PmagPy *Thellier GUI* (v.2.29)

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Contents

1 Introduction

The *Thellier GUI* is desiged for viewing, analyzing, and interpreting the experimental results of Thellier-type paleointensity experiments.
The *Thellier GUI* is a Python open code made part of PmagPy software(`http://earthref.org/PmagPy/cookbook/`).

If you use this program, you should cite the following reference:
Shaar, R., Tauxe, L., 2013. Thellier GUI: An integrated tool for analyzing paleointensity data from Thellier-type experiments. Geochem. Geophys. Geosyst. 14, 677-692, doi: 10.1002/ggge.20062.

The *Thellier GUI* currently supports the following PI protocols:

- ZI (the "Coe protocol" - Coe, 1967); IZ (the "Aitken Protocol" -Aitken et al., 1988), and IZZI (Tauxe and Staudigel 2004)

- The original Thellier Thellier protocol (Thellier and Thellier, 1959)

- Additional checks: pTRM checks (Coe, 1978), pTRM tail check (Riisager and Riisager, 2001), Additivity checks (Krasa et al., 2003).

- Microwave or thermal heatings.

- Other protocols will be added upon request.

The program uses MagIC formatted files. For details on the MagIC format see PmagPy cookbook in `http://earthref.org/PmagPy/cookbook/` . The *Thellier GUI* is part of the PmagPy GUI platform, hosted under Pmag GUI program.

To get started with Pmag GUI follow the tutorial on `http://earthref.org/PmagPy/cookbook/`).

Comments and suggestions are welcome. For requests, general support, and any comments, contact Ron Shaar (ron.shaar@mail.huji.ac.il) or Lisa Tauxe (ltauxe@ucsd.edu).

2 Running Pmag GUI and the example dataset

- **Running Pmag GUI:** All the relevant information on how to install PmagPy and run Pmag GUI is given in Chapter 1 and 2 in the PmagPy Cookbook: `http://earthref.org/PmagPy/cookbook/`

- **Example dataset:** The example dataset used in this manual is from Shaar et al. (2016). To download the data go to `http://earthref.org/MagIC/11028/` and save the txt file in the Data column in your MagIC project directory. The file can be unpacked by clicking the "unpack" button in the Pmag GUI.
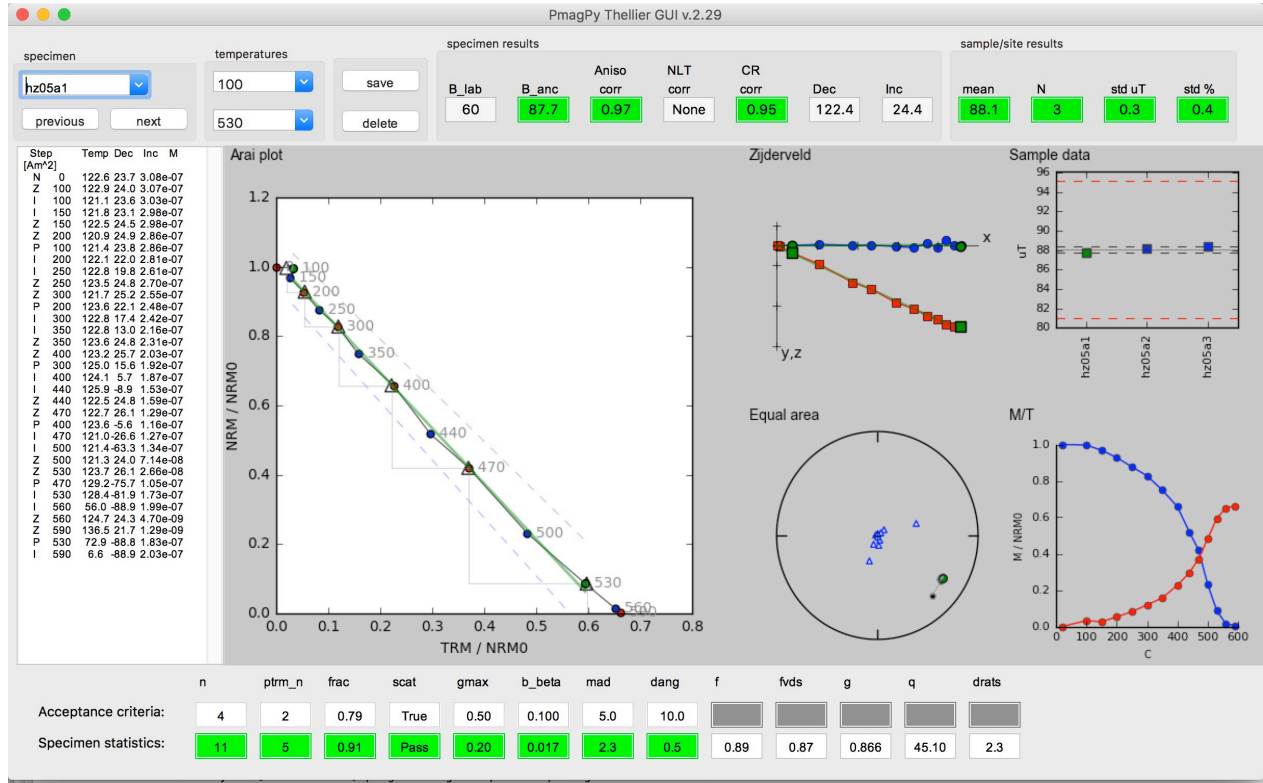
3 *Thellier GUI* main panel

