



TopShim

Automatic Shimming

Users Manual

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Chapter 1

Introduction

1.1 About *TopShim*

TopShim is a tool designed for easy and automatic shimming.

Functionality

The core method of *TopShim* is gradient shimming. This is complemented by a spectrum optimisation approach, where a quality criterion for the final lineshape ensures the best results for all possible situations.

Both 1D and 3D shimming modes are provided to adjust only the on-axis or both the on- and off-axis shim functions, respectively.

The acquisition of the B_0 field map data can be carried out with ^1H or ^2H observation, enabling the use of *TopShim* for protonated as well as deuterated solvents.

Optionally the additional tune functionality can be applied before and/or after gradient shimming in order to adjust low order shims for maximum lock level.

User Interface

In principle, *TopShim* is a push-button tool. The user has to decide only about the basic method to be used and thereupon all parameters are set automatically.

The simplest way of using *TopShim* is via the TOPSPIN command line. Alternatively, the *TopShim* GUI is also very easy to use, while providing some additional features. Moreover, with the command line parameter concept large flexibility is given to advanced users who want to adapt *TopShim* to their specific needs.

TopShim is also suitable to be used in NMR automation with ICON-NMR or other comparable tools.

1.2 Quick Guide

Probe Setup

- Always after changing the probe declare it with ***edhead***.
- Ensure the ^1H and ^2H 90° hard pulses are correctly defined in ***edprosol***.

Preparation

1. Open the data set of your planned NMR experiment.
2. Lock the sample using the ***lock*** command.

Shimming

TopShim can be controlled via the TOPSPIN command line. The basic commands are:

<i>topshim</i>	1D shimming
<i>topshim 3d</i>	3D shimming (only ^1H)
<i>topshim stop</i>	abort shimming
<i>topshim gui</i>	open the graphical user interface

Note the shimming procedure does not have a fixed duration but is continued until the optimum homogeneity has been achieved.

As a general rule please note that in order to work properly 1D shimming requires good 3D homogeneity. If necessary this can be provided by first running ***topshim 3d*** on a water sample and, after changing the sample, by adjusting the low order shims for maximum lock level.

Shimming a probe the first time

When shimming a probe the first time, the following preparative steps should be executed:

1. Enter a sample with solvent H₂O+D₂O, e.g. the standard sucrose test sample.
Lock, tune and match.
2. Perform 3D shimming: *topshim 3d*
3. Perform 1D shimming: *topshim*

Chapter 2

Prerequisites

TopShim works properly only if the spectrometer fulfils the prerequisites concerning hardware and software as described below.

2.1 Hardware

- **Spectrometer**
Avance AV, II, and III
- **Shim system**
All BOSS shim systems with electronic coding. These are
 - a) BOSS1-SB with 20 shim coils (not 13, 17, or 19)
 - b) BOSS1-WB ("WB17") with plug
 - c) BOSS2
 - d) BOSS-WB ("WB99")
 - e) BOSS3

As an exception also BOSS-WB without electronic coding are supported if declared manually with the part number of the shim system.

Find a complete list of part numbers of the supported shim systems in

```
$TOPSPINHOME/conf/instr/topshim/BOSS/BOSS.txt
```

- **RCB**
3D shimming requires the real-time control board (RCB) functionality. On some systems this might be provided by a 2H-TX board, or directly by some versions of the BSMS. Otherwise an RCB must be installed.
- **Lockswitch**
 ^2H shimming requires the lockswitch functionality in order to use the lock channel for standard acquisition. This feature is usually provided by a 2H-TX board, but on some systems may be part of the AQS or part of the RF amplifier. Otherwise a lockswitch board must be installed.
- **Gradient amplifier**
All types of GAB and GREAT are supported. The GREAT/E should have at least ECL01.
- **Probe**
The probe must be equipped with a Z or XYZ gradient. All high-resolution NMR probes produced by Bruker Switzerland and flow probes produced by Bruker Germany are supported.
- **Spectrometer PC**
At minimum a Pentium 4 Processor with 3 GHz and 1 GB RAM are advised.

2.2 Software

Note that generally after firmware changes *topshim cf* must be executed (see 3.2).

- **DRU firmware**
Use the web browser tool to check the DRU firmware version. It must not be older than 051205.
- **LCB firmware**
Use the **bsms** tool to check and update the current firmware settings on your system. The following LCB firmware (lock application software) versions are compatible with *TopShim*:
 - 000706 (lockak.hex) - 050324 (lockan.hex)
 - 060514 (lockap.hex) or later (preferred)



- **ELCB firmware**

Use the web browser tool to check the ELCB firmware version. The version should not be older than 070202.

Chapter 3

Setup

3.1 General Probe Setup

For the correct operation of *TopShim* the following standard procedures must be performed for each probe.

- After changing the probe it must always be declared using ***edhead***.
- For ^1H and ^2H shimming the respective ^1H and ^2H 90° hard pulses of a probe must be entered for the correct amplifier into the *prosol* table using ***edprosol***. Note that solvents with high conductivity may require individual pulses (see 4.6.2).

3.1.1 Probes with *CryoFit*

If your standard probe is operated as a flow probe using the *CryoFit* kit you need to declare that with the ***edhead*** tool.

In the ***Production Parameters*** set **use as flow probe** to **yes**. This gives you access to the ***Probe Flow Parameters*** that must be set correctly.

3.2 *TopShim* Spectrometer Setup

The *TopShim* setup procedure serves to determine features of the hardware present in the spectrometer. In principle, this procedure is fully automatic: each time after having performed **cf**, the setup procedure is executed when *TopShim* is started the next time.

