

Software from National Biomedical Center for Advanced ESR Technology[†]

ACERT – Jack H. Freed

This folder contains the ACERT software for simulation and analysis of ESR spectra. It includes:

1. Original versions of well-known programs described in the papers
"Calculating Slow Motional Magnetic Resonance Spectra: A User's Guide" by D.J. Schneider and J.H. Freed. Spin Labeling: Theory and Applications, Vol. III, *Biological Magnetic Resonance* **8**, 1-76 (1989) (Plenum, NY) and
"Nonlinear Least-Squares Analysis of Slow-Motional EPR Spectra in One and Two Dimensions Using a Modified Levenberg-Marquardt Algorithm" by David E. Budil, Sanghyuk Lee, Sunil Saxena and Jack H. Freed. J. Magn. Reson. A120, 155-189 (1996) and their most recent updates:
EPRL, PC, NLSL, PC.NEW, NL2DR, NL2DC
2. Basic programs for CW spectral fitting using the SRLS model as described in *"An Assessment of the Applicability of Multifrequency ESR to Study the Complex Dynamics of Biomolecules"*, Z. Liang and J.H. Freed, J. Phys. Chem. B, 103, 6384-6396 (1999): **NLSL.SLRS**
3. Software for Tikhonov regularization (TIKR) and maximum entropy (MEM) methods. The software was developed to extract pair distributions from pulsed ESR experiments. See: *"The Determination of Pair Distance Distributions by Pulsed ESR Using Tikhonov Regularization"* by Y.-W. Chiang, P.P. Borbat, and J.H. Freed, J. Magn. Reson. **172**, 279-295 (2005) and *Maximum Entropy: "A Complement to Tikhonov Regularization for Determination of Pair Distances Distributions by Pulsed ESR"* by Y.-W. Chiang, P.P. Borbat, and J.H. Freed, J. Magn. Reson. **177**, 184-196(2005): **PD_Tikhonov_pkg, DPD_pkg**

The programs are contained in the following subdirectories:

[EPRL](#) - the basic simulation programs for CW spectrum calculation including the program EPRL used to determine the truncated basis sets. A detailed description of the method and Version 1.0 of the program is given in the "User's guide" by Schneider and Freed (1989). See file UPDATE.DOC for cumulative changes through Version 1.6b that have been made in EPRL and related programs since the publication of Version 1.0.

[PC](#) - the original PC version of the CW spectrum simulation programs. (11/3/95).

[NLSL](#) - the least squares version of the above CW program described by Budil et al. (1996). See the subdirectory EXAMPLES for fitting examples to test.

[PC.NEW](#) - a version of the NLSL programs suitable for running on a PC with WINDOWS 98/2000/NT/XP. Besides executables and calculation examples the folder contains files, which are necessary for Fortran Powerstation 4.0 to compile and link the source files from [NLSL](#) folder. See README.TXT in this directory.

[NL2DC](#) - Contains the two-dimensional Fourier Transform (2D-FT) version of the least squares program using the conjugate gradients matrix solution method. For 2D basis set pruning see the subdirectory BASIS in NL2DR.

[NL2DR](#) - Contains the 2D-FT version of the least squares program using the Rutishauser matrix solution method. For 2D basis set pruning see the subdirectory BASIS.

The programs source codes for both **NL2DC** and **NL2DR** are designed for running under **LINUX**. They are stored in uncompressed format and may be obtained by ASCII ftp transfer. Tar files are provided for compressed data transfer and contain all files in the specific directories and subdirectories except the executables to save space.

READ.ME files are provided in each of the above directories giving further information on their contents and usage.

[NLSL.SRLS](#) contains the basic programs for CW spectral fitting using the SRLS model as described by Liang and J.H. Freed (1999). **NLSL.SRLS** is the fitting program, and **ESRBS.SRLS** is used to prune the basis set. **LBSR.SRLS** is for inputting all the parameters used in an **ESRBS.SRLS** calculation.

[PD_Tikhonov_pkg](#) package, includes all necessary functions required to extract the pair distributions from pulsed ESR experiments using the Tikhonov regularization method. MATLAB version 6.5 or higher is required to perform the task. PD_Tikhonov_pkg requires the use of the Regularization Toolbox package obtainable from the website: <http://www2.imm.dtu.dk/~pch/Regutools/index.html>. The toolbox is well documented with a detailed manual and illustrated with numerous examples. We strongly suggest users should first get acquainted with

the Regularization Toolbox. After un-zipping the package, please read **README.pdf** file.

[DPD_pkg](#) package, includes all necessary functions required to perform Tikhonov regularization (TIKR) method and maximum entropy method (MEM) to extract the pair distributions from pulsed ESR experiments. DPD_pkg can be considered an upgraded version of PD_Tikhonov_pkg package since both TIKR and MEM are included in the package. MATLAB version 6.5 or higher is required to perform the task. DPD_pkg requires the use of the Regularization Toolbox package obtainable from the website: <http://www2.imm.dtu.dk/~pch/Regutools/index.html> and which is very well documented with a manual and illustrated with numerous examples. We strongly suggest users should first get acquainted with the Regularization Toolbox. After un-zipping the package, please read **PD_demo.m** file.

Every effort has been made to ensure that these programs are correct and thoroughly tested. However, the programs are distributed "AS IS", and all warranties, whether expressed or implied, as to correctness or fitness for any specific purpose are specifically disclaimed. In no event shall the authors be liable for any direct, consequential or incidental damages arising from the use of these programs. Free use and distribution of these programs is permitted with suitable reference to the original publication (see above) in any published work resulting from the use of these programs or programs derived from them. The programs may be copied and distributed, so long as, 1) due credit is given by retaining the comment lines at the beginning of each source file in all copies; and 2) all copies must be distributed free of charge.

Questions and comments may be directed to ACERT at acert@cornell.edu, which will forward the correspondence to the most appropriate person.

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