ScanState

1. Introduction

ScanState is a MATLAB script for live monitoring of a running scan on Bruker ELEXSYS EPR spectrometers. It reads and analyses the Autosave-files generated by the Xepr software. Currently, the key features of the program are:

- Graphical remote live view of the current state of the scan.
- Output of parameters related to the current experiment, e.g. number of remaining scans, runtime of the experiment, predicted finishing time of the experiment. The approximate runtime t_{run} is computed via

  $$\mathbf{t_{run} = SRT \cdot NoP \cdot m \cdot n \cdot PC \cdot h}$$

  where SRT refers to the Shot Repetition Time, NoP to the Number of points recorded in the experiment, m to the steps of nuclear modulation averaging, n to the number of scans to be averaged, PC to the number of steps of the phase cycle, and h to the number of shots per point. All parameters except from m are reserved default parameters and will be extracted automatically from the .DSC file.
- Option to copy the Autosave-files to the local harddisk of the monitoring computer. This is especially useful if intermediate states of the experiment should be analyzed later (e.g. regarding changes of the SNR), or if spectrometer problems occur during the measurement adversely affecting the data quality (software errors, TWT errors, loss of proper tuning, temperature instabilities, e.g. due to shortage of liquid helium etc.).
- Option to export the current state of the scan graphically as image files and as ASCII-files.

2. Requirements

The minimum requirements to run the script are:

- Installation of Matlab ≥ version R2018a.
- Eprload files (eprload.p, eprload.m) distributed with the EasySpin package.[1] These have to be located in the same folder as the Scanstate.m file.
- Remote access to the HDD of the spectrometer computer which has to be accessible as a network drive.
- If the Autosave files are to be copied: sufficient free space on the local HDD (12 hours of logging generates roughly 1.6 GB of files on the HDD).

[1] S. Stoll, A. Schweiger, *J. Magn. Reson.* **2006**, *178*, 42–55. EasySpin can be downloaded at www.easyspin.org

3. Description of the program

As all MATLAB scripts, the program can be started by either clicking the "Run" button in the task bar of MATLAB or by pressing the "F5" key. This opens a window showing the current state of the scan.

At the beginning of the script, a few parameters have to be adapted to the custom settings of the local user. These are

a) General settings

1) pathname: In this string, the path to the acquisition folder on the computer running the Xepr software has to be set. Usually, it is located in the directory "computer:\XeprFiles\Acquisition\", where computer should be replaced by the letter representing the disk of the computer controlling ELEXSYS. Make sure to put a backslash (\) at the end of the path.
2) Updatefrq: This variable sets the period in seconds the script waits between two updates. By default, Xepr generates Autosave files every 60 seconds; however, this value can be changed in Xepr (Acquisition→Autosave Setup).
3) m: Number of modulation averaging steps used in PDS experiments to eliminate ESEEM. This number can be found in the .DSC file and is required for computing the runtime of the experiment. If your experiment does not include modulation averaging, set m=1.
4) Opengl hardwarebasic: This command makes the script use the hardware-accelerated version of OpenGL for graphics rendering, which is by default commented out. Especially if run via the Windows Remote Desktop environment, it may be necessary to uncomment this line in order to properly display the figures.

b) Save settings

If the script should save intermediate states of the scan to your local harddisk, the following parameters are to be set.

1) DestinationPath: Path to the folder in which the copied files should be stored. Make sure to put a backslash (\) at the end of the path.
2) Savemode (0, 1, 2): Sets the mode for saving the files to the local HDD.
   0: No files will be stored on the HDD.
   1: Only the last file of each scan will be stored on the HDD. If a single scan takes longer than the value set for Updatefrq, only the last file corresponding to each number of scans will be saved and the files will be called AUTOSAVE_1, AUTOSAVE_2, etc. This is especially useful for PELDOR experiments involving modulation averaging and several (hundreds of) scans.
   2: Every intermediate slice will be stored, and the files will be called AUTOSAVE_0_Date_Time etc. This is especially useful for long DQC/SIFTER/RIDME experiments involving time consuming phase cycling procedures, but only a few averages.
3) Figsave (0, 1, 2): Determines whether the script saves image files of the current state of the scan and copies them into the DestinationPath folder. It is coupled to the Savemode setting.
   0: No image files will be saved.
   1: Image files will be saved with the setting taken from Savemode.
   2: Image files without the textbox will be saved with the setting taken from Savemode.
4) datsave (0, 1): Determines whether the script saves ASCII-files of the current state of the scan and copies them into the DestinationPath folder. It is coupled to the Savemode setting.
   0: No ASCII-files will be saved.
   1: ASCII-files will be saved with the setting taken from Savemode.