If desired, the setup procedure can also be performed manually with

```
topshim cf
```

However, this is only required in specific cases, e.g. after firmware updates.

Nevertheless, some hardware components need manual interaction during the setup procedure as described below. For this reason after a **cf**, also a **topshim** or just **topshim cf** should be executed in order to avoid such queries interrupting e.g. an automation run.

3.2.1 Shim system BOSS1-SB

This section is only relevant for you if your spectrometer is equipped with a BOSS1-SB (standard bore) shim system and SCB13 shim current boards.

There are different types of BOSS1-SB shim systems that cannot be distinguished automatically. During the *TopShim* setup procedure you will be asked to provide the information necessary to detect the correct shim system. The description given in Figure 3.1 will help you to answer the questions correctly.

3.2.2 Shim matrix file

This section is only relevant for you if your spectrometer is equipped with a BOSS-WB matrix shim system and a BSMS with RS232 interface.

You have to make sure that the matrix file loaded into the BSMS is available in the TOPSPIN installation in the directory

```
$TOPSPINHOME/conf/instr/servtool/bsmstool/boss
```

Otherwise an error message will appear. In this case please follow the instructions given in the file `wb_inst_e.pdf` located in the subdirectory `wb`.

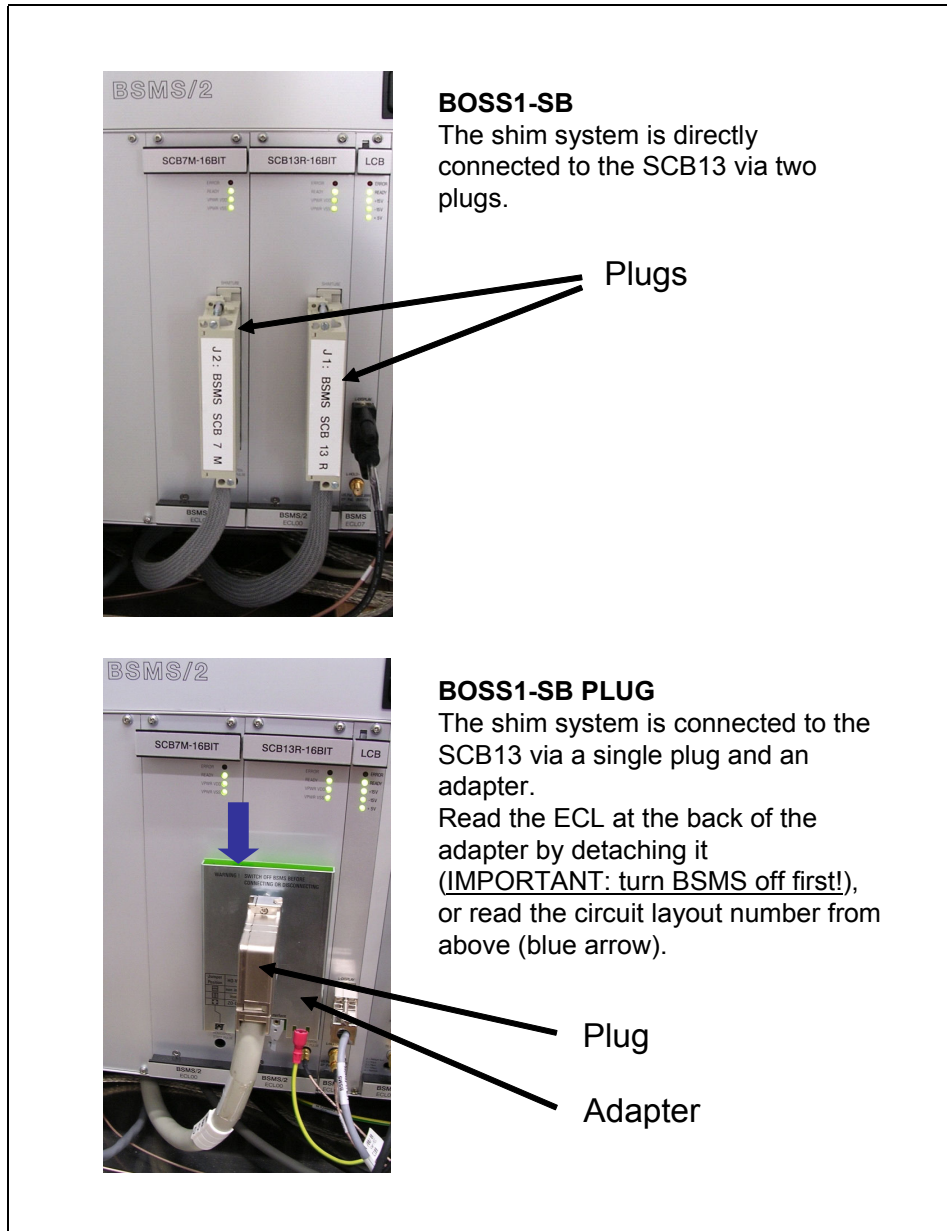


Figure 3.1 Connections of the BOSS1-SB shim system with the shim current boards SCB13

3.2.3 Multiple gradient amplifiers

This section is only relevant for you if there is more than one gradient amplifier available in your spectrometer.

The following two situations are possible:

1. Multiple GREAT

During the first *TopShim* setup procedure the currently connected GREAT is detected. If you switch to another GREAT by changing the wiring, you must perform *topshim cf* afterwards.

