) due to its prevalence of the relative Larmor frequency of protons in MR. The conversion back to other units, e.g. Tesla, is straightforward. Further units are defined and explicitly labeled as needed.

Tool Tips

Besides the detailed explanations on the BODETOX software provided in this manual, short summaries and reminders on the functionality at hand are added to most entry fields, flags, and buttons as tool tips. This information can be visualized by mousing over the button without clicking it. For further information about any single function, feel free to email me: christoph.juchem@columbia.edu.

Download, Installation and Use

The BODETOX software has been developed in MATLAB (MathWorks, Natick, MA, USA) and is currently distributed as a stand-alone executable program compiled in MATLAB version R2013b for 64-bit Windows, Apple Macintosh and Linux operational systems. It can be downloaded from the Columbia Technology Venture website under a limited-term academic license:

Juchem, C., BODETOX: B_0 detoxification software for magnetic field shimming. Columbia TechVenture license 17326 (2017), innovation.columbia.edu/technologies/CU17326_b0detox

The corresponding MATLAB Runtime environment needs to exist to provide the software with the required libraries. Detailed instructions on the installation of the MATLAB Runtime can be found at: <https://www.mathworks.com/help/compiler/mcrinstaller.html>.

It is important for Linux and Mac users to start the software via the provided shell script, i.e. the file ending with `.sh`, instead of e.g. double-clicking the BODETOX icon directly. This script opens a terminal window and dynamically links the necessary libraries before the software is started. All these settings are temporary and disappear when the software and the terminal window are closed. The terminal window corresponds to the Matlab command window and all info printouts are delivered to this window.

Step-by-step instructions for starting the BODETOX software via a shell script on Linux/Mac:

1) Place a copy of the provided BODETOX directory to your computer and make sure you have the permissions to access and execute the files. If needed, change the permissions with the Linux/Mac command `chmod`.

2) Identify the system's MCR root directory. This is typically something like `/usr/local/MATLAB/R2013b` on Linux or `/Applications/MATLAB/MATLAB_Runtime/v82` on Apple Mac

3) Run the shell script file with the MCR root directory as function argument, e.g.

`./run_BODETOX.sh /usr/local/MATLAB/R2013b` or similar for linux or

`./run_BODETOX.sh /Applications/MATLAB/MATLAB_Runtime/v82` or similar for Mac if you are currently in the BODETOX directory or from anywhere via the absolute path:

`/home/juchem/matlab_exe/BODETOX/run_BODETOX.sh /usr/local/MATLAB/R2013b`

If the assigned MCR root directory has been correctly input, the BODETOX software will start. You will then find a GUI of the software itself and a terminal window containing information printouts.

4) For convenience, I recommend including the MCR root directory information in the shell script itself, thereby rendering its assignment as function argument obsolete and enabling the execution of BODETOX by double-clicking the shell script file or a link to it.

To do so, open (a copy of) the shell script and confirm the existence of the paths containing the variable `MCRROOT`. If the paths exist, the software will be able to find the libraries and nothing needs to be changed. If not, adopt the path details after the `MCRROOT` variable to account for the MCR installation details on your computer. Once all paths are correct, calling the shell script alone without function argument will start the software correctly. For Mac OS, you will need to edit the file to something like this:

```
#!/bin/sh
# script for execution of deployed applications
#
# Sets up the MATLAB Runtime environment for the current $ARCH and
executes
# the specified command.
#
```

```

exe_name=$0
exe_dir=`dirname "$0"`
echo "-----"
if [ "$1" = "*" ]; then
echo Usage:
echo $0 \<deployedMCRroot\> args
else
echo Setting up environment variables
MCRROOT="$1"
MCRROOT=/Applications/MATLAB/MATLAB_Runtime/v82;
echo ---
DYLD_LIBRARY_PATH=.:${MCRROOT}/runtime/maci64 ;
DYLD_LIBRARY_PATH=${DYLD_LIBRARY_PATH}:${MCRROOT}/bin/maci64 ;
DYLD_LIBRARY_PATH=${DYLD_LIBRARY_PATH}:${MCRROOT}/sys/os/maci64;
export DYLD_LIBRARY_PATH;
echo DYLD_LIBRARY_PATH is ${DYLD_LIBRARY_PATH};
shift 1
args=
while [ $# -gt 0 ]; do
    token=$1
    args="${args} \"${token}\""
    shift
done
eval "\"${exe_dir}/BODETOX.app/Contents/MacOS/BODETOX\" " $args
fi
exit

```

Note that you need to tell your Mac to execute the shell script if you double-click it. Otherwise, the file will be opened for editing in a text editor. To do so, go to *Open with* and select an iTerminal.

5) If you link the shell script to an icon or a command name, it can be executed easily to start up the software. For Linux, this can be achieved by adding a symbolic link to the */usr/bin* directory connecting a command name to the location of the script:

```
In -s /usr/local/juchem/matlab_exe/BODETOX/run_BODETOX.sh BODETOX
```

Note that root permissions are required for the creation of such a link; please, therefore, ask your system administrator for help if needed. Once the link has been created, you can (run the script and thereby) start the software from any terminal window simply by typing *BODETOX* followed by the return key.

Before you start

The manual is organized into chapters that resemble the page structure of the software. General aspects and core features, e.g. some of the display settings, are shared across pages. They are described in full with their first use and treated with greater brevity thereafter; it is, therefore, advisable to read the manual from the beginning. In the following, the individual subsections of

BODETOX are described in more detail. Further information and hints on the functionality of individual buttons can be visualized by placing the mouse over them.

Also of note is the information provided in the last few paragraphs of the manual, especially the call to join us in the fight against multiple sclerosis (MS) as well as some remarks on academic merit and legal aspects of software use.

I The Data Page

The data page is used to define and load the experimental B_0 field map data. Field maps are regular images that are acquired at various echo times. As such, the magnetization phase becomes a function of the apparent magnetic field in individual voxels and thereby allows the calculation of full magnetic field distributions in three dimensions.

The *Data* page is used to assign and load experimentally acquired B_0 information.

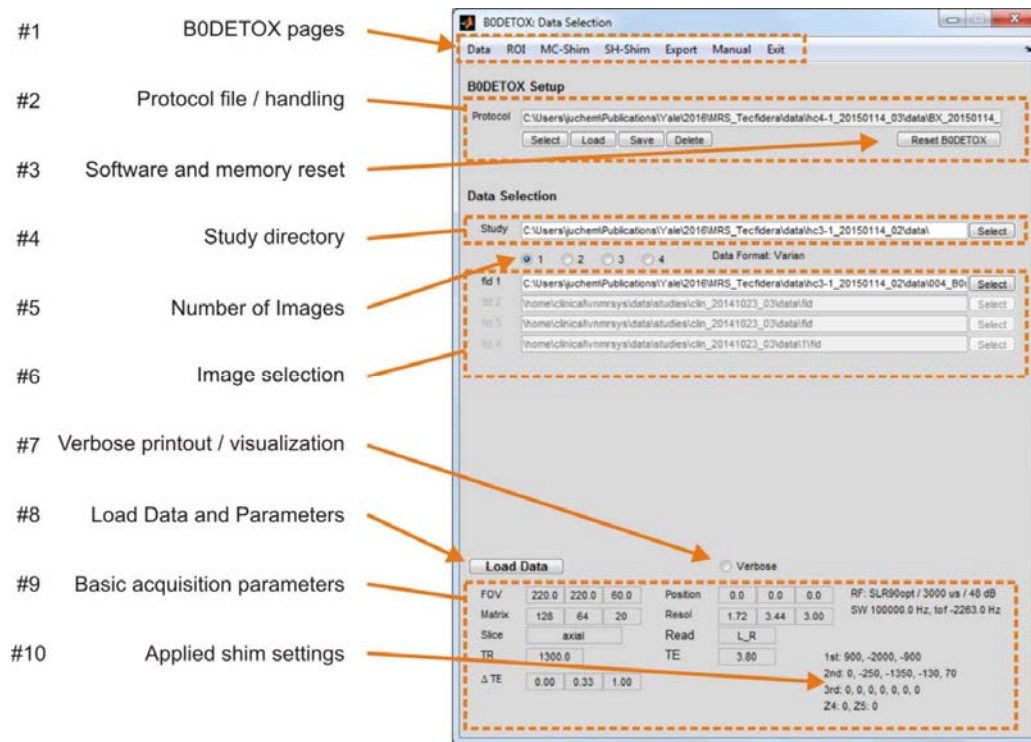


Fig. 1.1: *Data* and parameter loading page.

