

DEER analysis report on dataset DEER_71_205_MTSL_EMCV_d2_12us_spec

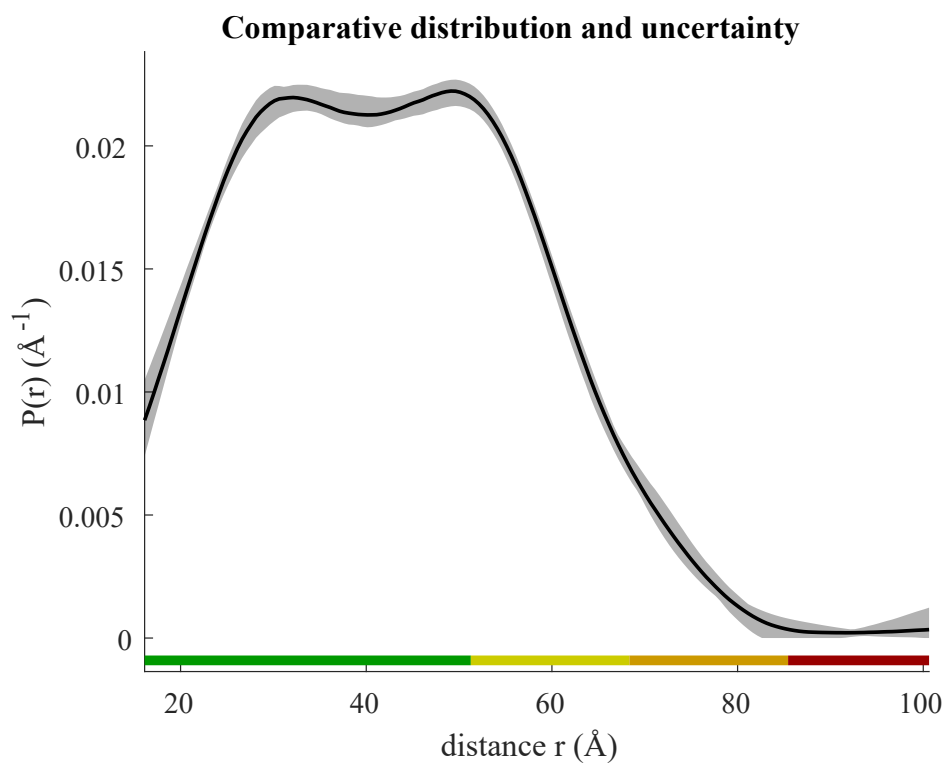
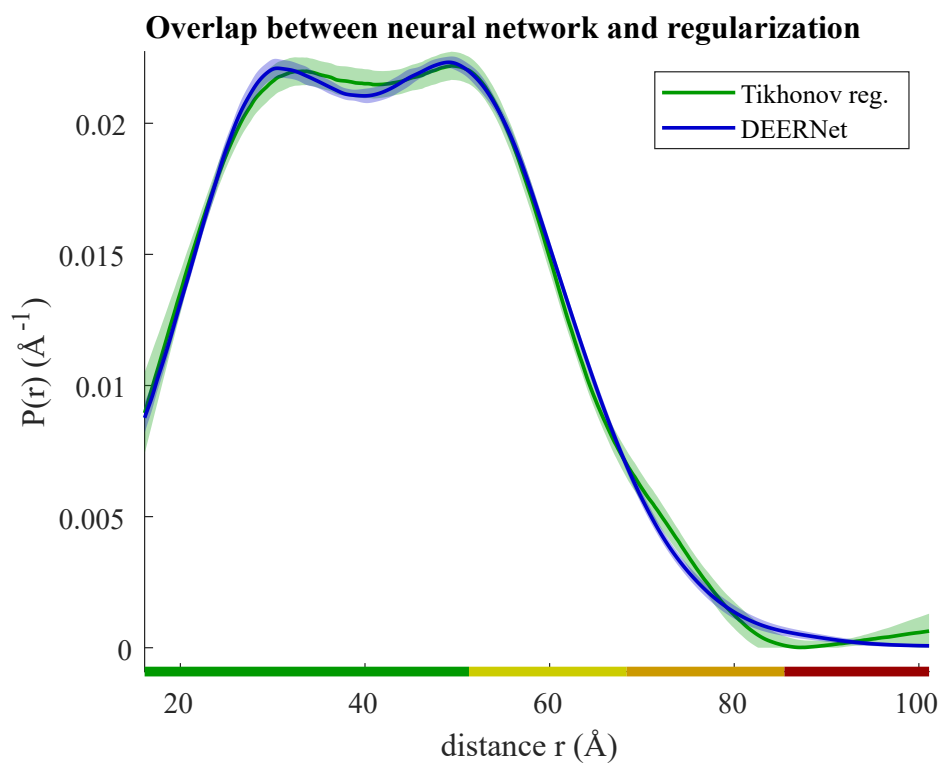
**DEERNet Spinach SVN Rev 5662 and DeerLab
0.9.1 Tikhonov regularization**

