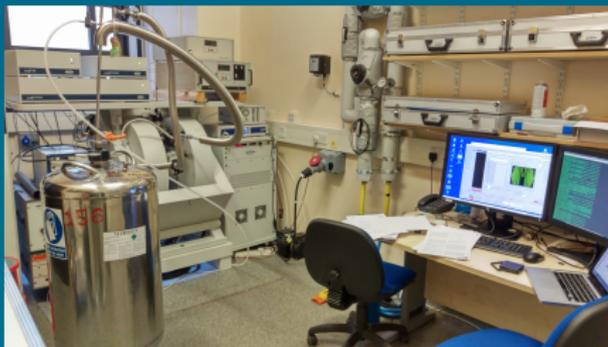


Optimising an Echo with Feedback Control

optimal control with Bruker SpinJet-AWG

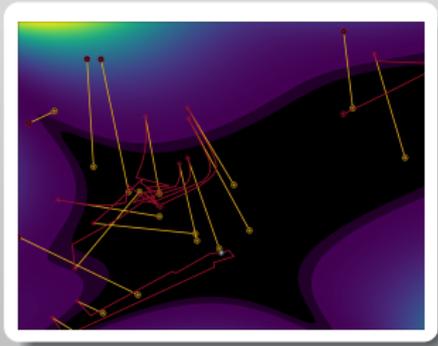
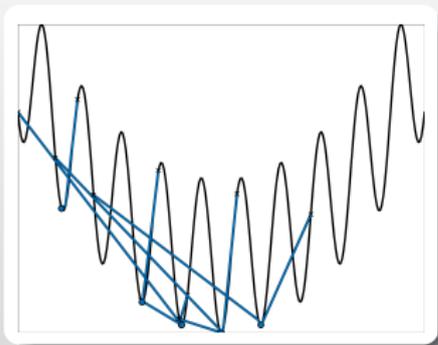
David L. Goodwin,
William Myers,
Christiane Timmel,
& Ilya Kuprov

d.goodwin@soton.ac.uk



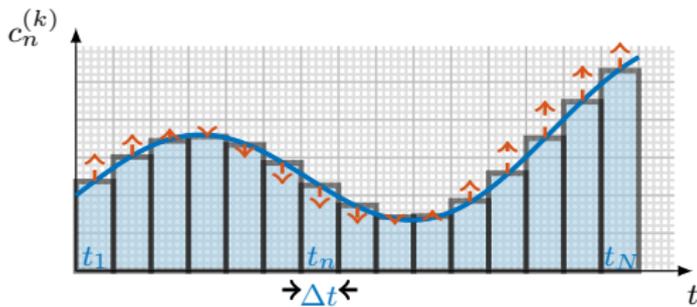
RSC@Sussex, Wednesday 4th April 2016





- ▶ We always minimise a number (or minimise the negative of a number - maximising).
- ▶ This number can be created in any way - it is only a metric (although it can have a physical significance).
- ▶ Minimising many variables can be equivalent to minimising the sum of those elements (usually with normalisation i.e an average).
- ▶ Usually, we minimise this metric as the output of a function.
- ▶ These functions can be “physics” or even “a black-box machine”.
- ▶ Essentially - we can treat any well behaved functions as a “black-box” - with only inputs and outputs seen by the optimisation algorithm.
- ▶ Analytically, the overlap between two states can be maximised: $\langle \text{DESIRED STATE} | \text{CURRENT STATE} \rangle$.

PIECEWISE CONSTANT APPROXIMATION IN A GRAPE SIMULATION



$$\begin{aligned} & \left\langle \text{DESIRED STATE} \left| \hat{\mathcal{P}}_N \hat{\mathcal{P}}_{N-1} \cdots \hat{\mathcal{P}}_2 \hat{\mathcal{P}}_1 \right| \text{CURRENT INITIAL STATE} \right\rangle \\ & = \left\langle \text{DESIRED STATE} \left| \text{CURRENT FINAL STATE} \right. \right\rangle \end{aligned}$$