Figure 1: Thellier GUI main panel

The *Thellier GUI* main panel is shown in Figure 1

graphics:

- **Arai plot:** The Arai plot shows NRMs versus pTRMs, normalized by NRM_0. Blue circles are zerofield-infield (ZI) steps, red circles are infield-zerofield steps (IZ), triangles are pTRM checks, blue squares are tail checks, diamond are additivity checks. Temperatures can be displayed near data points (depending on your preferences (see Chapter 9). pTRM checks and tails checks can be connected to the temperature in which they were carried out (depending on your preferences, Chapter 9). Temperature bounds and best fit line are marked in green. 'SCAT box' (related to SCAT statistics) is marked with dashed lines. You can zoom into the figure by placing the mouse cursor over the Arai plot and "drawing" a line from top left to bottom right. Zooming out is by "double click" .

- **Zijderveld plot:** The directions of the NRMs are displayed on the Zijdreveld plot. The x axis is rotated to the direction of the NRM . Blue symbols are the x-y projection, and red symbols are the x-z projection. The direction of the best fit line is shown in green. Temperatures can be displayed near data points (depending on your preferences, Chapter 9).You can zoom into the figure by placing the mouse cursor over the Zijderveld plot and "drawing" a line from top left to bottom right. Zooming out is by "double click" .

- **Equal area plot:** The lower hemisphere equal area projection shows the direction of the NRMs (by default) as closed (positive inclinations) and open (negative inclinations) circles.

The direction of the best fit line is shown in green circle. The direction of the pTRMs can be displayed (depending on your preferences) with triangles.

- **Moment-temperature plot:** The normalized moments of NRMs and pTRMs, normalized by NRM_0 are shown in blue and red, respectively.

- **Sample/site data:** If at least two specimens from the same sample/site have a saved interpretation, then their values are displayed on this plot. The mean $\pm$ standard deviation of the mean are marked as horizontal dashed lines. The bounds for the standard deviation in the selection criteria are marked with red dashed lines. The current specimen in marked in green.

- **Non-linear TRM:** If the specimen has non-linear TRM data (Selkin et al., 2007; Shaar et al., 2010), then the NLT data can be displayed instead of the Moment-Temperature plot Figure 2. The plot shows the the moments of each NLT measurements, normalized by the inferred moment at the lab field (see examples in Shaar et al., 2010). Dashed line shows the assumption of linearity (a line that connects the origin and [lab field, 1.0] point). The green line show hyperbolic tangent best fit to the data. The green circle shows the paleointensity calculated using the NLT correction. The horizontal distance between the dated line and the green circle is the difference between the NLT-corrected result, and the non-corrected.
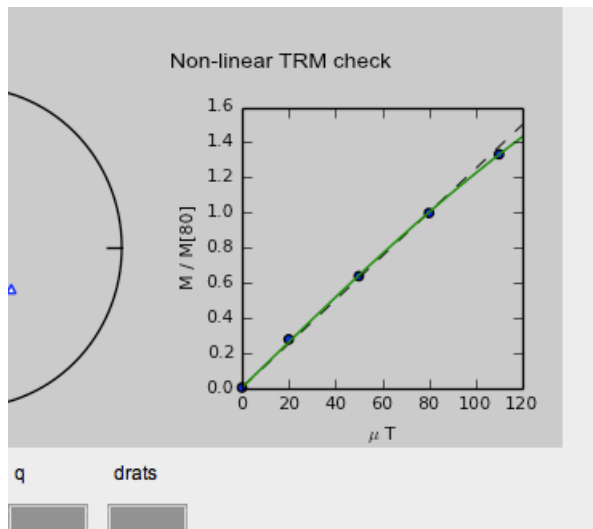

