

DEER analysis report on dataset DEER_Q235C_S475C_IA_EMCV_in_D2O_d 2_14us_spec

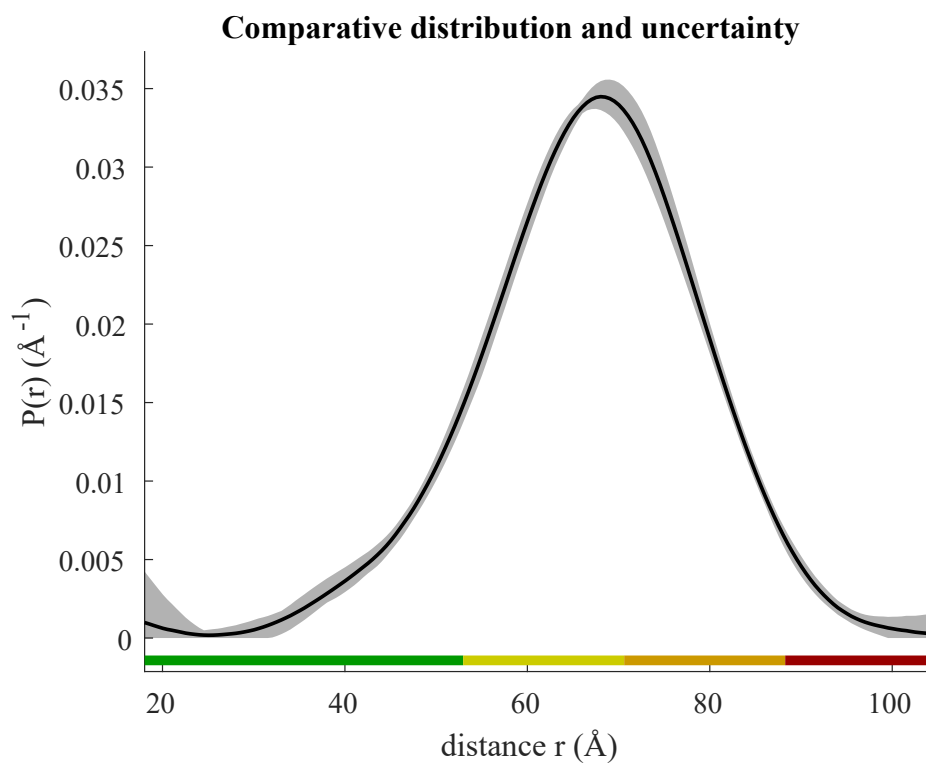
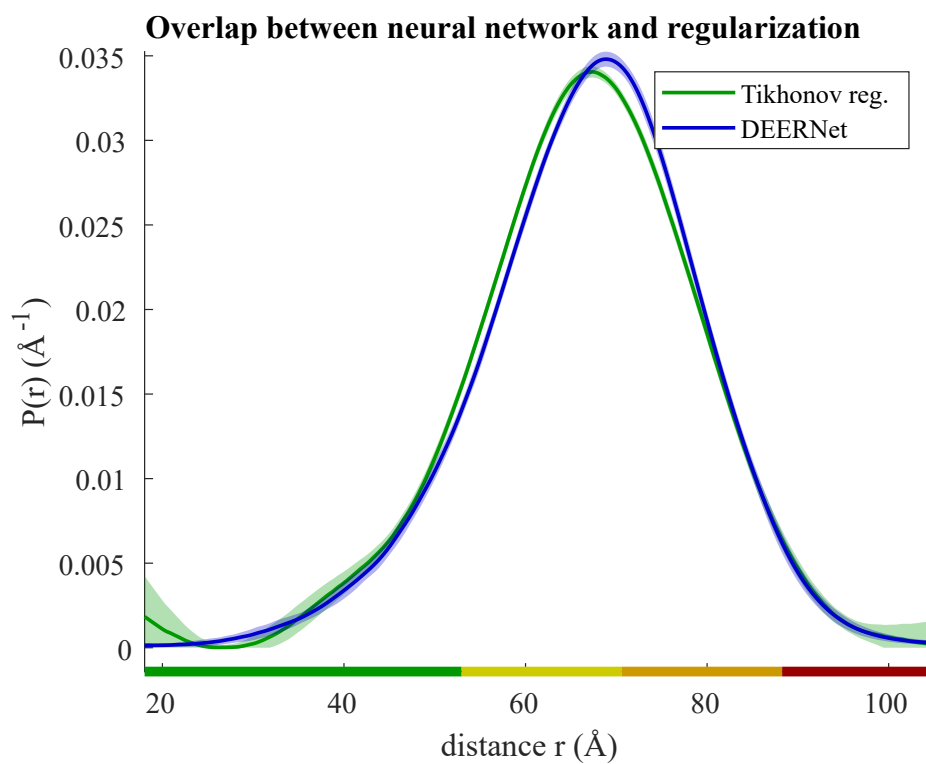
**DEERNet Spinach SVN Rev 5662 and DeerLab
0.9.1 Tikhonov regularization**

