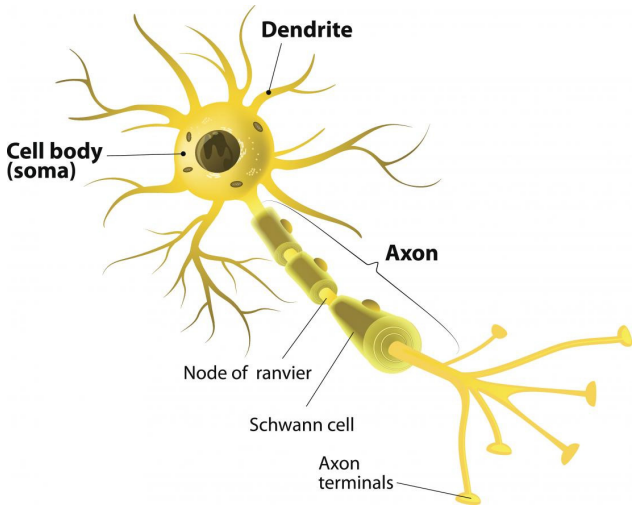
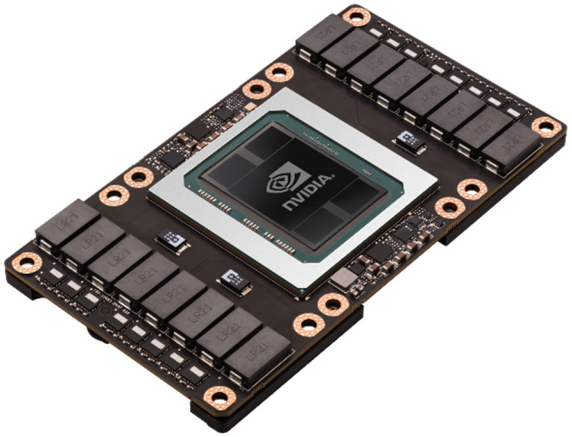




Hands-on tutorial: making (up) an AI training database

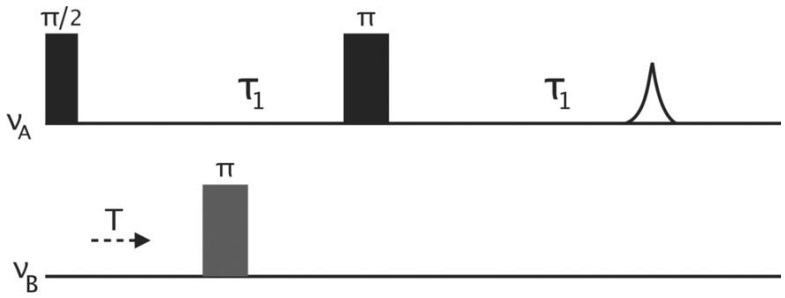
NMR/EPR simulation tools are very accurate – just sprinkle some noise and instrumental artefacts

Prof Ilya Kuprov, Weizmann Institute of Science, 2025

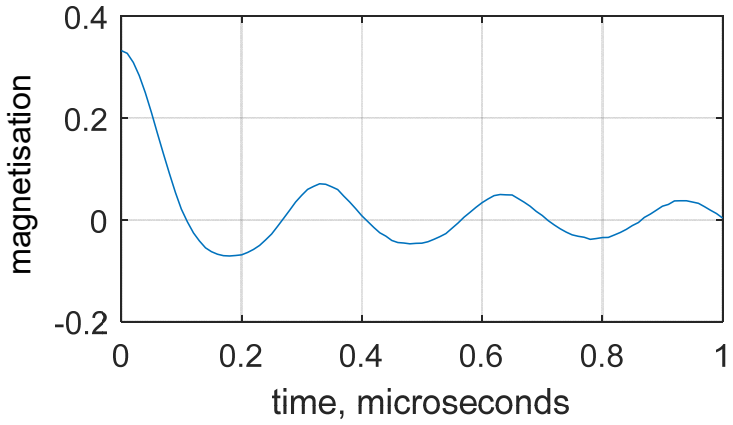
For all lecture notes and video records see https://spindynamics.org