Figure 2: *Thellier GUI* TRM data plot

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- **Cooling rate data:** If the specimen has cooling rate experiment data then the it can be displayed instead of the Equal Area plot Figure 3. Cooling rate experiment data is displayed as TRM (normalized to the TRM in the lab's cooling rate) versus ln(lab cooling rate oven / cooling rate). Following halgedahl (1980) the relation should be linear and therefore, the cooling rate correction is calculated by linear extrapolation to the ancient cooling rate (red circle is Figure 3).

measurements text panel (left penal):

- four columns of text display the measurement data:
  - Step: "N" for NRM, "Z" for zero field step, "I" for infield step, "P" for pTRM check, and "T" for tail check, "A" for additivity check.
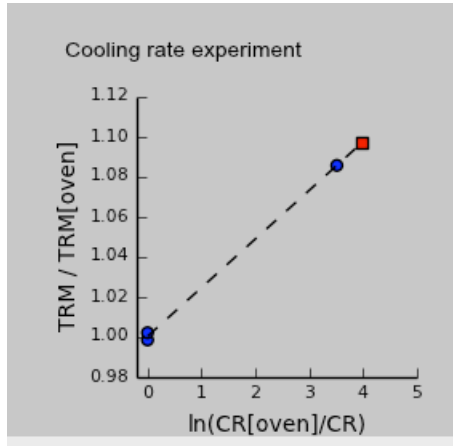
5

Figure 3: *Thellier GUI* cooling rate plot

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  – Temp: temperature in C

  – Dec: declination

  – Inc: inclination

  – Moment: magnetic moment in units of Am^2

specimen box (top left controls):

- **Specimen:** a dropdown menu for choosing a specimen from the list of all the specimens (sorted by name).

- **Previous/next:** buttons to move forward and backward in the specimens list.

- **Moving with the keyboard:** (option does not work on all operating systems) Previous/next buttons can be also activated from the left/right buttons on the keyboard.

temperature box :

- temperature bounds can be manually selected using the two selection boxes.

Save/Delete box:

- **save/delete:** Save or delete the currently displayed interpretation. The saved interpretation are not written to a file, and when exiting the GUI they will be unavailable. For saving the interpretations into files see section 8.

specimen results:

- **B_lab:** laboratory field in units of μT.

- **B_anc:** specimen's paleointensity in units of μT. If this window is colored in green it means that the interpretation passed the selection criteria. Red means that the interpretation failed the criteria.

- **Aniso Correction:** anisotropy correction factor. If this window is colored in red it means that there is an error or warning related to the anisotropy correction.

- **NLT Correction:** Non-Linear TRM (NLT) correction factor.

- **CR Correction:** Cooling rate correction factor.

- **Dec/Inc:** Ancient declination/inclination calculated by PCA of the NRM in the selected temperature bounds.

sample results:

- **mean:** sample mean in units of μT.

- **N:** number of specimens used for calculating the mean.

- **std uT:** standard deviation of the sample mean in units of μT.

- **std %:** standard deviation of the sample mean devided by the mean in units of percentage.

