DEER analysis report on dataset DEER_complex_EMCV_DtoF_T109_Q235_IAproxyl_new_26uM_spec

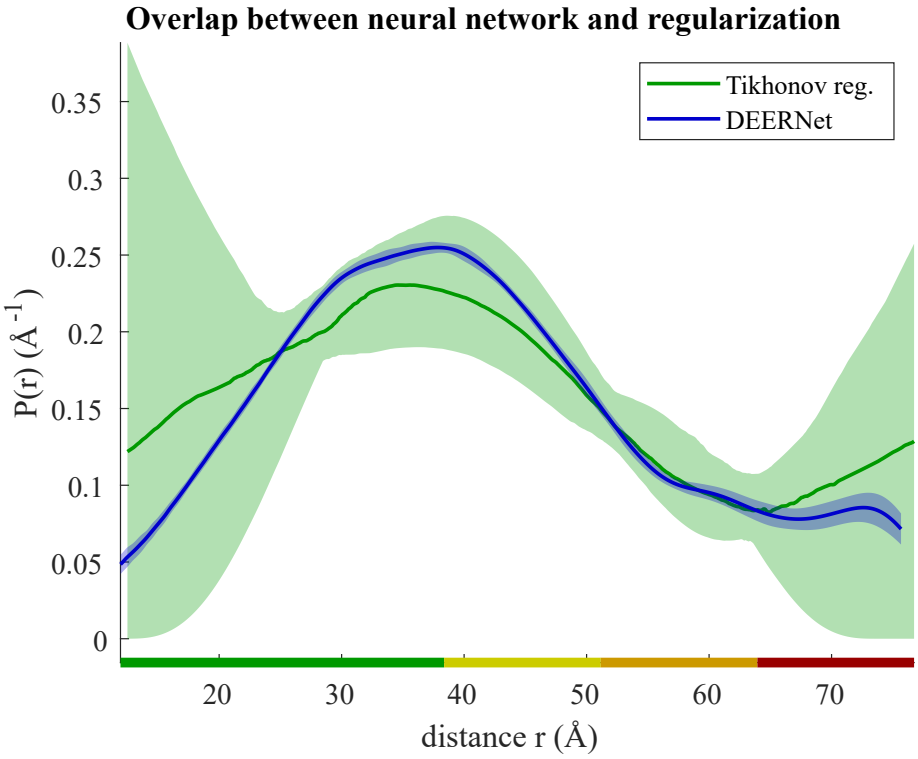
DEERNet Spinach SVN Rev 5662 and DeerLab 0.9.1 Tikhonov regularization

