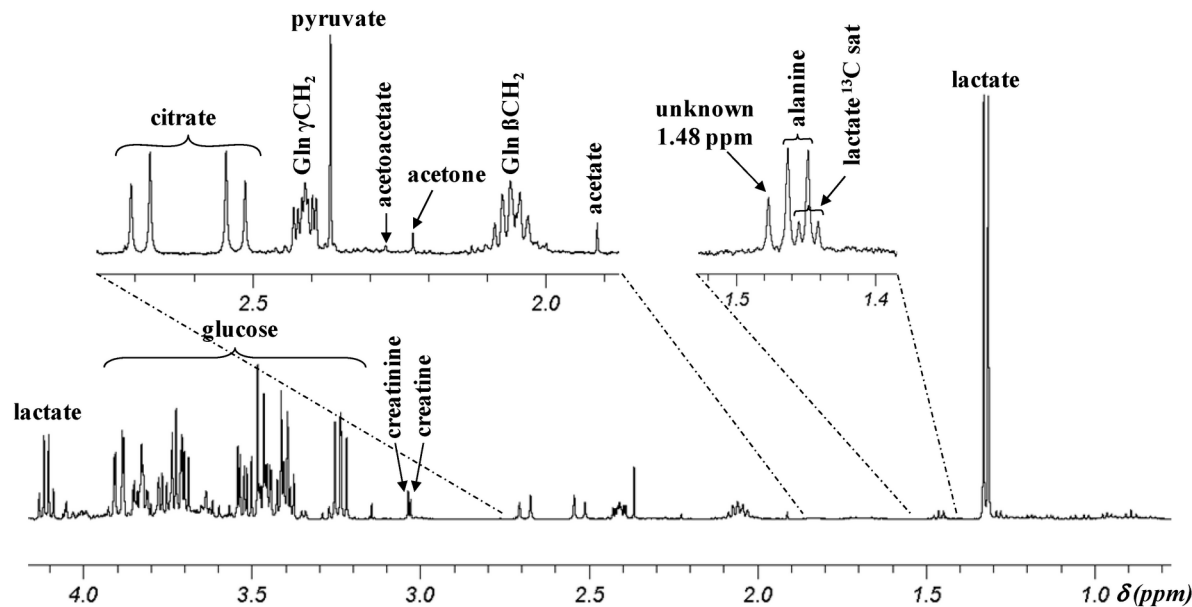
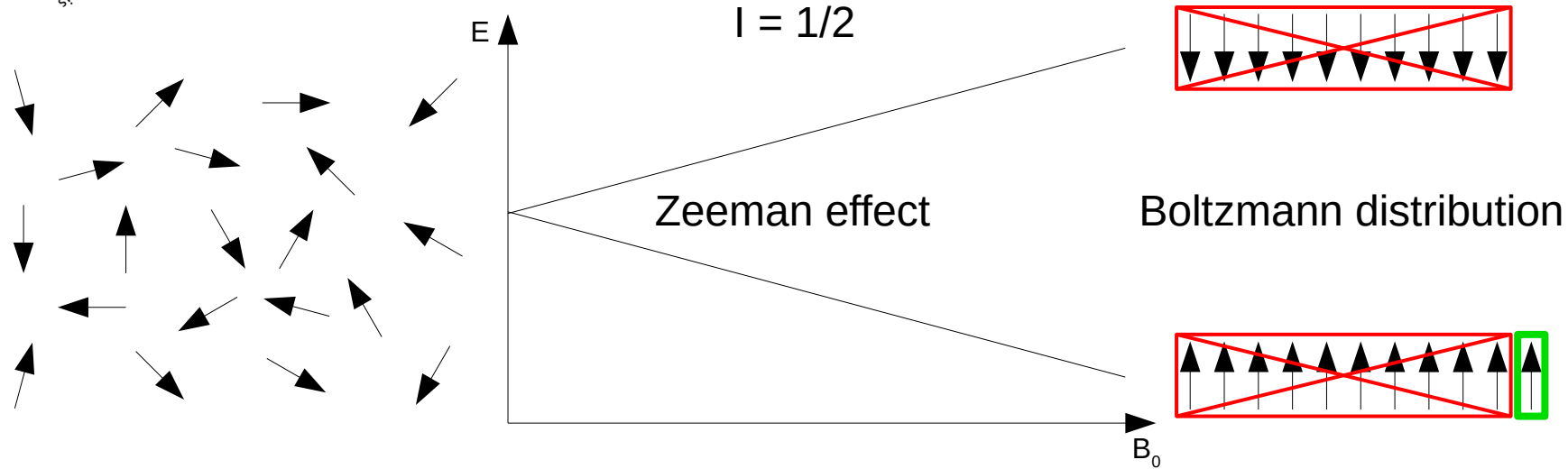


Simulating and denoising NMR spectra under Python

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Nuclear magnetic resonance (NMR)

