DEER analysis report on dataset 220531_KAq195.6_DEER_208032_66pc_pi
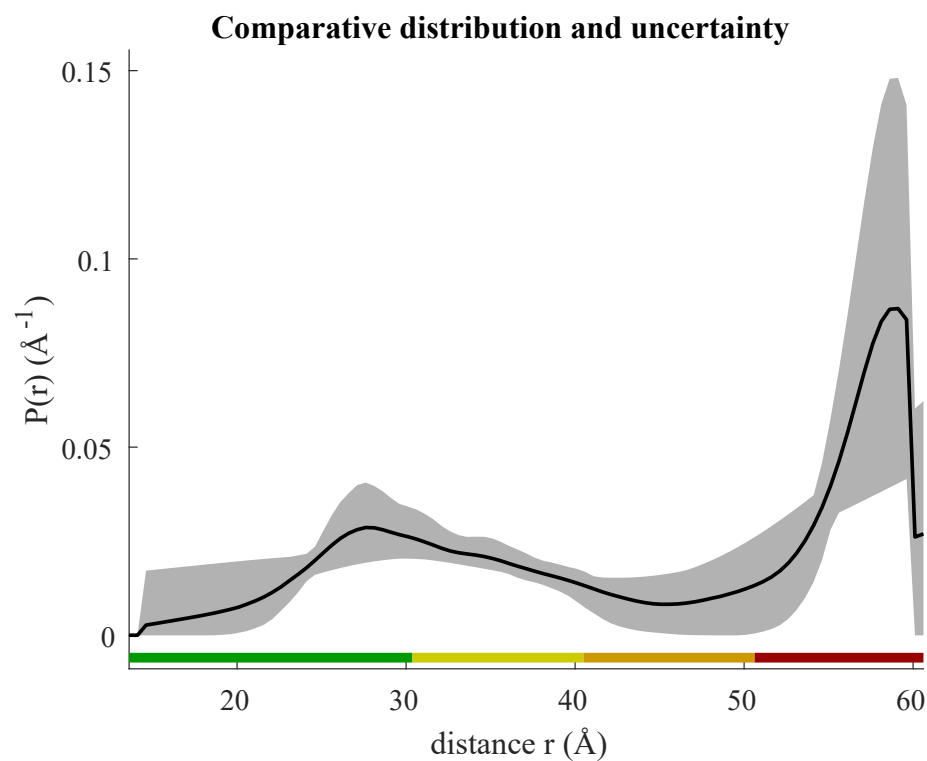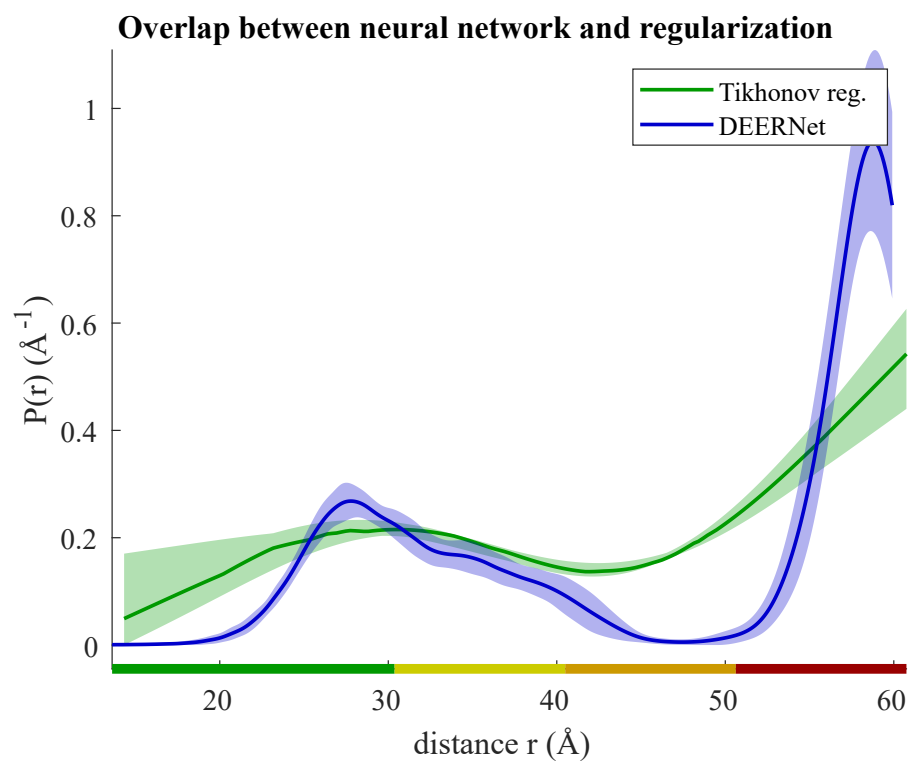
DEERNet Spinach SVN Rev 5662 and DeerLab 0.9.1 Tikhonov regularization