Double electron-electron resonance

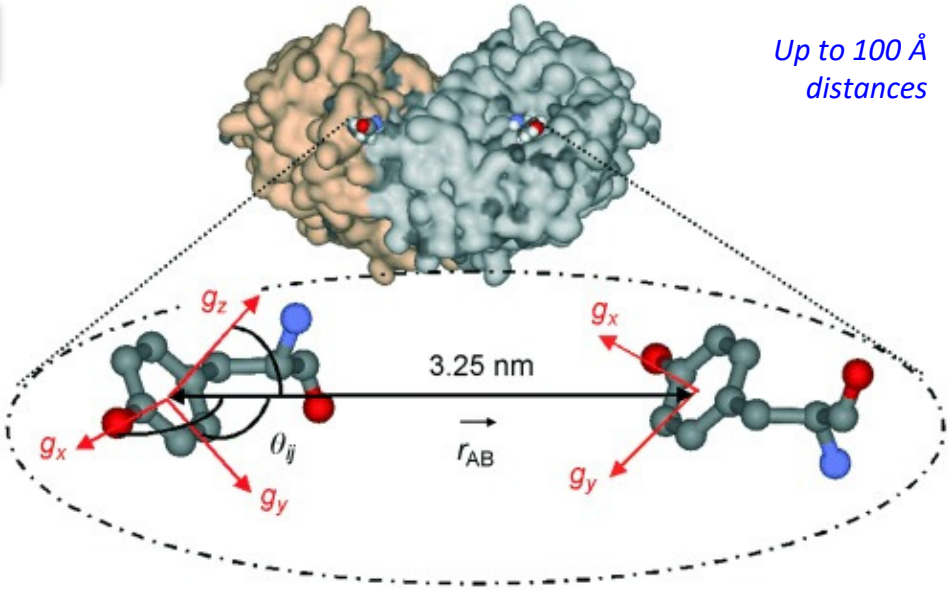
Echo modulation by dipolar coupling:



+ many technical refinements.

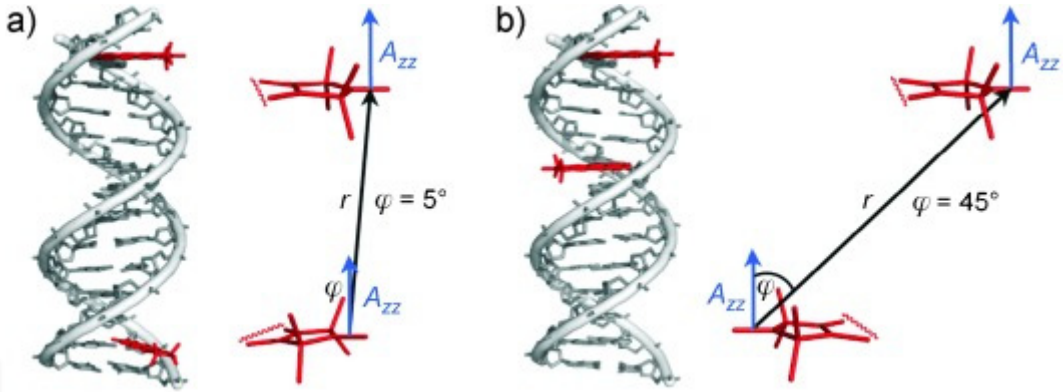


+ much statistics and DSP work.



