

DEER analysis report on dataset DEER_71_388_IAP_D2O_EMCV_after_SEC_ d2_9us_10scs_spec

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

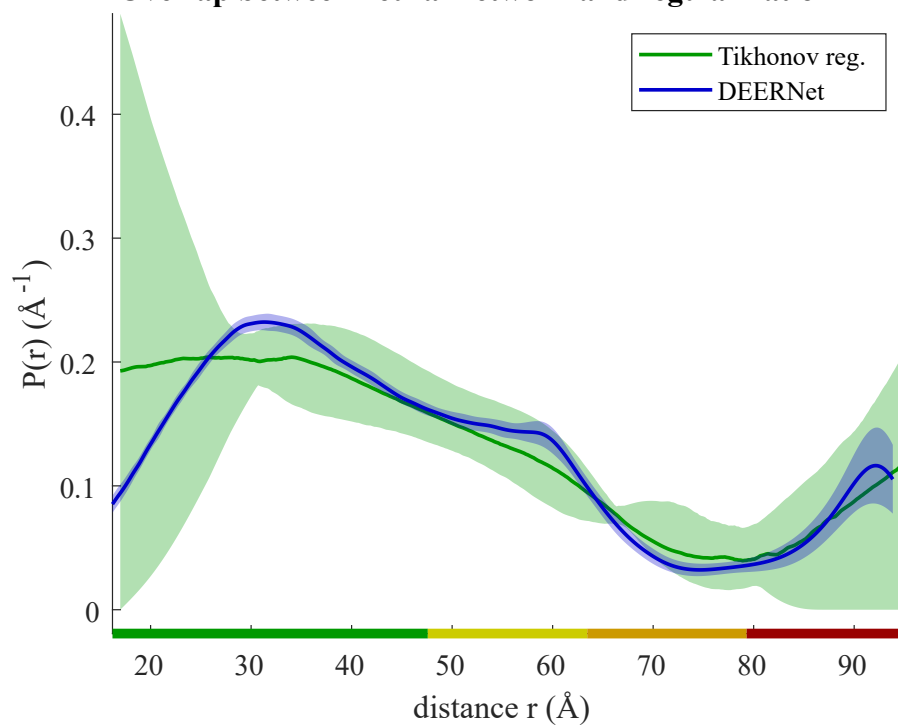
ComparativeDEERAnalyzer version 2.0

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

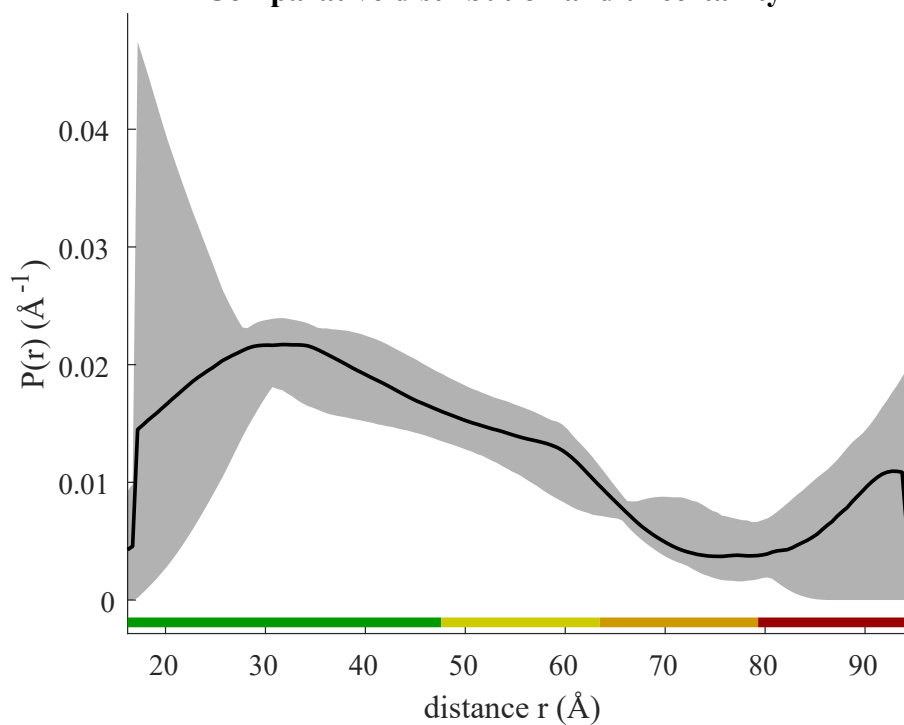
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1. Distance distributions