Protocol

The analysis of B_0 field maps relies on a wealth of chosen parameters. The BODETOX software accounts for this by saving the entire parameter selection to protocol files. These protocols can be loaded to restore all parameter settings to previously selected values. While all software and processing parameters are written to file, the decision has been made to exclude larger data structures such as the field maps themselves, thereby keeping the size of the resultant protocol files to a minimum, typically to a few kilobytes. Explicit export options are available to save the data to file (compare *Export* page). Notably, protocols are saved in MATLAB (.mat) format. Besides convenience, the reloading of tailored protocol files can be used to ensure consistent data processing of various experiments throughout a study.

There are two different protocol options with identical file format: 1) A general default file and 2) user-defined protocols. Parameter settings are inherently saved to a general default file when the software is properly closed via the *Exit* button (#1, rightmost page option) and it is strongly advised to do so. One default parameter file exists for every BODETOX installation. This background file is shared across users and overwritten every time the software is closed. In addition, parameter settings can be saved to protocol files designated by the user in the protocol section (#2). The *Select*, *Load*, *Save*, and *Delete* functionalities provide handling options for the selected protocol file.

Note that closing BODETOX through the operating system's Close button (x) in the upper right corner of the window is not advised as parameter settings are thereby lost.

Reset BODETOX

Processing B_0 maps and optimized shim settings requires a multitude of intermediate steps and data. Sometimes the status of the current data in memory becomes unclear, such as when a new field map is to be analyzed. The *Reset BODETOX* button restarts the software (#3). All parameter settings are kept, but the data memory is freed, thereby returning to a well-defined starting point.

Verbose

BODETOX can provide detailed information on every processing and analysis step to enable the user to access the processing stream and to evaluate intermediate results. While this information is always available, its display might not always be warranted. A situation-dependent balance exists between the provided level of detail and the risk of overloading the result display. If the *Verbose* flag (#7) is selected, detailed information is provided, e.g. for more comprehensive data analysis and experiment debugging. If the flag is not selected, only overview and summary data are shown instead.

Data Selection

The calculation of a B_0 field information is based on a phase difference acquired over a given echo time delay. BODETOX therefore supports the use of a series of 2 to 4 individual images that are saved separately as individual data files (#5, options 2-4). In practice, it is more convenient to acquire the images at varying echo time in a single scan and to save the resultant information in a single file. Option 1 in #5 allows reading the required phase information from a single multi-echo scan. Note that the software imposes no limit on the number of echo time delays if all data are contained in a single file.

Once the data format (#5) and file location(s) (#6) have been selected, the data can be loaded from file by pushing the *Load Data* button. Relevant acquisition parameters are automatically read from the corresponding parameter files when B_0 data are loaded. A selection of them, e.g. basic experiment conditions (#9) and apparent shim settings (#10), are displayed in the BODETOX

window for convenience. Explicit user-input for the definition of the data set at hand is not required.

For all file formats explained below, loading of both the magnitude and the field map information is achieved by pushing the *Load Data* button. It is advisable to always keep an eye on the terminal window as details of the data loading and format as well as potential problems will be shown here. Note that all relevant scan characteristics such as field-of-view, echo time delays or spatial resolution are read from the data header or associated parameter file and no manual assignments are necessary. If the loading has been successful, the info fields at the lower end of the *Data* page will be populated. Note that besides basic acquisition characteristics (#9), this will also entail the SH shim settings applied during B_0 field mapping.

The reading routines work have been tested for the data formats that have come my way. If you encounter problems with the specific data format you use, please get in touch with me (christoph.juchem@columbia.edu) and we will work it out.

Supported Data Formats, Data Selection and Loading

1) General Electric (GE) .MRDC format

GE's standard B_0 mapping sequence *GEMS B0map* saves the magnitude and field map information in a series of DICOM images in .MRDC format. To read such B_0 maps with BODETOX, copy these files to a single folder in the overall study directory (#4). Then select the single image option (#5, left-most flag 1) as all information originates from a single scan and data set. This choice will prepopulate the data path of *fid 1*. In a last step, push the *Select* button of *fid 1* in section #6, go into the scan directory and select any of the .MRDC files. Finally, read the files as detailed above.

Note that while the first-order terms, i.e. linear shims, are written to the file headers by default, this is not the case for the higher order terms. We therefore added such functionality to GE's standard B_0 mapping sequence and are happy to share this extension with the community upon request.

2) Siemens .IMA format

Siemens' standard B_0 mapping sequence *AdjGre* saves the magnitude and field map information in DICOM .IMA format in two consecutive directories. To read such B_0 maps with BODETOX, place copies of these two directories into the study directory (#4) and select the two image option (#5). Then push the *Select* button of *fid 1* (#6), go to the scan directory containing the field map information, i.e. the larger scan number, and select any of the .IMA found there. In a second step, push the *Select* button of *fid 2* (#6), go to the scan directory containing the magnitude images, i.e. the smaller scan directory number, and select any .IMA file there. Finally, read the files as detailed above.

3) Bruker and Varian FID format

BODETOX is capable of reading the Bruker and Varian raw file format *fid*, reconstructing the resultant images and extracting both magnitude and field map information. To do so, place copies of the scan directories contain both the raw data and the corresponding parameter files (Varian: *procpa*, Bruker: *acqp/method*) into the study directory. Based on the apparent data format, select either the one or the multiple scan option. Then select the *fid* data files for each of the experiments. Note that the corresponding parameter files are expected to be located in the same scan directories. Finally, read the files as detailed above.

II The Region-of-Interest (ROI) Page

2.1 General

The *ROI* page enables definition of the shim ROI by combining selection criteria that are based on geometry, (magnitude) image or magnetic field properties. All selected criteria are calculated individually and then combined by a Boolean AND operation. In other words, only voxels that fulfill all conditions are considered valid and become part of the final ROI. The only exception to this rule is the cluster condition (*Min. Neighbors*) which applies a minimum neighbor threshold search once to the final ROI.

Voxel: Cubic volume selection defined by its position, size and rotation (#1)

Slices: Image slice selection along the x, y and z direction (#2)

Ellipsoid: Ellipsoid volume selection defined by position, radius and rotation (#3)

Signal: Absolute value imaging signal (#4, 1st)

SNR: Signal-to-noise ratio. By default, a small square area in one of the outer corners is used to determine the noise floor. Selection of the attached flag allows manual definition of the noise region (#4, 2nd)

Segmentation: Brain segmentation option (#4, 3rd) via Brain Extraction Tool (BET) [8, 9]. BET is a powerful method developed at the University of Oxford for the separation of brain voxels from the surrounding skull and air (S.M. Smith. Human Brain Mapping, 17(3):143-155, November 2002). It is not part of the BODETOX software distribution and separate conditions apply (e.g. compare <https://fsl.fmrib.ox.ac.uk/fsl/fslwiki/BET>).

Grad.: Voxel-specific field gradient (1st derivative), consistency criterion to sort out outliers (#4, 4th)

G. Dev.: Voxel-specific 2nd derivative of field distribution, consistency criterion to sort out outliers (#4, 5th)

Frequ.: Frequency range criterion, only values between these limits are considered (#4, 6th)

Error: Error of the voxel-specific linear regression-based magnetic field calculation in Hertz (#4, 7th)

Manual: Manual slice-by-slice ROI selection through polygon drawing. Assigned are the first (left) and the last (right) slice to be considered. If the slice step size (center) is larger than 1, the ROI is interpolated for intermediate slices for which no explicit manual ROI assignment has been performed (#4, 8th)

Min. Neighbors: Cluster criterion based on minimum number of valid neighbors, limits: [1, 9+8+9=26] (#4, 9th). Note that this is the only condition that is not determined individually and combined with the individual results from the other conditions, but applied once in the very end to the (Boolean AND-combined) outcome of all other conditions.