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

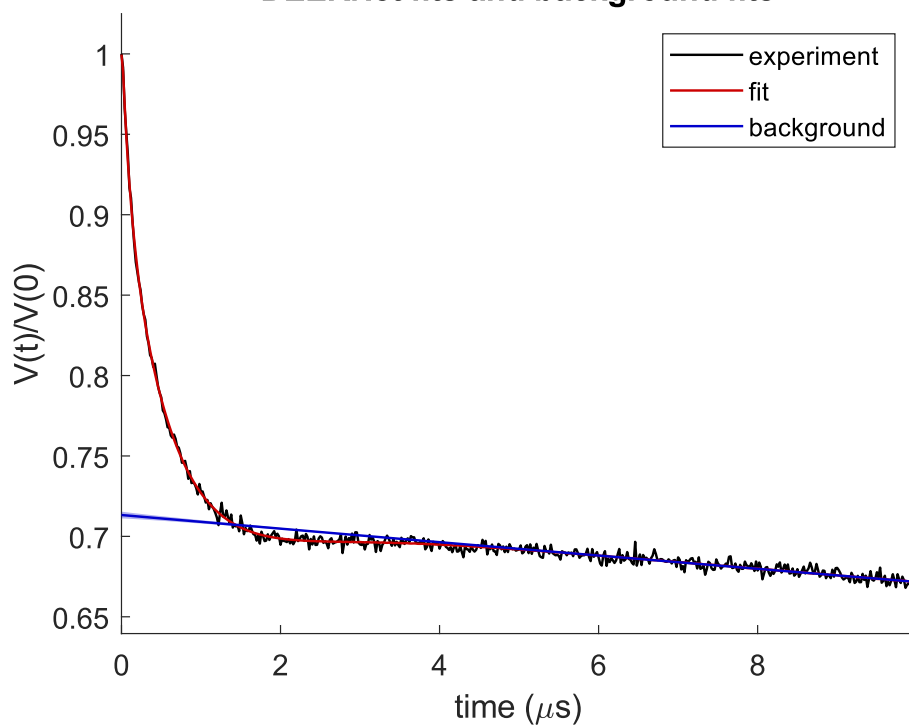
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1. Distance distributions

