

# **DEER analysis report on dataset 220705\_BEBQ71.89\_DEER**

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

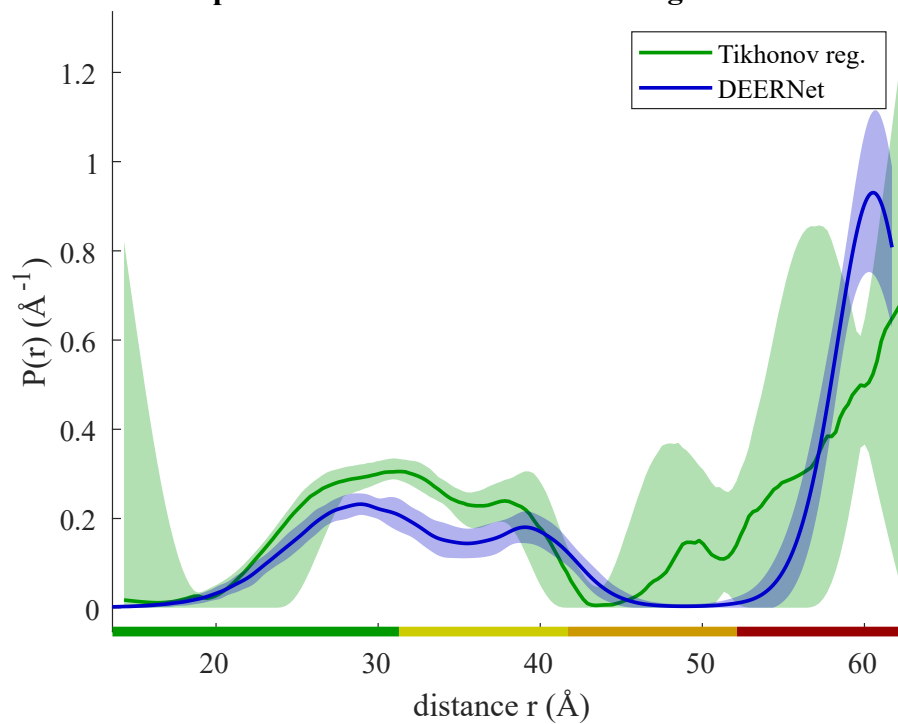
**ComparativeDEERAnalyzer version 2.0**

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

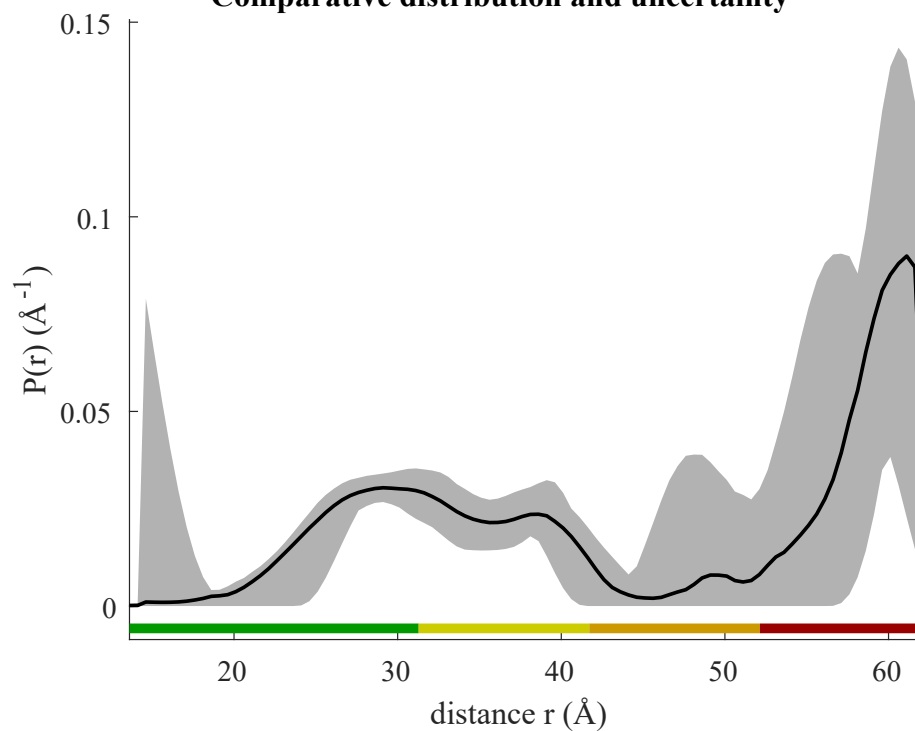
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## 1. Distance distributions

