

DEER analysis report on dataset DEER_Q152C_Q235C_MTSL_EMCV_d2_6u s_spec

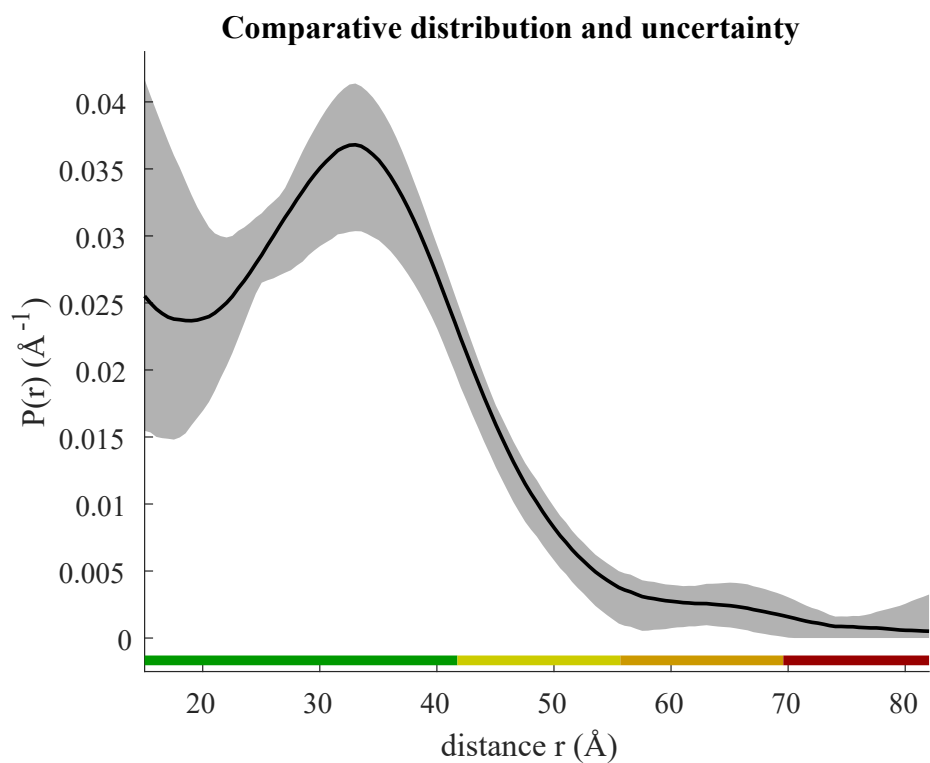
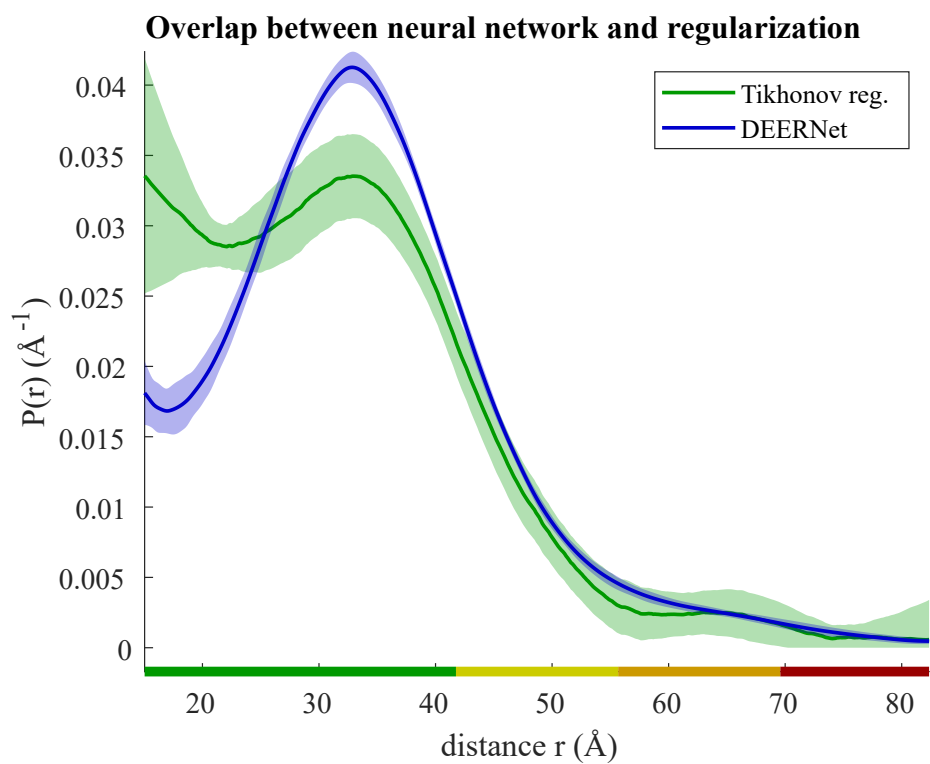
**DEERNet Spinach SVN Rev 5662 and DeerLab
0.9.1 Tikhonov regularization**