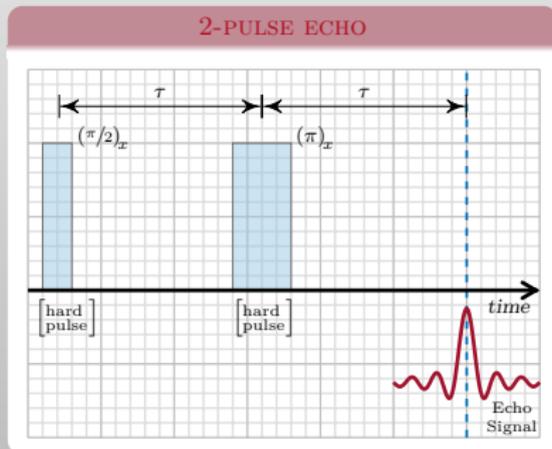
- ▶ Propagator over a time slice: $\hat{\mathcal{P}}_n = \exp \left[-i \left(\hat{H}_0 + \sum_k c_n^{(k)} \hat{H}_k \right) \Delta t \right]$
- ▶ Optimality conditions, $\frac{\partial J}{\partial c_k(t)} = 0$ at a minimum.

Optimising an Experiment

Using PulseSPEL variables

- ▶ matlab function forms the objective function of an optimisation algorithm
- ▶ python scripts are invoked by matlab, using data saved by matlab
- ▶ commands sent to modify PulseSPEL files from python a script
- ▶ send new PulseSPEL variables to experiment and run the experiment with another python script
- ▶ read the signal produced from these new variables