4 Paleointensity statistics

The *Thellier GUI* program support the specimen paleointensity statistics listed in the official "Standard Paleointensity Definitions" (SPD), written and maintained by Grieg Paterson. The current version of SPD can be found in:
`http://www.paleomag.net/SPD/`.
Currenly, there are about 40 different statistics in SPD.1.0.
The bottom panel of the *Thellier GUI* program shows the default *Thellier GUI* statistics (or the ones that the user chose in the past and saved in PmagPy folder). To change the statistics list: choose tom the menubar Preferences → Specimen paleointensity statistics from SPD list. From the dialog window (Figure 4) choose your preferred set of paleointensity statistics, and save the file in the main PmagPy folder. The program needs to restart before seeing this change.
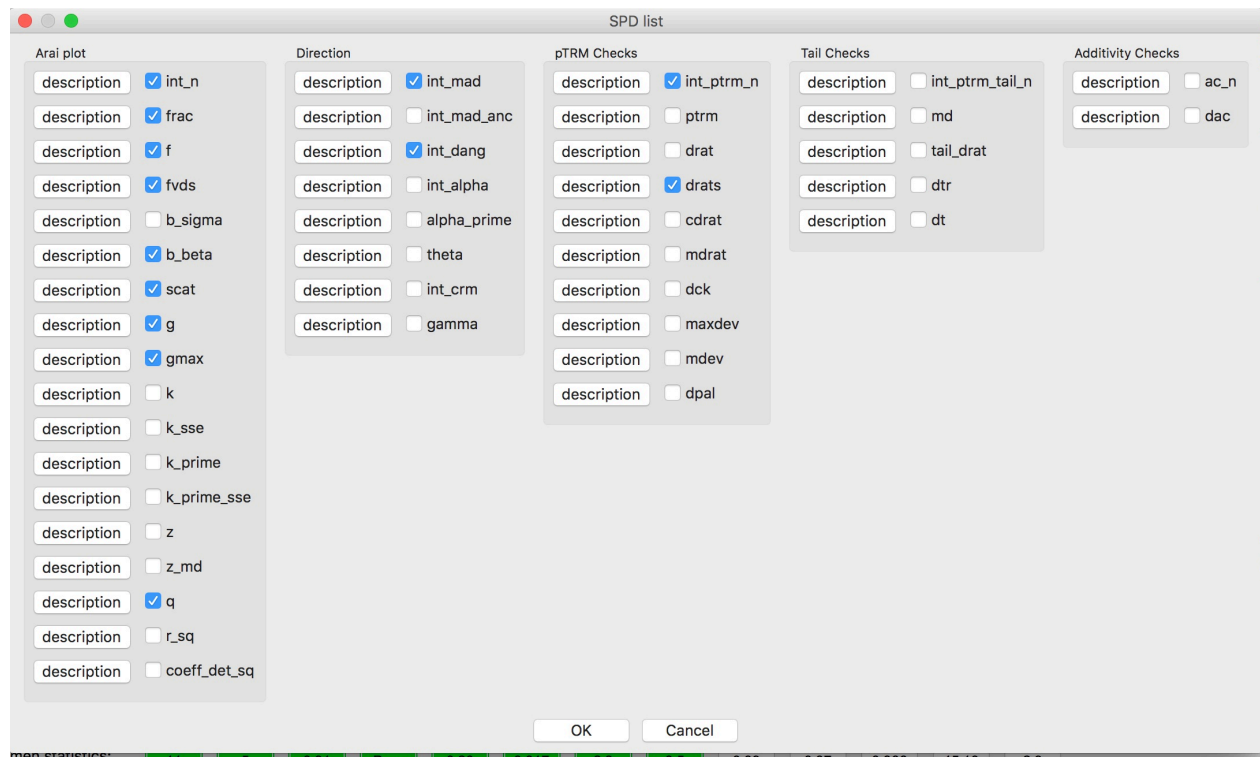

Figure 4: specimen paleointensity preferences window

5   Acceptance criteria

Figure 5: *Thellier GUI* Acceptance criteria dialog window

To change the acceptance criteria choose from the menubar: Analysis → Acceptance criteria → Change acceptance criteria. Figure 5 shows the acceptance criteria dialog window.

The dialog window is separated to six groups of criteria as listed below:

Specimen acceptance criteria

The acceptance criteria dialog window shows the specimen paleointensity statistics displayed on the bottom panel of the *Thellier GUI* . To add or remove specimen paleointensity statistics see Section 4.

Anisotropy criteria

- **F-test checkbox:** By checking this box, the program will use the anisotropy F-test (Hext, 1963) as a selection criterion. If the specimen's F-test is below the threshold value for anisotropy at the 95% confidence level, the anisotropy tensor will not be used to correcting the paleointensity result.

- **Alteration check threshold value %:** For ATRM only. The program checks the relative difference between four pairs of ATRM measurements: (+x,-x), (+y,-y), (+z,-z), (first measurement, alteration check measurement). If relative difference in units of % ($100 \frac{B1,B2}{mean(B1,B2)}$) of at least one of these pairs is lower than the threshold value then the anisotropy tensor is discarded and is not used to correct the paleointensity result.

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Sample acceptance criteria

- **int_n:** minimum number of specimens for sample mean calculation

- **int_outlier_check:** A minimum number of specimens for outlier check. An outlier is a specimen whose all paleointensity 'acceptable' values are not in the interval define by the mean $\pm 2\sigma$. If only one specimen in the sample meets this definition, then this specimen is discarded from sample mean calculation.

STDEV-OPT:

- **STDEV-OPT checkbox:** The STDEV-OPT (standard-deviation-optimal) algorithm per mutates all the acceptable paleointensity values at the specimen level and choose for each specimen the interpretation that results with the minimum standard deviation of the sample means (see Shaar and Tauxe, 2013 for details).

