DIELECTRIC SPECTROSCOPY GUI manual

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This manual explains the operation of the MATLAB graphical user interfaces (GUIs) functions developed to load, process and interpret dielectric spectroscopy data collected by Solartron systems. There are three primary functions:

1. `load_solartron_gui` is an interface GUI that loads and pre-processes the Solartron and temperature data into a consistent MATLAB format for use by the later GUIs.
2. `merge_solartron_gui` is an interactive GUI for merging dielectric spectra from individual temperatures.
3. `inv_cole_gui` is an interactive GUI for inverting the dielectric spectra for multiple Cole–Cole dielectric relaxations and DC conductivity. The Optimization Toolbox is required for this GUI.

Additional sub-functions (`chisq`, `delta_chisq`, `fm_cole`, `fm_cole_sep`, `read_meta`, `read_solartron_csv`) that must be available within the user's path to ensure correct operation of the above primary functions. Up-to-date versions of these GUIs and the sub-functions are available through Github, including version control: https://github.com/joemacgregor/dielectric_spectroscopy_gui. This repository also includes data examples and calibration files for a sample from the Vostok 5G ice core

All functions have help documentation associated with them that can be accessed either by opening the file in Editor or using `help` in the command line. This inline documentation is presented in the standard MATLAB format and is meant to be exhaustive for all sub-functions . For the GUIs, their operation is documented below.

These GUIs were designed on a Mac using a large monitor. The appearance of the GUIs differs slightly between Mac and Windows, but the behavior is the same. Depending on the system, `load_solartron_gui` will change the default display of figures to ensure that its size is maximized within the Figure Toolbar, using `set(0, 'DefaultFigureWindowStyle', 'docked')`. However, it cannot adjust the location of the Figure Toolbar, which may be docked within a single MATLAB window. Undock the Figure Toolbar to maximize the GUI's size. To restore normal figure display behavior in MATLAB, enter `set(0, 'DefaultFigureWindowStyle', 'default')` in the command line.

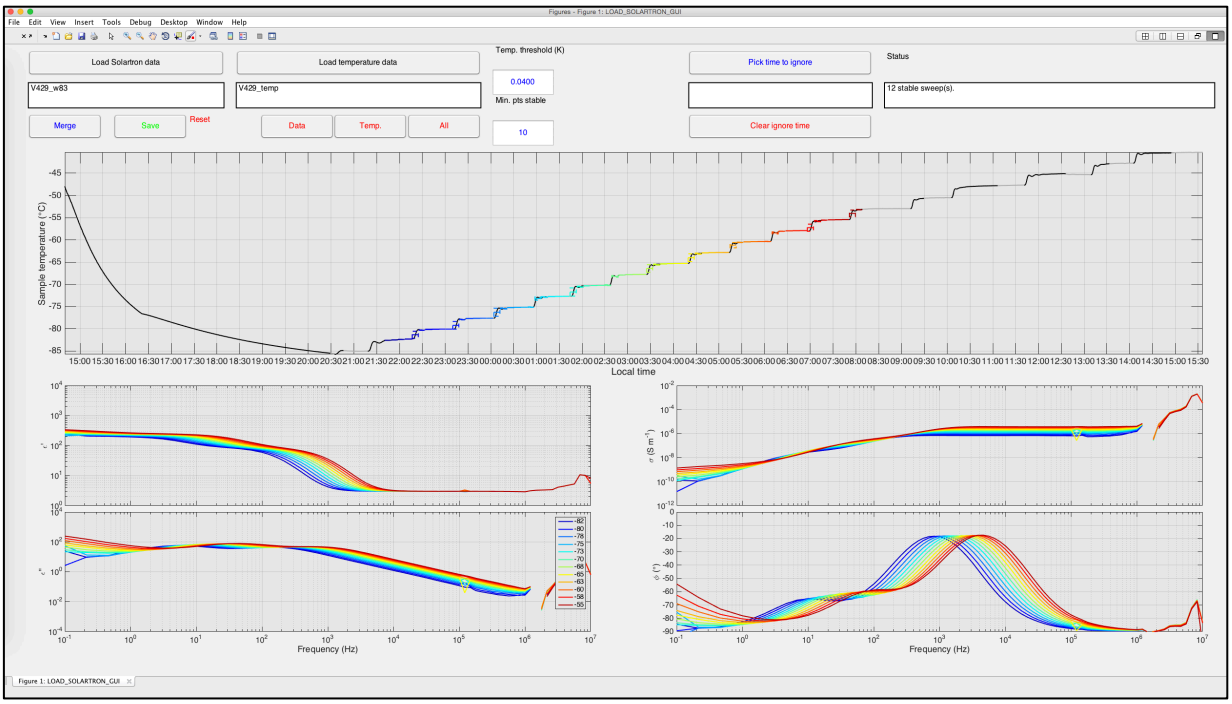
All operations that manipulate the data are organized above the data windows. **Black** text coloring signifies loading data operations, **blue** signifies data manipulation, **red** signifies resetting and **green** signifies saving.