- ▶ Simple, 2-pulse echo experiment.
- ▶ Aim to find an optimised echo.
- ▶ Maximise the area under the real part of the echo signal.
- ▶ Vary the time between pulses, τ .



```
; FT-EPR package
;
; PulseSPEL variable
; definitions & conventions
begin defs

; Variables ; Comments:

p0 = 16 ; 90 pulse length
p1 = 32 ; 180 pulse length
p4 = 100 ; laser trigger

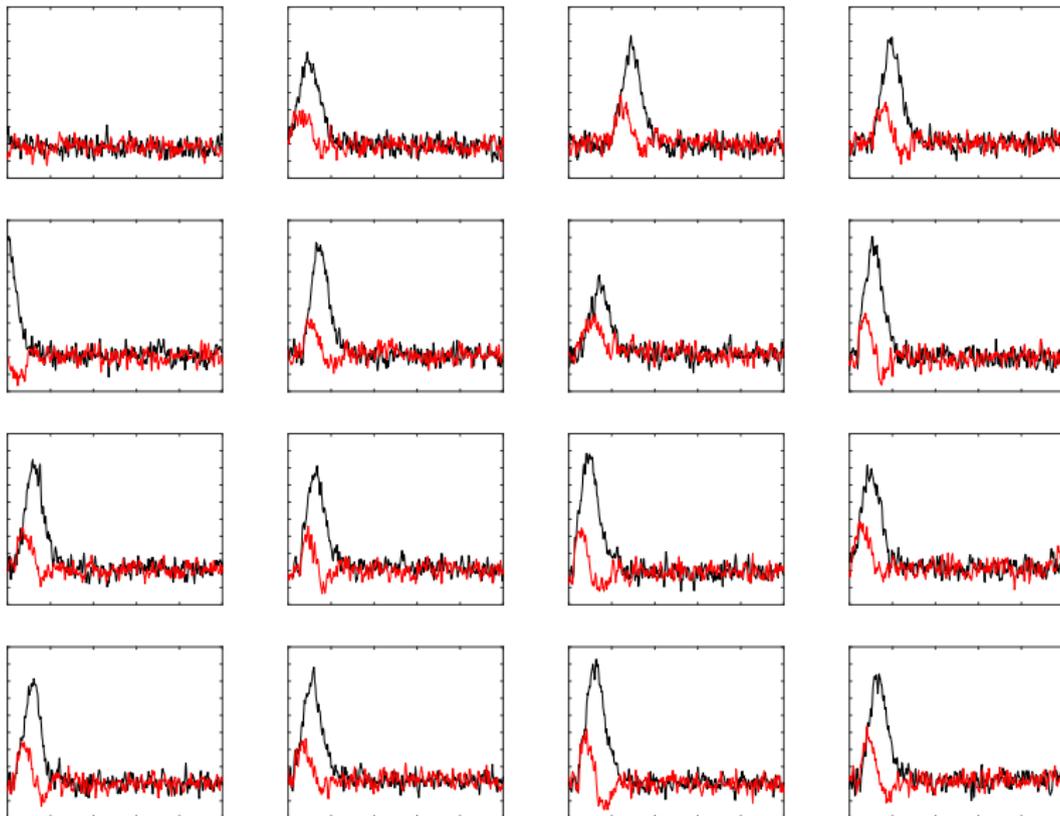
d0 = 400 ; Acquisition delay
d1 = 260 ; tau

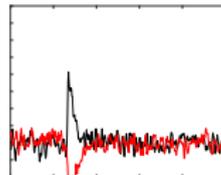
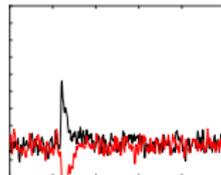
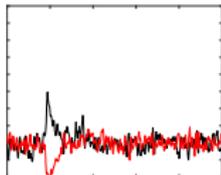
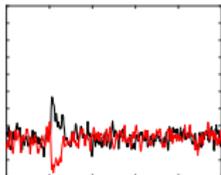
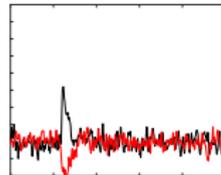
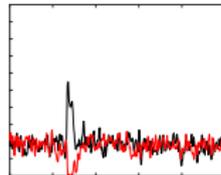
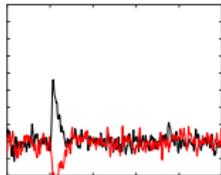
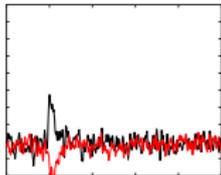
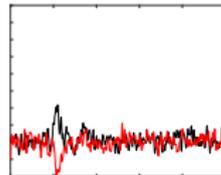
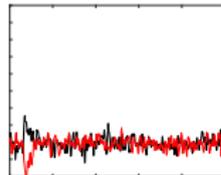
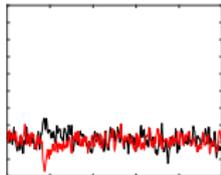
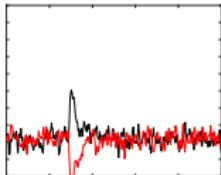
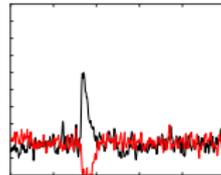
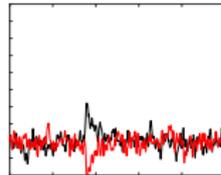
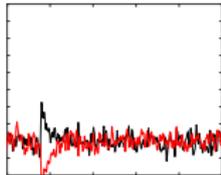
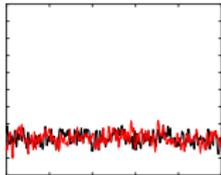
aa0 = 13 ; amplitude
aa1 = 20 ;

ap11 = 0 ; phase pulse 1
ap12 = 180 ;
ap13 = 90 ;
ap14 = 270 ;

ap21 = 0 ; phase pulse 2
ap22 = 180 ;
ap23 = 90 ;
ap24 = 270 ;

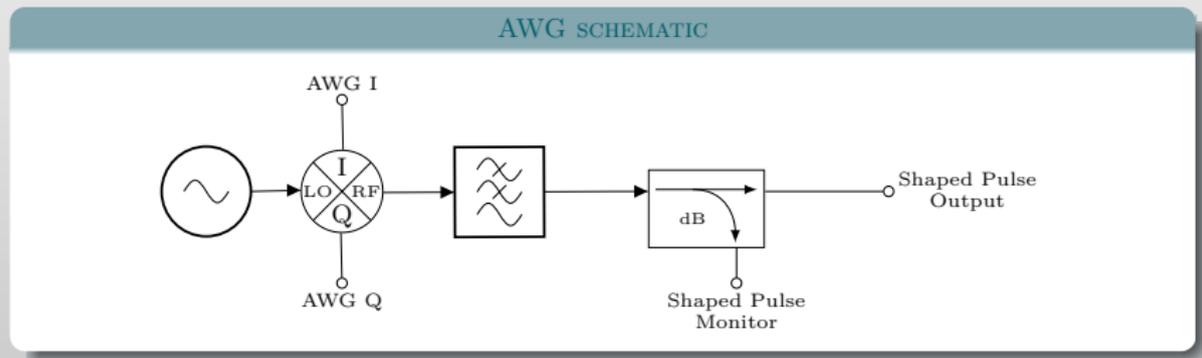
as0 = 0 ; AWG pulse shapes
as1 = 83 ;
end defs
```





- ▶ Newton based methods have good convergence properties, but all need a gradient.
- ▶ Gradient-free optimisation can make an estimate of the gradient through finite differences - but this is usually expensive with little or no gains from an inexact gradient.
- ▶ Simplex methods find better points at each iterate - but convergence is not guaranteed.
- ▶ Simplex methods do not work well with bounds.
- ▶ Most optimisation methods work on smooth function.
- ▶ Optimising an integer variable digitises the surface, potentially creating false stationary points.