- **int_sigma_uT:** standard deviation of the sample mean in units of μT. NOTE: int_sigma_uT is combined with int_sigma_perc with logical OR: (int_sigma_uT OR int_sigma_perc)

- **int_sigma_perc:** standard deviation of the sample mean in units of %. NOTE: int_sigma_uT is combined with int_sigma_perc with logical OR: (int_sigma_uT OR int_sigma_perc)

- **int_interval:** The interval between acceptable interpretation (interpretation that pass the acceptance criteria) in units of μT. NOTE: int_interval and int_inteval_perc is combined with logical OR: (int_interval OR int_inteval_perc).

- **int_inteval_perc:** The interval between acceptable interpretation (interpretation that pass the acceptance criteria) in units of %. NOTE: int_interval and int_inteval_perc is combined with logical OR: (int_interval OR int_inteval_perc).

- **aniso_threshold_perc:** The STD-OPT algorithm calculates the mean anisotropy degree ($\frac{\tau_1}{\tau_2}$) of all the specimens in the sample. If the mean anisotropy degree of the sample is larger than aniso_threshold_perc, then any specimen with no anisotropy correction (was not measured, or rejected) will be discarded.

Bootstrap:

- **Enable BS checkbox:** Simple bootstrap. use discrete values of all the possible poaleintensities at the specimen level.

- **Enable BS-PAR checkbox:** Parametraic bootstrap. use a uniform distribution between B_{max} and B_{min}, where B_{max} and B_{min} are the maximum and the minimum acceptable paleointensity values of the specimen.

- **specimen_int_max_slope_diff:** specimens with $\frac{slope_{max}}{slope_{min}} >$ specimen_int_max_slope_diff are discarded from bootstrap calculation.

- **int_BS_68_uT:** 68% confidence interval of the sample bootstrap paleointensity in units of μT.

- **int_BS_68_perc:** 68% confidence interval of the sample bootstrap paleointensity in units of %.

- **int_BS_95_uT:** 95% confidence interval of the sample bootstrap paleointensity in units of μT.

- **int_BS_95_perc:** 95% confidence interval of the sample bootstrap paleointensity in units of %.

6 Manual interpretation

Manual interpretation is the conventional approach of interpreting the data. It is done by manually selecting the temperature bounds for each specimen separately.

To manually interpret your dataset choose the temperature bounds from the temperature boxes. To save or delete your interpretation press on the save/delete buttons.

Before exiting the GUI make sure that all the interpretations are saved. To learn how to save data see section 8.

7 Automatic interpretation: *Thellier Auto Interpreter*

The *Thellier Auto Interpreter* is a tool for automatic interpretation based on given paleointensity statistics as acceptance criteria. The concept of this tool is explained in details in Shaar and Tauxe (2013). Before running the *Thellier Auto Interpreter* the program needs to know the relationship between specimens, samples, and sites. The program takes this information from the columns "er_specimen_name", "er_sample_name", and "er_site_name" in the magic_measurements.txt file. If the relationship between sites, samples and specimens was not completely defined in the process of converting your measurement file format to MagIC format (Section **??**) then use the Earth REF builder in the Pmag GUI..

1. **Prepare the required inputs**
   Open from the menu-bar the paleointensity statistics dialog window by choosing "Analysis" → "Acceptance criteria" → "Change acceptance criteria". The first row shows the specimen acceptance criteria. The se cond row shows the criteria related to anisotropy at the specimen level. The third row shows sample/site acceptance criteria. Fill these lines with the criteria that you want to apply. For more explanation on acceptance criteria dialog box see section 5.

2. The *Thellier Auto Interpreter* uses three different algorithms: STDEV-OPT (optimal standard deviation), BS (bootstrap) and BS-PAR (parametric bootstrap). For most application STDEV-OPT is the recommended option. The STDEV-OPT does the following tasks:

   (a) The program analyzes all the possible best-fit lines of each Arai plot separately and isolates the interpretations that pass the specimen selection criteria.

   (b) Each interpretation is corrected for anisotropy effect, cooling rate effect (for slow-cooled samples such as pottery), and if needed, non-linear-TRM (NLT).

   (c) The program calculates all the possible sample/site means and isolates the means that pass sample/site acceptance criteria.

   (d) The most likely sample/site mean is calculated by choosing from all the means that passed the criteria the one with the lowest standard deviation.

   (e) The uncertainty bounds of the sample/site paleointensity are calculated by finding from all the means that passed the criteria the two end case interpretations: the one with the lowest paleointensity ($B_{min} \pm \sigma_{min}$), and the one with the highest ($B_{max} \pm \sigma_{max}$). The error envelope is [B_{min} - σ_{min}, $B_{max} + \sigma_{max}$].

