

DEER analysis report on dataset DEER_t109C_S500C_d20_MTSL_EMCV_na t_d2_14us_110scsc_spec

**DEERNet Spinach SVN Rev 5662 and DeerLab
0.9.1 Tikhonov regularization**

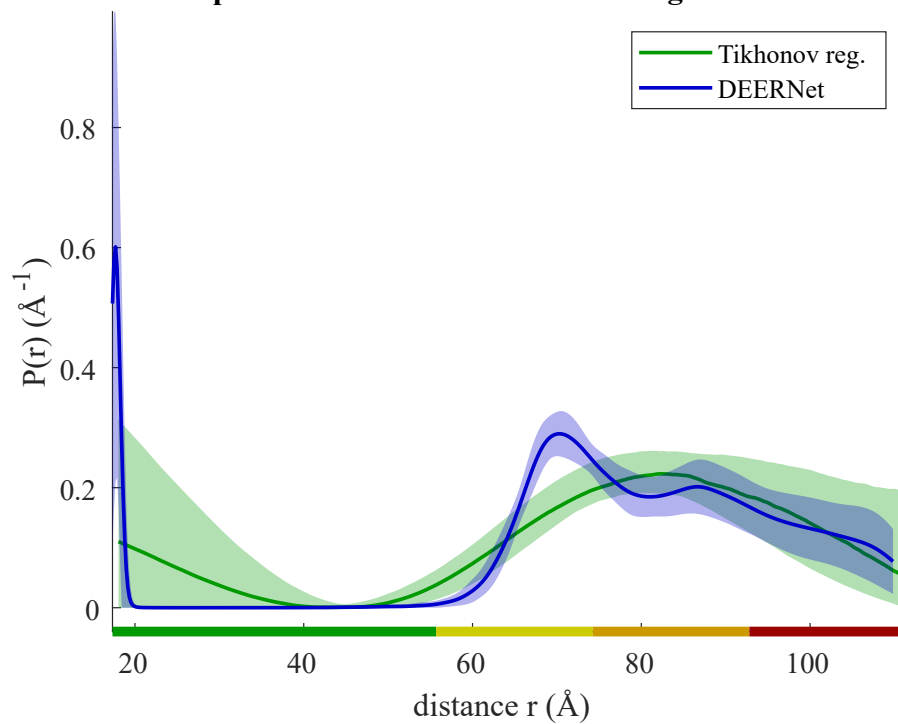
ComparativeDEERAnalyzer version 2.0

see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/
mr-1-209-2020

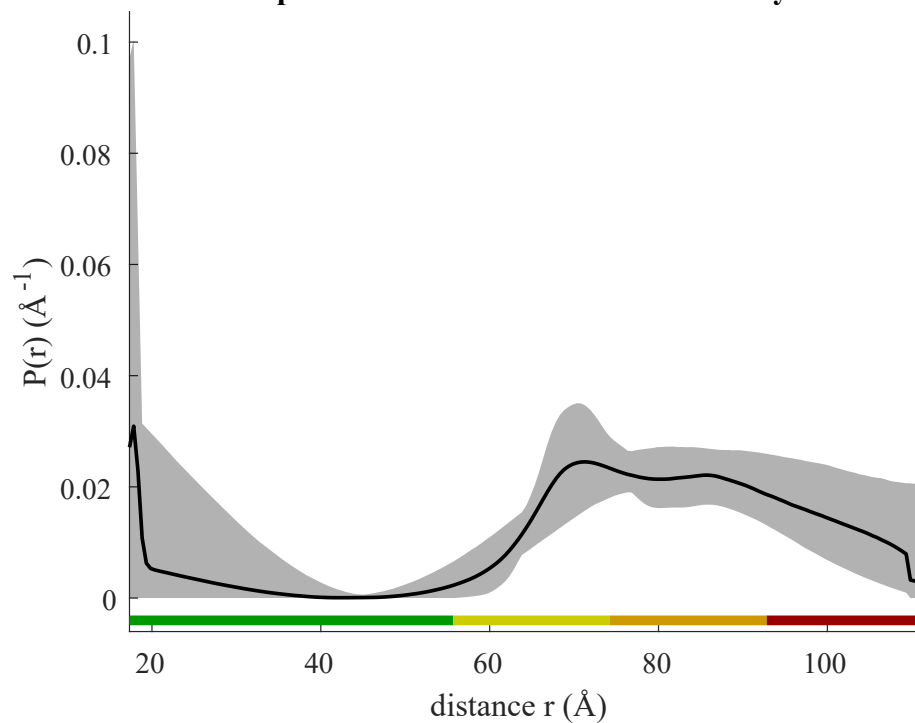
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1. Distance distributions

