

# DeerStitch and DADeers GUIs

## User Manual

### 1 Introduction

Reference (please cite if package is used): J. E. Lovett, B. W. Lovett and J. Harmer, DEER-Stitch: Combining three- and four-pulse DEER measurements for high sensitivity, deadtime free data, *Journal of Magnetic Resonance*, **223** (2012) 98-106.

The DEER Stitch method has been developed to combat the sensitivity issue of the 4p-DEER method for samples where a short phase memory time ( $T_m$ ) precludes the collection of sufficient data for accurate distance distribution analysis. It combines a 3p-DEER time trace with a short 4p-DEER time trace so as to give good quality deadtime free DEER time traces. This manual expects the user to be proficient in the DEER (PELDOR) experiment. DeerStitch relies on the *epload* function from the EasySpin package to open .dta binary file format from Bruker (see S. Stoll and A. Schweiger, EasySpin, a comprehensive software package for spectral simulation and analysis in EPR, *Journal of Magnetic Resonance*, **177** (2005) 390-403). Thus EasySpin must be installed and a path set to it. Further, DADeers GUI uses distance distributions in a format outputted by the DeerAnalysis program (see G. Jeschke, V. Chechik, P. Ionita, A. Godt, H. Zimmermann, J. Banham, C. R. Timmel, D. Hilger and H. Jung, DeerAnalysis2006 - a comprehensive software package for analyzing pulsed ELDOR data, *Applied Magnetic Resonance*, **30** (2006) 473-498).

DeerStitch and DADeers were written in Matlab R2012a for Mac using GUIDE and released January 2013. This is the April 2013 (1.1) version. DeerStitch/DADeers 1.1 includes a linux/windows version which should display better. To use these simply remove DeerStitch.fig and DADeers.fig and rename DeerStitch-windows-linux.fig as DeerStitch.fig and similar for DADeers.

If problems are encountered when using the programs or if you have comments, suggestions or require further assistance please e-mail janet.lovett@ed.ac.uk.

For flexible working, please set the Matlab path to the downloaded DEERS folder. The GUIs can be initialised by typing their name (either “DeerStitch” or “DADeers”) in the Matlab command line.

### 2 DeerStitch

Figure 1 shows the initial DeerStitch GUI. To start load the 3p DEER and 4p DEER data in .dta/.dsc Bruker format using the interactive buttons. You can change directories to find the data. Once uploaded you will see the real (in-phase) and imaginary (out-of-phase) parts of each dataset. It is recommended that the data is taken such that the imaginary part is zero but this is not always possible and some basic phase correction can be applied in DeerStitch to correct for a (reasonably) constant offset.

The next stage is to check the 3p and 4p DEER parameters. The short names for the parameters are derived from G. Jeschke’s Deer4p pulspel program for running the DEER experiment:

**d1** is the time between the first and the second observer pulses in 4p DEER (named  $\tau_{4a}$  in the DEER-Stitch paper). Default is 400 ns;

**d3** is the deadtime in the experiment, the time between the start time for the  $\pi$  pump pulse and the time that data acquisition starts. Default is 80 ns for 4p DEER and 0 ns for 3p DEER;

**d30** is incremental time for the pump pulse and therefore defines the experimental resolution. Default is 8 ns;

**p0** is the duration of the observer  $\frac{\pi}{2}$  pulse. In G. Jeschke’s Deer4p program this value is the same for both observer pulses. Default is 32 ns;

**p2** is the duration of the pump  $\pi$  pulse. Default is 12 ns;

**dim** is the expected background dimension of the sample. Homogeneous samples will have a 3-dimensional (i.e. exponential) background. Default is 3;