2. GAB and GREAT

The two types can be detected simultaneously via BSMS and the serial interface RS232, respectively. Hence, during the *TopShim* setup procedure, you will be asked which one of the two amplifiers is actually connected to the probe gradient. If you later switch from GAB to GREAT or vice versa, you must set the routing again with *topshim setgradamp*.

3.3 *TopShim* Probe Setup

The *TopShim* probe setup procedure collects information about the current probe, i.e. the last one declared with *edhead*. This procedure is performed automatically when a probe is shimmed with *TopShim* the first time.

The probe setup can always be repeated with

```
topshim edhead
```

This is required after modifications to the probe e.g. during a service.

3.3.1 Probes without PICS

Since about the year 2000 all Bruker probes are equipped with a PICS (Probe Identification and Control System). The PICS also stores information used by *TopShim* about the gradient and RF coils.

In case a probe does not carry a PICS, this information must be provided by using the *edhead* tool. The following description assumes that your probe has already been added to the probe list.

1. Start *edhead*.
2. Select your probe.

-
3. Select *Edit probe parameters*.
 4. Select *Production Parameters*.
 5. Set the **Gradient System**.
 6. Enter **Part Number** and **Serial Number** of your probe.
The serial number must consist of four digits. Add leading zeros to fill up shorter numbers, e.g. write "0012" instead of "12".
 7. Select *Coils Parameters*.
 8. As far as known, enter the nuclei available on the inner and the outer coil. Of particular importance are ^1H and ^2H .
 9. Press *Apply*, *OK*, and *Exit*.

Chapter 4

Using *TopShim*

4.1 General

4.1.1 User interface

The principle of *TopShim* is to provide a push-button functionality where only the very basic decisions have to be made by the user.

There are two ways of using *TopShim*: via the TOPSPIN command line or the graphical user interface (GUI).

The command line version enables very fast and direct operation. Furthermore, if desired a large number of parameters can be easily accessed. The basic commands are:

<i>topshim</i>	1D shimming (^1H or ^2H according to solvent)
<i>topshim 3d</i>	3D shimming (only ^1H)
<i>topshim stop</i>	abort shimming

Alternatively, the simple and easy-to-use GUI serves to give access to the most important parameters. Furthermore, the process of shimming is documented perpetually. The GUI can be opened with the command *topshim gui* or from the

TOPSPIN menu: *Spectrometer* → *Shim control* → *Automatic Shimming*. See 4.4 for a detailed description of the GUI.

4.1.2 Basic functionality

The core functionality of *TopShim* is based on gradient shimming (see Refs. [1-3]). The two main methods are 1D and 3D shimming.

1D shimming is able to adjust the on-axis shim functions. These are the axially symmetric functions Z, Z2, Z3, etc. 1D shimming can be performed using ^1H or ^2H data acquisition, hence samples with protonated or deuterated solvents can be used. The duration of 1D shimming will vary from several seconds up to a few minutes depending upon the available signal strength.

3D shimming uses all shim functions, i.e. the on-axis as well as the off-axis shim functions, such as X, Y, XZ, etc. 3D shimming can only be performed on samples having a strong reference signal, hence only with ^1H data acquisition, and only on aqueous samples or samples providing an alternative strong ^1H signal. 3D shimming takes between 5 and 30 minutes, depending on the initial B_0 homogeneity.

The default shimming method is 1D, with the nucleus used for data acquisition (^1H or ^2H) selected automatically based on the lock solvent name. 3D shimming, or other non-default methods, can be selected via command line options or using the graphical interface to *TopShim*.

4.1.3 Shimming

For shimming successfully with *TopShim* please always follow the steps described below.

1. Open the data set of the planned NMR experiment

TopShim reads the observe nucleus of the planned experiment, the *NMR nucleus*, to determine the coil used for the spectrum optimisation procedure performed during shimming (see 4.2). If no data set is open, the inner coil is used by default. Alternatively, the NMR nucleus can be set manually (see 4.5.2).



2. Lock the sample for the correct solvent using the *lock* command

TopShim usually requires the system to be locked in. As *TopShim* reads the name of the last used lock solvent and then makes many different optimisations accordingly (see 4.6) it is important that the solvent name used for locking is

correct. Note in particular that the shimming method for D₂O or H₂O+D₂O will be different (²H and ¹H respectively).

3. Perform shimming

Type the desired *TopShim* command in the TOPSPIN command line or open the GUI and start shimming.

TopShim will finish after the optimum shim has been obtained. The required number of iterations is not known a priori, hence the "residual time" in the "acquisition information" of the acquisition status bar is described as „unknown“.

4.1.4 Important rules

For optimum performance of *TopShim* please note the following rules:



- **1D shimming generally requires good 3D homogeneity**

Therefore 3D shimming on a water sample should be performed at least once on a probe. After changing the sample the low order shims should be readjusted, e.g. by using the *TopShim* tune functionality (see 4.3). If the sample is spinning this requirement is not quite as crucial.

- **Sample spinning state**

1D shimming should always be performed in the same sample spinning state as the planned NMR experiment. For 3D shimming spinning will be switched off.

- **Initial homogeneity**

3D shimming can be performed starting from a relatively bad initial homogeneity. However, at least the low order shims should be adjusted beforehand.

- **Repeating shimming**

In general after a single run the optimum homogeneity should have been found. Hence usually starting *TopShim* with the same parameters again will not bring any further improvement and shimming should stop after acquisition of the first field map. However, there may be rare cases where repeating the identical procedure can have a positive effect.

- **Sample temperature**

After changing the sample you need to wait for a sufficiently long time (e.g. 60 to 120 sec) to allow the sample to reach a stable temperature, depending on the difference of the room and the sample target temperature. Otherwise a shim setting optimal at the initial temperature may not be appropriate at a later stage. Furthermore, operating close to the boiling point of a sample should be avoided

as this may cause serious signal loss during the shimming acquisition due to convection. The latter problem can also be associated with temperature gradients in the probe.