Some clinical MR scanners (e.g. GE) move the patient bed to account for offset positions along the z-axis, e.g. of MR spectroscopy voxels, instead of applying the physical offset in the MR experiment itself. If such bed shift is applied, it needs to be taken into account in the B_0 shim calculation as the position of the subject relative to the MR scanner and its SH shim coils is affected and thereby no longer identical between the B_0 mapping experiment and, for example, the intended MR spectroscopy scan. This position mismatch is considered in BODETOX by selecting the *Bed Centering Z* flag (#10). The required shift information is assigned as the original z-coordinate of, for instance, the MRS voxel at hand. Note that the position-based criteria such as the cubic or ellipsoid volume conditions can still be used; their z-coordinate now refers, however, to the new bed center position. For instance, assume that B_0 shimming is performed for an MRS voxel located at $x/y/z = 10/20/30$ mm. If bed position is not adjusted, an ellipsoid of appropriate dimensions located at the same 10/20/30 mm position can be used for ROI selection. By contrast, if the bed position is centered around the voxel position, the *Bed Centering Z* flag should be selected, the original 30 mm offset position along z should be assigned. Since the MRS voxel is located at the 10/20/0 mm physical position during the scan, these coordinates ought to be used for geometry-based conditions such as the ellipsoid-based volume selection.

Focus Removal: Removal of spherical foci. Sometimes useful for the exclusion of extreme artifacts e.g. in the prefrontal cortex or the temporal lobes (#11)

Manual/Direct: Assignment mode of focus removal (#11)

N: number of foci to be removed (#11)

Calc ROI button: Perform ROI calculation and visualization. The result of this calculation is automatically forwarded for shim field analysis on the *MC-Shim* or *SH-Shim* pages (#6)

Show ROI button: Only visualizes the current ROI without recalculation. This button is preferable when only display parameters have been changed (#7)

The *ROI File Handling* enables saving a derived ROI to file or to load an ROI from file. This functionality is useful when, for example, an ROI has been derived manually and the same ROI needs to be available for multiple field maps, such as for the experimental confirmation of the predicted B_0 shim outcome. In addition, the basic combination of the current ROI with an ROI on file can be realized via a Boolean *AND* (#12)

Plot Field / Auto-Setup: Flag to enable the visualization of the ROI selection on top of the B_0 field map. Pushing the *Auto-Setup* button pre-selects display parameters typical for field mapping (#5)

Plot Image / Auto-Setup: Flag to enable the visualization of the ROI selection on the (TE-averaged) magnitude image (#13). Field and image visualization typically require different display settings. The *Auto-Setup* button applies default settings for the visualization via MRI and, together with the corresponding button for field map-based ROI visualization (#5), allows easy switching between both modes

Transp.: Transparency of the ROI overlay on the field map or magnitude image, 0: fully transparent, i.e. the ROI is not visible, 1: fully opaque, i.e. only the ROI is visible, suggestion: 0.2

In general, four different modes are supported for the visualization of images and field maps (#8):

- 1) *Slice*: Single slice mode (axial/coronal/sagittal)
- 2) *All*: Display of all slices of the available data set (axial/coronal/sagittal)
- 3) '*3D*': Pseud-3D mode consisting of three orthogonal slice sections (x=sagittal, y=coronal, z=axial). Pushing the (A) button will determine the center-of-mass of the current ROI selection and center the pseudo-3D display on the ROI.
- 4) *3D*: True 3-dimensional visualization

Four modes can be chosen for the color limits defining the range of MRI signal intensities or B_0 field values (#9):

- 1) *Auto*: Automated estimation of amplitude range to include most voxels
- 2) *Global*: Cover the data sets' full numeric range defined by the minimum/maximum values
- 3) *Slice*: Employs the minimum/maximum search to the single slice selected under *Slice*
- 4) Extra flag (o): Direct assignment of minimum/maximum values to be used

The color schemes *jet*, *hsv* and *hot* (#15) are supported as, depending on the field distribution at hand, small effects can be more apparent with one than another

Supported color modes are (#16):

Gray: Gray scale, cannot be combined with colorbar visualization

Color, Color mode, *Colorbar* can be added

Position / Distance: Positions and distances can be measured directly (#17) if single slice mode is selected (compare #8)

Black / White: The details of an ROI selection are sometimes difficult to spot with the overlay of MRI or field map and ROI. The *Black* and *White* options (#17) allow suppression of non-ROI background via overlay with a black or white mask, respectively.

Section: The visualization of slice sections corresponding to the pseudo-3D ('*3D*') data visualization mode is sometimes good to have, while other times it might be in the way. This flag (#17) enables the addition or removal of labels indicating the slice positioning in both MRI and B_0 field maps.

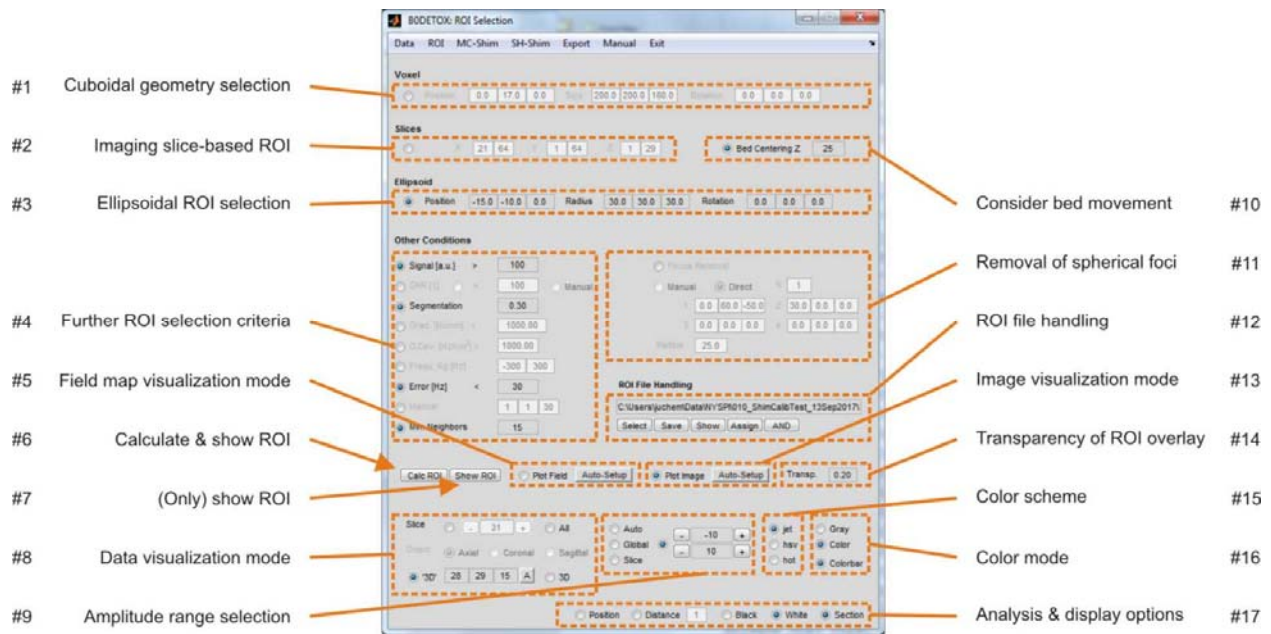


Fig. 2.1: Region-of-Interest (ROI) page.

Note that BODETOX checks for the existence of data relevant for a given processing step before it is executed. If the necessary data do not exist, they are loaded or reconstructed automatically in a recursive fashion. For instance, the use of an image-based ROI criterion like the SNR requires the existence of the corresponding MRI data. If this data are not found, they are reconstructed first. If the raw data and MRI parameters for this image reconstruction are not found, the data are loaded from file. Similarly, the use of the voxel-specific error of the linear regression employed for frequency calculation necessitates that this analysis has been done already. However, if no B_0 map (remember: in Hertz) is found, it is automatically calculated along with an earlier step, e.g. data loading, if needed.

2.2 Usage Example: ROI Selection for Single-Voxel MRS

The combination of a spherical volume at the intended MRS voxel position (-3/52/22 mm) and a selection of basic quality criteria, e.g. error of the voxel-specific B_0 field calculation <30 Hz, allows the extraction of a frontal brain region surrounding the MRS voxel geometry at hand. The '3D' display mode allows an easy assessment of the selected ROI. Note that the automated center-of-mass calculation (#8, A button) hereby centers the orthogonal slice sections to the ROI at hand. The ROI selection is shown as purple overlay onto the magnitude image (upper right) as well as the apparent B_0 field distribution (lower right) based on the predefined parameter defaults available via the *Auto Setup* buttons.