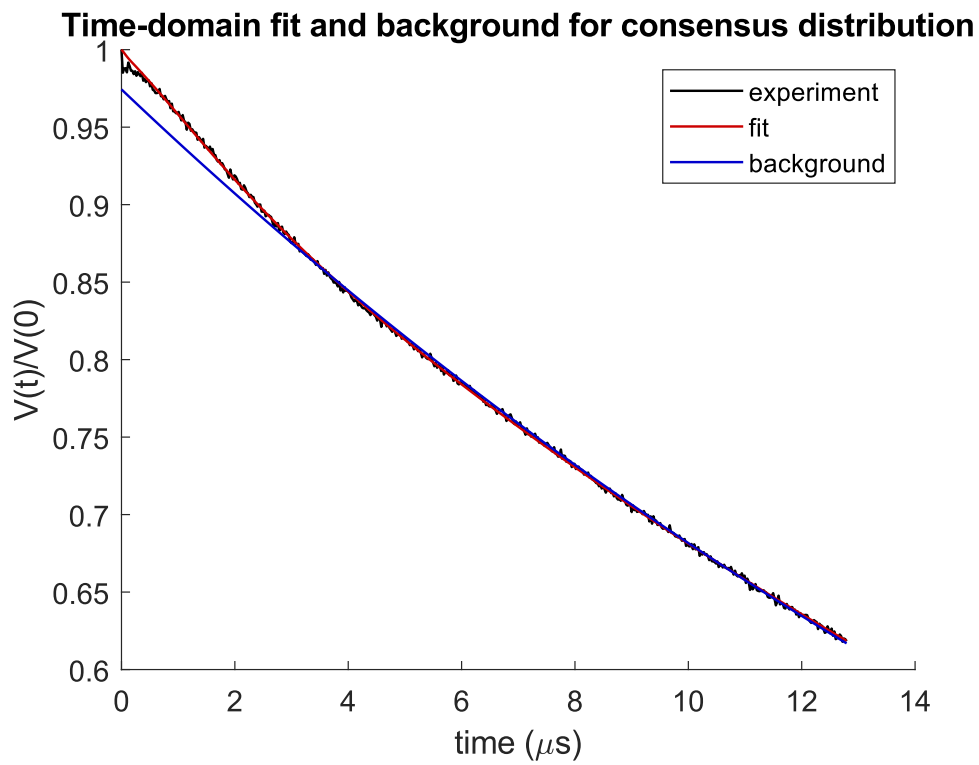
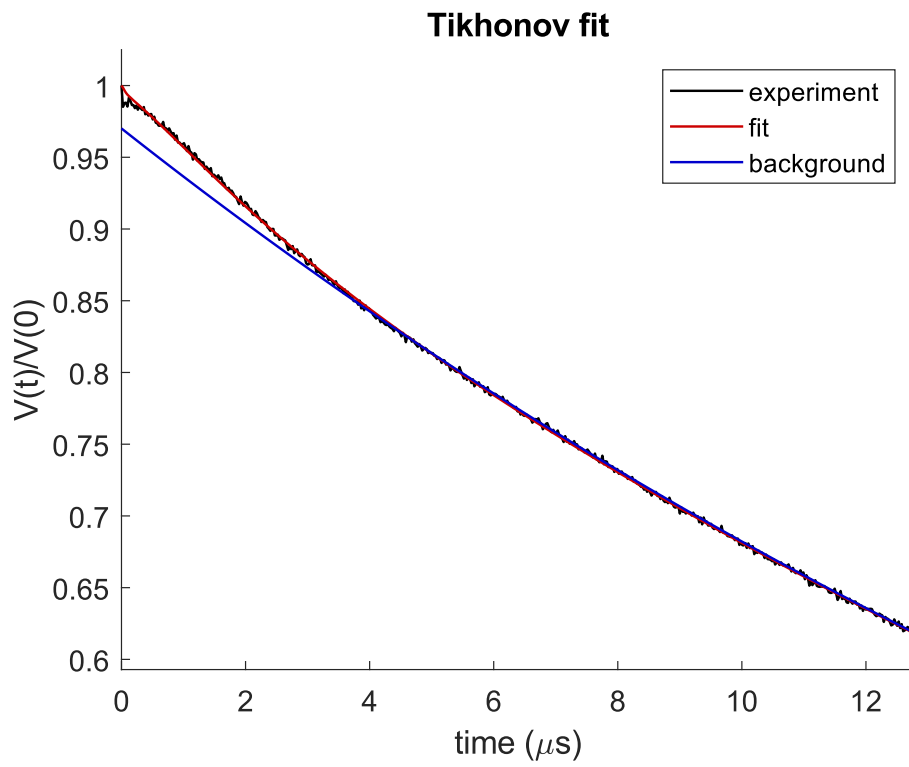
Overlap between neural network and regularization



Comparative distribution and uncertainty



2. Fits of time-domain data



3. Experimental and processing parameters

Please consider improving signal-to-noise ratio (below 20)

DEERNet background not provided, as it was considered unreliable.

Modulation depth: 0.026

Signal-to-noise ratio: 15.9 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00782

From Tikhonov fit: 0.00194

Zero time: 0 ns

Maximum time: 12792 ns

The last 7 % of the data was cut off

Time increment: 24 ns

Phase: -1.1 degree

Ensemble of 32 neural networks

Background separation by DeerLab bilevel optimization

Background dimension: 3

Regularization parameter by best overlap with neural network solution

Regularization parameter used: 50.48

Reg. par. initial estimate by lr: 6.31

Overlap between DEERNet and regularization solutions: 0.822

Predicted overlap of consensus solution with ground truth: 0.70...0.87

Mean distance: 82.2 Å

Distance standard deviation: 16.5 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_t109C_S500C_d2O_MT
SL_EMCV_nat_d2_14us_110scsc_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_t109C_S500C_d2O_MT
SL_EMCV_nat_d2_14us_110scsc_spec_consensus_DEER_distribution.csv

3. Experimental and processing parameters

Fit and background in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_t109C_S500C_d2O_MT
SL_EMCV_nat_d2_14us_110scsc_spec_consensus_DEER_fit.csv

Metadata:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_t109C_S500C_d2O_MT
SL_EMCV_nat_d2_14us_110scsc_spec_comparative_DEER_meta_data.csv