Up to 100 Å distances

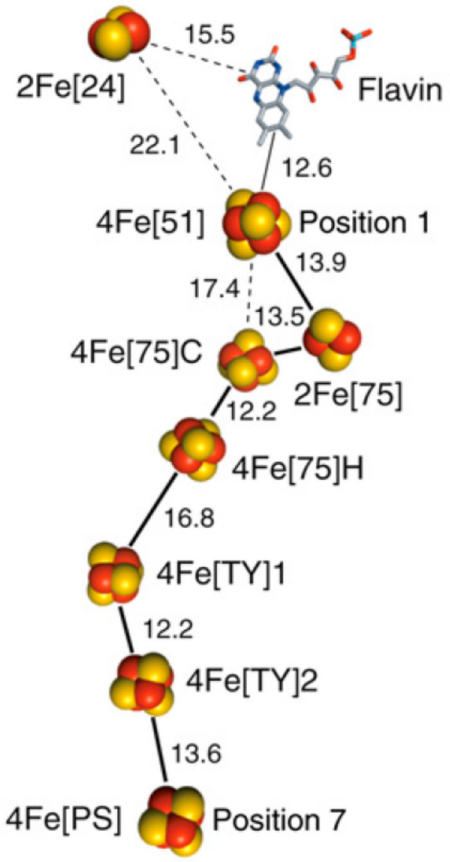
V. Denysenkov, D. Biglino, W. Lubitz, T.F. Prisner, M. Bennati - 2008

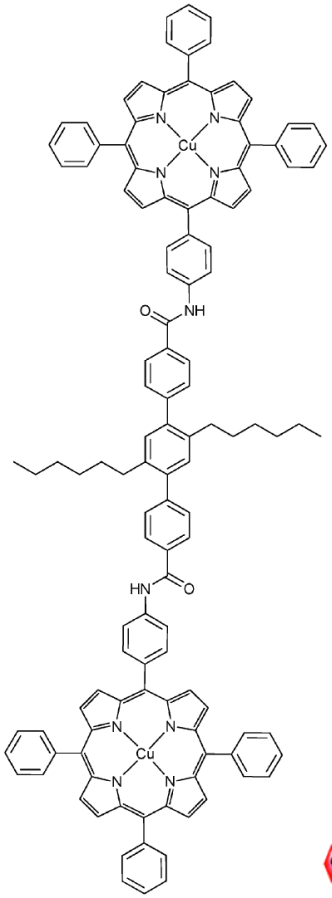


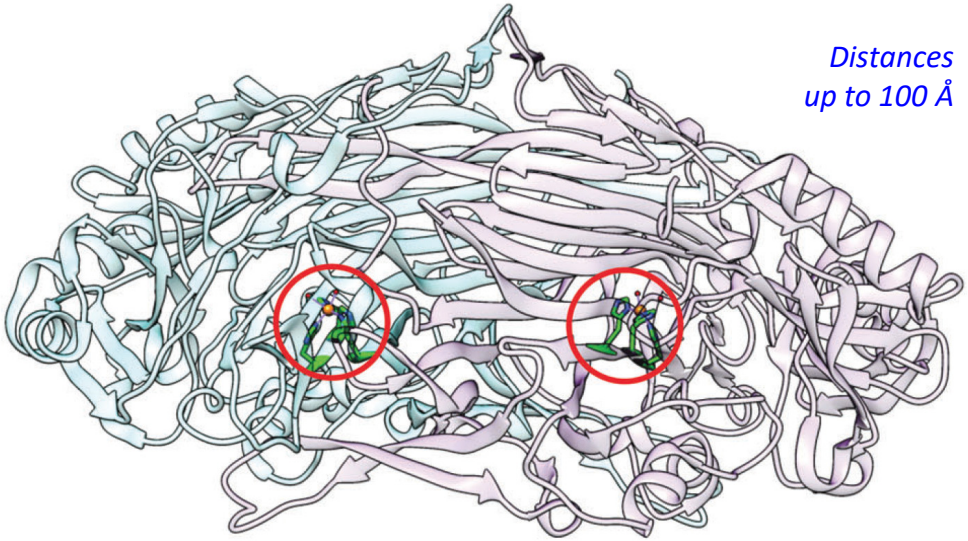
O. Schiemann, P. Cekan, D. Margraf, T.F. Prisner, S.Th. Sigurdsson - 2009