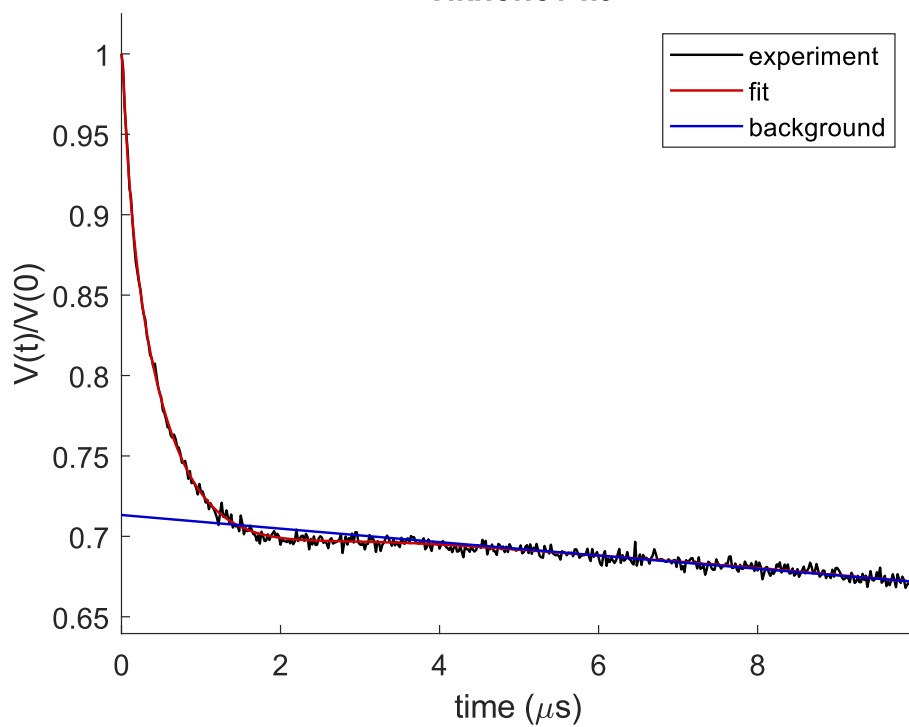


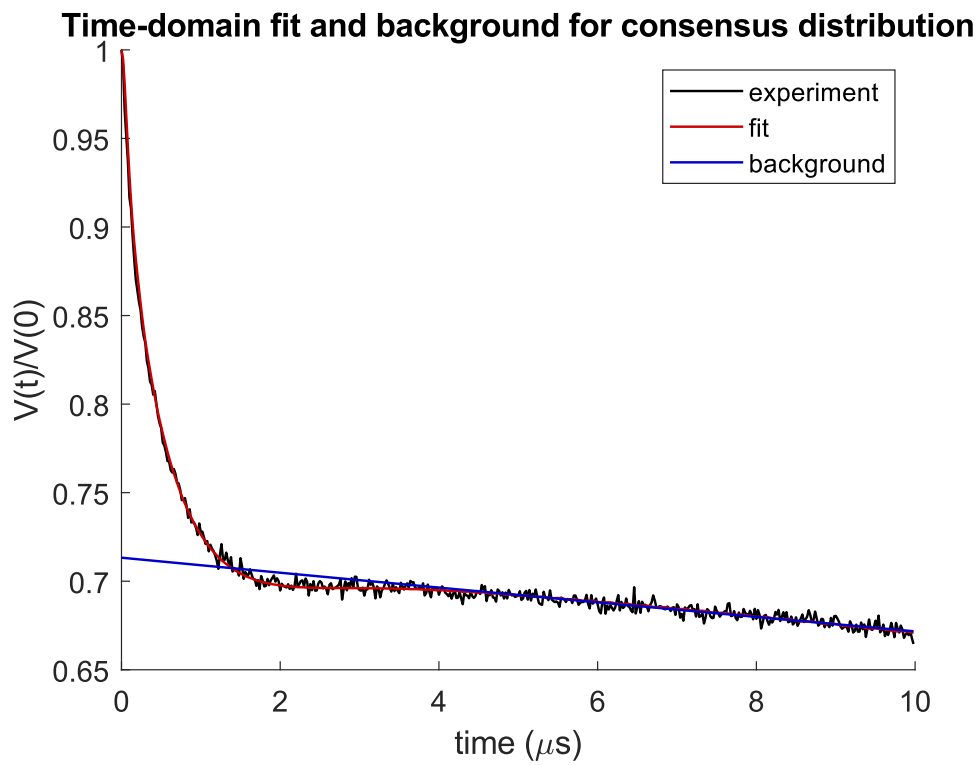
2. Fits of time-domain data

DEERNet fits and background fits



Tikhonov fit





3. Experimental and processing parameters

Modulation depth: 0.286

Signal-to-noise ratio: 104.3 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00667

From DEERNet fit: 0.00275

From Tikhonov fit: 0.00316

Zero time: 126 ns

Maximum time: 9980 ns

The last 14 % of the data was cut off

Time increment: 20 ns

Phase: 20.2 degree

Ensemble of 32 neural networks

Background separation by neural network

Background dimension: 3

Regularization parameter by best overlap with neural network solution

Regularization parameter used: 19.86

Reg. par. initial estimate by L-curve corner: 79.43

Overlap between DEERNet and regularization solutions: 0.986

Predicted overlap of consensus solution with ground truth: 0.85...1.00

Mean distance: 38.8 Å

Distance standard deviation: 18.6 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_205_MTS�_EMCV_d
2_12us_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_205_MTS�_EMCV_d
2_12us_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_71_205_MTSL_EMCV_d
2_12us_spec_consensus_DEER_fit.csv

Metadata:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_205_MTSL_EMCV_d
2_12us_spec_comparative_DEER_meta_data.csv