

# **DEER analysis report on dataset DEER\_80\_388\_MTSL\_EMCV\_d2\_9.5us\_spe c**

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

**ComparativeDEERAnalyzer version 2.0**

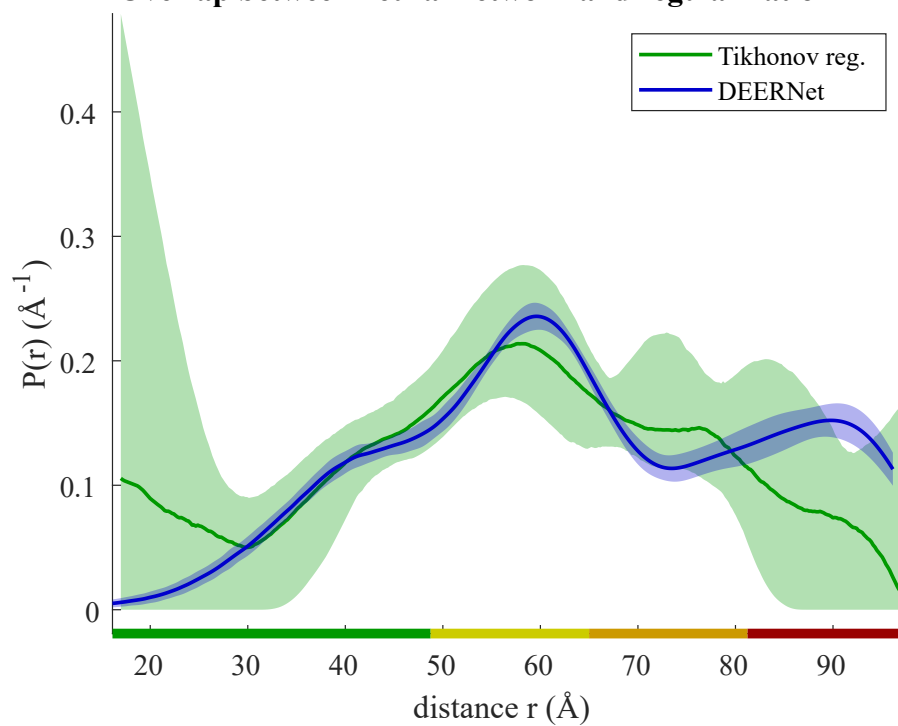
see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/  
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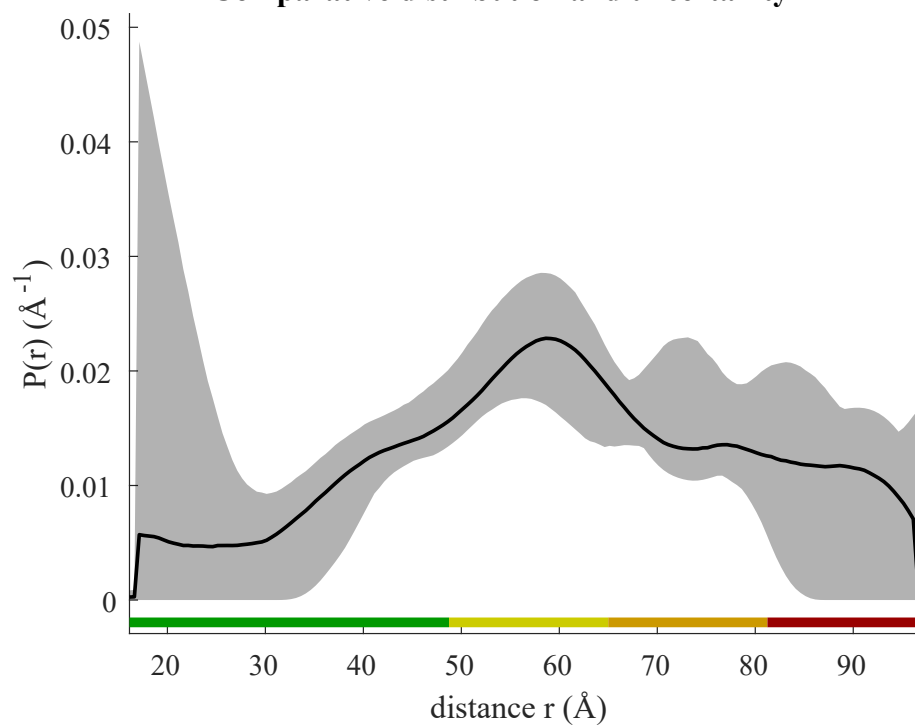
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## 1. Distance distributions