Finally, you should always make sure that the gas flow is set correctly as specified for your probe.

4.1.5 Shimming a probe the first time

As noted above, 1D shimming generally requires good 3D homogeneity. Therefore, 3D shimming should be performed on a water sample before 1D shimming, in case the off-axis shims are not optimal yet.

Furthermore, during the first 1D run of *TopShim* for a probe several calibration steps will be performed. This has to be done with ^1H acquisition, i.e. also on a water sample. Again a good 3D homogeneity is important for this step.

Hence, when using *TopShim* the first time on a probe the following procedure should be executed:

1. Use a sample with the solvent $\text{H}_2\text{O}+\text{D}_2\text{O}$, e.g. the standard sucrose sample used for water suppression tests. The sample should have the largest diameter used with this probe. Furthermore it should be filled not less than given by the filling height specified for the probe. The spinning state does not matter.
Lock, tune and match.
2. Perform 3D shimming: *topshim 3d*
3. Perform 1D shimming: *topshim*

The command *topshim calinfo* shows if the calibration has already been performed for the current probe. If ever the calibration procedures were performed with a bad 3D shim, they can always be repeated on a water sample with *topshim cal*. Alternatively, the calibration data can be deleted by executing *topshim calreset*.

Note that spectrum optimisation (4.2) will be skipped for shimming before the probe calibration in order to improve the quality of the latter. Hence if spectrum optimisation is desired *topshim* can be repeated directly after the calibration run.

4.1.6 Selection of shim functions used

The set of shims actually used for shimming is selected based on the respective situation. If a shim is modified or not, depends on its effectiveness in the sensitive

sample volume in relation to the current B_0 homogeneity. Hence also the size of the sample and the RF coil play a role for this selection.

The set of shims used for shimming is constantly updated while the homogeneity improves. Therefore shimming can also be started with bad initial homogeneity.

There is an upper limit defined for the order of the shim functions used by *TopShim*. See the description of **ordmax** in 4.5.2 for further explanation.

The role of Z6

Sometimes the Z6 shim plays a particular role. It may happen that the optimum shim settings for slightly different situations show large differences in the Z6 values without a considerable influence on the spectrum quality. On the other hand large changes of Z6 can affect the optimum setting of low order shims due to an interaction with the environment. Therefore it is common to keep an already established value of Z6 for a certain probe and perform shimming without the latter.

By default *TopShim* is not using Z6. In order to use this shim it can be activated with

```
topshim z6
```

This can be necessary if a probe is shimmed from scratch or if lineshape, resolution, or water-suppression are not satisfactory.

Note that different from the behaviour described above, in TOPSPIN 2.0 the Z6 shim was used by default by *TopShim*.

4.2 Spectrum Optimisation

Based on the mapped B_0 field *TopShim* performs an optimisation of a criterion for the quality of the spectral line [4]. Of course the aim is to obtain a narrow and smooth line without the presence of false peaks. Within this framework there is still some freedom to shape the line in order to emphasise particular properties, such as a narrow line width or hump, or good solvent suppression. Three such shapes are prepared to meet the specific needs of an NMR experiment and/or probe.

<i>ls</i>	lineshape with narrow width
<i>lshump</i>	lineshape with narrow hump
<i>ss</i>	solvent suppression
<i>optoff</i>	no optimisation, use standard spatial weighting

The parameters can be added after the *TopShim* command, e.g.

```
topshim lshump
```

or

```
topshim 3d optoff
```

The default shape is selected based on the current solvent (see 4.6). For the solvents H₂O+D₂O, CH₃CN+D₂O, and CH₃OH+D₂O the default is ***ss***, for all other solvents ***ls*** is used.

The spectrum optimisation uses the B₁ sensitivity profile of the coil that is used for observation in the planned NMR experiment. Therefore, as described above the nucleus is read from the currently active data set.

4.3 Tune

In some cases it is advantageous to support the standard *TopShim* gradient shimming methods by the integrated tune procedure. This procedure modifies shim values for maximum lock level similar to the TOPSPIN ***tune*** command. By default tune is switched off.

Two main cases apply:

1. Tune *before* gradient shimming can be used to prepare the best off-axis shims before running a 1D *TopShim* (e.g. after 3D shimming on a sample in a different solvent, or when starting from a relatively poor reference shim set).
2. Tune *after* gradient shimming can be used ensure the absolute best shims when some residual shim gradients might remain.

In the table shown below the sets of shims provided for tune, the respective commands, and a short description are summarised. See 4.3.1 and 4.3.2 for a more detailed explanation.

Set of shims	Before	After
Z	tunebz no specific purpose	tuneaz remove possible residual Z gradient
Y	tuneby no specific purpose	tuneay 3D: remove possible residual Y gradient
X	tunebx no specific purpose	tuneax no specific purpose
Z-X-Y	tunebxyz 1D: remove gradients after solvent change	tuneaxyz 1D: remove possible gradients after large changes of Z6 3D: remove possible residual gradients
Z-X-Y-XZ-YZ	tuneb 1D: remove gradients after solvent change 3D: improve initial homogeneity	tunea 1D: remove possible gradients after large changes of Z6

The tune parameters can be added after the *TopShim* command, e.g.

topshim 3d tuneb or

topshim tunebxyz tuneaz

The duration of the tune procedure depends on the number of shims and the response time of the system. It ranges from a few seconds to several minutes. For optimum performance tune is always preceded by ***autogain*** and ***autophase***.

