

DEER analysis report on dataset DEER_71_240_MTSL_EMCV_d2_6us_115sc s_spec

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

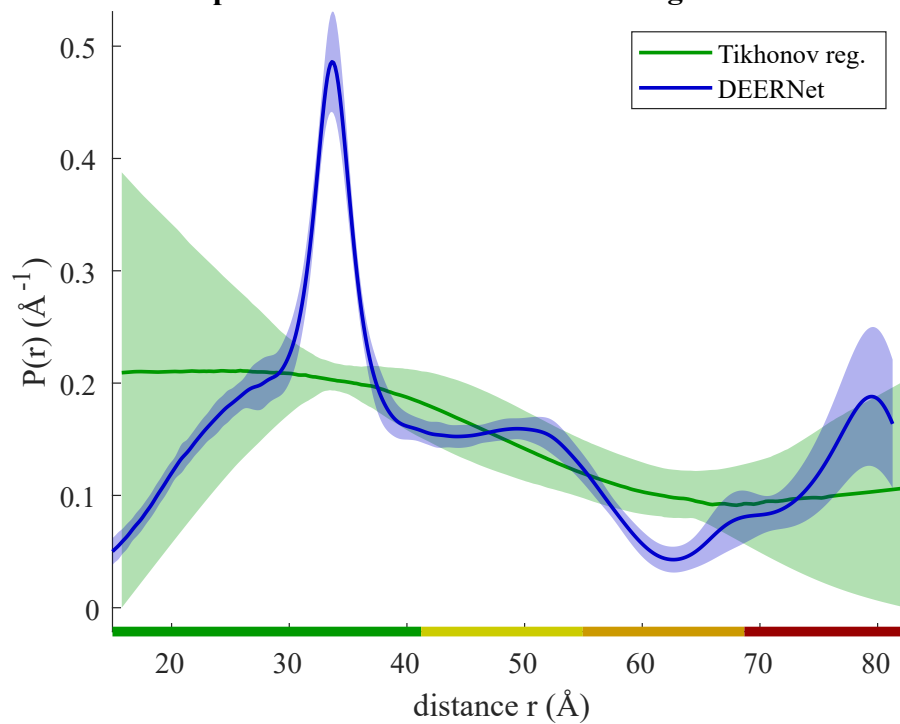
ComparativeDEERAnalyzer version 2.0

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

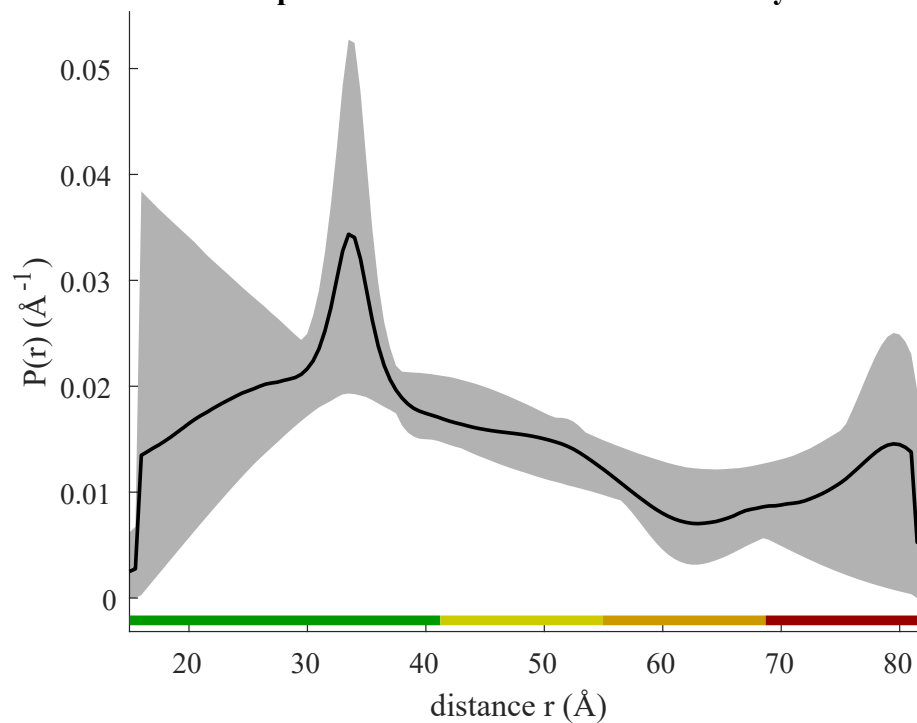
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1. Distance distributions