Details in Gunnar Jeschke's review (https://doi.org/10.1146/annurev-physchem-032511-143716)

Double electron-electron resonance

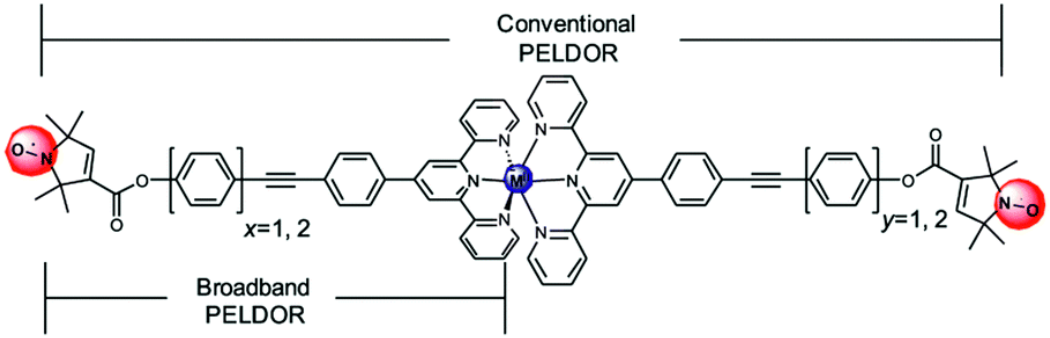






Distances up to 100 Å

A.M. Bowen, M.W. Jones, J.E. Lovett, T.G. Gaule, M.J. McPherson, J.R. Dilworth, C.R. Timmel, J.R. Harmer - 2016



M.M. Roessler, M.S. King, A.J. Robinson, F.A. Armstrong, J. Harmer, J. Hirst – 2009

J.E. Lovett, A.M. Bowen, C.R. Timmel, M.W. Jones, J.R. Dilworth, D. Caprotti, S.G. Bell, L.L. Wong, J. Harmer - 2009

A. Giannoulis, K. Ackermann, P.E. Spindler, C. Higgins, D.B. Cordes, A.M.Z. Slawin, T.F. Prisner, B.E. Bode - 2018

Details in Gunnar Jeschke's review (https://doi.org/10.1146/annurev-physchem-032511-143716)

Double electron-electron resonance

For two spin ½ particles at a specific distance, in the $\Delta\omega \gg D$ limit:

$$\gamma(r,t) = \sqrt{\frac{\pi}{6Dt}}\left(\cos[Dt]\,\mathrm{FrC}\left[\sqrt{\frac{6Dt}{\pi}}\right] + \sin[Dt]\,\mathrm{FrS}\left[\sqrt{\frac{6Dt}{\pi}}\right]\right)$$

Fresnel function — *dipole coupling (depends on distance)*

Add a distance distribution:

$$\int p(r)\,\gamma(r,t)\,dr$$

distance density

Add imperfect pulses:

$$(1-\mu) + \mu\int[\cdots]\,dr$$

modulation depth

Add finite concentration:

$$[\cdots]\exp\left[(-kt)^{N/3}\right]$$

background decay — *magic number*

With ensemble effects, concentration effects, and instrumental noise:

$$\left[(1-\mu) + \mu\int p(r)\,\gamma(r,t)\,dr\right]\exp\left[(-kt)^{N/3}\right] + n(t) = s(t)$$

