DeerLab
Basics

1 Initialize

```python
import numpy as np
import matplotlib.pyplot as plt
import deerlab as dl
```

2 Load data

```python
t,V = dl.deerload("dataset.DTA")
Vexp = dl.correctphase(V)
Vexp = Vexp/np.max(Vexp)
```

3 Zerotime correction

```python
deadtime = 0.3  # µs
t = t - t[0]
t = t + deadtime
```

4 Experiment

```python
r = np.linspace(2,5,50)
tau1 = 0.4  # µs
tau2 = 3.5  # µs

my4pdeer = dl.ex_4pdeer(
            tau1, tau2, pathways=[1,2,3])
```

5a Model (non-parametric)

```python
Vmodel = dl.dipolarmodel(
            t, r, experiment=my4pdeer)
```


5b Model (parametric)

```python
Pmodel = dl.dd_gauss2

Vmodel = dl.dipolarmodel(t, r, pmodel=Pmodel,
                    experiment=my4pdeer)
```

6a Fitting

```python
results = dl.fit(Vmodel, Vexp)
print(results)
results.plot(xlabel="Time ($\mu s$)")
```

6b Fitting with compactness

```python
compactness = dl.dipolarpenalty(
        Pmodel=None, r=r, type='compactness')
results = dl.fit(
        Vmodel, Vexp, penalties=compactness)
print(results)
results.plot(xlabel="Time ($\mu s$)")
```

7a Extracting distance (non-parametric)

```python
P = results.P
Puq = results.PUncert
Pci95 = Puq.ci(95)
```

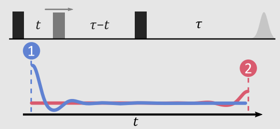
7b Extracting distance (parametric)

```python
Pfit = results.evaluate(Pmodel, r)
scale = np.trapz(Pfit, r)
Puncert = results.propagate(
                Pmodel, r, lb=np.zeros_like(r))
Pfit = Pfit / scale
Pci95 = Puncert.ci(95) / scale
```

Experiment

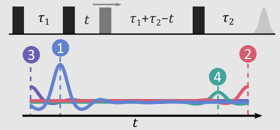
3 pulse DEER

```python
dl.ex_4pdeer(tau, pathways,
    pulselength)
```



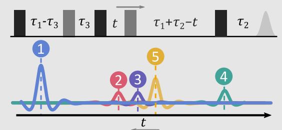
4 pulse DEER:

```python
dl.ex_4pdeer(tau1, tau2,
    pathways, pulselength)
```

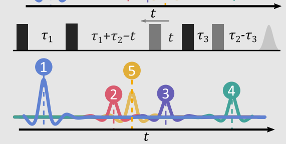


5 pulse DEER

```python
dl.ex_fwd5pdeer(tau1, tau2,
tau3,   pathways,pulselength)
```

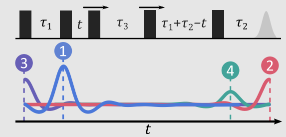


```python
dl.ex_rev5pdeer(tau1, tau2,
tau3,   pathways, pulselength)
```



RIDME

```python
dl.ex_ridme(tau1, tau2, tau3,
    pathways, pulselength)
```

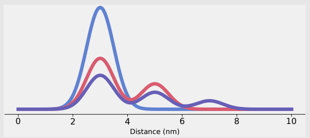


Other Experiments Models are available...

Distance Models

Gaussian

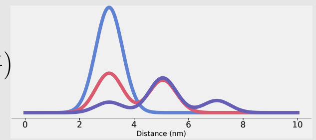
$$P(r)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{(r-\langle r\rangle)^2}{2\sigma^2}\right)$$



```python
dl.dd_gauss(r, mean, std)
dl.dd_gauss2(r, mean1, std1, amp1, mean2, std2, amp2)
dl.dd_gauss3(r, mean1, std1, amp1, mean2, std2, amp2, …)
```

Rice

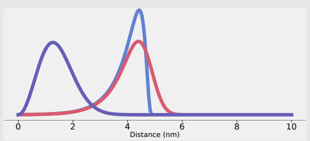
$$P(r)=\frac{\nu^{n/2-1}}{\sigma^2}r^{n/2}\exp\left(-\frac{(r^2+\nu^2)}{2\sigma^2}\right)I_{n/2-1}\left(\frac{r\nu}{\sigma^2}\right)$$



```python
dl.dd_rice(r, location, spread)
dl.dd_rice2(r, location1, spread1, amp1, location2, spread2, amp2)
dl.dd_rice3(r, location1, spread1,  amp1, location2, spread2, amp2, …)
```

