DEER analysis report on dataset 220707_BEBQ71.97_DEER

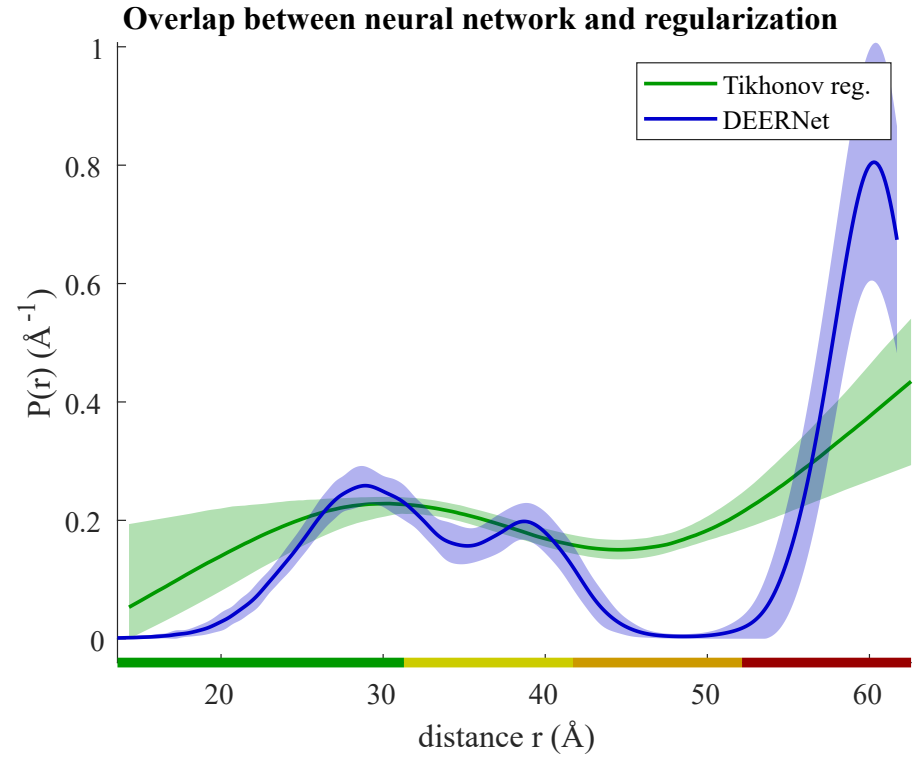
DEERNet Spinach SVN Rev 5662 and DeerLab 0.9.1 Tikhonov regularization