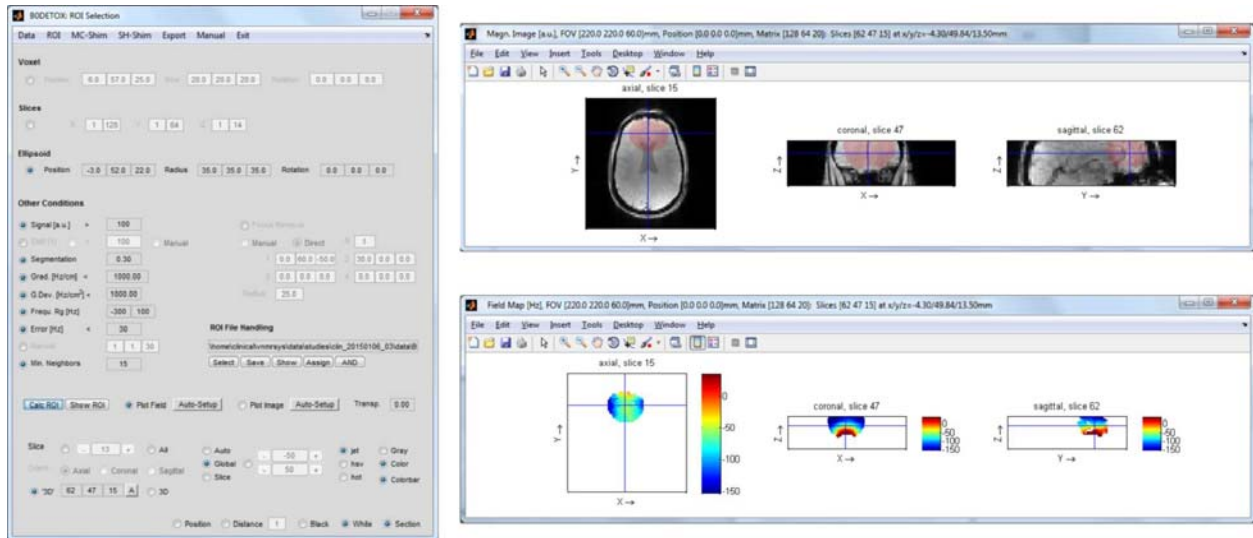


Fig. 2.2: Usage example of region-of-interest selection.

Note that the magnitude and B_0 field information loaded on the *Data* page (via the *Load Data* button) is automatically transferred to the *ROI* page and used for this analysis. If no field information was found, the corresponding data loading and image/ B_0 processing required to obtain such information is performed automatically.

In the same vein, the derived ROI is automatically transferred to the *MC-* and *SH-Shim* pages for further analysis.

III The Multi-Coil (*MC-Shim*) Page

The setup of the *MC-Shim* page follows the steps necessary to convert a B_0 field distribution to a set of multi-coil (MC) hardware settings for its compensation with B_0 shimming. The definition of the MC system at hand is followed by the field analysis, before the current settings of the resultant optimized MC shapes are written to file for application to the amplifier electronics.

3.1 General

Multi-coil shimming requires calibration information from the applied MC system at the geometry of the applied B_0 map. This information needs to be derived with the first use (#9), after which it can be reloaded from file (#1). The necessary steps are:

- 1) Acquire a B_0 map to characterize the field inhomogeneity at hand
- 2) Select *Derive* to translate the geometry of the MC calibration fields to the geometric conditions of the B_0 field map acquired for shimming (#10)
- 3) Select the applied MC system (7T 1st, 7T new, 9.4T Mouse,...)
- 4) Assign the geometry of the applied B_0 map (from the *Data* page) by pushing the vertical (*L*) button next to the FOV, position and matrix entry fields. Notably, any geometry can be used when FOV, position and matrix size are entered directly.
- 5) Press the *Derive* button to resample the original calibration maps to the geometry of the provided B_0 map.
- 6) This information can be used for the subsequent MC shim analysis and by saving it to file for any future analysis that is based B_0 maps with the same geometry.

If such calibration is available with subsequent experiments, selecting the *Load* radiobutton instead of *Derive* allows you to select and upload this information directly from file.

For MC shimming, two different modes are available, *Global* (i.e. static) and *Dynamic* shimming. Global shimming optimizes the B_0 field over the selected ROI as a whole to derive one set of shim currents corresponding to one (static) shim field. Dynamic shimming breaks the ROI to be shimmed down to slice-specific subvolumes and optimizes them in a serial fashion. The result is a set of shim currents (corresponding to a single shim field) for every slice. Further literature on the principles of static and dynamic shimming can be found in the reference list at the end of this manual.

3.2 Global/Static MC Shimming

For global/static shimming of the ROI defined on the *ROI* page:

- 1) Select the *Global* radiobutton (#3)
- 2) Select the *Write* flag to automatically write the modeling/fitting result to file (#13, left)
- 3) Select the file to which the derived shim currents should all be written to (#13)
- 4) Push the *Do Analysis* button (#5) to perform an ROI-specific analysis of the original magnetic field distribution and write the corresponding (single) set of MC currents to file
- 5) For the MC installation environments established at Yale and Columbia University, this file needs to be uploaded as event 0 (static, immediately applied) in the B_0 mapping method to physically apply the shim field.

3.3 DYNAMITE Shimming

For slice-specific dynamic shimming of the selected ROI assigned on the *ROI* page:

- 1) Select the *Dynamic* radiobutton (#3)
- 2) Select the *Write* flag to automatically write the modeling/fitting result to file (#13, left)
- 3) Select the file the derived shim currents shall be written to (#5)
- 4) Select the fitting format parameters *Slices*, *Range*, *Step* and *Orientation* (#11) based on the geometry of the B_0 mapping with respect to the geometry of the target application. For instance, let's assume that we want to derive dynamic shim fields for an axial EPI experiment with 5 slices, 1.5 mm thick. In principle, you could map the B_0 field at the identical geometry. The corresponding parameter settings would be *Slices* 1..5, *Range* 0..0 (i.e. slices to be included in the field optimization before and after the considered one), *Step* 1 (i.e. every slice of the B_0 mapping experiment is considered). In practice, such choice would be suboptimal, however, since the B_0 field would be optimized only within the slice (in the x-y plane). Potential through-slice components along z would not be corrected and could jeopardize the experiment. The inclusion of multiple slices from either within the considered EPI slice or its surroundings considers through-slice field components and is therefore the preferable approach. The appropriate B_0 mapping experiment could use 15 slices with 0.5 slice thickness. The fitting parameters *Slices* 2..14, *Range* 1..1, *Step* 3 then consider ROI contributions of the three B_0 mapping slices that contribute to every EPI slice to derive the corresponding shim field. To further emphasize the minimization of through-slice components one could also map the B_0 field on 17 slices with 0.5 mm thickness and apply the settings *Slice* 3..15, *Range* 2..2, *Step* 3. In this case, the ROI volume considered for slice-shimming considers not only the 3 slices within the EPI slices, but furthermore includes one more B_0 mapping slices on each side. This example also demonstrates that the geometry of the B_0 mapping should be chosen based on the geometry of the target application of dynamic shimming, here EPI. Notably, the FOV and matrix sizes (i.e. the in-plane resolution) do not need to be matched.
- 5) Pushing the *Do Analysis* button (#5) performs the dynamic MC shim analysis and writes all sets of shim currents to file since the *Write* option is selected.

6) For the MC installation environments established at Yale and Columbia University, this file needs to be uploaded to the events 1..n in the B₀ mapping method to dynamically apply the derived slice-specific shim fields during MR sequence execution.

Slices are renumbered for sparse slice sampling (*Step* > 1) to match the slice numbering of the target application. For instance, since the target EPI application in the above example uses 5 slices, the corresponding shim results need to be written to the events 1..5 even if they were derived from B₀ slices 2..14 or 3..15. If the flag *Full* is selected, the reordering is disabled and intermediate slices are assigned sets of zero current.

Before (#12): Shows the original magnetic field map to be shimmed as it has been measured, i.e. before any manipulation

Best Fit (#12): Shows the best possible modeling result for the applied MC shim device. Notably, the identical shape with reversed polarity is applied for shimming. The comparison with the best fit to the original problem enables the user to evaluate the adequacy of the applied shimming.

After (#12): Shows the theoretical/calculated magnetic field distribution in the presence of the calculated shim corrections. This map allows outcome prediction of the applied shimming and should be extremely similar to the map that is obtained when the original field mapping experiment is repeated in the presence of the determined shim field.

By default, the field maps of the best fit and the projected residual are assigned to the center slice of optimized group of slices only to allow a meaningful visualization in the regular scenario in which overlapping groups are used (e.g. *Range* 1..1, *Step* 1). In the 2nd example above (*Slices* 2..14, *Range* 1..1, *Step* 3) one might want to assess the quality of the achieved shim throughout the entire EPI slice is and therefore visualize all three slices of each optimized group. The flag *Keep Selected* allows this.