- ▶ The AWG can shape the phase and amplitude of a pulse.
- ▶ Used in many optimisation models to send shaped pulses to the experiment.
- ▶ Chirped pulses and Wurst pulses are successful examples.
- ▶ The sent shaped pulse may not be exactly what the experiment sees - may need to create a response function.



[2] P. E. Spindler, Y. Zhang, B. Endeward, N. Gershernzon, T. E. Skinner, S. J. Glaser and T. F. Prisner, *J. Mag. Reson.*, 2012, **218**, 49–58.

[3] P. E. Spindler, S. J. Glaser, T. E. Skinner and T. F. Prisner, *Angew. Chem. Int. Ed.*, 2013, **52**, 3425–3429.

[4] T. Kaufmann, T. J. Keller, J. M. Franck, R. P. Barnes, S. J. Glaser, J. M. Martinis and S. Han, *J. Mag. Reson.*, 2013, **235**, 95–108.

[5] A. Doll, S. Pribitzer, R. Tschaggelar and G. Jeschke, *J. Mag. Reson.*, 2013, **230**, 27–39.

[6] A. Doll and G. Jeschke, *J. Mag. Reson.*, 2014, **246**, 18–26.

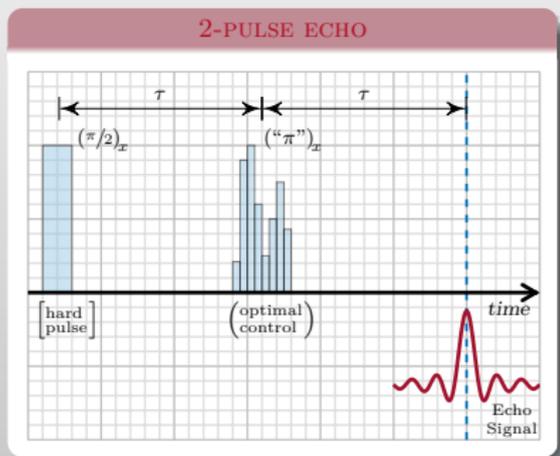
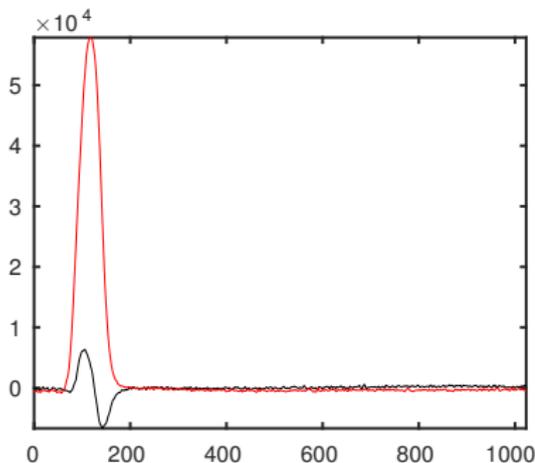
[7] P. Schöps, P. E. Spindler, A. Marko and T. F. Prisner, *J. Mag. Reson.*, 2015, **250**, 55–62.