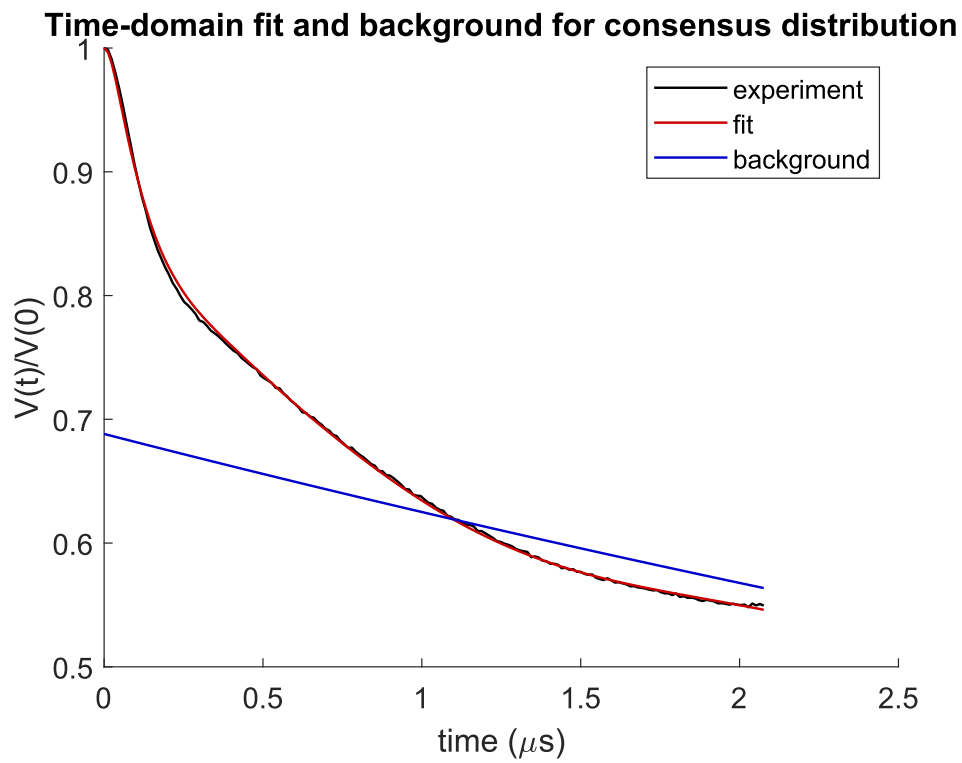### ComparativeDEERAnalyzer version 2.0

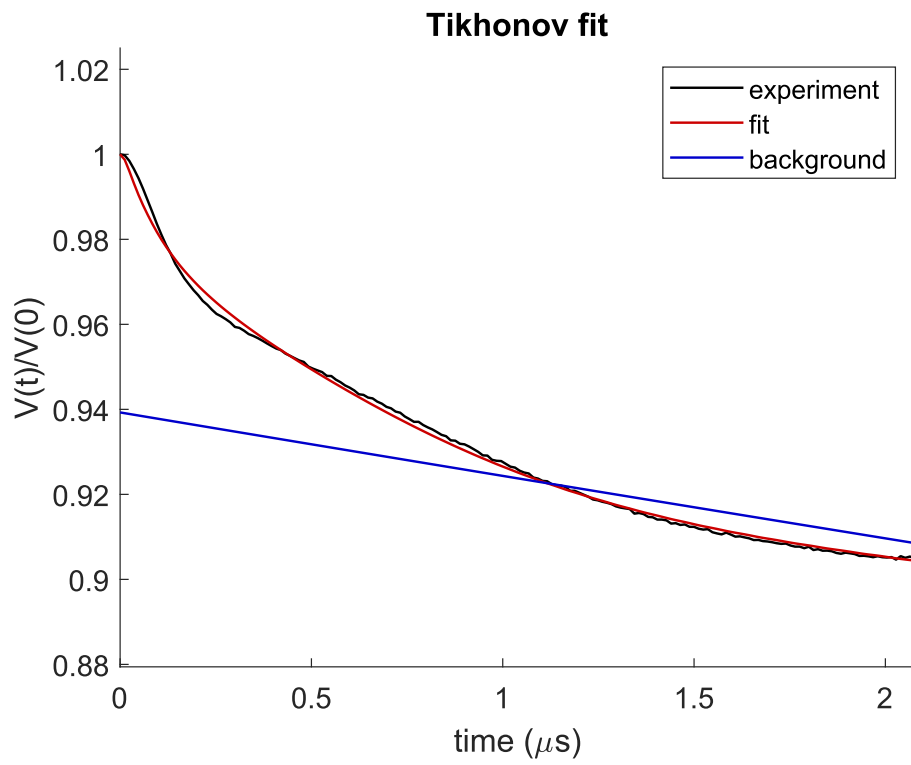07-Jun-2022 15:01:52

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

Ghost suppression for a 7-spin system was applied.

Modulation depth: 0.312

Signal-to-noise ratio: 216.7 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00152

From Tikhonov fit: 0.00633

Zero time: 288 ns

Maximum time: 2076 ns

Time increment: 12 ns

Phase: -2.8 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: 8.04

Reg. par. initial estimate by lr: 0.25

Overlap between DEERNet and regularization solutions: 0.689

Predicted overlap of consensus solution with ground truth: 0.57...0.74

Mean distance: 43.9 Å

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

Distance standard deviation: 13.6 Å

Full data set in Matlab format: C:\Users\Katrin\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\KAq195\220531_KAq195.6_DEER_208032_66pc_pi_comparative_DEER_analysis.mat

Distance distributions in text format: C:\Users\Katrin\Documents\OneDrive - University of St

Andrews\StAndrews\Work\BEB\Projects\CP_div\MscS\MscS_D67R1_M47R1_Mary_220518\
KAq195\220531_KAq195.6_DEER_208032_66pc_pi_consensus_DEER_distribution.csv

Fit and background in text format: C:\Users\Katrin\Documents\OneDrive - University of St
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