3. **Run the *Thellier Auto Interpreter*** After you set the acceptance criteria, run the interpreter by choosing from the menu-bar "Auto Interpreter" → "Run Thellier Auto Interpreter". The runtime of the program may take between few seconds for small datasets to few minutes for large datasets with hundreds to thousands of specimens.

4. **Output files**
   The *Thellier Auto Interpreter* produces the following output files in a directory named "thellier_interpreter":

   - **thellier_interpreter.log**
     A log file. Each line in the log file starts with -I- (Information), -W- (Warning), or -E- (Error). The first massages include general messages and acceptance criteria. Then, each trial (a pair of temperature bounds) is given, for example:

-I- specimen su100301a (200-500) FAIL on: specimen_frac= 0.799844,

-I- specimen su100301a (200-515) PASS

The end of the log files shows the samples/sitees mean calculation.

- **thellier_interpreter_specimens_bounds.txt:**
  A summary file that lists the minimum and the maximum of the 'acceptable interpretation' (for specimens that have at least one 'acceptable' interpretation). The first four lines in the file are the acceptance criteria used. The next line is a header, and then the data for all the specimens: sample name, specimen name, anisotropy correction factor, anisotropy correction type, NLT correction factor, lab field (uT), STDEV-OPT minimum 'acceptable' interpretation, maximum 'acceptable' interpretation, and Warning. This file is useful for inspecting the behavior of the dataset in general.

- **thellier_interpreter_all.txt** A file that contains all the accepted interpretations (temperature bounds, paleointensity values, and statistics) for all the specimens. There may be more than one 'acceptable' interpretation for each specimen.

- **thellier_interpreter_STDEV-OPT_specimens.txt:**
  A list of the specimen's interpretations that were chosen by STDEV-OPT algorithm to produce the STDEV-OPT sample/site mean, and the paleointensity statistics.

- **thellier_interpreter_STDEV-OPT_samples.txt or thellier_interpreter_STDEV-OPT_sites.txt**:
  A summary file with all the samples/sites that passed the criteria. The first four lines are the acceptance criteria used in the interpretation. Then, the following information is given: sample/site name, number of specimens used in the calculation, the STDEV-OPT paleointensity in units of μT, standard deviation of the sample mean in units of μT, standard deviation divided by the mean in units of %, the minimum acceptable sample/site mean and its standard deviations, the maximum acceptable sample/site mean and its standard deviations, the interval of accepted means in units of μT, Interval of accepted means divided by the sample's mean in units of %, Warning. This information is useful for generating a table for a publication.

- **thellier_interpreter_STDEV-OPT_redo**:
  A "redo" file. This is a tab-delimted text file with three fields: the first field is specimen name, the next is minimum temperature bound (in Kelvin, whereas NRM is 273), and the third field is the maximum temperature bound. If you quit the program you can load the interpretation of the last *Thellier Auto Interpreter* run by loading this file (From the menu-bar "Analysis" → "Import previous interpretation").

- **thellier_interpreter_BS_samples.txt**:
  A summary file with all the samples that passed the criteria in the bootstrap method (only if BS method is used for sample calculation).

- **thellier_interpreter_BS-PAR_samples.txt**:
  A summary file with all the samples that passed the criteria in the parametric bootstrap method only if (BS-PAR method is used for sample calculation).

8 Save interpretations

The interpretations (done manually or by *Thellier Auto Interpreter*) can be saved in different forms as explained below.
There are two different ways to save your interpretations as described below

1. Analysis → Save current interpretation.
   the following file will be saved:

   - thellier_GUI.redo. A redo file is a tab-delimted text file with three fields: the first field is specimen name, the next is minimum temperature bound (in Kelvin, whereas NRM is 273), and the third field is the maximum temperature bound. If you quit the program you can load the interpretations on the next time you open it by importing this file (From the menu-bar "Analysis" → "Import previous interpretation (redo file)").

2. File → Save MagIC Pmag tables.
   This saves all the results in MagIC pmag format. These files can be later uploaded to the MagIC database. The MagIC pmag table includes three files:

   - pmag_specimens.txt: The final result at the specimen level. For details see `http://earthref.org/MAGIC/metadata.htm`
   - pmag_samples.txt or pmag_sites.txt: The final result at the sample or site level. For details see `http://earthref.org/MAGIC/metadata.htm`
   - pmag_results.txt: The final result table to be used by the MagIC database For details see `http://earthref.org/MAGIC/metadata.htm`

   When the *Thellier GUI* programs starts up it searches for pmag_specimens.txt and import the interpretations saved in this file.

