Supporting Information for "Magnetic unmixing of first-order reversal curve diagrams using principal component analysis"

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Introduction

The supporting online material for this paper consists of (i) instructions on how to run FORCem (FORC environmental magnetism), a program designed to automatically

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upload and analyze a suite of raw FORC files that have been measured using **identical experimental protocols**, (ii) two *.mov files with animations of the three-dimensional PCA space and mixing tetrahedron for the quaternary mixture, and (iii) a zip file containing two Igor Pro experiments: a) FORCem.pxp, a fully self-contained and compiled code used to analyze the data presented in this paper, and b) FORCem_demo.pxp, containing uploaded data from core SHAK-10-9M-F.

Quickstart Guide to FORCem (FORC environmental magnetism)

Before using FORCem, it is recommended that one or more samples be analyzed using FORCinel[1] to determine optimal parameters for smoothing, ridge extraction, grid definition, etc. These parameters should then be used on the entire dataset when running FORCem.

1. System requirements

FORCem is a self-contained package written using Igor Pro by WaveMetrics (`www.wavemetrics.com`). Although Igor Pro is a commercial package, a fully functioning demo version can be downloaded for free for Mac and Windows. This will allow you to explore FORCem, but will not allow you to export results after 30 days. FORCem has been written using Igor Pro version 6.36, on a Mac Mini with a 2.6 GHz Intel Core i7 processor and 16 GB RAM, running OS X version 10.8.5. The program has also been tested successfully on a MacBook Pro with a 2.2 GHz Intel Quad Core i7 processor and 4 GB RAM. Although cross platform is usually trouble free, functionality cannot be 100% guaranteed on other systems using different software versions.

2. Running FORCem

After downloading the FORCem.pxp file (`www.esc.cam.ac.uk/nanopaleomag`), simply double click to open it within Igor Pro. You should see the following windows: Data Browser, FORC Control Panel, PCA Control, Define Endmembers, and the FORCem command window. If not all the windows are visible on your screen, go to the menu bar and click Windows>Control>Retrieve All Windows in order to move them into visible positions.

2.1. Loading FORCs

To load the suite of raw FORC files, press **Load multiple FORCs** in the FORC Control Panel. (Note that in Igor, before pressing a panel button, the respective window needs to be selected.) The ensuing dialog window asks for the folder containing the raw FORC files to be analyzed. All the files should have an extension, typically *.frc or *.forc. The next dialog box asks for this extension name. Note that data from all the files with the specified extension in the selected folder will be uploaded.

The user is then prompted to choose whether certain actions should be performed, or to input some processing parameters. The succession of dialog boxes contains the following operations:

1. Perform drift correction
2. Remove first point artefact
3. Remove lower branch
4. Input VARIFORC smoothing parameters
5. Indicate wave name containing sample masses (optional)

6. Extract central ridge

All of the above are standard FORCinel 2.0 operations, except for item 5. If used, the wave containing the sample masses should be created or imported in the *Results* folder (see Data Browser window).

Depending on the size and number of data files, the uploading and processing of the FORC data may take several hours (to get a rough estimate multiply the total processing time of one data file in FORCinel by the number of files to upload).

The upload procedure will create a series of waves in *Results*, among which is a 3D wave called *totalstack*, in which each layer will contain one processed FORC diagram (the equivalent of the wave *variforc_raw* in FORCinel). This wave will be used in the PCA.

2.2. PCA Procedures

Once the data are uploaded, press **PCA Grid** in the PCA Control window, and input the grid dimensions (in T). For typical magnetite-bearing samples a resampling resolution of 0.005 T is recommended for short processing times. A resolution of 0.002 T can be employed for small grids ($<0.1 \times 0.1$ T). For higher coercivity minerals a resolution of 0.01 T is recommended. The individual grids are redimensioned and placed into a wave called *Dat_matrix*, in which each line is an unfolded grid presented as a succession of vertical profiles (the so-called PCA spectrum). The subtraction of the mean PCA spectrum produces the wave *meanmatrix*, which will be used in the PCA. Both *Dat_matrix* and *meanmatrix* are plotted at the end of the gridding procedure.