The tune procedure can also be used without gradient shimming by using the parameter ***tune***, e.g.

topshim tune tunea.

Note that if the sample is spinning, only on-axis shims will be used by tune.

4.3.1 Before

1D shimming: After changing the solvent, off-axis gradients may have to be readjusted. This must be performed before 1D gradient shimming as a good 3D homogeneity is required. Adjusting the off-axis shims is preceded by optimisation of Z to improve the sensitivity of the lock level to changes of the off-axis shims.

3D shimming: Generally, 3D shimming can be started from a relatively bad initial homogeneity. Nevertheless, it can still be advantageous to adjust the very basic shims prior to gradient shimming.

4.3.2 After

1D shimming: Due to interaction of the shim system with the magnet and other hardware effects it may happen that there are residual field gradients present after gradient shimming. Primarily, this can be a gradient along Z. However, after application of large Z6 changes also low-order off-axis shims such as e.g. X, Y, XZ, or YZ can be affected.

3D shimming: After 3D shimming with RCB, a residual Y gradient may be present, in very rare cases also an X gradient.

4.4 Graphical User Interface (GUI)

You can open the GUI in two ways:

- from the TOPSPIN command line by typing
topshim gui
- from the TOPSPIN menu with
Spectrometer → *Shim control* → *Automatic Shimming*.

The GUI can be opened even if *TopShim* is currently running.

In the following the elements of the GUI shown in Figure 4.1 are shortly described. Each element is also supported by a tool tip.

4.4.1 The Shim panel

The **Shim** panel gives access to the basic parameters, displays real-time information about the shimming process, and shimming can be started or aborted.

In the **SHIM** box, parameters concerning gradient shimming are accessible:

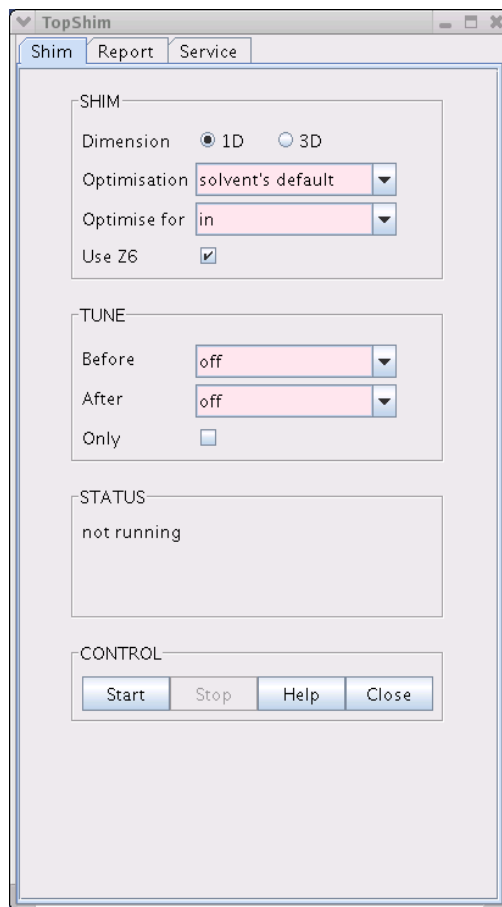


Figure 4.1 The *TopShim* GUI.

The **Dimension** radio button selects between 1D or 3D shimming (see 4.1.2).

The **Optimisation** pull-down menu gives access to the various types of spectrum optimisation (see 4.2).

The parameter labelled with **Optimise for** should be set to the observe nucleus of the planned NMR experiment. From this nucleus the RF coil B_1 profile is derived that is used for the spectrum optimisation. Normally this is set automatically, according to the NMR dataset from which the GUI was started.

Use Z6 can be activated to enable changes of this shim.

The **TUNE** box enables application of the *TopShim* tune functionality **Before** or **After** gradient shimming (see 4.3). With the **Only** box being selected, gradient shimming is skipped completely.

The box **PARAMETERS** is only accessible if it is enabled in the **PREFERENCES** in the **Service** panel (4.4.3). The text line serves to define additional parameters as described in 4.5.2. Multiple parameters are separated by a space. Note that options (see 4.5.1) cannot be entered here. The additional parameters will only be used if the check box is enabled. Thus you can leave frequently used parameters in the line and just disable them in case they are not required.

The **STATUS** lines inform the user if *TopShim* is currently running or not, display important parameters (e.g. the used solvent), show the task currently dealt with, and keep the user posted about acquisition and processing steps.

The **CONTROL** box provides four buttons with basic control functionality:

After pressing **Start** the shimming procedure is started immediately with the parameters set above. You can also start from the command line while the GUI is open. However, in this case *TopShim* is started with the parameters as set in the command line and the GUI is used only as a display tool.

By pressing **Stop** the shimming procedure is aborted immediately. The best shim values found so far will be set.

Pressing **Help** will display this manual.

The **Close** button closes the GUI. If *TopShim* is running, it will not be aborted.

4.4.2 The Report panel

The **Report** panel collects the most important information about parameters and results of the current shimming run. Alternatively, the most recent report can always be displayed with *topshim report* or with the **Report** button in the **Service** panel.

4.4.3 The Service panel

The **Service** panel serves to give direct access some of the options described in 4.5.1 and to setup the GUI.

The box **GENERAL** provides the buttons **About** to show the current *TopShim* version and **Help** to display this manual also from this panel.