1. `load_solartron_gui`

To start, either type `load_solartron_gui` in the command line or run it from the Editor after having opened it. If you start it from the command line, `load_solartron_gui.m` must either

be in a directory in your path or your current directory must be where the file is located, which is standard MATLAB behavior.

1.1. GUI layout



This GUI has buttons on top, the temperature history in the middle, and a plot of the last recorded dielectric spectrum for each set-point temperature on the bottom (explained below), decomposed into four parts (left column: real and imaginary parts; right column: real conductivity and phase). This breakout for the dielectric spectra is consistent across all GUIs.

There are two user-editable variables displayed in the GUI, whose names are given above those fields. To adjust them, enter a new value in the appropriate units and then press “enter” or “return”.

The reset buttons are somewhat superfluous at this point, as each time either Solartron or temperature data are loaded, the reset functions are called.

Below the primary functions of `load_solartron_gui` are explained. For each sub-section header, a simple description of the operation is given, followed by the button name in the GUI and the key sub-functions within `load_solartron_gui.m` that it calls.

1.2. Load Solartron data (*Load Solartron data*; `load_solar`)

The first step is to load Solartron data that has been collected by pressing *Load Solartron data*, specifically a `.csv` file. For reference, the file’s name, minus the .csv extension, is displayed immediately below this button. Nothing else will be displayed immediately.

1.3. Load temperature data (*Load temperature data*; `load_temp`)

Next, load a temperature file (either .csv or .mat format) that contains the temperature time series recorded separately during Solartron data acquisition. Again, the name of the temperature file (without the extension) will be displayed immediately below this button and nothing else will be displayed immediately.

1.4. Merge/process Solartron and temperature data (*Merge*; `do_merge`)

Once both the Solartron and temperature data have been loaded successfully, they must be merged ("processed"). The title of this operation is vestigial and is distinct from the merging process that occurs in the next GUI. This process first involves loading the open/short calibration data contained in `path_os`. Then, if the data are to be ignored after a certain time (selected separately), then this operation is performed. The measured complex impedance spectra are then converted into complex capacitance and permittivity. Each frequency sweep is evaluated for temperature stability, as determined by comparing the prescribed temperature threshold (assigned separately) and the standard deviation of temperature during this period. For each Solartron set-point temperature (i.e., the desired measurement temperature, prescribed beforehand), only the last temperature-stable sweep is preserved when saving.

The temperature time series is shown in the temperature window as a black line. Colored horizontal lines indicate the mean temperature during a sweep. A different color is used for each set-point temperature. The surrounding colored box indicates the range of the mean ± standard deviation during this period. If a sweep is deemed temperature-stable, then this box is a solid line. Otherwise, it is a dashed line. All sweeps are shown. Below, the last temperature-stable complex permittivity spectrum for each set-point temperature is shown, using the same color set as for the temperature time series.

1.5. Pick time after which to ignore data (*Pick time to ignore*; `do_ignore`)

In certain circumstances, it may be necessary to ignore the data after a certain point in time. Use this tool to select the point along the *x*-axis after which the temperature data will be ignored, and hence no stable sweeps can be preserved. The local time after which this will occur is displayed immediately below the button.