**cut** defines the number of ns of data to remove from the 4p DEER, if required. The “cut” 4p DEER data

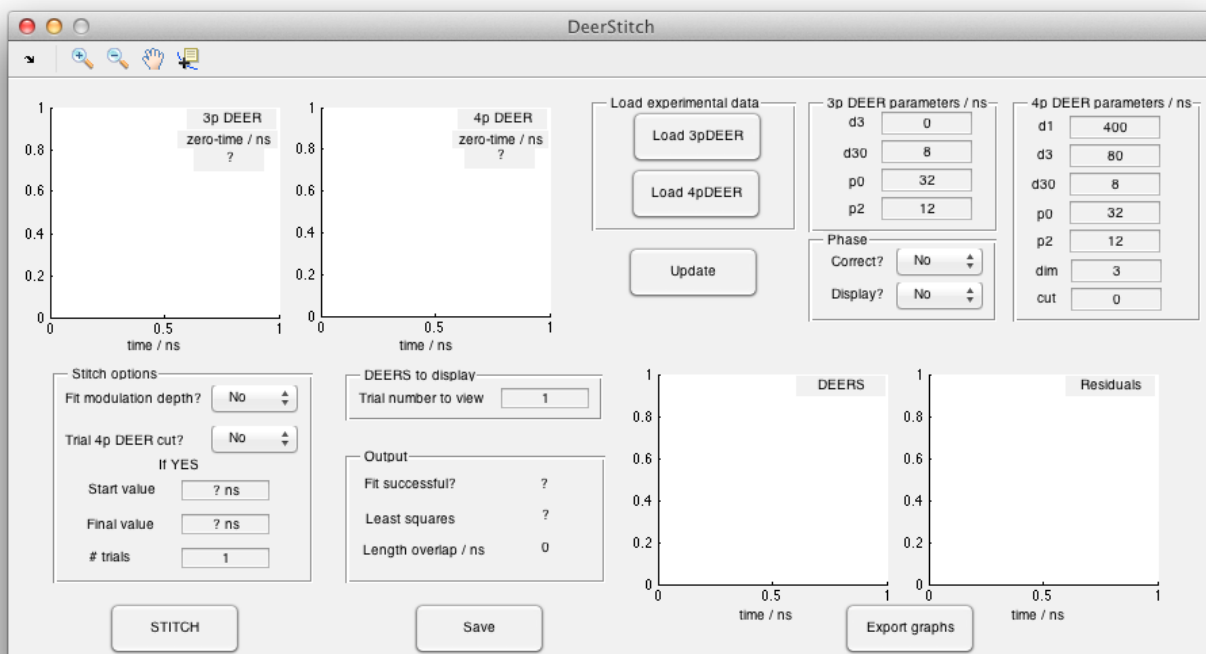


Figure 1: The DeerStitch GUI

will be displayed. Default is 0 ns;

The DEER time traces can be phase corrected if necessary and the imaginary part can either be displayed or hidden. The Stitch procedure does not use the imaginary part.

Once the parameters have been defined the Update button will re-draw the time trace graphs and the calculated zero-time will be displayed. This can be repeated, particularly useful to explore the value of the cut parameter.

The next stage is to define the Stitch options. The modulation depth of the 4p DEER time trace can be fitted to the 3p DEER data by choosing “Yes” from the drop down menu. By choosing to trial 4p DEER cut the 4p DEER time trace will be cut sequentially by the number of ns defined in start value through to the finish value with a step sized determined by the number of trials desired. This will alter the overlap region between the 3p and 4p DEER and thus offer a method for determining the robustness of the resulting DEERS. If the option to trial is not chosen then the cut value from the initial parameters will be used in the Stitch procedure. It is strongly recommended that the the overlap region is tested and that the 4p-DEER is measured to as long as is feasible with good signal-to-noise. The DEER-Stitch paper contains more detail about this procedure.

With options chosen, the STITCH button can be pressed and the Stitch method will be run. The axes labelled DEERS will show four time traces. The first is the overlay of the cut 4p DEER (red) on the 3p DEER (black). The next (green) is a DEERS time trace where only the distorted part of the 3p DEER time trace is replaced (DeerStitch calculates this as  $\frac{p_0}{2} + \frac{p_2}{2} + 8$  ns from the zero-time). The final trace (blue) is the DEERS time trace where the full length of the 4p DEER data replaces the 3p DEER.

The DEERS from the trials can be viewed separately, along with their vital statistics (did the fit converge? what is the least squares value in the 3p and 4p DEER overlap region (for the non-normalized data)? and, what is the length of the overlap?) by inputting a trial number into the DEERS to display panel and pressing carriage return within the Trial number to review box (this needs to be done to see the residuals and other values, even if there was only one Stitch carried out). The DEERS axes now includes the residuals in cyan. The Residuals axes shows a histogram plot of the residuals with normal distribution of equal standard deviation but centred around zero for comparison. If the residuals do not form an approximate normal distribution centred around zero then extra caution should be exercised in interpreting the DEERS time

trace. However, remember that as the overlap region becomes smaller the residuals will naturally become more random. Hence the residuals should be used as a guide along with the stability of the DEERS time traces with altering overlap length.