Overlap between neural network and regularization

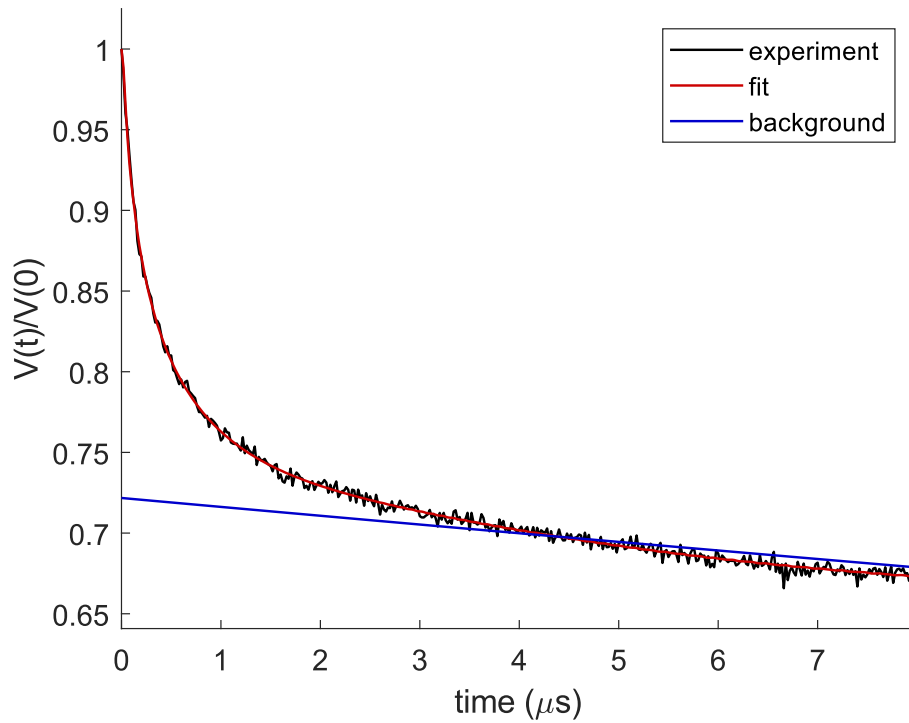


Comparative distribution and uncertainty

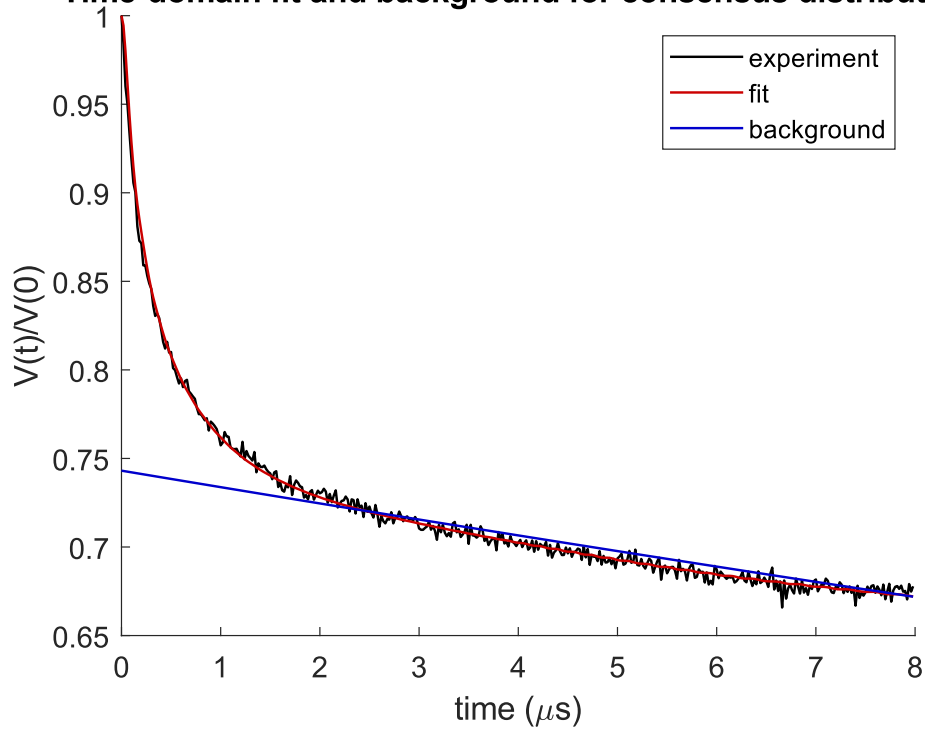


2. Fits of time-domain data

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: 0.257

Signal-to-noise ratio: 81.9 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00272

From Tikhonov fit: 0.00355

Zero time: 123 ns

Maximum time: 7980 ns

The last 8 % of the data was cut off

Time increment: 20 ns

Phase: -4.9 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: 28.42

Reg. par. initial estimate by lr: 2.51

Overlap between DEERNet and regularization solutions: 0.937

Predicted overlap of consensus solution with ground truth: 0.80...0.98

Mean distance: 46.5 Å

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

Distance standard deviation: 20.6 Å

Full data set in Matlab format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_388_IAP_D2O_EMC
V_after_SEC_d2_9us_10scs_spec_comparative_DEER_analysis.mat

Distance distributions in text format:

G:\projects\Christoph_Gmeiner\modelling\master_shot\Deer\DEER_71_388_IAP_D2O_EMC
V_after_SEC_d2_9us_10scs_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_388_IAP_D2O_EMC
V_after_SEC_d2_9us_10scs_spec_consensus_DEER_fit.csv

Metadata:

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V_after_SEC_d2_9us_10scs_spec_comparative_DEER_meta_data.csv