To perform the PCA press **Run PCA** in the PCA Control window. The end of the run (which can last for a few minutes if *meanmatrix* is large) is signalled by the display of a table containing the cumulative variance of the PCs. The next step is to press **num**

of PCs to use in the PCA Control window. The number of PCs used is subject to user interpretation of the dataset and of the values in the displayed table. The software currently accepts values of 1, 2, or 3, corresponding respectively to binary, ternary, and quaternary mixtures.

After selecting the number of significant PCs, press **Plot PCs** in the PCA Control window to display the PC score plot(s) and a general FORC diagram calculated using user-defined PC scores values. These PC scores are controlled by a moveable cursor ($\oplus$) within the score plot. After selecting the score plot window, move the cursor either by using the arrow keys, or by clicking and dragging it to the desired position. The FORC diagram will be automatically updated.

2.3. Selecting End Members and Calculating Proportions

If there is only one significant PC, all the data points can be expressed as linear combinations of two end members (EMs) with PC 1 values outside the interval spanned by the data. The cursor movement in the score plot will only relay values in the horizontal direction. Move the cursor beyond the data interval in one direction until a physically realistic EM FORC topology is attained (graph axes can be rescaled if necessary). Select the Define Endmembers window and press **Set EM1**. A table called End Member PCs containing EM score values will be displayed. Select the score plot and move the cursor beyond the data interval in the opposite direction until a second suitable EM is obtained. Select the Define Endmembers window and click **Set EM2**, making sure that the score value has registered in the table. Then press **Calculate Proportions**. A graph with proportion values for each EM will be displayed, along with calculated FORC diagrams for each EM.

If there are two significant PCs, the data points can be expressed as linear combinations of three EMs. The cursor will register score values for both PC 1 and PC 2, which will be used to calculate the general FORC diagram. Apply the procedure described above to select and display the three end members. After calculating proportions, a red triangle will be displayed in the score plot. Check that all non-outlying data points are contained within this triangle. If necessary adjust EMs and recalculate proportions. In addition to the proportions graph, one can plot this triangle as a ternary diagram, by going to the menu and clicking Windows>New>New Ternary Diagram, and then selecting the A, B, and C components as the waves *em1*, *em2*, and *em3* found in the *Results* folder. The value in the box labeled "Select Z Data (for Contour Plot)"can be left as "_none_".

If there are three significant PCs, the data points can be expressed as linear combinations of four EMs. In addition to the PC2 vs. PC1 score plot and the general FORC diagram, a PC3 vs. PC1 score plot and a 3D plot of the score space will be displayed. These additional graphs are intended to help better visualize the three dimensional score space and assist with EM selection. The second score plot contains a cursor (⊞) that controls PC 3 score values, which can only be moved in the vertical direction. The ⊞ cursor moves automatically in the horizontal direction when moving the ⊕ cursor in the first score plot. PC 3 values can also be controlled by manually changing the value in the PC3 box that now appears in the PC2 vs. PC1 score plot. After settling on suitable EMs and calculating proportions, the 3D score plot will be updated with a triangular pyramid whose vertices are the four EMs. Projections of this pyramid will appear in the 2D score plots. Check that all non-outlying data points are contained within this pyramid. An additional 3D

plot of the quaternary mixing diagram is displayed. In this case the pyramid is a regular tetrahedron, with the data points situated at proportional distances from the vertices.

Movie S1. Animation of the 3D PCA space in the case of the quaternary mixture considered in Fig. 10 of the main text.

Movie S2. Animation of the quaternary mixing diagram displayed in Fig. 10b of the main text.

Notes

1. FORC processing software suites can be found at `www.esc.cam.ac.uk/nanopaleomag`