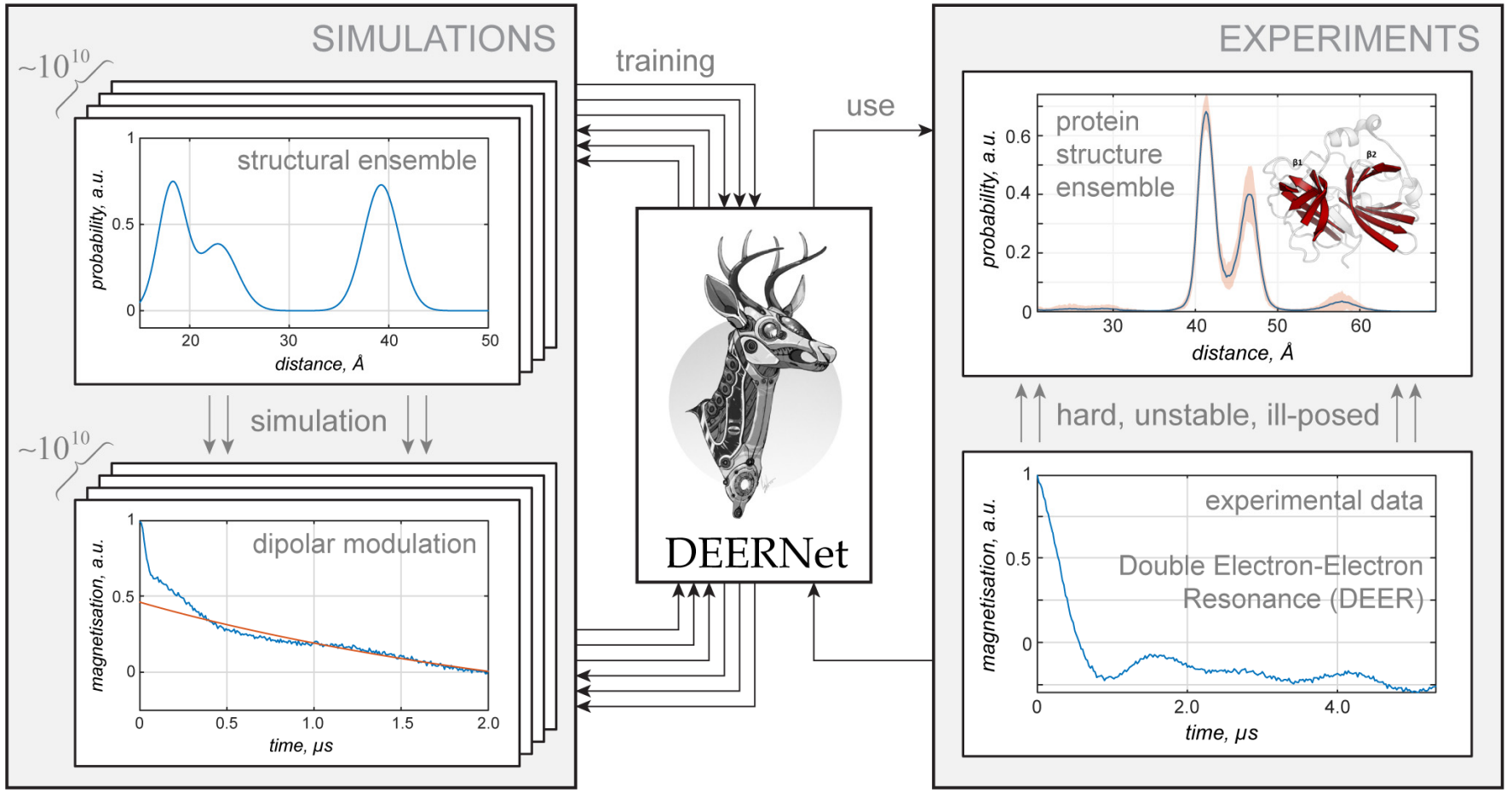
modulation depth — *distance distribution* — *kernel* — *overall decay* — *effective dimension* — *noise* — *being measured*

Fredholm integral equation of the second kind

Details in Gunnar Jeschke's review (https://doi.org/10.1146/annurev-physchem-032511-143716)

Training set generation

Not enough DEER data in the world. Try to train a neural net on simulations?



"Hmm… this creates effectively an infinite training dataset!" – Jake Keeley

Spinach library: 20 years of research and programming (https://spindynamics.org).