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

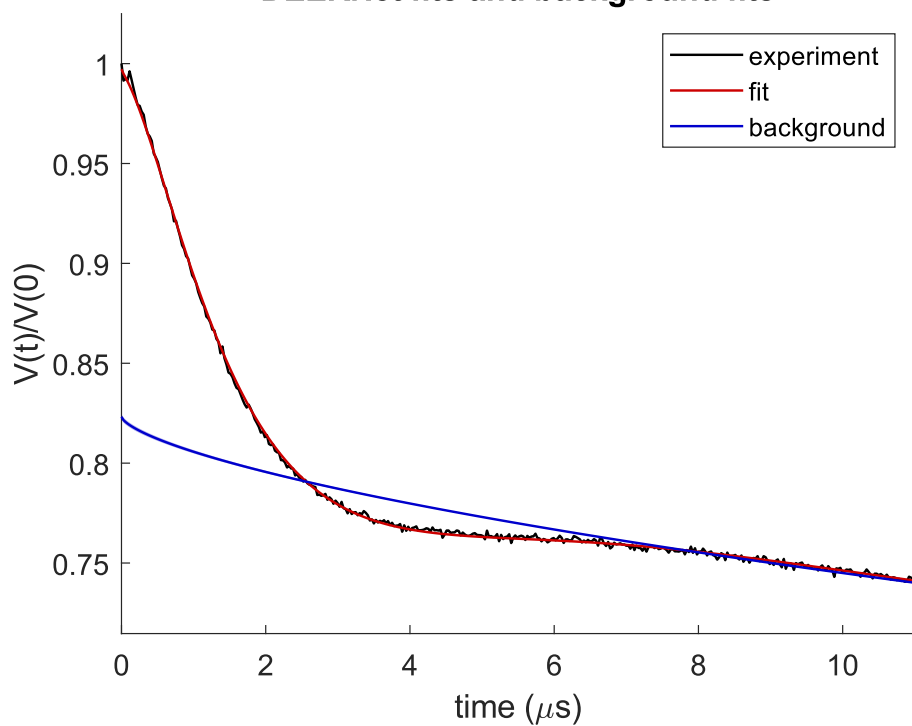
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1. Distance distributions