1.6. Saving reformatted Solartron and temperature data (*Save*; `do_save`)

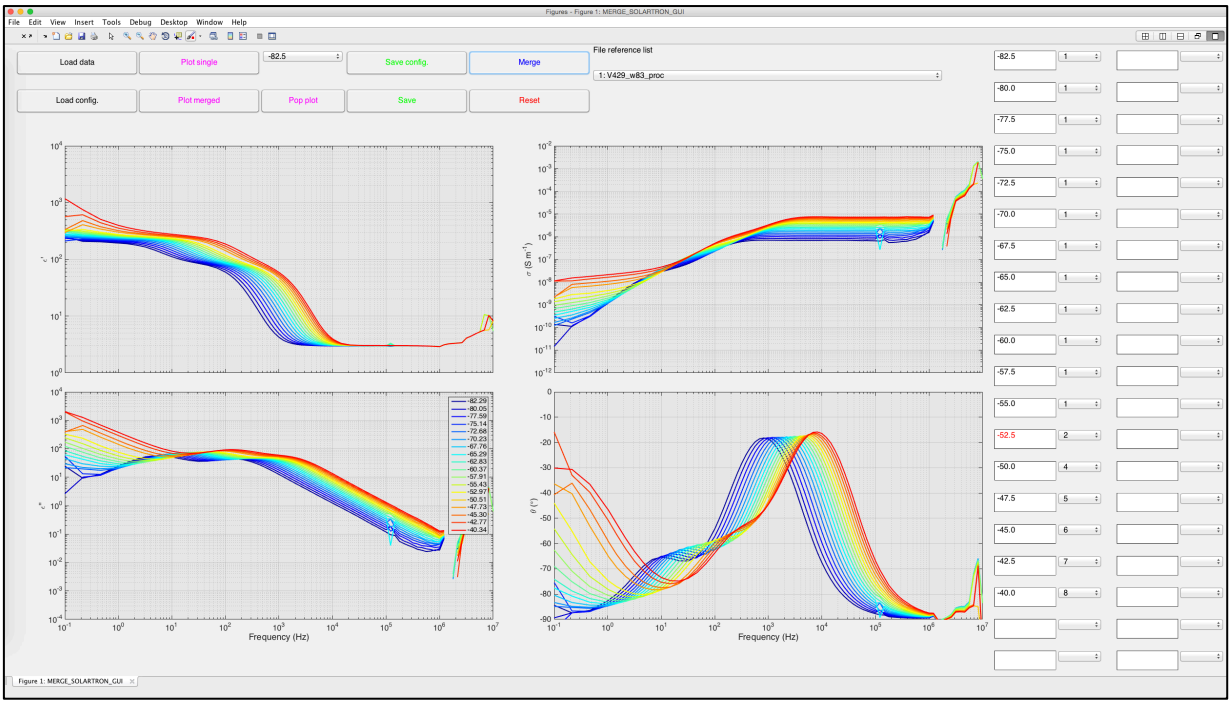
Once it is clear that the data have been loaded correctly and the measurement period has been constrained suitably, the processed data should be saved in MATLAB .mat format. For simplicity, all variables inside the GUI workspace (not directly visible to the user) are saved in the resulting file, including some that are not strictly necessary going forward. The suggested name for the file to be saved is appended with "_proc" to indicate that it has been processed.

2. `merge_solartron_gui`

Once all the files have been processed by `load_solartron_gui`, it is then necessary to merge them into a single file appropriate for the inversion. In this step, multiple measurements from different files may have been made at the same set-point temperature. In such a case, it is

necessary to select which measurement to keep to then represent that temperature. `merge_solartron_gui` then homogenizes the data into a single file that can read directly by `inv_cole_gui`, saving only the necessary variables to interpret the temperature time series.

Again, action buttons and lists are on top. The complex permittivity spectra are in the lower left, and the list of different temperatures is shown in the right. If more than 40 processed files are to be loaded, then set `do_big = true;` in `merge_solarton_gui.m`'s preamble. This will increase the number to 100 and affect the display, but may be much slower.



2.1. Load processed Solartron/temperature data (*Load data*, *Load config.*; `load_data`, `load_cfg`)

The first step is to load processed Solartron/temperature data generated through `load_solartron_gui`. Multiple files can be selected simultaneously. The range of temperatures in ºC will be listed in the first dropdown list. The second dropdown list (labeled File reference list) assigns a number to each loaded file. These numbers are then used in the boxes on the right to distinguish the origin of the spectrum for each temperature. If a temperature is colored in red, then more than one measurement at that temperature was made. Be sure to select the appropriate file for that temperature before proceeding. Choosing the "0" option, available for each temperature, means that any measurement at that temperature will not be included in the merged file. Nothing else will be displayed immediately.