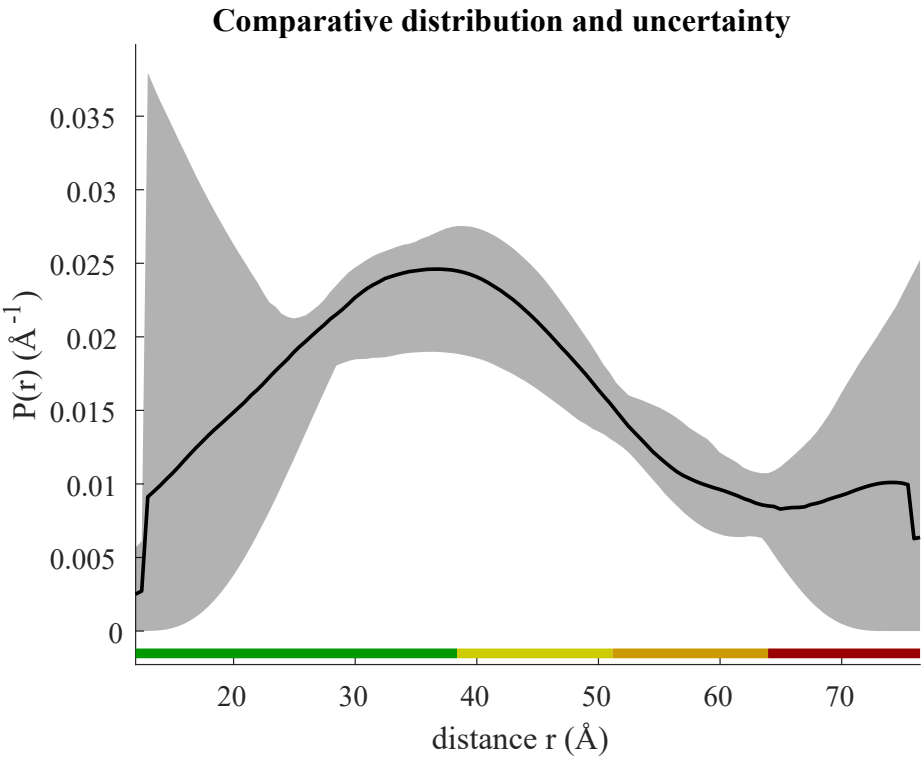
ComparativeDEERAnalyzer version 2.0

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

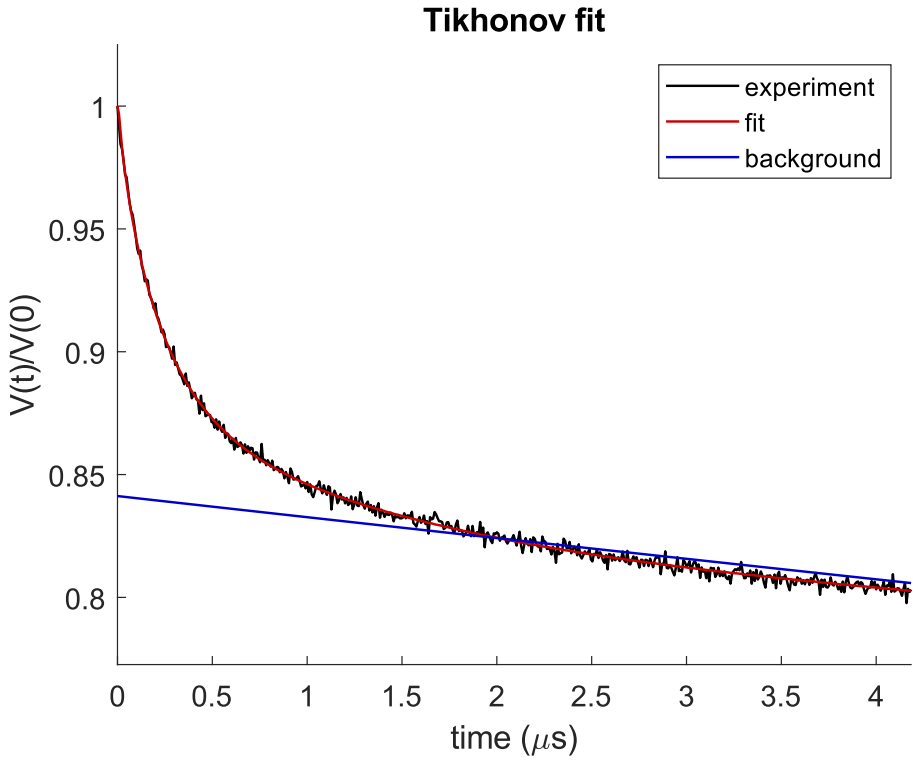
24-Feb-2022 10:51:19

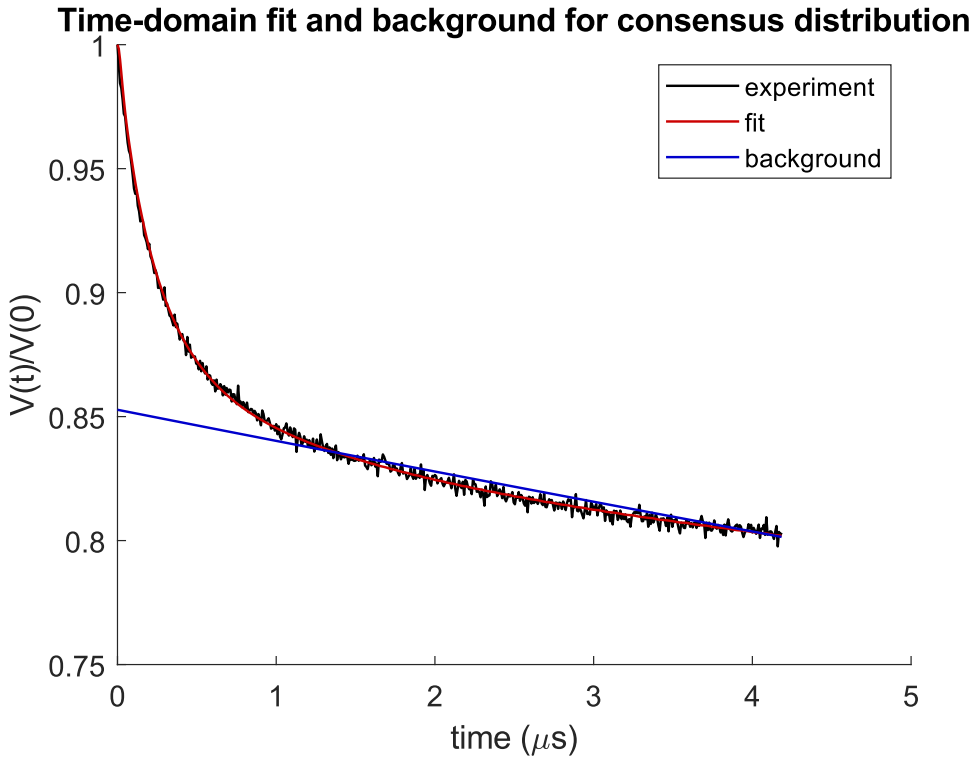
1. Distance distributions





2. Fits of time-domain data





3. Experimental and processing parameters

DEERNet background not provided, as it was considered unreliable.

Modulation depth: 0.147

Signal-to-noise ratio: 74.4 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00256

From Tikhonov fit: 0.00203

Zero time: 121 ns

Maximum time: 4184 ns

The last 11 % of the data was cut off

Time increment: 8 ns

Phase: -0.3 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: 56.57

Reg. par. initial estimate by lr: 10.00

Overlap between DEERNet and regularization solutions: 0.930

Predicted overlap of consensus solution with ground truth: 0.80...0.97

Mean distance: 40.9 Å

Single Gaussian provided different mean distance. Distribution may be incomplete.

Distance standard deviation: 16.0 Å

Full data set in Matlab format:
G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_complex_EMCV_DtoF_T109_Q235_IAproxyl_new_26uM_spec_comparative_DEER_analysis.mat

Distance distributions in text format:
G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_complex_EMCV_DtoF_T109_Q235_IAproxyl_new_26uM_spec_consensus_DEER_distribution.csv

Fit and background in text format:
G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_complex_EMCV_DtoF_T109_Q235_IAproxyl_new_26uM_spec_consensus_DEER_fit.csv

Metadata:
G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_complex_EMCV_DtoF_T109_Q235_IAproxyl_new_26uM_spec_comparative_DEER_meta_data.csv