9 Appearance preferences

Some appearance preferences can be changed by choosing from the menu bar: Preferences → Appearance preferences. (Figure 6).
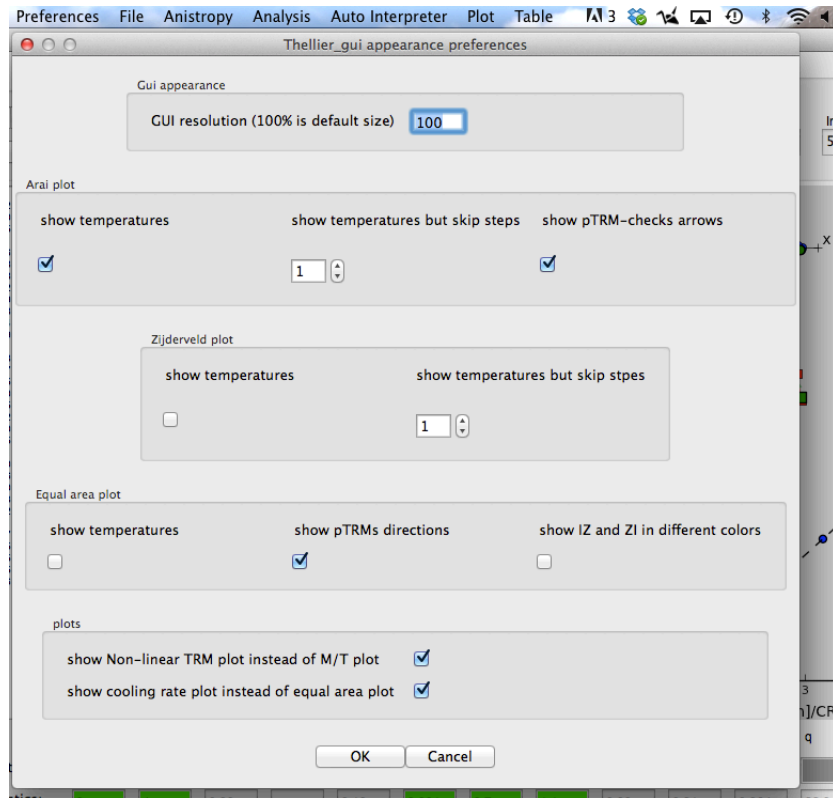

Figure 6: Appearance preferences window

- **adjusting window size**. The default resolution (the size of the screen) is 100% . To change that pick a number not larger than 130%.

- **Arai plot**. The temperature can be visible or invisible. Also, the temperature can be displayed every n steps. The arrows connecting pTRM cheks to the starting temperature can be also visible or invisible.

- **Zijderveld plot**. The temperature can be visible or invisible. Also, the temperature can be displayed every n steps.

- **Equal area plot**.
  - show temperature: show the temperature.
  - show pTRMs direction: show the direction of the 'pTRM gained' (not anly the 'NRM lost').
  - show IZ / ZI in different colors.

- **additional plots**. As there is room only for five plots, choose which of the additional plot you want to see in the bottom row.

10 Remanence anisotropy correction

To calculate remanence anisotropy tensors Select from the menu-bar Anisotropy → Calculate anisotropy tensors. Two files will be crated in the MagIC project folder: rmag_anistropy.txt and rmag_results.txt. For explanation on the format of these files see: `http://earthref.org/MAGIC/metadata.htm`.

The *Thellier GUI* supports two types of anisotropy calculations: ATRM in 6 directions, and AARM in 6,9,or 15 directions.

After calculation of the anisotropy tensor check Errors and Warnings by choosing the menubar: Anistropy → Show anisotropy calculation warnings/Errors.
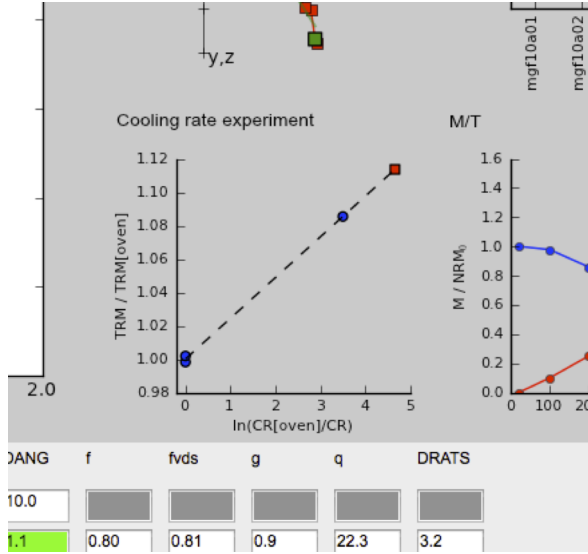
11   Cooling rate corrections

Figure 7: cooling rate correction calculation

The algorithm of the cooling rate correction follows Figure 4 in Halgedahl et al. (1980). To show the cooling rate data on the *Thellier GUI* main panel, the appearance statistics should be set to "show cooling rate plot instead of equal area plot". To do that choose from the menu-bar Preference → Appearance preferences.