If that data have loaded and saved previously, then a merged configuration file will also have been generated. The key aspects of the saved configuration are which temperatures from which files are used.

2.2. Plot single temperature (*Plot single*; `plot_single`)

For temperatures with multiple measurements, use *Plot single* to plot only the measurements at that temperature. A legend will be provided for each file showing the name of the file and the mean ± standard deviation of the temperature during the measurement sweep.

2.3. Merge data (*Merge*, *Plot merged*; `do_merge`, `plot_merge`)

Once the data are loaded and the preferred measurement has been selected for each temperature, then should then be merged. The resulting range of complex permittivity spectra will then be displayed. Each color represents a distinct temperature, and the mean temperature for that measurement will be given in a legend. If necessary, you can return to this plot using *Plot merged*.

2.4. Save merged data (*Save*, *Save config.*; `do_save`, `do_save_cfg`)

Once successfully merged, the merged data should then be saved. The merged "configuration" will also be saved, representing the selection of temperatures from different files. If only the configuration needs to be saved, use *Save config.*. It is recommended to save the merged data with a filename that ends in "_merge".

2.5. Plot data separately (*Pop plot*; `plot_pop`)

A figure can be generated separately that shows the dielectric spectra for either a single temperature or the merged set (depending on which is currently displayed). This figure does not include the GUI elements and is more appropriate for saving an image.

3. `inv_cole_gui`

This GUI is used to invert measured complex permittivity spectra from a range of temperatures for multiple Cole–Cole inversions. This GUI is the most complex of the three, but it is also the most generalized. In other words, if a MATLAB .mat file can be generated that is comparable to that generated by `merge_solartron_gui` (but collected with a different system), then it is compatible with `inv_cole_gui` and can be used to perform Cole–Cole inversions.

There are two GUIs generated. The first (labeled INV_COLE_GUI) is the primary GUI and the only one in which any action can be performed. The second (INV_RESULTS) shows the Arrhenius (1000 / T in K) temperature dependence of the inversion results for several model parameters. For relaxation frequency (top middle), some reference patterns are also shown for ice (*Auty and Cole* [1952]: cyan; *Kawada* [1978]: green; Cl^--saturated ice from *Stillman et al.* [2013]: gray).

As before, action buttons are concentrated in the top and right. The complex permittivity spectra are displayed as for the first two GUIs. This GUI includes multiple slider bars for key model parameters.

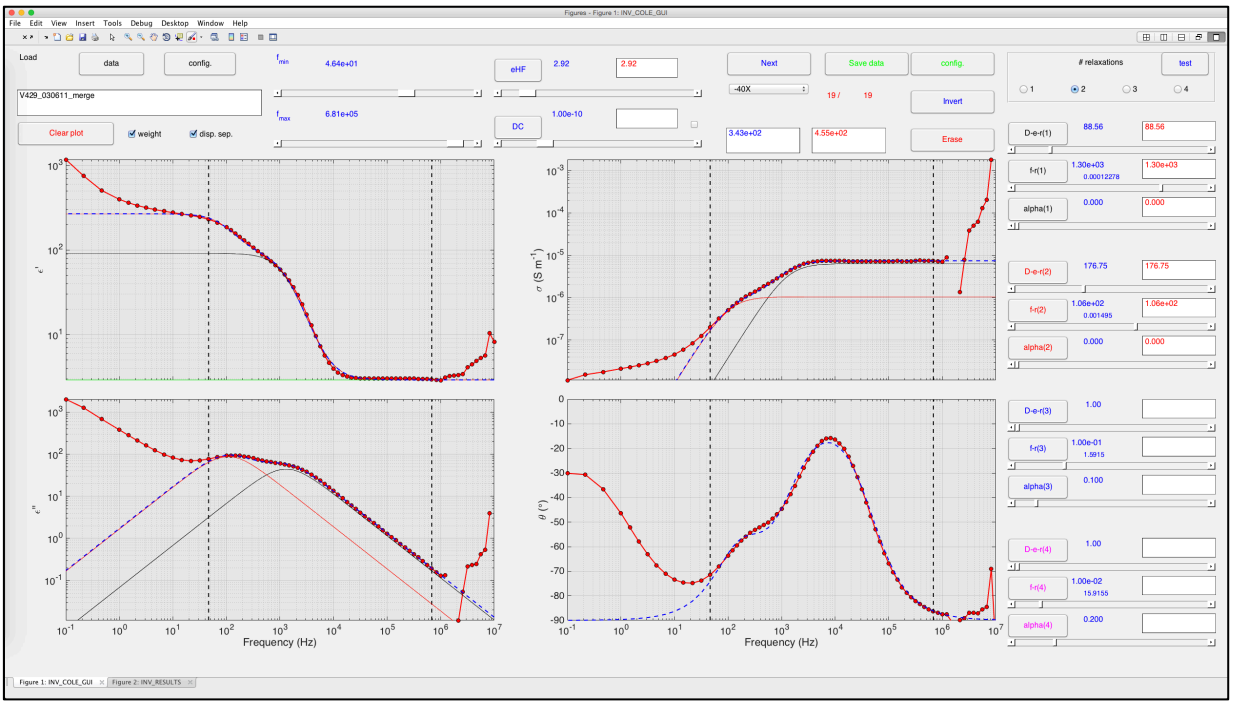
For all button labels, due to a MATLAB oddity, button labels cannot be shown using intuitive symbology. *eHF* represents the real part of the high-frequency permittivity, *DC* represents the