**Overlap between neural network and regularization**



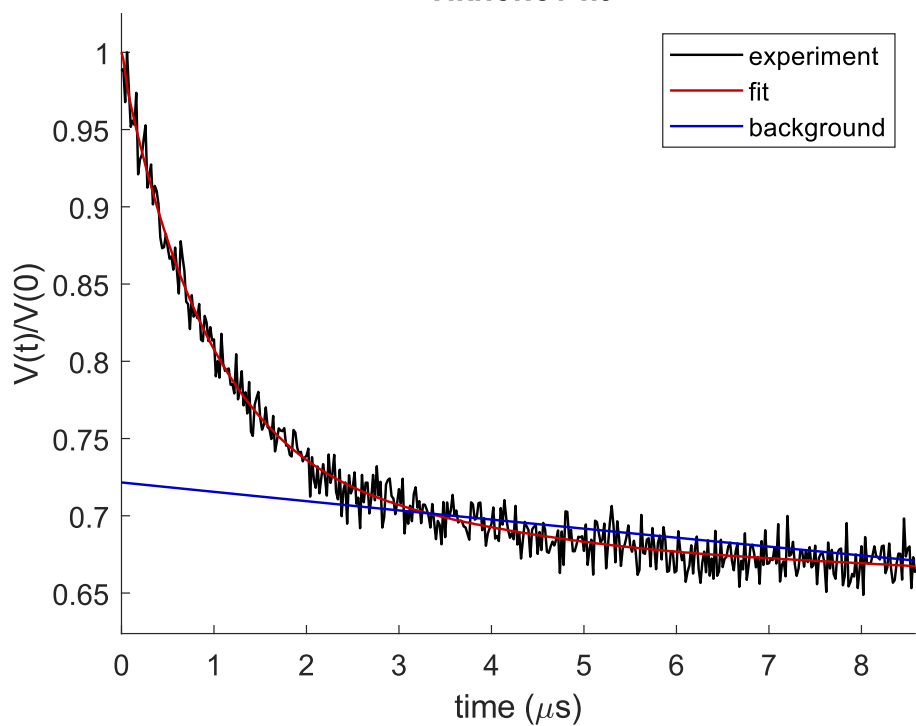
**Comparative distribution and uncertainty**



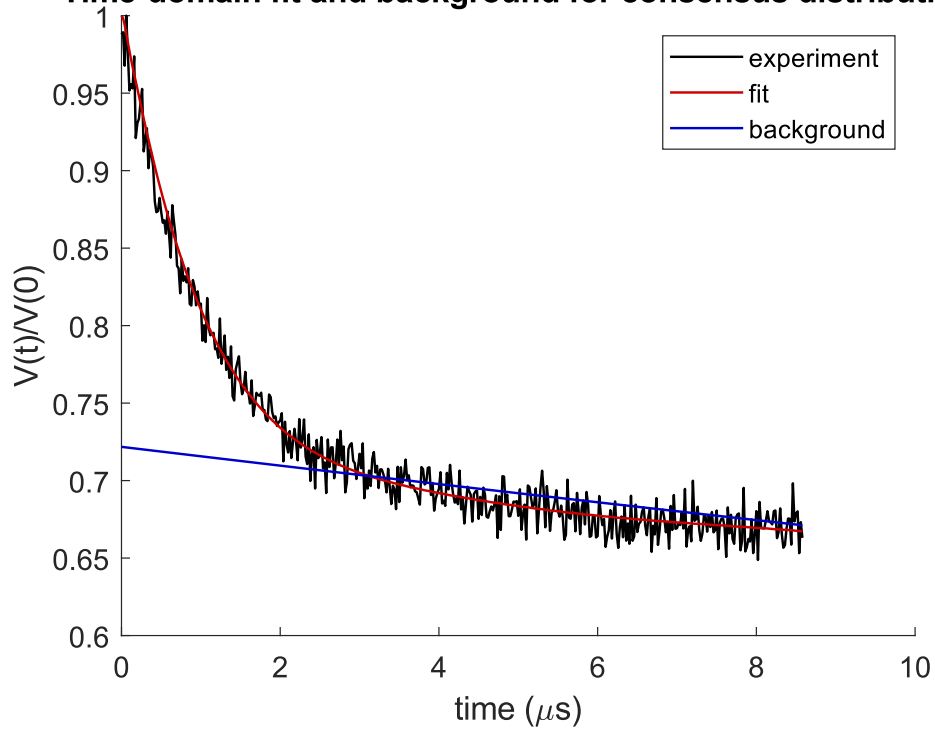
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## 2. Fits of time-domain data

**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.**

Modulation depth: 0.278

Signal-to-noise ratio: 27.0 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.01240

From Tikhonov fit: 0.01029

Zero time: 146 ns

Maximum time: 8580 ns

The last 6 % of the data was cut off

Time increment: 20 ns

Phase: -2.3 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: 22.41

Reg. par. initial estimate by lr: 15.85

Overlap between DEERNet and regularization solutions: 0.879

Predicted overlap of consensus solution with ground truth: 0.75...0.92

Mean distance: 61.2 Å

Distance standard deviation: 28.1 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_80\_388\_MTS�\_EMCV\_d  
2\_9.5us\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_80\_388\_MTS�\_EMCV\_d  
2\_9.5us\_spec\_consensus\_DEER\_distribution.csv

### 3. Experimental and processing parameters

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Fit and background in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_80\_388\_MTSL\_EMCV\_d  
2\_9.5us\_spec\_consensus\_DEER\_fit.csv

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_80\_388\_MTSL\_EMCV\_d  
2\_9.5us\_spec\_comparative\_DEER\_meta\_data.csv