**Overlap between neural network and regularization**



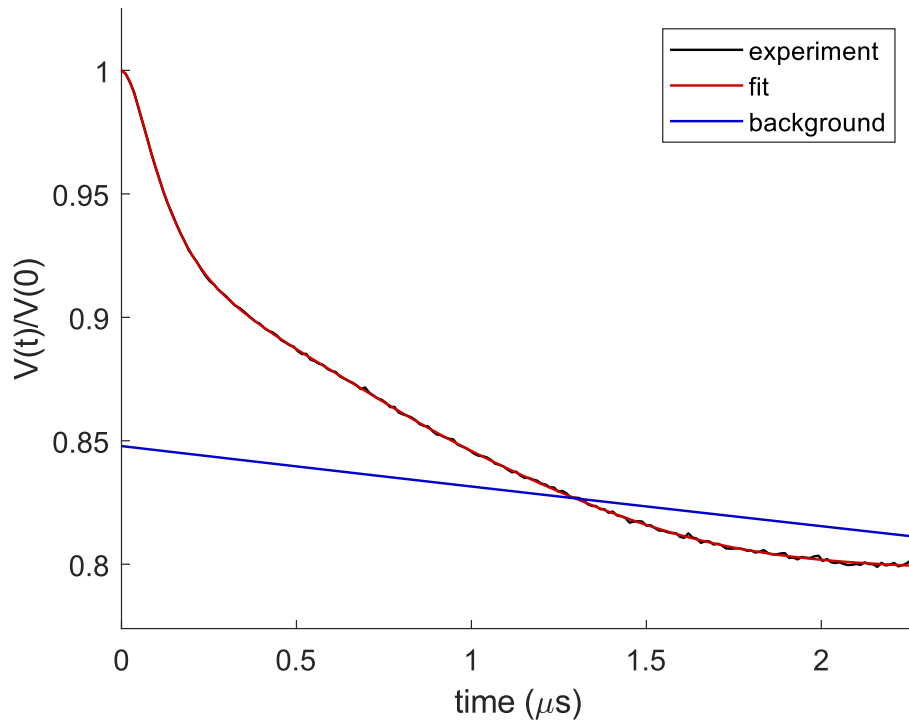
**Comparative distribution and uncertainty**



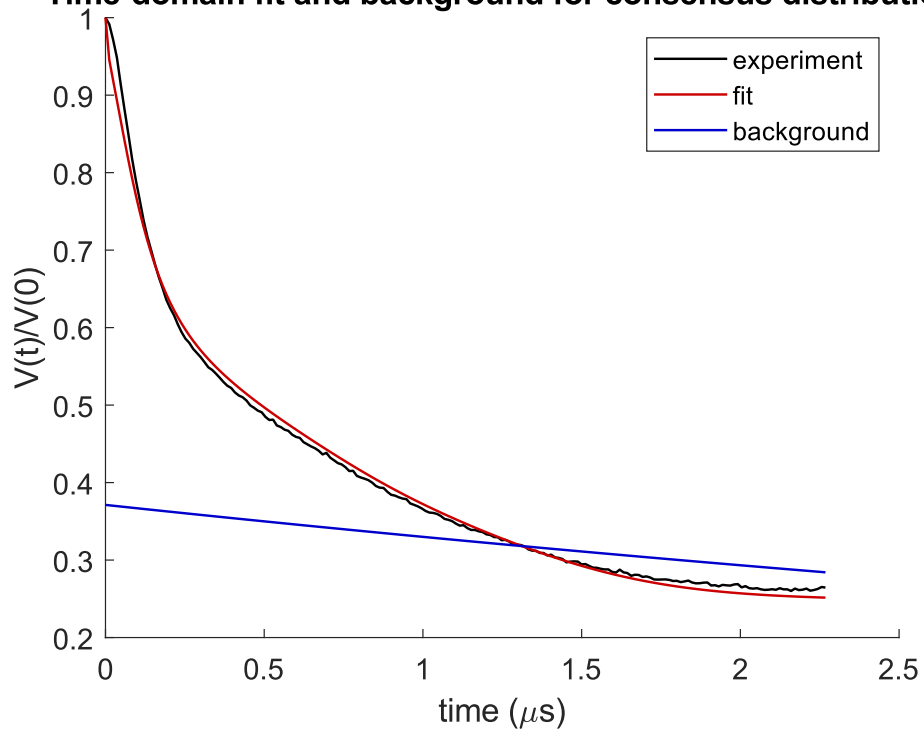
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## 2. Fits of time-domain data

**Tikhonov fit**



**Time-domain fit and background for consensus distribution**



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### 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: 0.629

Signal-to-noise ratio: 229.8 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00345

From Tikhonov fit: 0.00850

Zero time: 18 ns

Maximum time: 2.268000e+03 ns

Time increment: 12 ns

Phase: 4.6 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: 0.25

Reg. par. initial estimate by lr: 1.00

**Overlap between DEERNet and regularization solutions: 0.769**

Predicted overlap of consensus solution with ground truth: 0.65...0.82

**Mean distance: 45.0 Å**

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

Distance standard deviation: 14.1 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\BEB\_Q71\_M47\220705\_BEBQ71.89\_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\BEB\_Q71\_M47\220705\_BEBQ71.89\_DEER\_consensus\_DEER\_distribution.csv

### 3. Experimental and processing parameters

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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\BEB\_Q71\_M47\220705\_BEBQ71.89\_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\BEB\_Q71\_M47\220705\_BEBQ71.89\_DEER\_comparative\_DEER\_meta\_data.csv