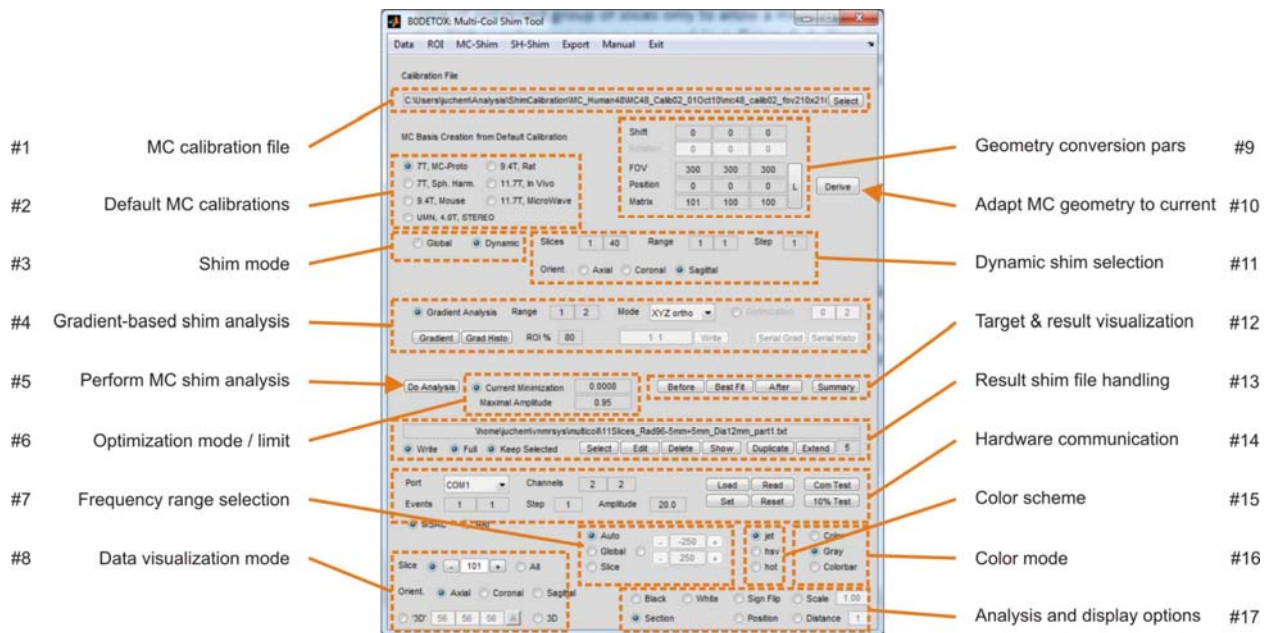


Fig. 3.1: Main Multi-Coil Shim (MC-Shim) page.

3.4. Result Visualization and Documentation

The performance of the shim optimization is analyzed and a series of quality measures are returned in the main window. In addition, all three fields from the field optimization, i.e. the original target field, the best fit and the predicted residual field deviation after shimming, are available. Each of these fields can be exported and saved to file for documentation or further analysis (compare *Export* page).

3.5. Usage Example: DYNAMITE Shimming of the Rat Brain

An example of DYNAMITE shimming of the *in vivo* rat brain at 11.7 Tesla with a 48-channel MC setup (from [5]) is summarized below. The ROI selection of brain slices 1..24 on the ROI page is shown as array of slices (Figure 3.2) along with the corresponding B_0 field distributions before shimming (Figure 3.3). The simulation of slice-specific DYNAMITE shimming on the BODETOX *MC-Shim* page predicts largely homogeneous B_0 conditions in the rat brain throughout the selected range of slices (Figure 3.4, third row) based on the close resemblance of the apparent B_0 background field (first row) with MC-generated field shapes (second row). Note that the corresponding 24 sets of slice-specific 48 coil currents are automatically written to file and can be subsequently uploaded to the amplifier electronics via serial communication software installed on the console computer or directly by BODETOX.

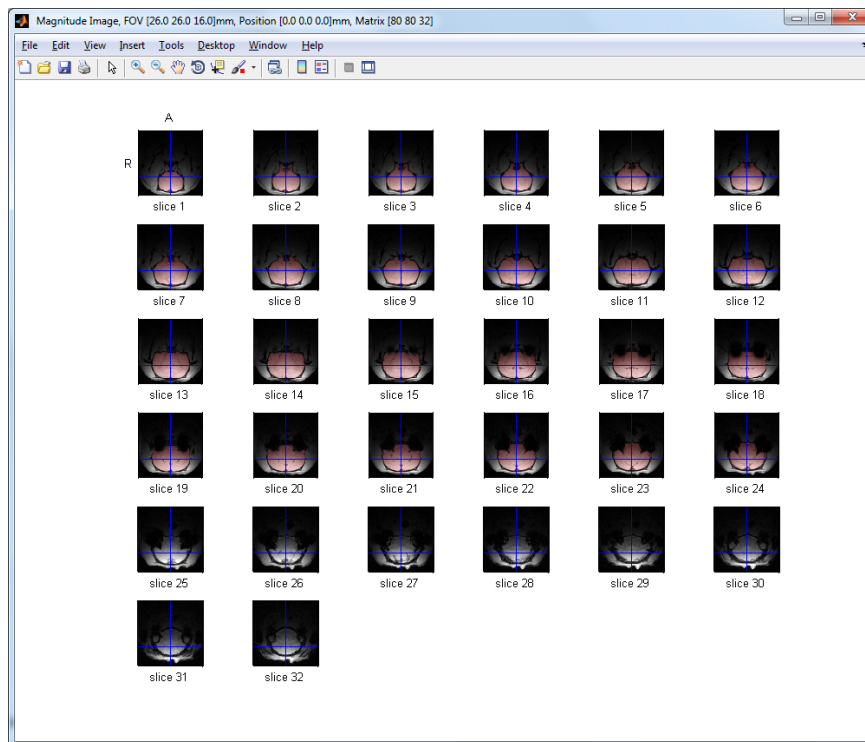


Fig. 3.2: ROI selection of a frontal part of the rat brain (arrayed visualization format: *A/R*).

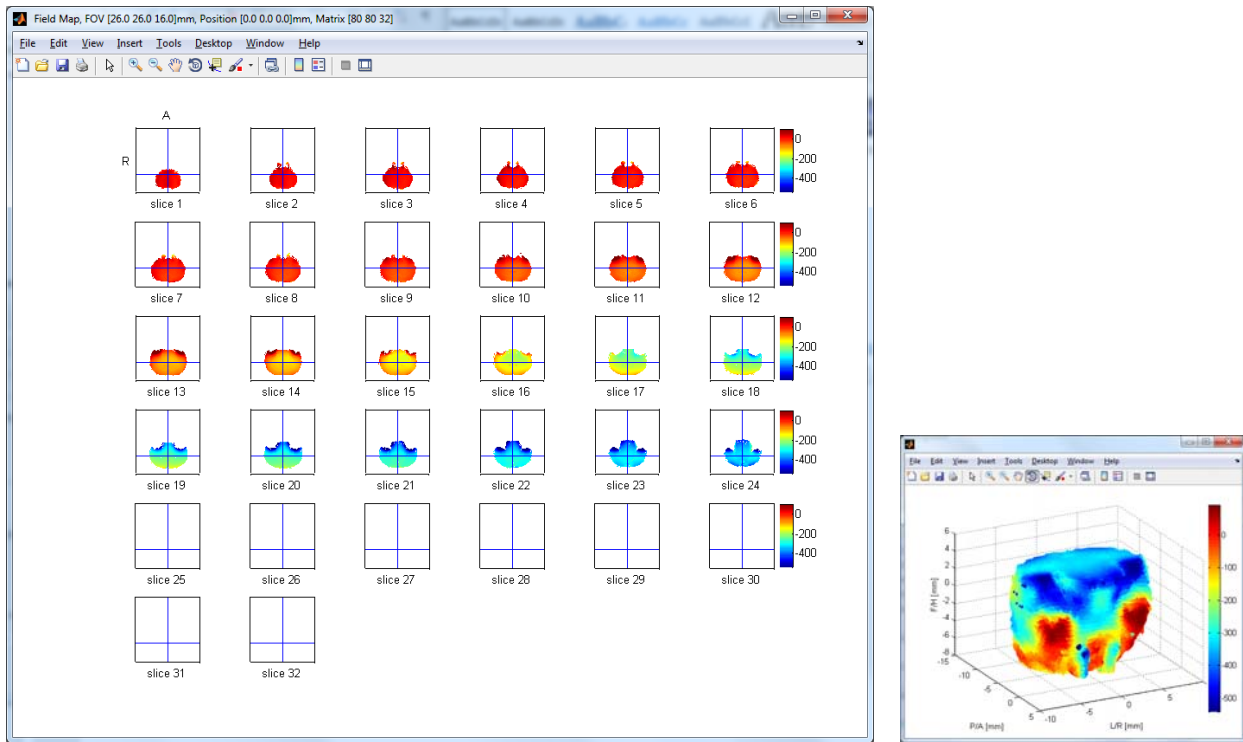


Fig. 3.3: B₀ field conditions in the *in vivo* rat brain at 11.7 Tesla before shimming (left: All, right: 3D).