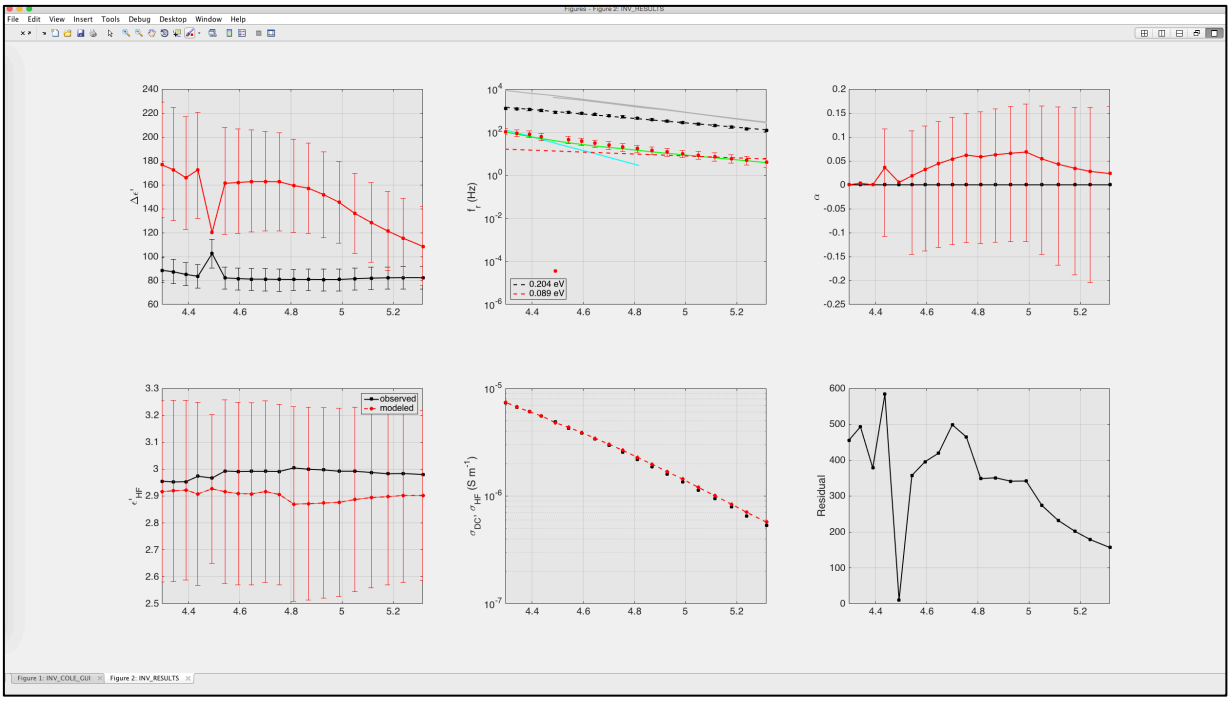
DC conductivity, *D-e-r* represents the dielectric susceptibility, i.e., the difference the real part of the static and high-frequency-limit permittivity, *f-r* is the relaxation frequency and *alpha* is the Cole–Cole distribution parameter.