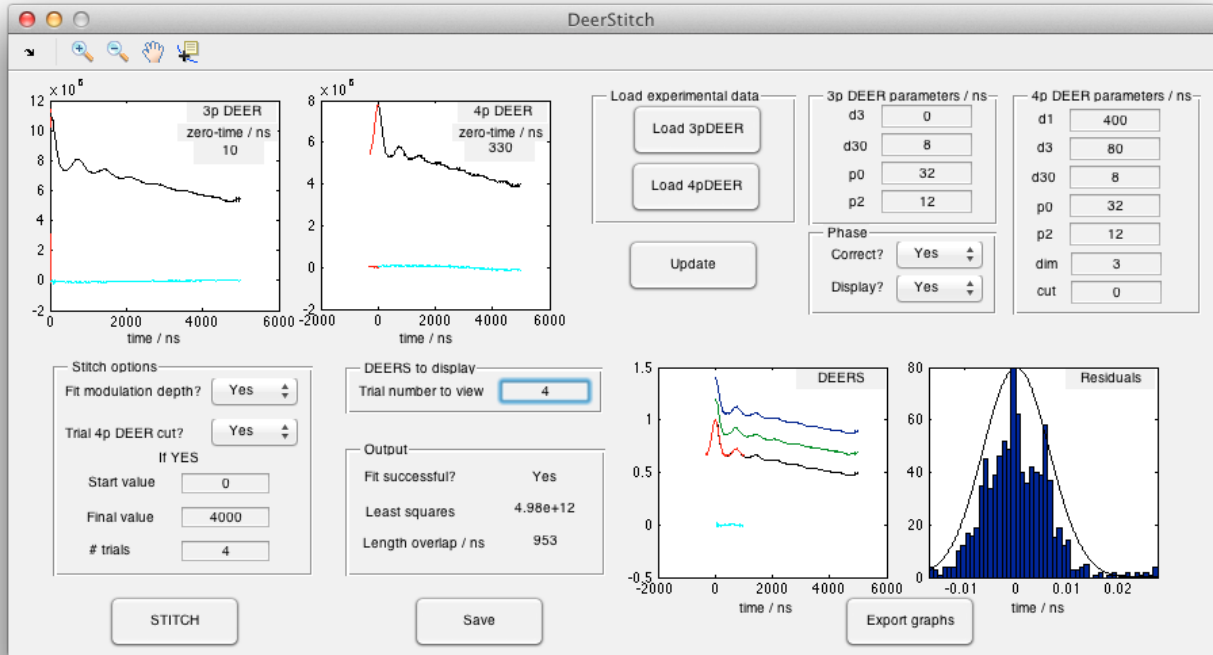


Figure 2: Example of DeerStitch using the data set available in the Examples folder.

Example 3p and 4p DEER data is included in the Example folder and this can be uploaded to demonstrate the effect of changing the parameters, phase correction, modulation depth fitting and trialling the cutting region. This is shown in figure 2

Pressing the Save button will save all trials as separate asciis with set filenames. The desired directory for saving the data can be pointed to during the Save operation but must already exist. The files contain the following (in all cases *ANS* is yes or no to fitting the modulation depth and *NUM* is the number of ns overlap between the 3p and 4p DEER):

*deers\_RepLong\_modfit\_ANS\_ol\_NUMns.txt* - DEERS time trace where the entire length of the 4p DEER has been used to replace the 3p DEER. The imaginary part is zero. This file can be opened by DeerAnalysis;

*deers\_RepShort\_modfit\_ANS\_ol\_NUMns.txt* - DEERS time trace where only the distorted part of the 3p DEER has been replaced by the 4p DEER. The imaginary part is zero. This file can be opened by DeerAnalysis;

*residuals\_modfit\_ANS\_ol\_NUMns.txt* - the residuals between the fitted 4p DEER and the 3p DEER time trace;

*deer4p\_fitted\_modfit\_ANS\_ol\_NUMns.txt* - the fitted 4p DEER time trace;

*deer3p\_modfit\_ANS\_ol\_NUMns.txt* - the 3p DEER time trace starting from the first “undistorted” time point.

The Export Graphs button displays the DEERS time traces and Residuals plots as separate Matlab figures.

### 3 DADeers

It may be convenient to use DeerAnalysis to extract distance information from the DEERS time traces. DADeers is a simple GUI to take results from DeerAnalysis for multiple sets of DEERS data (at least a *\_RepLong\_* and corresponding *\_RepShort\_*) and plot the “background-corrected” time traces and average, maximum and minimum (the latter two referring to intensities) distance distributions. To use this GUI please upload the DEERS time trace files outputted from DeerStitch into DeerAnalysis one at a time. Analyse for a distance distribution in the most appropriate way and save the data using the default settings. In DADeers select whether the modulation depth was fitted in DeerStitch and whether a trial was run for the