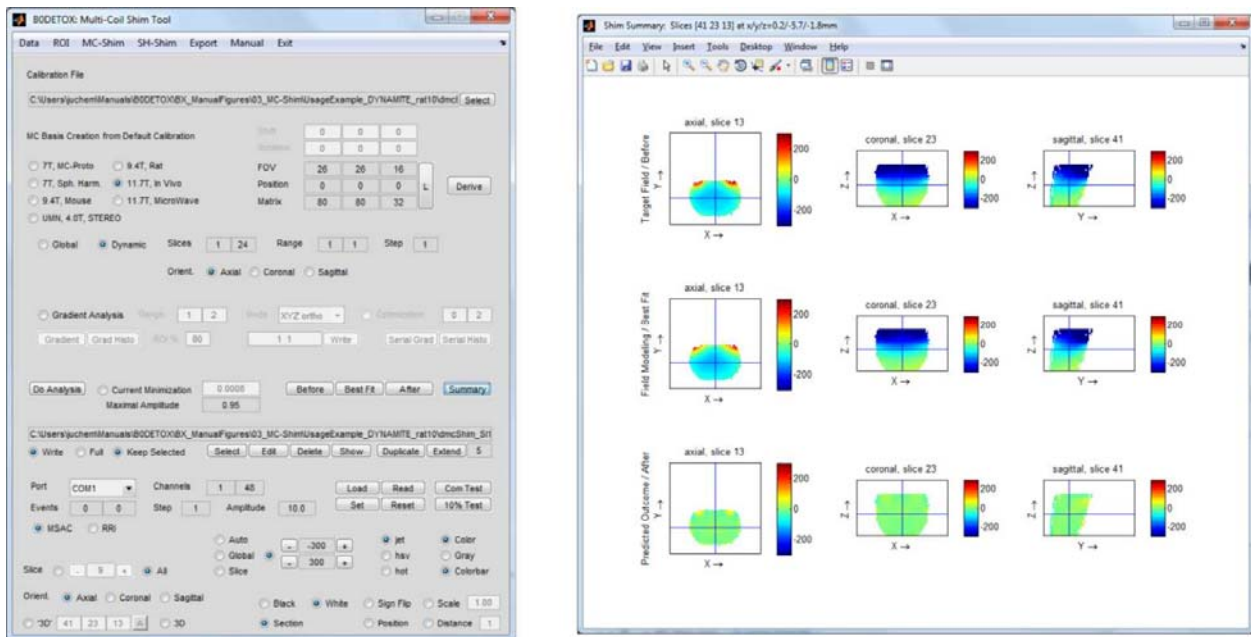


Fig. 3.4: DYNAMITE B₀ field analysis with BODETOX and predicted shim performance (Before, Best Fit, Predicted).

IV The Spherical Harmonics (*SH-Shim*) Page

The calculation of optimized spherical harmonic (SH) shim settings consists of two steps: 1) The decomposition of the apparent field distribution in a basis of SH fields shapes supported by the shim system, and 2) the translation of the optimized correction field in shim settings for the SH system at hand. While the outcome of the decomposition is a set of field amplitudes in Hz/cmⁿ units, the second step results in a vector of SH coil currents in Ampere or (arbitrary) hardware units.

Section 4.1. describes the general setup and use of the *SH-Shim* page. The characterization of the SH system for the MR scanner at hand is summarized in section 4.2. The remaining sections of this chapter contain selected usage examples for commonly applied B₀ shim scenarios.

4.1. General

The setup of the *SH-Shim* page follows the steps necessary to convert a B₀ field distribution into a set of hardware settings for its homogenization with B₀ shimming. The definition of the shim system at hand is followed by the SH field analysis, before the resultant SH shapes are converted to SH coil currents and written to file in MR vendor-specific formats for their subsequent application to the shim hardware.

SH Calibration (#1): BODETOX comprises a library of calibration files for precalibrated MR scanners. If *Auto* is selected, the software identifies the apparent shim system and the calibration information is retrieved from file. The calibration information from other shim systems needs to be loaded directly from *File* after the corresponding path (#2) has been assigned (#9).

Shim Order (#10): Spherical harmonics order to be applied for shimming. If the selected order exceeds the capability of the shim system at hand, it will be automatically adopted to account for the available hardware.

Do Analysis (#4): Perform ROI-specific B₀ shim analysis of the original magnetic field distribution up to the selected spherical harmonic order and calculate the corresponding shim fields and settings for the shim system at hand. Note that both the ROI and the B₀ field map are automatically transferred from the *ROI* page.

Before: Shows the original magnetic field map before any manipulation

Best Fit: Shows the best possible modeling result for the applied spherical harmonics order. Notably, the identical shape with reversed polarity is applied for shimming. The comparison of the best fit and the original problem, i.e. the target B₀ shape to be shimmed, enables evaluation of the adequacy of the applied shim functions and order.

After: Shows the theoretical/calculated magnetic field distribution in the presence of the calculated shim corrections. This map facilitates outcome prediction of the applied shimming and should be extremely similar to the map that is obtained when the original field mapping experiment is repeated in the presence of the determined shim field.

BODETOX converts the best available shim field to hardware settings that can be applied experimentally. As such, shim fields have to be calculated, loaded to the *Applied* fields (i.e. these are the settings that are used) and then written to a text file that can be loaded and applied by the MR scanner software. The normal shimming procedure is to be done as follows:

1) Define the spherical harmonics *Shim Order* (#10)

2) Select the SH analysis mode as either unrestricted fit assuming infinite dynamic range on all supported SH terms or restrict the SH field analysis to the limitations of the employed shim system (#14). The unrestricted fit allows unbiased analysis of the field distribution at hand. The consideration of the shim system at hand is necessary, however, for meaningful experimental shimming. Note that the limitation also already considers the lack of individual terms, i.e. incomplete SH orders.

3) Perform the field analysis and calculation of the corresponding shim fields (*Do Analysis*, #4)

4) Any calculation of absolute shim settings has to consider the shim currents/setting that were applied during the B_0 field mapping as the performed shim analysis is relative. This is achieved by loading the background shim settings present during B_0 map acquisition (*Load Exp. Shim to Applied*, #13) before the necessary changes determined by the shim analysis are added in the following step.

5) Load the derived shim settings to the *Applied* fields by pushing the *Add to Applied* button (#13). Note that every button press adds another copy of the last shim analysis; the button must therefore be pressed only once.

6) Define/*Select* a text file to which the shim settings should be written (#15)

7) Pushing the *Write* button (#15, right) will then save the shim settings to file.

8) The shim file then needs to be transferred to the MR systems' shim folder and loaded; i.e. the fields have to be applied.