The buttons in the box **GUI DEFAULTS** enable the user to define new default values for the parameters settings in the **Shim** panel (see 4.4.1). With the button **Save** the current settings are stored as default values. They will be loaded when the GUI is opened. Alternatively they can always be reloaded with the **Load** button. The button **Restore** enables to restore the factory default settings. By pressing this button the values are loaded into the GUI. In order to make them the default settings again, you have to press **Save** afterwards.

The box **SETUP** contains three buttons **Cf**, **Edhead**, and **Gradamp** for the *TopShim* specific spectrometer setup (see 3.2).

In the box **PROBE CALIBRATION** the **Info** button displays the calibration status for the current probe. With **Reset** these calibration values can be deleted. This is required if a) the calibration was performed with a bad 3D homogeneity (see 4.1.4) or b) hardware components such as magnet, gradient system or shim system have been changed since the last calibration. After the reset shimming on a water sample must be performed to redo the calibration (see 4.1.5).

In the box **DIAGNOSTICS** with the button **Report** the results of the last *TopShim* run can be displayed. Pressing the button **Logfile** shows the disk location of the current *TopShim* logfile. This is useful if problems occur during shimming and you want to report them to the Bruker service (see 5.2).

Finally, in the box **PREFERENCES** the functionality of the GUI can be modified. Setting the check box **External** releases the GUI from the TOPSPIN main window. The check box **Additional parameters** controls if in the **Shim** panel the optional parameter line is available (see 4.4.1). The chosen preferences will be remembered after closing the GUI.

4.5 Options and Parameters

Options and parameters serve to change the behaviour of *TopShim* in the desired manner. They can be added after ***topshim*** in the TOPSPIN command line.

4.5.1 Options

These options do not start shimming, but execute other tasks such as e.g. performing configuration or providing information. Options must be added directly after the ***topshim*** command separated by a space:

topshim <*option*>

The following options are available:

<i>gui</i>	open graphical user interface
<i>stop</i>	<p>abort shimming</p> <p>A parameter can be added to determine the shim values set after abortion:</p> <p><i>optimum</i> → best setting found so far (default)</p> <p><i>current</i> → current setting</p> <p><i>original</i> → original setting</p> <p>Example: <i>topshim stop original</i></p>
<i>help</i>	display this manual
<i>about</i>	display the version information
<i>report</i>	display the report of the latest run of <i>TopShim</i>
<i>logfile</i>	display the location of the <i>TopShim</i> log-files
<i>edhead</i>	perform the <i>TopShim</i> probe setup procedure (see 3.3)
<i>cf</i>	perform the <i>TopShim</i> spectrometer setup procedure (see 3.2)
<i>setgradamp</i>	set the <i>TopShim</i> gradient amplifier routing (see 3.2.3)
<i>calinfo</i>	display calibration information for the current probe (see 4.1.5)
<i>calreset</i>	reset all calibration results for the current probe (see 4.1.5)
<i>edpar</i>	create or modify parameter file (see 4.5.3)

4.5.2 Parameters

Although not required in most cases, there are a number of parameters that can be set by the user to control the behaviour of *TopShim*.

An arbitrary number of parameter expressions can be added after the ***topshim*** command in the command line, each of them separated by a space:

```
topshim <par1> <par2> ...
```

The priority of the parameter expressions increases from left to right, i.e. the last expression has the highest priority. This hierarchy is required if a parameter occurs more than once.

There are two types of parameter expressions: parameter file names and explicit parameter settings. With parameter files one or multiple parameters can be set. An example is the parameter file ***lshump*** that changes several parameters for the spectrum optimisation. In contrast explicit parameters serve to set the value of a single parameter. The syntax for setting a parameter explicitly is:

```
<parameter_name>=<parameter_value>
```

Note that there must not be spaces in such an expression. An example for performing *TopShim* for a flow application using both types of parameter expressions is:

```
topshim lockoff o1p=1.95 rga
```

Here, *TopShim* is executed with the lock switched off, the resonance frequency set to 1.95 ppm, and with receiver gain optimisation.

In the following table a number of available parameter expressions are listed.

General	
<i>1h</i>	use ¹ H field mapping requires strong ¹ H signal, e.g. in a water sample default: defined by solvent.
<i>2h</i>	use ² H field mapping requires a deuterated solvent default: defined by solvent

coil=	<p>sets the NMR nucleus</p> <p>NMR nucleus = observe nucleus of the planned NMR experiment that defines the RF B₁ coil profile used in the spectrum optimisation (see 4.2)</p> <p>possible values: all nuclei available on the probe; in = inner coil; out = outer coil</p> <p>default: observe nucleus of the active data set; if no data set is active, the inner coil is used</p> <p>example: coil=13c</p>
z6	also use Z6 for shimming
ordmax=	<p>set maximum total order of shim functions</p> <p>There is an upper limit defined for the order of the shim functions used by <i>TopShim</i>. This limit is given separately for on- and off-axis shims. By default the highest on-axis order is 5, i.e. Z1 ... Z5 are used. The default for the total off-axis order is 7, i.e. the highest order shims used are (X2-Y2)Z5 and XYZ5.</p> <p>A restriction of the maximum order can e.g. be employed to avoid usage of Z4 with 1 mm probes.</p> <p>Examples:</p> <p>ordmax=3 → use Z1 ... Z3 for 1D or 3D shimming</p> <p>ordmax=4, 5 → maximum on- and off-axis order for 3D shimming</p> <p>default: ordmax=5, 7</p>
Fast	
ldfast	<p>perform fast 1D shimming</p> <p>only one optimisation loop and at maximum 3 fit iterations; maximum duration per 1D map is 40 sec</p> <p>The homogeneity must already reasonable and enough signal strength must available.</p>