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

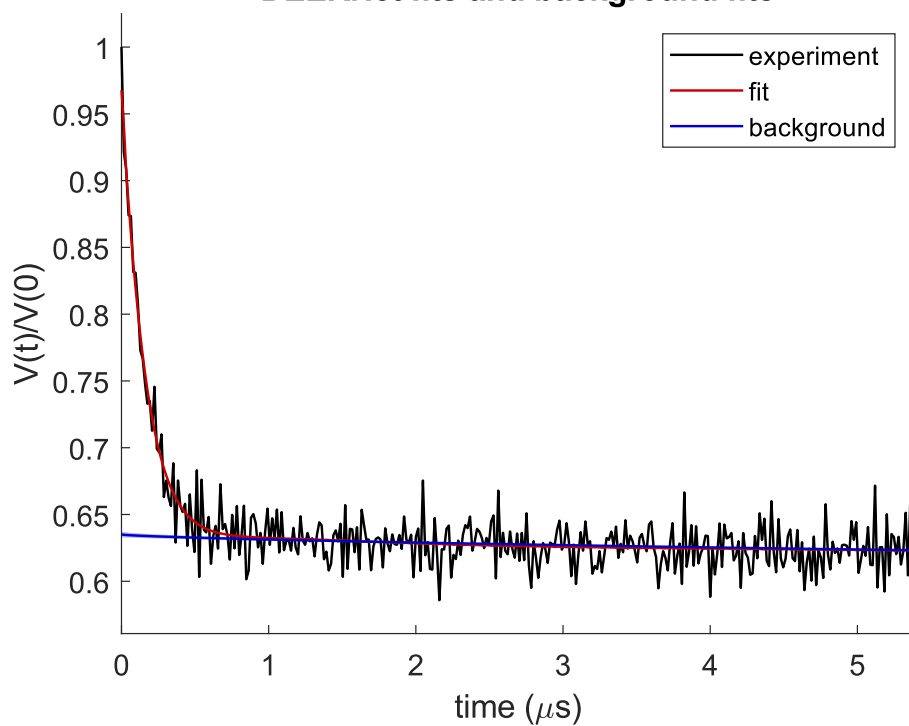
24-Feb-2022 08:34:57

1. Distance distributions

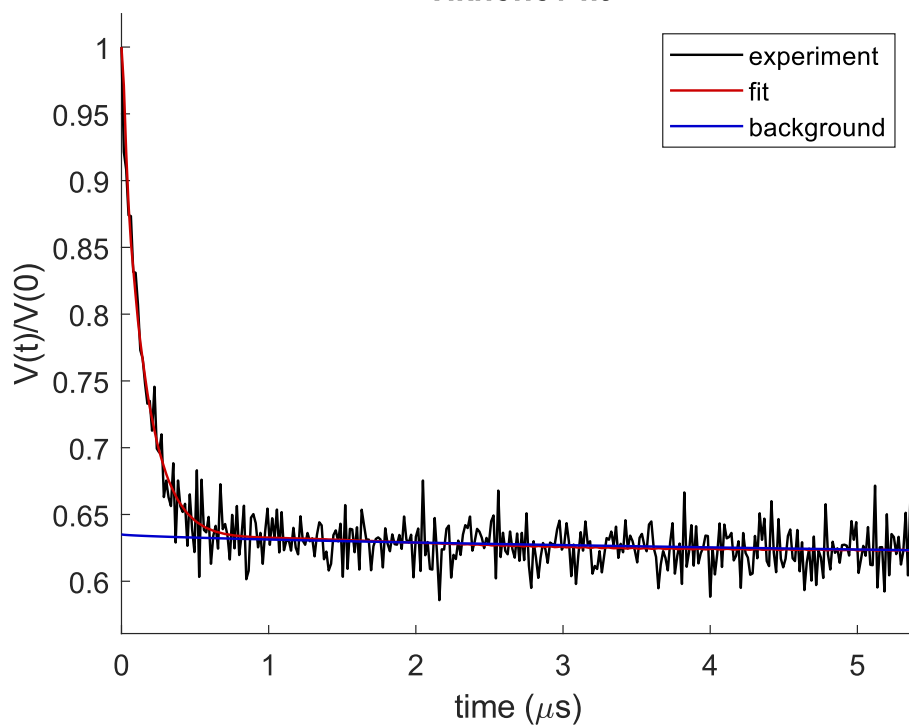


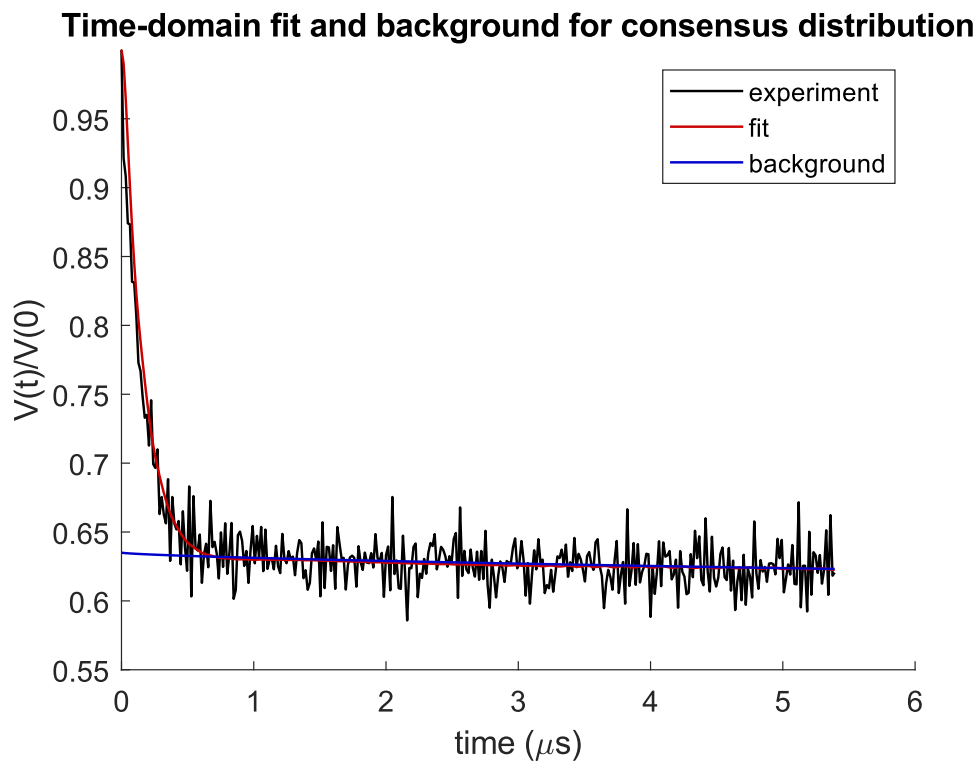
2. Fits of time-domain data

DEERNet fits and background fits



Tikhonov fit





3. Experimental and processing parameters

Modulation depth: 0.344

Signal-to-noise ratio: 22.3 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.01412

From DEERNet fit: 0.01542

From Tikhonov fit: 0.01643

Zero time: 120 ns

Maximum time: 5392 ns

The last 5 % of the data was cut off

Time increment: 16 ns

Phase: -19.8 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: 40.00

Reg. par. initial estimate by L-curve corner: 10.00

Overlap between DEERNet and regularization solutions: 0.897

Predicted overlap of consensus solution with ground truth: 0.77...0.94

Mean distance: 33.4 Å

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

Distance standard deviation: 11.7 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q152C_Q235C_MTSL_E
MCV_d2_6us_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q152C_Q235C_MTSL_E
MCV_d2_6us_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_Q152C_Q235C_MTSL_E
MCV_d2_6us_spec_consensus_DEER_fit.csv

Metadata:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_Q152C_Q235C_MTSL_E
MCV_d2_6us_spec_comparative_DEER_meta_data.csv