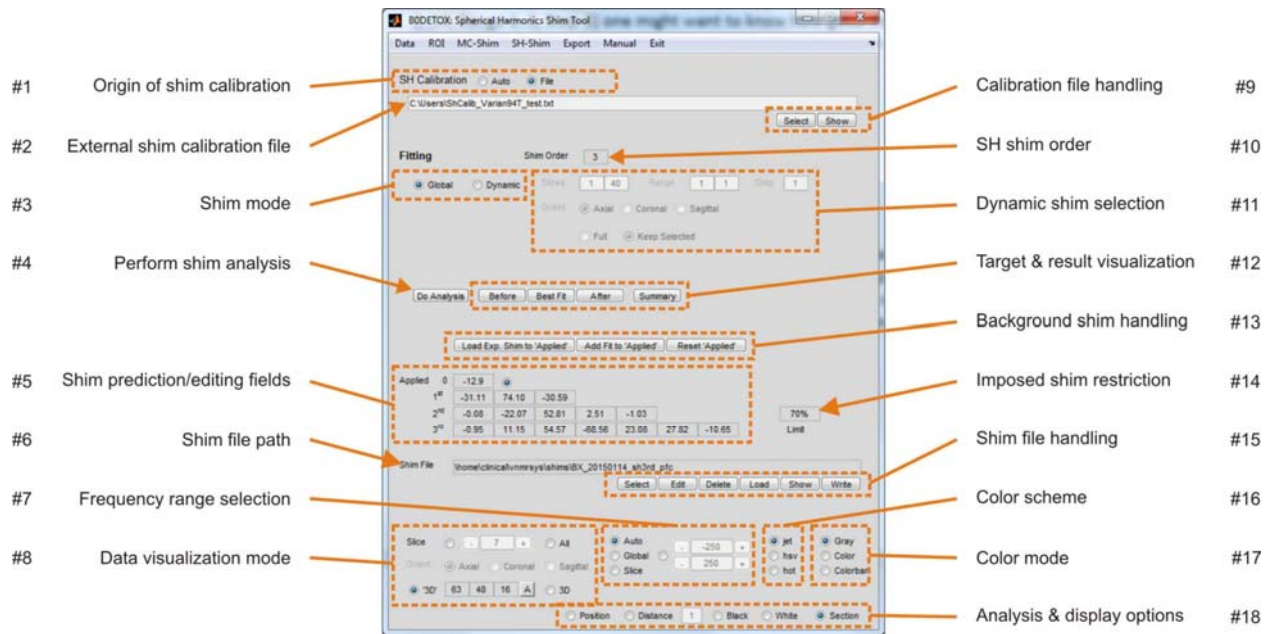


Fig. 4.1: Main Spherical Harmonics Shim (*SH-Shim*) page.

4.2. Calibration of SH Shim System

The reliable characterization of the SH shim system serves two purposes and is essential for good B_0 shim performance:

- 1) Characterization of SH field shapes along with their static imperfections, i.e. their cross-terms.
- 2) Determination of the available dynamic range, including the translation factor or link between the applied arbitrary hardware units and the resultant field amplitudes in Hz/cm^n .

The resultant calibration matrix in Hz/cm^n per 1% of the available dynamic range is used by BODETOX to translate the optimized SH shim field in a set of SH hardware settings as first described in [7]. The nominal dynamic range of the employed SH coils therefore corresponds to the diagonal elements multiplied by 100. The coils' imperfections (or cross-terms) can be found as off-diagonal elements and should be small for well-designed, constructed and implemented SH coil systems. Note that the derivation of shim settings via the shim system's full correlation matrix minimizes shape imperfections of individual SH channels by other available coils and thereby allows reliable SH B_0 shimming in a one-step process.

Spherical Harmonic Calibration Analysis

The goal of the SH shim calibration is to determine the available SH field amplitude per employed coil current or hardware setting, i.e. the bang for the buck. To this end, a series of B_0 field maps is acquired for every SH shape at varying shim settings. The decomposition in all SH shapes up to the supported SH order of the shim system at hand provides the desired SH shapes (as diagonal elements) as well as its imperfections or cross-terms expressed in terms of the other available SH

shapes (as its off-diagonal elements). Note that BODETOX can be used for this analysis. Besides the regular SH result format (compare Usage Example in section 4.4.), a single-line printout formatted for direct copy/paste, e.g. to Microsoft Excel, is available with the selection of the *Excel Format* flag on the *SH-Shim* page. Linear regression of the applied percentage of the available dynamic range (in [%]) and the SH field amplitude (in [Hz/cmⁿ]) then reveals the desired calibration information. The detailed description of the do's and don'ts of a high-quality B₀ shim calibration is beyond the scope of this manual. Feel free to contact me directly; I am happy to guide you through it.

Spherical Harmonic Calibration File

BODETOX recognizes a series of specific MR scanners and shim systems that have been calibrated previously. These systems are recognized automatically (if the *Auto* flag is selected) and employed to derive optimal shim fields for the MR system at hand. For all other MR systems, the corresponding calibration information has to be made available to BODETOX (*File*).

Shim calibration files contain the following components:

- 1) A potential file header. Lines starting with a percentage sign (%) are interpreted as comments and not considered for further analysis.
- 2) An identifier *Name* of the MR system can be assigned to serve as label for further analysis and result printouts.
- 3) The vendor of the MR system to be employed for shimming is required for the translation of the derived shim fields to hardware-specific shim settings (or currents) in a format that is accepted by the MR scanner software. The resultant shim fields are reported in a text output and written to file for direct upload and use on the MR console computer. Supported vendor names are 'Varian', 'Bruker', 'Siemens', 'General Electric' (or 'GE').
- 4) The specific MR scanner model or *System* needs to be assigned for accurate scaling from SH shim terms to hardware units, e.g. for Siemens shim systems. Supported systems so far include *Prisma*, *Prisma_fit*, *Investigational_Device_7T* (Siemens) and *SIGNA* (GE).
- 5) The maximal order of the SH shim system at hand can be assigned directly in the calibration file to guide the BODETOX software. If this parameter is lacking, it is derived automatically from the calibration information.
- 6) The calibration information is reported as a quadratic 25x25 matrix in Hz/cmⁿ for 1% of the dynamic range capable of describing SH shim systems of up to the fourth order. SH orders in BODETOX are consistently structured in ascending order *n* with terms listed from *-n* to *n*. The first row therefore corresponds to the effect of the application of a B₀ coil on the other SH shapes. Rows two to four reflect the linear gradients X (*m*=1), Z (*m*=0) and Y (*m*=-1) and their effects on the other SH shapes, followed by the second order terms X²-Y² (*m*=2), ZX (*m*=1), Z⁰ (*m*=0), ZY (*m*=-1) and XY (*m*=-2), the third order terms X³ (*m*=3), Z(X²-Y²), Z²X, Z³, Z²Y, ZXY and Y³ (*m*=-3). An ideal coil system would have non-zero entries only along the matrix' diagonal representing the field amplitude that is generated per % of its dynamic range. In reality, however, the shapes of individual coils do not fully resemble the target shape at hand, reflected by non-zero off-

limited to the installation of different hardware components such as coils or amplifiers, i.e. the obvious. Minute variations in the positioning of the shim system within the gradient coil or reversed polarity of the coil connections render the use of a generic shim calibration suboptimal and in many cases impossible. It is therefore strongly recommended *not* to solely rely on generic information but to perform a dedicated calibration of every individual SH shim system to be used. In reality, no two implementations are truly alike.

Note that Siemens employs a few additional, system-specific scaling factors along the process. I am happy to work them out with you for the shim system you use. Please get in touch.

4.3. SH Shim File Handling

The resultant shim outcome is written to text files in an MR system and vendor-specific format based on the encountered source data format. While SH settings for static B_0 shimming are save to file when users push the *Write* button (#15), all shim settings are saved automatically with dynamic shimming.

4.4. Usage Example: Static SH Shimming for Single-Voxel MRS

For the region-of-interest selection from the *ROI* page, the corresponding SH shim analysis results in:

3rd order analysis (offset, X, Z, Y, X2-Y2, ZX, Z2, ZY, XY, X3, Z(X2-Y2), Z2X, Z3, Z2Y, ZXY, Y3):

```
[-93.46869 6.60929 -82.40274 83.97081 ...
```

```
1.39530 2.30433 28.02777 -2.10814 -0.82643 ...
```

```
-0.00815 0.07006 -0.06966 -1.47615 -0.55138 -0.01800 -0.03122] Hz/cm^n
```