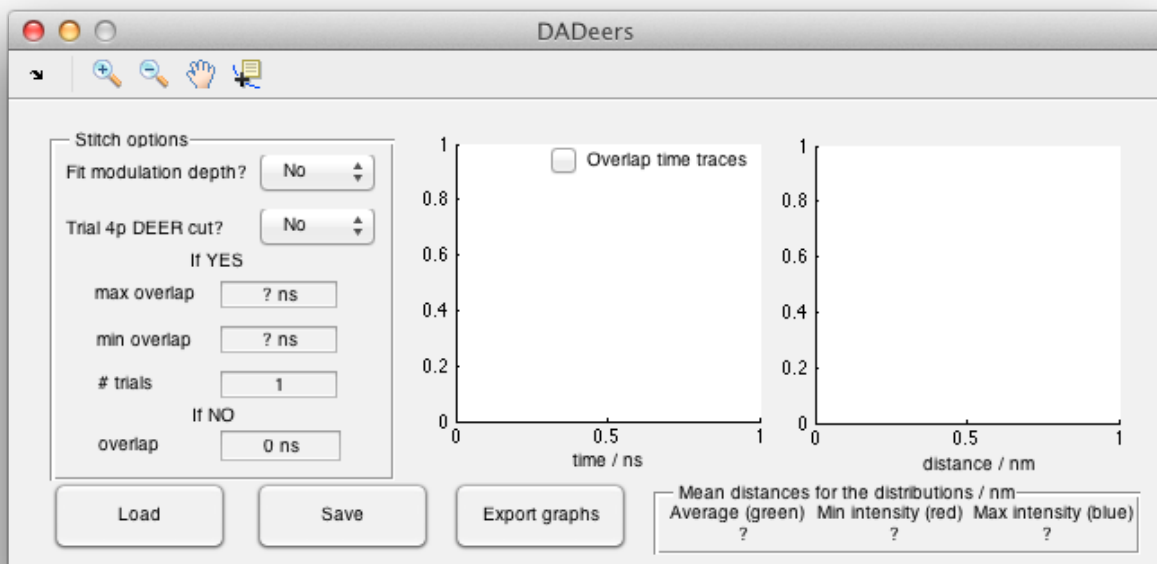


Figure 3: The DADeers GUI

4p DEER cut (i.e. if the trial number was greater than one). If trials were run then fill in the maximum number of ns overlap, the corresponding minimum (these values are in the filenames of the DEERS data) and the number of trials that were run. If the cut value was not varied then simply fill in the number of ns overlap in the bottom editable box. This allows DADeers to read the filenames. Once this information is filled in then the Load button should be pressed. You will be directed to the current directory and you can navigate to the directory containing the results, note that at this point it does not matter which filename you double-click. The time traces and the average, maximum and minimum time traces will be plotted. Additionally the average (mean) distance for the three distance distributions are given at the bottom right. An example is shown in figure 4.

The time traces can be viewed either offset from each other or overlaid by unpicking/ticking the box at the top of the axes. Pressing the Export graphs button will show the two plots as independent figures. The Save button will save the average, maximum and minimum distance distributions in ascii format with the filename you wish.

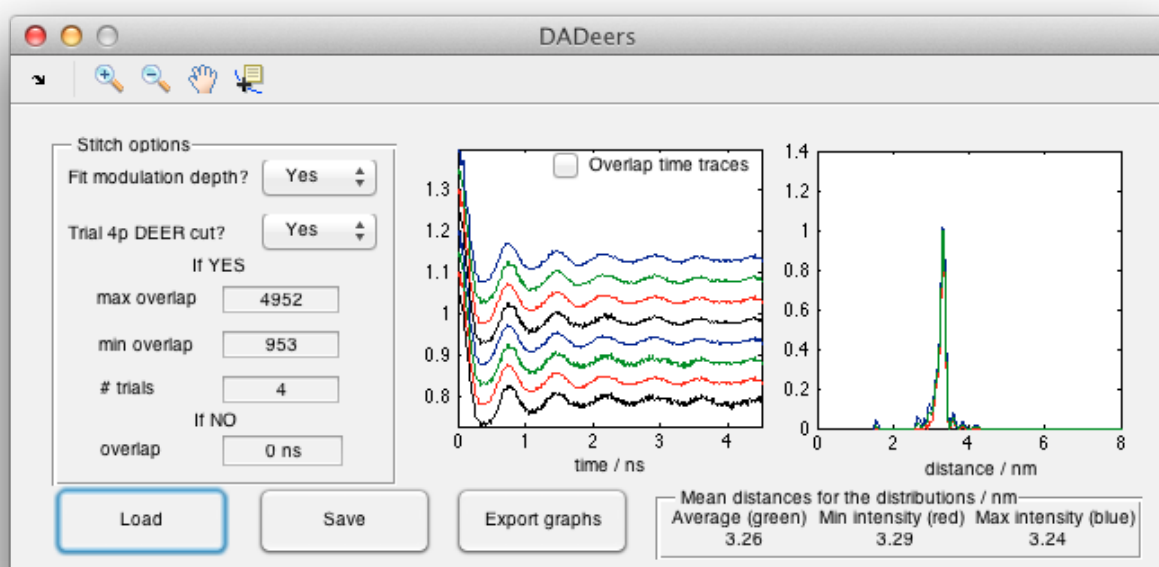


Figure 4: DADeers with processed DEERS files from DeerAnalysis loaded. These results were originally generated from the 3p and 4p DEER data in the Example directory and can be found in the Processed directory.