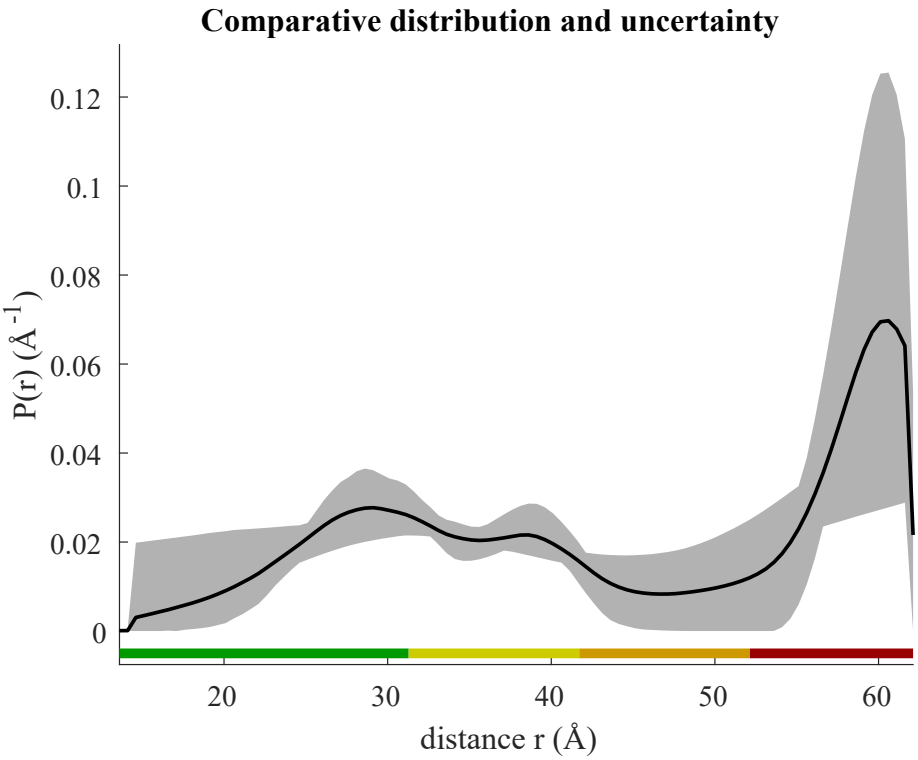
ComparativeDEERAnalyzer version 2.0

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

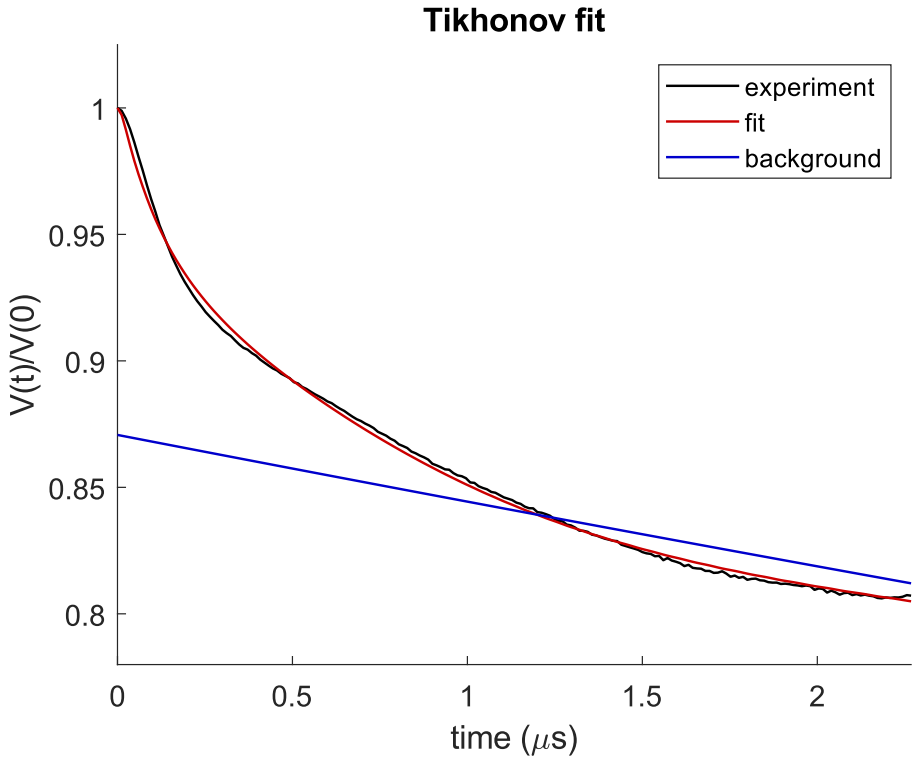
08-Jul-2022 10:24:52

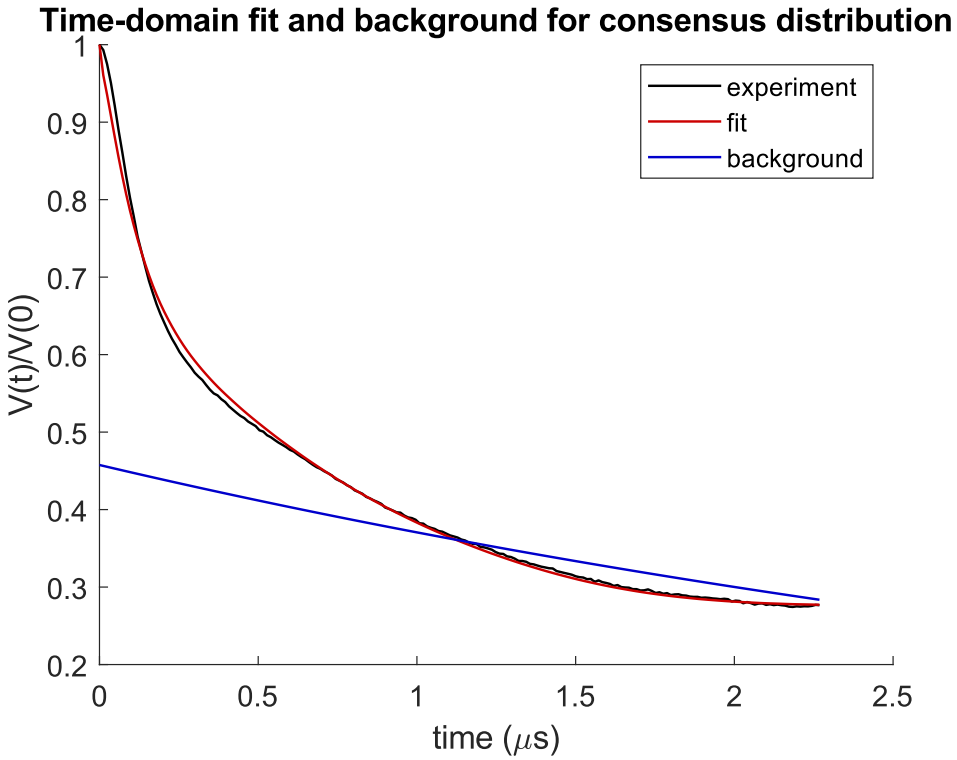
1. Distance distributions





2. Fits of time-domain data





3. Experimental and processing parameters

DEERNet background not provided, as it was considered unreliable.

Ghost suppression for a 7-spin system was applied.

Modulation depth: 0.542

Signal-to-noise ratio: 256.3 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00300

From Tikhonov fit: 0.01126

Zero time: 18 ns

Maximum time: 2.268000e+03 ns

Time increment: 12 ns

Phase: 6.7 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: 20.24

Reg. par. initial estimate by lr: 0.32

Overlap between DEERNet and regularization solutions: 0.704

Predicted overlap of consensus solution with ground truth: 0.58...0.76

Mean distance: 43.7 Å

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

Distance standard deviation: 14.2 Å

Full data set in Matlab format: C:\Users\ka44\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_for_paper\BEBQ71_M47\220707_BEBQ71.97_DEER_comparative_DEER_analysis.mat

Distance distributions in text format: C:\Users\ka44\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_for_paper\BEBQ71_M47\220707_BEBQ71.97_DEER_consensus_DEER_distribution.csv

Fit and background in text format: C:\Users\ka44\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_for_paper\BEBQ71_M47\220707_BEBQ71.97_DEER_consensus_DEER_fit.csv

Metadata: C:\Users\ka44\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_for_paper\BEBQ71_M47\220707_BEBQ71.97_DEER_comparative_DEER_meta_data.csv