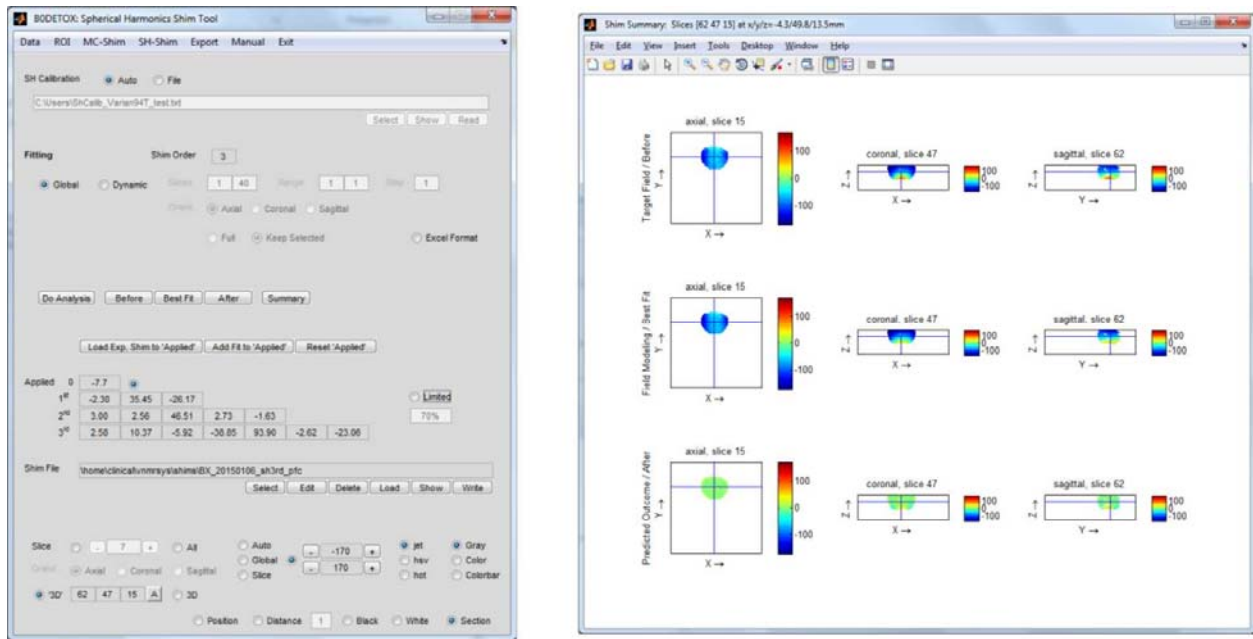


Fig. 4.2: Static B_0 shimming of spherical ROI in the human frontal brain (compare usage example from *ROI* page).

The outcome of this theoretical SH shim assessment represents the best-case scenario for the SH shim system at hand. If the SH calibration has been successful, the resultant B_0 field distribution in the presence of the experimental shim corrections will resemble these predictions largely down to the noise level. If they do not, something is not right.

V The *Export* Page

Anatomical images and field maps can be saved to file for further analysis and documentation. Every such data set consists of the data itself, e.g. a B_0 field map, along with an ROI that goes with it. The origin of this data is selected separately via the *Data Selection* flags (#1) and the *ROI Selection* flags (#2). Within each of these pages, the last data set that has been visualized is the one that is exported to file. This easy trick allows the user to easily select any data structure, e.g. the optimized shim field or the predicted residual after shimming with the display of *Best Fit* or *After* (#12) on the SH shim page, respectively.

In most cases, full 3-dimensional data sets are exported and written to a specific file (#5) that is located in a given directory (#4). In this case, the *All* option should be selected to export all slices of the data set, i.e. full 3D (#3). In order to save a single slice to file, this mode needs to be selected and the corresponding slice number assigned (#3, left). A variety of data formats, comprising both numeric and image types, is supported.

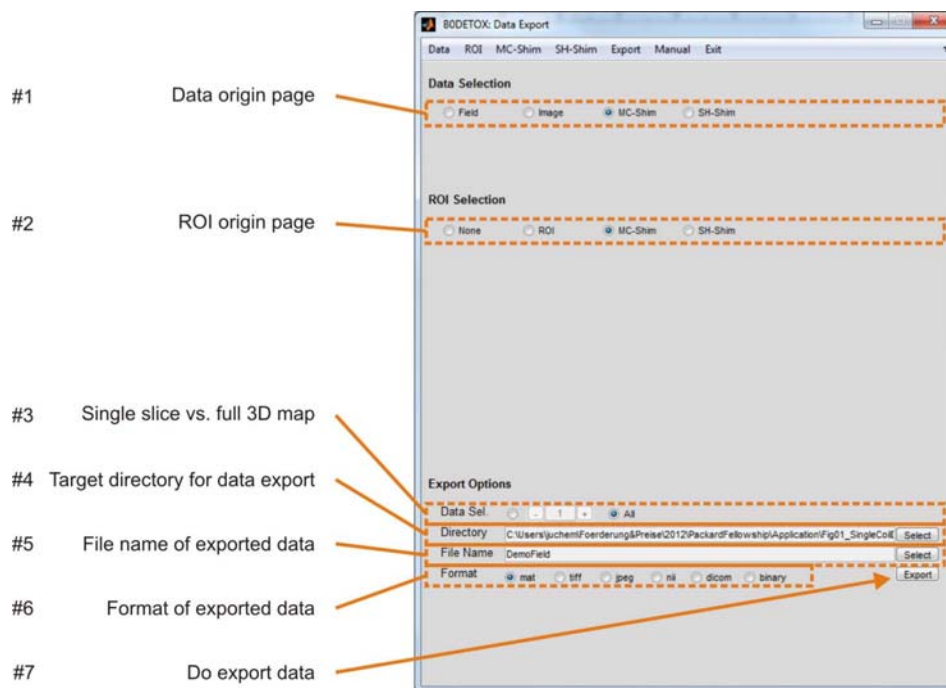


Fig. 5.1: The *Export* page.

VI The *Manual* Page

The *Manual* tab of the BODETOX window does not switch to other pages but opens the software manual that you are currently reading in Adobe Acrobat© if available. You can place the PDF file of the manual that comes with the software anywhere on your computer. The first time you press the *Manual* tab, you are prompted to select the file location. This location is remembered by the software and the manual will be opened immediately with subsequent use.

VII The *Exit* Page

The exit tab does not open up a full page the way the *Data*, *ROI* and *Analysis* tabs do. Instead, the software is exited and all parameters are saved to a default protocol file. At restart, BODETOX opens in the exact same window and re-loads all parameters from this file. Closing BODETOX through the [x] button in the upper right corner of the window will also exit the software; however, the parameter settings are not kept. Note that the explicit loading of specific protocols on top of the default protocol via the *Data* page is always possible.

The *Exit* tab saves all current parameters to a default protocol file and subsequently closes the program. This procedure allows BODETOX to reopen in the page that was used last with all parameter settings as selected previously. Closing BODETOX through the operating system's Close button in the upper right corner of the window is not advised as parameter settings are thereby lost. Note that explicitly loading a specific protocol on the *Data* page is always possible.

VIII Supported Data Formats

The BODETOX software supports the processing of both standard and home-grown B₀ mapping data in a variety of formats from a variety of vendors:

- 1) Varian: FID files
- 2) Bruker: FID files
- 3) Siemens: DICOM. IMA files
- 4) General Electric: DICOM .MRDC files

The software automatically retrieves the parameters describing the experimental data set as well as a variety of additional information relevant for the understanding of the data at hand including the echo time spacing and the employed B₀ shim settings. The corresponding parameter files

therefore have to exist and are expected to be located in their usual file location with the raw/image data.

BODETOX works reliably for the data sets of above formats that have come my way. However, it is unlikely that all potential constellations are covered, especially if customized MRI sequences are used. Therefore, feel free to contact me if your specific vendor or data format is not yet supported. I am more than happy to work with you!

X Terms of Use and Additional Remarks

Purpose and Liability

The BODETOX software is meant for research purposes only. Neither the creator, Christoph Juchem, nor Columbia University assumes any responsibility of any kind. Please refer to the license agreement for further details.

Legal and Academic

BODETOX software is made publically available under a term-limited license. The software can be used free of charge in a non-commercial academic setting with the understanding that it is referenced properly in any publication for which it has been used, e.g. as

Juchem C, Herman P, Sanganahalli BG, Nixon TW, Brown PB, McIntyre S, Hyder F, de Graaf RA. (2014) Dynamic Multi-Coil Technique (DYNAMITE) Shimmied EPI of the Rat Brain at 11.7 Tesla. NMR Biomed 27:897-906.

If the software has been instrumental to your research, please consider offering the creator of the software, Christoph Juchem, an authorship on the first publication for which BODETOX has been used.

Join Us in the Fight against Multiple Sclerosis

The National Multiple Sclerosis Society (NMSS) and patient advocate groups such as the Nancy Davis Foundation (*Erase MS*) provide instrumental support for MS patients and researchers aiming to end this devastating disease. While we do not ask for monetary contributions for ourselves, we encourage you to consider a donation to these organizations. If you chose to support their invaluable efforts based on the free use of the BODETOX software, please assign *Juchem Laboratory* as the occasion of the donation.

<http://www.nationalmssociety.org/Donate>

<http://www.erasems.org/donate/>

Questions and Feedback

The development of the BODETOX software is still a work in progress. Questions and feedback are always welcome.

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XI References

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