<i>3dfast</i>	perform fast 3D shimming only one optimisation loop and at maximum 3 fit iterations Can be applied if the 3D homogeneity is already quite good.
Calibration	
<i>cal</i>	force the execution of all calibration procedures for the current probe; a water sample must be used usually a part of initial calibration
<i>phcal</i>	force probehead position calibration May be used after reinserting the probe. usually a part of initial calibration
Various	
<i>lockoff</i>	enable shimming while the lock is switched off The user must ensure that the excitation frequency is on resonance. Hence the lock field value must be set on resonance and/or the resonance frequency <i>o1p</i> must be set manually (see below). Furthermore the solvent must be set correctly. By default the solvent is determined according to the last <i>lock</i> command performed. Alternatively, it can be set using the <i>solvent</i> parameter (see below).
<i>o1p=</i>	set the excitation frequency <i>o1p</i> [ppm] manually Example: <i>o1p=1.95</i> Default: depending on solvent, usually BSMS lock shift
<i>o1pget</i>	read the excitation frequency <i>o1p</i> [ppm] from the currently active data set Performing the shimming acquisition on a desired peak can be accomplished by 1) acquisition of a spectrum, 2) setting <i>o1p</i> in the acquired spectrum to the desired peak using <i>.cal</i> , and 3) by starting shimming with <i>topshim o1pget</i> .

<i>solvent=</i>	set the solvent Example: <i>solvent=CH3CN+D2O</i> Default: <i>auto</i> , i.e. determined from last <i>lock</i> command
<i>rga</i>	force receiver gain optimisation before shimming
<i>autogain</i>	perform autogain for the lock after shimming By default autogain is executed only before the tune procedure.
<i>selwid=</i>	set width of selective excitation [ppm] and switch it on Example: <i>selwid=0.5</i> Default: depending on solvent, or 1 ppm
<i>shigemi</i>	eliminate unreliable data at axial Shigemi tube walls in case of 1D shimming
<i>astm</i>	perform ¹ H shimming on ASTM sample Used for shimming of 10 mm probes. See 4.7.2.
Diagnostics	
<i>map</i>	acquire field map without shimming Serves for diagnostics. Can be performed for 1D and 3D. The raw, magnitude and field map data is stored in data sets for the user <i>topshimData</i> .
<i>plot</i>	create graphical output during shimming Serves for diagnostics. The intermediate and final raw, magnitude and field map data is stored in data sets for the user <i>topshimData</i> . Should not be used routinely as large amounts of data are created, in particular for 3D.

4.5.3 Creating parameter files

Initially please note that parameter files should be created only by experienced users.

If a certain setting of one or multiple parameters should be used repeatedly it can be stored in a new parameter file. Parameter files are located in

```
$TOPSPINHOME/conf/instr/topshim/parameters
```

New parameter files should be stored in the subdirectory `user`. The general procedure for creating a new parameter file should be:

1. Open an available parameter file, e.g. `default.par`, that contains all possible parameters.
2. Save the file with a new name `myfile.par` in the subdirectory `user`.
3. Delete all lines with parameters that should not be modified.
4. Make the desired changes to parameter values.
5. Save and exit.

In principle, any text editor can be used. However, *TopShim* offers the option ***topshim edpar*** that leads through the described procedure.

The new parameter values can be used by adding the parameter file name without the extension in the command line, i.e. ***topshim myfile***.

4.6 Solvents

Knowledge of the solvent is the most important source of information for *TopShim*. Therefore it is essential to lock correctly before shimming. The following parameters are derived from the solvent.

- nucleus used for field mapping (^1H or ^2H)
- optimum 2H flip angle
- use of selective excitation
- receiver gain
- type of spectrum optimisation (see 4.2)

For most solvents, the shim nucleus is ^2H and spectrum optimisation is performed for lineshape with narrow width. Only for the protonated solvents $\text{H}_2\text{O}+\text{D}_2\text{O}$, $\text{CH}_3\text{CH}+\text{D}_2\text{O}$, and $\text{CH}_3\text{OH}+\text{D}_2\text{O}$, the nucleus is ^1H and the lineshape optimisation aims at solvent suppression.

The optimum flip angle is determined from the pulse repetition time of the field mapping sequence and from calibration data specific for each solvent (see 4.6.1).

Selective excitation is used in cases where multiple lines of comparable size are expected. An example is MeOD.

The receiver gain is calculated based on the expected relative signal strength.

The required information is available for all solvents found in the default solvents table that can be accessed using **edsolv**.

4.6.1 Solvent setup

To allow optimum *TopShim* performance specific solvent properties have to be known. These have been pre-defined for all standard solvents (those named in the default Bruker solvent table), but to use other solvent names with *TopShim* they must first be configured. In all cases the new solvent name must first have been created with **edsolv**, and a suitable entry made in the lock table with **edlock**.

The command for creating the *TopShim* solvent settings is

```
topshim solvcal
```

The associated procedure has two parts, A) definition the solvent properties and B) the flip angle calibration (^2H only).

Part A only

In the following cases it is sufficient to execute part A only:

- ^1H is used for field mapping (part B will automatically be skipped). Example: H₂O+D₂O
- Concerning shimming the new solvent has the same properties as an existing one. Example: New solvent Urine+D₂O, copy from H₂O+D₂O.
- Only minor changes have to be applied with respect to an existing solvent. Example: New solvent: H₂O+EtOH+D₂O, copy from H₂O+D₂O and change to selective excitation.