For each of these model parameters, the slider bar is used to adjust the starting model guess prior to inversion. After the inversion is complete, the best-fit value is reported within the associated text box in red and the slider bar is adjusted to that value. Units are S.I. only. Pressing on these buttons opens up a dialog box in which the range of the inversion to test can be adjusted. For the three Cole–Cole model parameters that can be different for each relaxation (up to four), these parameters are listed in the right-hand column. The number of relaxations to use in the inversion is set by the radio button in the top right. For the relaxation frequency, the value of the relaxation time ($f_r = 1/2\pi\tau$) is also shown in a smaller font immediately below the current relaxation-frequency value.

f_{min} *and* f_{max} are the minimum and maximum frequencies of the bandwidth to be used in the inversion, whose values can be adjusted using the slider bars.

The checkboxes below the data loading buttons toggle whether to weight the inversion as a function of frequency and whether to display each inverted relaxation separately.





This GUI makes use of hotkeys for shortcuts, listed below in Table 1.

Table 1. `inv_cole_gui` hotkeys

Key	Action
1	Set number of relaxations to fit to 1
2	Set number of relaxations to fit to 2
3	Set number of relaxations to fit to 3
4	Set number of relaxations to fit to 4
5	Toggle display of master radargram
6	Toggle display of intersecting radargram
c	Load inversion configuration
d	Toggle inversion switch for DC conductivity
e	Delete model inversion for current temperature
g	Toggle grid lines
i	Do inversion for current temperature with current initial model parameters
l	Load merged data file
n	Switch to next (higher) temperature in file and perform inversion
o	Save inversion configuration for all temperatures
p	Toggle display of inversion separated by each relaxation and DC conductivity
r	Remove current plot
s	Save inverted model parameters
w	Toggle frequency-dependent inversion weighting
↑	Switch to next temperature
↓	Switch to previous temperature
spacebar	Switch between GUIs (applies to both GUIs)

3.1. Load merged data/configuration (*Load…data*, *config.*; `load_merge`)

First, load a merged data file generated by `merge_solartron_gui`. If this file has already been partly or fully inverted and saved, then an inversion configuration file (*_inv_cfg.mat) will also have been generated. This file can be loaded using *config.* after the merged data have been loaded. The filename is displayed below these buttons, and the dielectric spectrum of the first temperature is displayed.

The data themselves are shown as both a red line with red circles overlain upon it. f_{min} *and* f_{max} are shown as vertical dashed black lines. Even if an inversion has not yet been performed, the forward model using the default model parameters (unboxed text next to each button) will be shown. The sum of this model's relaxations and/or DC conductivity is shown as a blue dashed line. If the *disp. sep.* checkbox is checked, then each component of this forward model (`do_fm`, `fm_cole`, `fm_cole_sep`, `res_cole`, `chisq`, `delta_chisq`) is also shown separately as a thin solid line. The color scheme for each relaxation follows the text color of the button. Additionally, *eHF* is shown in green and *DC* in cyan. Note that these individual components are not broken out for phase (lower right). The data–model residual value of this forward model is shown in blue in the leftmost of two text boxes in the top right. It is automatically updated as the forward model is adjusted.

The total number of temperatures in the merged file is listed in the upper right, along with the number that have been inverted successfully (e.g., 10/19). The temperature set is listed in a dropdown menu.

3.2. Invert merged data for a given temperature (*Invert*, *Next*, *Erase*; `do_inv`, `do_activ`, `inv_report`, `nuke_inv`)

Press *Invert* to use the current model parameters as the initial guess in an inversion for the best-fit model parameters. The resulting inversion results will then be shown in both GUIs, with the residual shown in red in the rightmost of the two text boxes in the top right. In dropdown menu, this temperature will now be listed with an "X" to indicate that it has been inverted. If you do not wish to preserve this inversion, press *Erase*.

Pressing *Next* moves on to the next temperature in the list and immediately uses the inversion results for the current parameter as the model guess for the next temperature to then invert. This approach speeds up the inversion of an entire dataset, especially if the temperature pair is not so far apart as to be overly sensitive to the differences in their spectra.

3.3. Save inversions and/or configuration (*Save data*, *config.*; `save_cfg`, `save_cfg_vars`, `save_inv`, `save_inv_vars`)

As before, both the inversions and their configuration using *Save data* and *config.*, respectively. The suffixes "_inv" and "_inv_cfg" will be suggested, respectively.