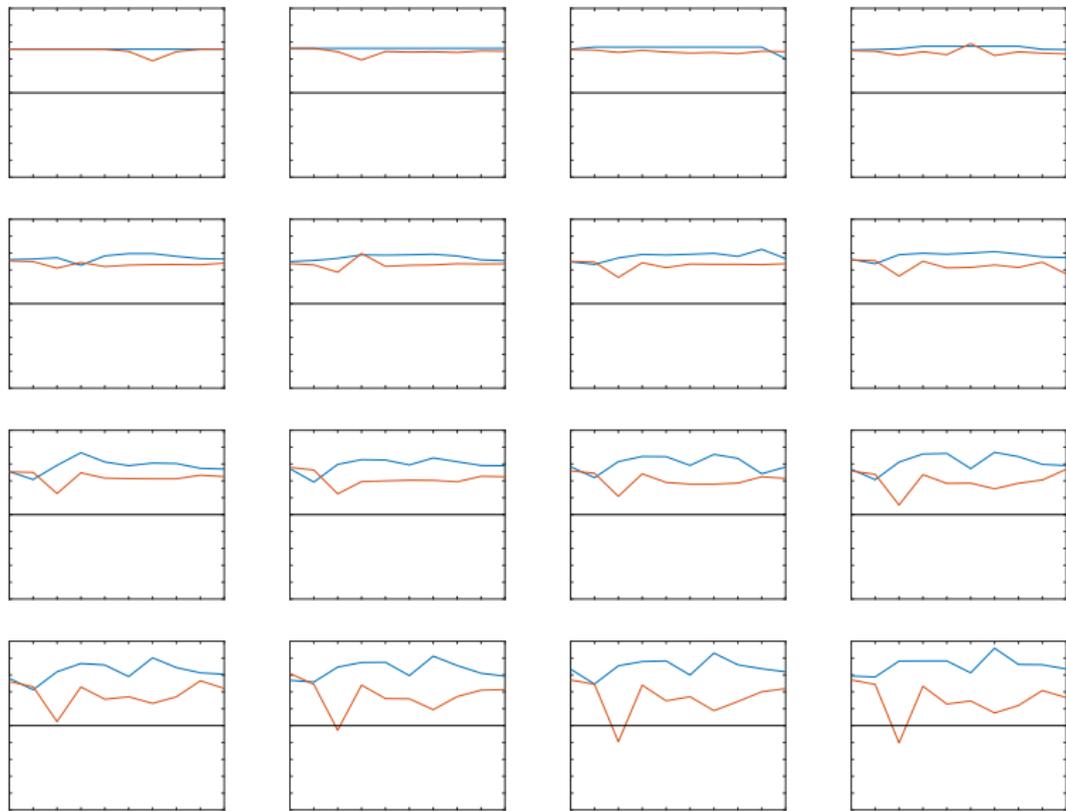
[8] G. Jeschke, S. Pribitzer and A. Doll, *J. Phys. Chem. B.*, 2015, **119**, 13570–13582.

Optimising an Echo

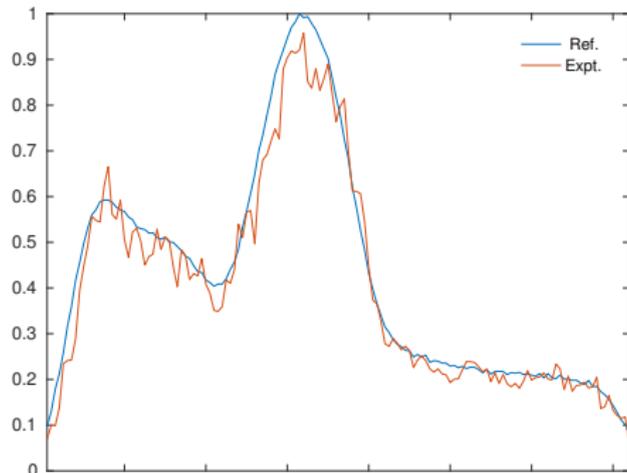
Using a Shaped Waveform

- ▶ Simple, 2-pulse echo experiment.
- ▶ Aim to find an optimised echo.
- ▶ Maximise the area under the real part of the echo signal.
- ▶ Vary the shape of the soft π -pulse.
- ▶ Many pulses take a long time to optimise (as opposed to a chirped pulse which have only 3 or 4 variables to optimise)





- ▶ Another measure to optimise could be the shape of the signal.
- ▶ Requires a reference shape, that which we would like the signal to mimic.
- ▶ Optimise:
 $\langle \text{REFERENCE PLOT} | \text{CURRENT PLOT} \rangle$
- ▶ Any information that can be mathematically extracted from the signal can be optimised (better optimisation if normalised).



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- (4) A. Doll, S. Pribitzer, R. Tschaggelar and G. Jeschke, *J. Mag. Reson.*, 2013, **230**, 27–39.
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- (7) G. Jeschke, S. Pribitzer and A. Doll, *J. Phys. Chem. B.*, 2015, **119**, 13570–13582.
- (8) T. Kaufmann, T. J. Keller, J. M. Franck, R. P. Barnes, S. J. Glaser, J. M. Martinis and S. Han, *J. Mag. Reson.*, 2013, **235**, 95–108.