There are two ways to start the setup procedure for part A only. Either you lock on the new solvent and then execute **topshim solvcal**, or you tell *TopShim* the solvent name in the command line with

```
topshim solvcal solvent=<newsolventname>
```

(where **<newsolventname>** is the name of your solvent exactly as entered in **edlock**). Then you enter the requested informations. In case of ^2H shimming the

setup procedure must be cancelled before the calibration.

Part A and B

For a novel solvent used for ^2H shimming and with unknown properties the following procedure applies:

1. The 3D homogeneity should be already good.
2. Insert a sample with the new solvent.
3. Lock for the previously defined solvent.
4. Perform basic shimming, either manually or using a tune.
5. Start the solvent setup using *topshim solvcal*.
 - a) Initially select a solvent that is closest in character to your new solvent, and answer other questions.
 - b) Start the flip angle calibration test (note this can take between 10 and 60 minutes to complete).

4.6.2 Solvent-specific pulses

TopShim calculates pulses depending on the 90° hard pulse given in the *edprosol* tables. These pulses must be correct to obtain the optimum efficiency of the shimming procedure. Therefore it is important to provide solvent-specific pulses in cases where considerable differences are expected for the same nucleus.

For example this may be necessary for salty water samples with high conductivity. In such a case a new solvent must be defined and the pulse must be determined and entered in the *edprosol* table for this specific solvent.

4.7 Specific probes and tubes

4.7.1 1 mm probes

In principle, 1D and 3D *TopShim* can be used with 1 mm probes as usual. Due to the length of the RF coil the highest on-axis shim order chosen is usually Z3 or Z4 (see 4.1.6). However, in rare cases Z4 may be chosen although its application leads to excessive shim values. In such a situation the maximum on-axis shim order can be restricted manually by using

```
topshim ordmax=3
```

Similarly, 1.7 mm probes may require preventing the use of Z5, i.e.

```
topshim ordmax=4
```

See also 4.5.2 for a detailed description of the parameter.

4.7.2 10 mm probes

Samples with a large diameter are prone to convection in the sample which may hamper the gradient shimming procedure. Therefore, it is advantageous to perform 3D shimming on a sample which has a higher viscosity than H₂O. A very good candidate is the Bruker standard sample ASTM consisting of 40% p-dioxane in 60% C6D6. With this sample field mapping is performed on the ¹H peak at 3.475 ppm which is achieved with the following command:

```
topshim 3d 1h o1p=3.475
```

Alternatively, the already provided parameter file can be used

```
topshim 3d astm
```

See also 4.5.2 for a detailed description of the parameters.

4.7.3 Shigemi tubes

For shimming Shigemi tubes please follow these rules:

- The filled tube range should not be less than about 7 mm.
- Centre the filled tube range well with the probe centre using the sample gauge.
- For 1D shimming add the parameter **shigemi** to the *TopShim* command, which will eliminate unreliable data at the axial tube walls.

4.8 Automation

TopShim is ready for easy shimming in automated NMR. The command line interface is suitable for this purpose without modifications. The basic command with or without parameters can be used with tools such as macros or AU programmes.

In ICON-NMR the default 1D *TopShim* method is already provided by the shim command **TOPSHIM**. Additional new methods can be defined by adding parameters to

this command

```
TOPSHIM <par1> <par2> ... e.g.
```

```
TOPSHIM 3d tunea
```

or by describing an new shim command with

```
CPRW topshim <par1> <par2> ... e.g.
```

```
CPRW topshim 3d tunea
```

Alternatively, user-defined macros or AU programmes can be used, e.g.

```
CPRW my_topshim_macro
```

```
XAU my_topshim_au
```

Chapter 5

Various

5.1 What is new in *TopShim* for TOPSPIN 2.1?

The following new features and modifications have been implemented for the present version:

- GUI: A service panel was added, user default settings can be stored, the GUI can be made external, and additional parameters can be used. See 4.4.
- By default Z6 is not used anymore. See 4.1.6 and 4.5.2.
- The new parameter *shigemi* facilitates shimming of Shigemi tubes. See 4.7.3.
- The new parameter *autogain* adjusts the lock level after shimming. By default autogain is only executed before the tune procedure. See 4.7.3.
- Editing user parameter files is possible with the option *edpar*. See 4.5.3.
- The parameters *map* and *plot* are diagnostic tools.

5.2 Support

In case of problems please first check for known bugs and possible fixes on the Bruker knowledge base

<http://www.bruker-biospin.de/shell/bkb/index.cgi>

To report problems please email

`nmr-software-support@bruker-biospin.de`

making sure to describe the problem as fully as possible and including the *TopShim* logfile

`topshim<date>.log`

as well as the TOPSPIN history file

`history`

both located in

`$TOPSPINHOME/prog/curdir/<user>`

5.3 References

The following references are the original publications about gradient shimming for high resolution liquid NMR and about the spectrum optimisation method.

1. M.G. Prammer, J.C. Haselgrove, M. Shinnar, and J.S. Leigh. A new approach to automatic shimming, *J. Magn. Reson.* 77 (1988) 40-52
2. P.C.M. Van Zijl, S. Sukumar, M. Johnson, P. Webb, R.E. Hurd, Optimized shimming for high-resolution NMR using three-dimensional image-based field mapping, *J. Magn. Reson. A* 111 (1994) 203-207
3. S. Sukumar, M.O. Johnson, R.E. Hurd, P.C.M. Van Zijl, Automated shimming for deuterated solvents using field profiling, *J. Magn. Reson.* 125 (1997) 159-162
4. M. Weiger, T. Speck, M. Fey, Gradient shimming with spectrum optimisation, *J. Magn. Reson.* 182 (2006) 38-48

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