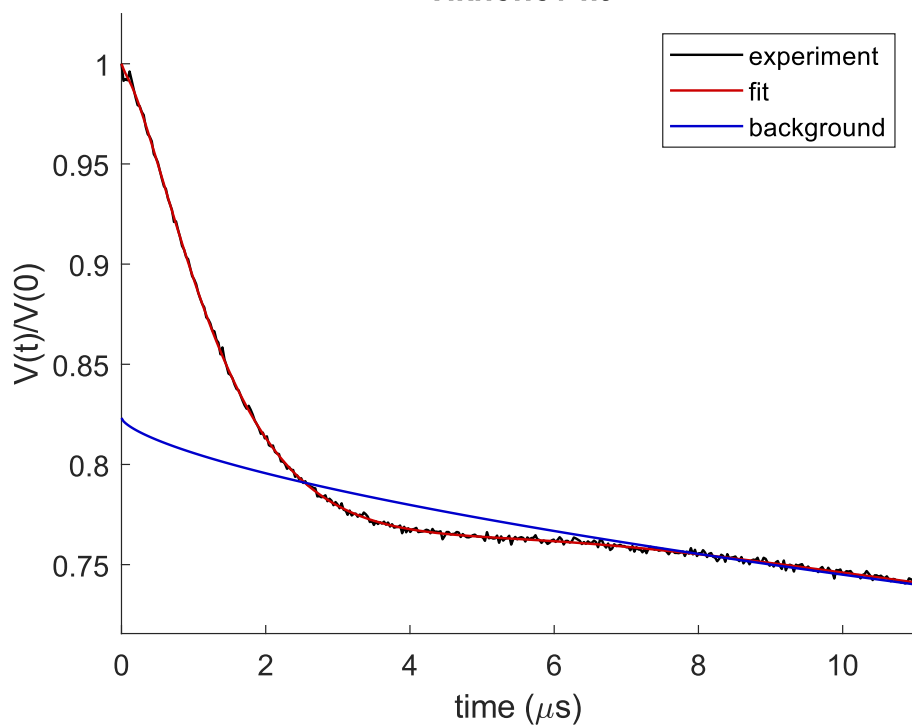


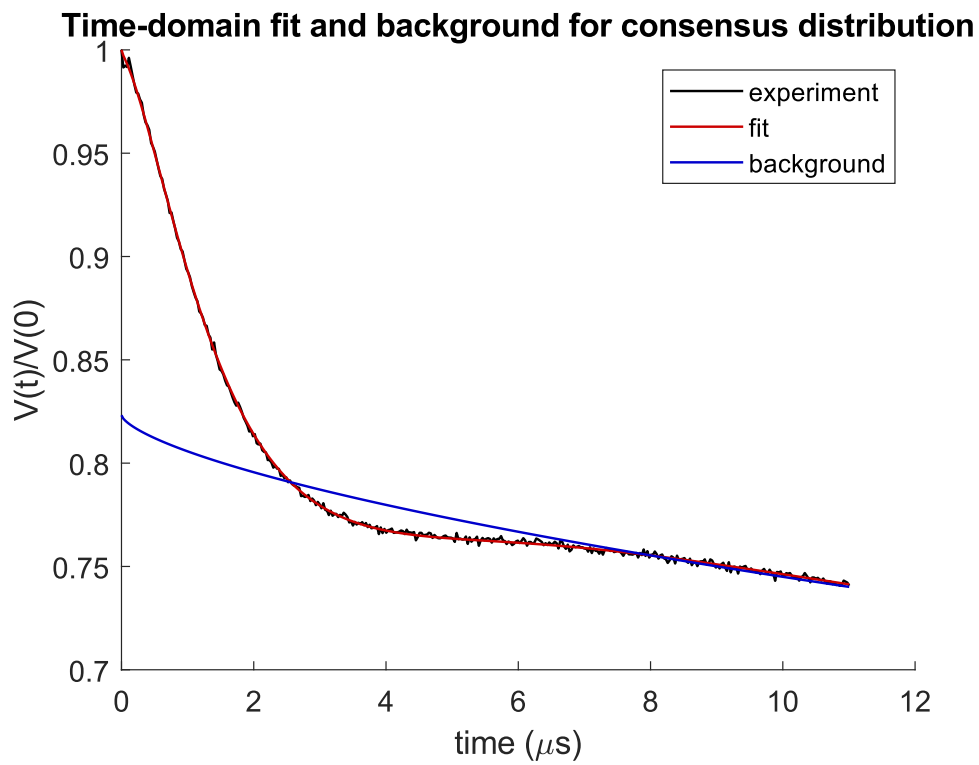
2. Fits of time-domain data

DEERNet fits and background fits



Tikhonov fit





3. Experimental and processing parameters

Modulation depth: 0.175

Signal-to-noise ratio: 121.2 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00146

From DEERNet fit: 0.00144

From Tikhonov fit: 0.00122

Zero time: 0 ns

Maximum time: 11004 ns

The last 21 % of the data was cut off

Time increment: 28 ns

Phase: 29.2 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: 11.18

Reg. par. initial estimate by L-curve corner: 31.62

Overlap between DEERNet and regularization solutions: 0.969

Predicted overlap of consensus solution with ground truth: 0.83...1.00

Mean distance: 66.8 Å

Distance standard deviation: 11.9 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q235C_S475C_IA_EMC
V_in_D2O_d2_14us_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q235C_S475C_IA_EMC
V_in_D2O_d2_14us_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_Q235C_S475C_IA_EMCV_in_D2O_d2_14us_spec_consensus_DEER_fit.csv

Metadata:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q235C_S475C_IA_EMCV_in_D2O_d2_14us_spec_comparative_DEER_meta_data.csv