Overlap between neural network and regularization

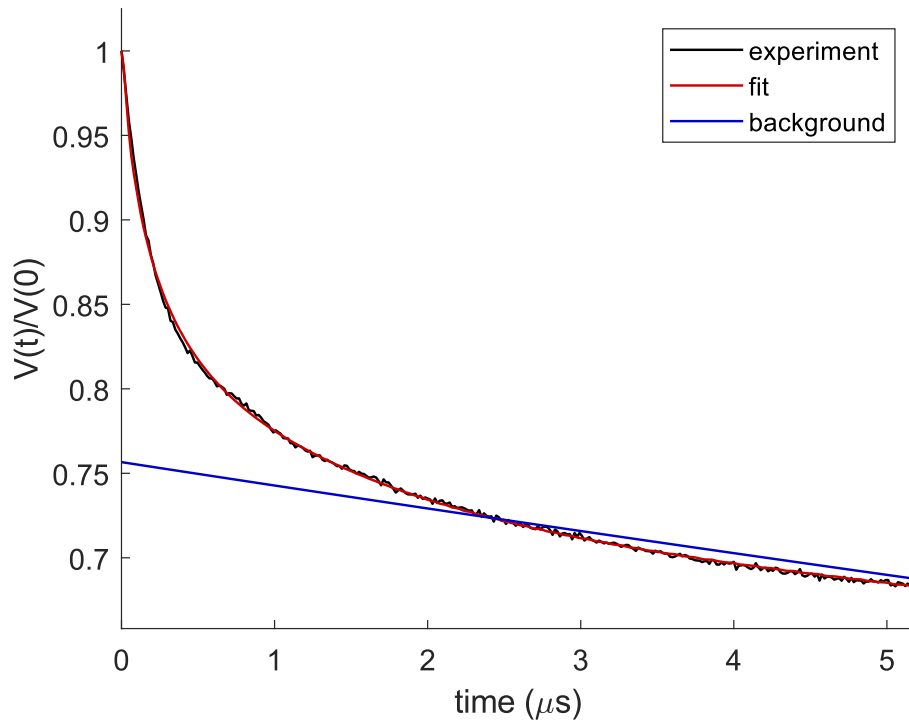


Comparative distribution and uncertainty

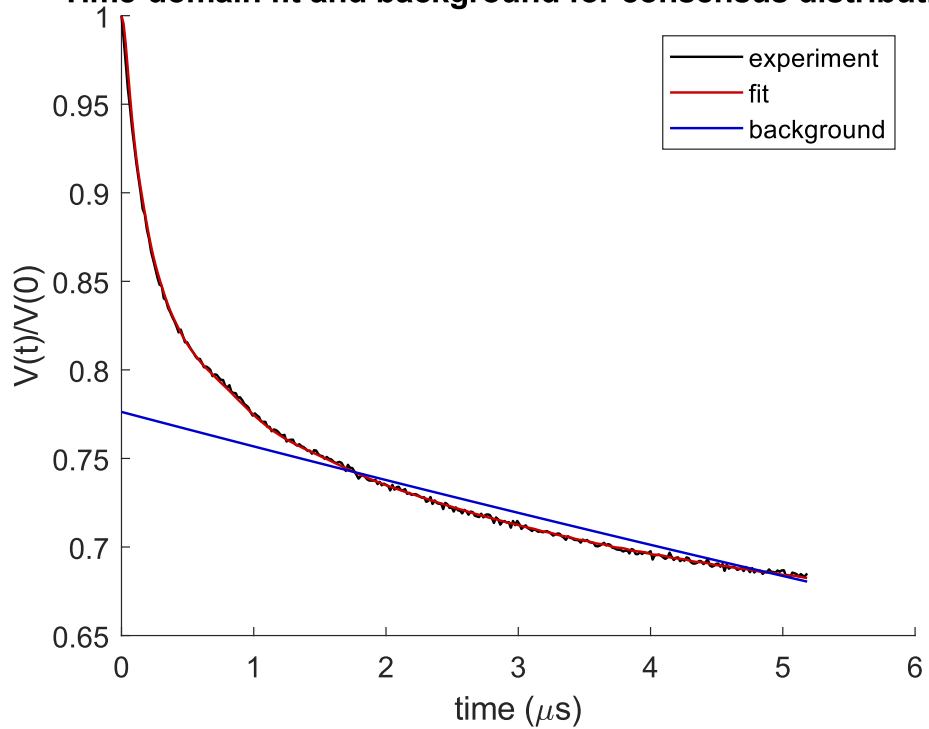


2. Fits of time-domain data

Tikhonov fit



Time-domain fit and background for consensus distribution



3. Experimental and processing parameters

DEERNet background not provided, as it was considered unreliable.

Modulation depth: 0.224

Signal-to-noise ratio: 150.5 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00133

From Tikhonov fit: 0.00195

Zero time: 124 ns

Maximum time: 5184 ns

The last 9 % of the data was cut off

Time increment: 16 ns

Phase: 6.3 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: 127.70

Reg. par. initial estimate by lr: 2.00

Overlap between DEERNet and regularization solutions: 0.844

Predicted overlap of consensus solution with ground truth: 0.72...0.89

Mean distance: 43.8 Å

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

Distance standard deviation: 18.3 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_240_MTS�_EMCV_d
2_6us_115scs_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_240_MTS�_EMCV_d
2_6us_115scs_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_240_MTSL_EMCV_d
2_6us_115scs_spec_consensus_DEER_fit.csv

Metadata:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_240_MTSL_EMCV_d
2_6us_115scs_spec_comparative_DEER_meta_data.csv