Disordered physical models

```python
dl.dd_wormchain(r, contour,
                persistence)
dl. dd_wormgauss(r, contour,
                persistence, std)
dl.dd_randcoil(r, Nres, scaling,
                length)
```



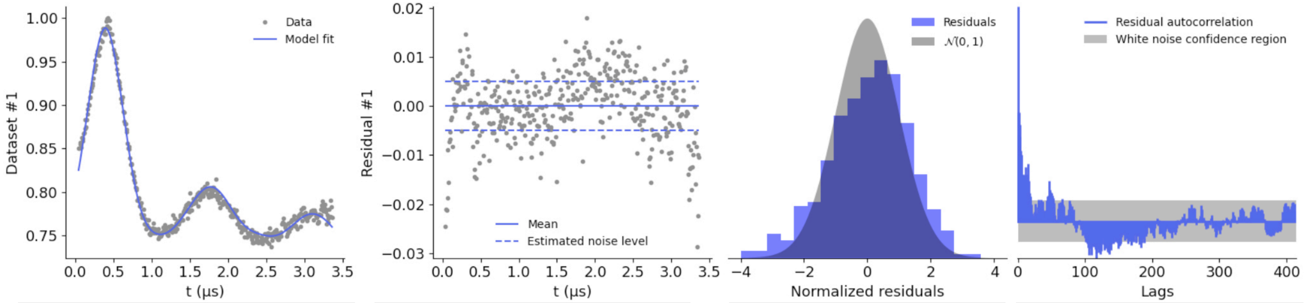
DeerLab Advanced

Other useful functions

... bootstrap sampling?
→ `dl.fit(**, bootsrap=200, bootcore=4)`
... distribution statistics?
→ `dl.diststats(r, P, Puq=Puq, verbose=True)`
... fit statistics?
→ `dl.goodness_of_fit(data, results.model, Ndof, noiselvl)`
... save object?
→ `dl.store_pickle(object, "filename")`
... load object?
→ `dl.load_pickle(object, "filename")`
... profile likelihood analysis?
→ `dl.profile_analysis(model, y, parameters=["lam1"])`
... save plot?
→ `plt.save_plot("filename", dpi)`

Fit Statistics

```
results.plot(xlabel="Time ($\mu s$)", gof=True)
```



Fit
1. Does the line fit the data?
↳ Check if parameter have hit limits
↳ Include more pathways

Residuals
1. Are the residuals random or is there a pattern?
↳ Check if parameter have hit limits
↳ Include more pathways

Residuals Distribution
1. Is the distribution shifted compared with noise?
↳ Check if parameter have hit limits
↳ Include more pathways

Residual Autocorrelation
1. Is the autocorrelation within the white noise?
↳ Check if parameter have hit limits
↳ Include more pathways

Background Models

```
dl.fit(**, Bmodel=dl.bg_hom3d, **)
```

Physical Models

```
dl.bg_hom3d(t, conc, lam)
dl.bg_hom3dex(t, conc, rex, lam)
dl.bg_homfractal(t, fconc, fdim, lam)
```

Phenomenological Models

```
dl.bg_exp(t, decay)
dl.bg_strexp(t, decay, stretch)
dl.bg_prodstrexp(t, decay1, stretch1, decay2,
                 stretch2)
```

Exporting data

... Text files
→ `np.savetxt('filename', array)`

... Matlab files
→ `from scipy.io import savemat`
→ `savemat('filename.mat', array1, array2, ...)`

Global Fitting

1. Build individual Models
```
Vmodels = []
Vmodels.append(modelA)
...
```

2. Put data into a list
```
Vs = []
Vs.append(dataA)
...
```

3. Make the global model by joining the individual models
```
globalmodel = dl.merge(*Vmodels)
```

4. Link the distance distribution into a global parameter
```
globalmodel = dl.link(globalmodel,
P=['P_1','P_2'])
```

5. Adjust weights in fit (optional)
```
results = dl.fit(globalmodel, Vs, weights=[1,1])
```

Model Manipulation

... extract a parameter?
→ `model.param  # e.g. Model.conc, model.lam1`
... freeze a parameter?
→ `param.freeze(value)  # e.g. lam1.freeze(0.25)`
... unfreeze a parameter?
→ `param.unfreeze()`
... set the initial value?
→ `param.set(par0=value)`
... set the limits?
→ `param.set(lb=0.1, ub=np.inf)`

... link two parameter?
→ `dl.link(model, newparam=['paramA','paramB'])`
... merge two parameter?
→ `dl.merge(model1, model2)`
... relate two parameter?
→ `dl.relate(model, paramA=lambda paramF: fcn(paramF))`

... linear combine two models?
→ `dl.lincombine(model1, model2, model3)`
... copy a model?
→ `from copy import deepcopy`
→ `deepcopy(modelA)`