Figure 7 show the cooling rate correction calculation. In this example there are three measurements: the first is the fast (oven) cooling rate, the second is a slow cooling rate, and the third is an alteration check measurement in the fast (oven) cooling rate. The oven magnetization (TRM_{lab}) is calculated by the average of the first and the alteration check measurements. The x-axis in the plot is $ln(\frac{\text{oven's cooling rate}}{\text{cooling rate}})$ the y-axis is $\frac{\text{TRM}}{TRM_{lab}}$. The red point is an extrapolation using an estimated cooling rate of the ancient TRM.

IMPORTANT NOTES:

- **Alteration check:** The threshold for alteration check if 5%. If the relative change between the first and the alteration-check measurements is higher than 5%, then the cooling rate correction factor will not be used to correct the paleointensity data and the cooling plot data will not be shown.

- **Inferred cooling rate correction:** If at least one specimen out of all the specimens in the sample have cooling rate correction, then the cooling rate correction for the other specimens that do not have cooling rate correction is the mean of the cooling rate correction of the sister specimens that have cooling rate correction.

12 Plot paleointensity curve

If the interpretations were saved as MagIC pmag tables, then the paleointensity curve can be displayed. To plot paleointensity curve choose from the menubar Plot → Plot paleointensity curve. To add location map check the "show location map" box. One option is to use "auto-scale". The other option is to specify the lat/lon bounds.
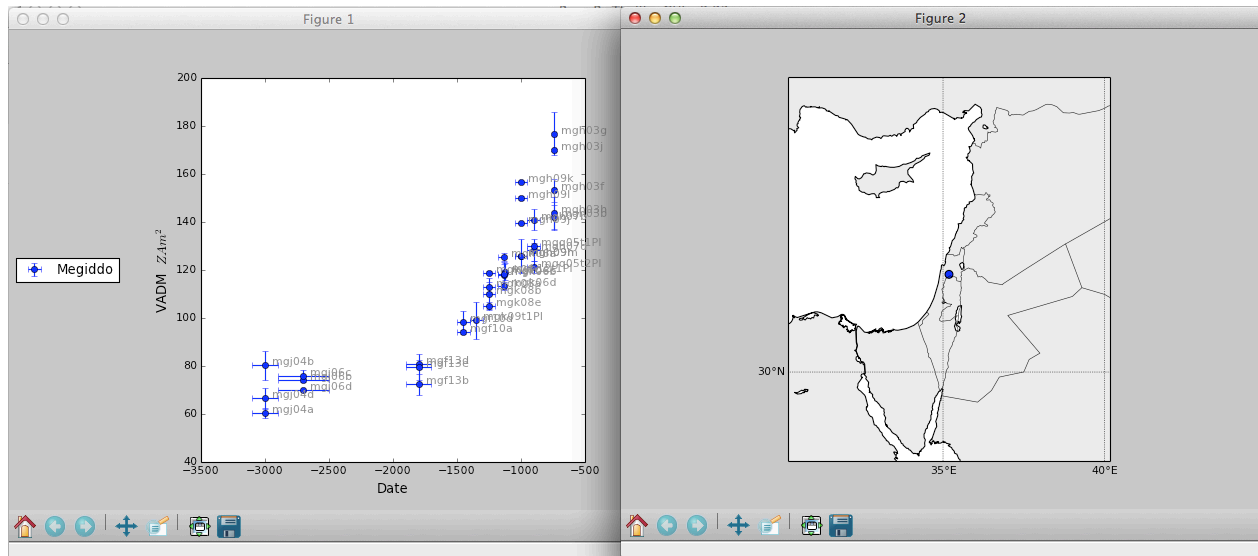

Figure 8: paleointensity curve of Megiddo dataset

13 Save figures

To save plots choose from the menubar: File → Save plot. The figure that on the display will be saved. So, if the interpretation is already displayed on the plot, it will be saved with the interpretation. The default options for saving the figures are pdf, svg, and eps. To save in another format the appropriate suffix should be added to the file name (python supported formats are emf, eps, pdf, png, ps, raw, rgba, svg, svgz).