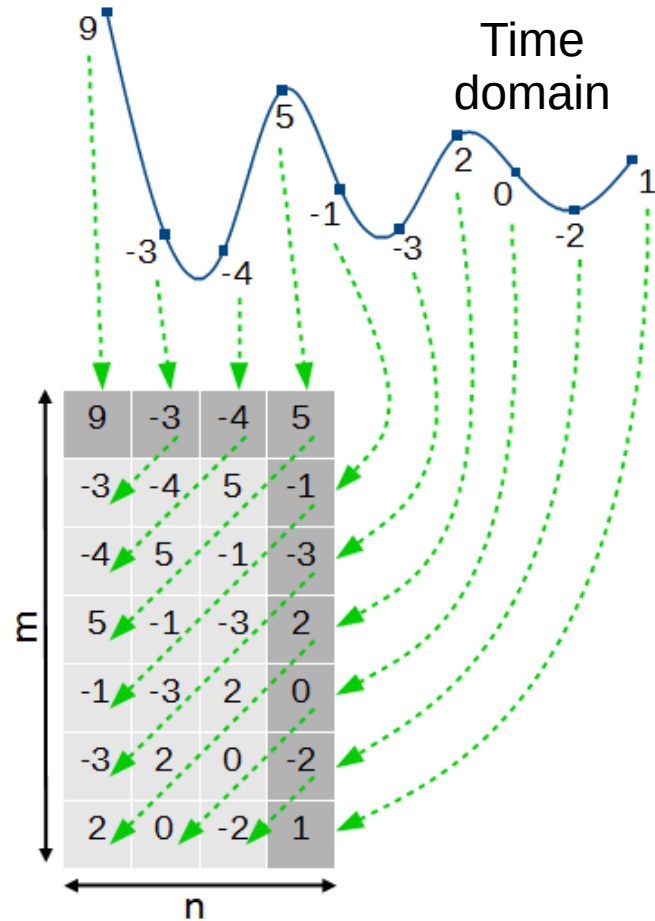


One nucleus over 10^5 is visible
Poor sensitivity

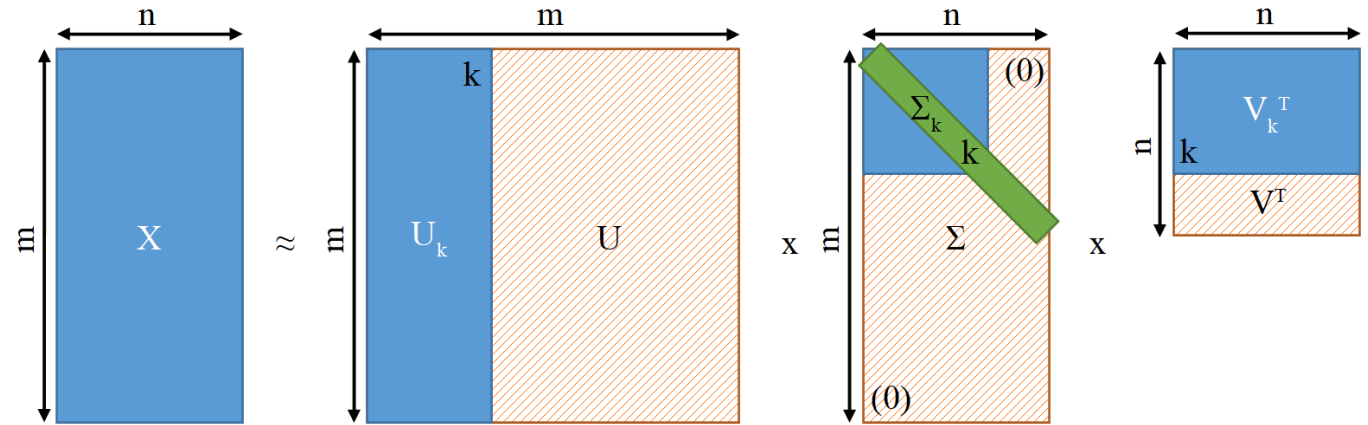
Spectroscopy
Powerful local probe

Ex: Alzheimer disease

Singular Value Decomposition (SVD) JDEV



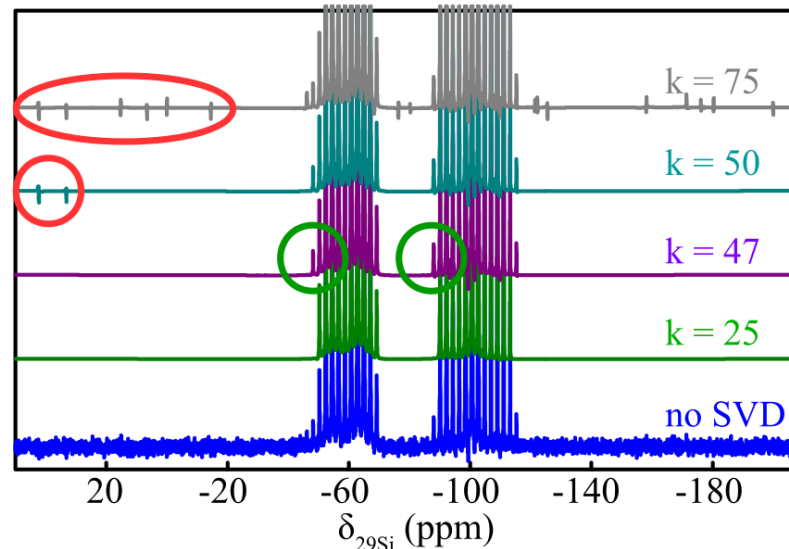
M. A. Arbib and E. G. Manes, *J. Comput. Syst. Sci.*, 20, 3, 330–378 (1980).



Low rank matrix approximation

D. W. Tufts *et al*, *P. IEEE*, 70, 6, 684–685 (1982).
 J. A. Cadzow, *IEEE T. Acoust. Speech*, 36, 1, 49–62 (1988).

Frequency domain



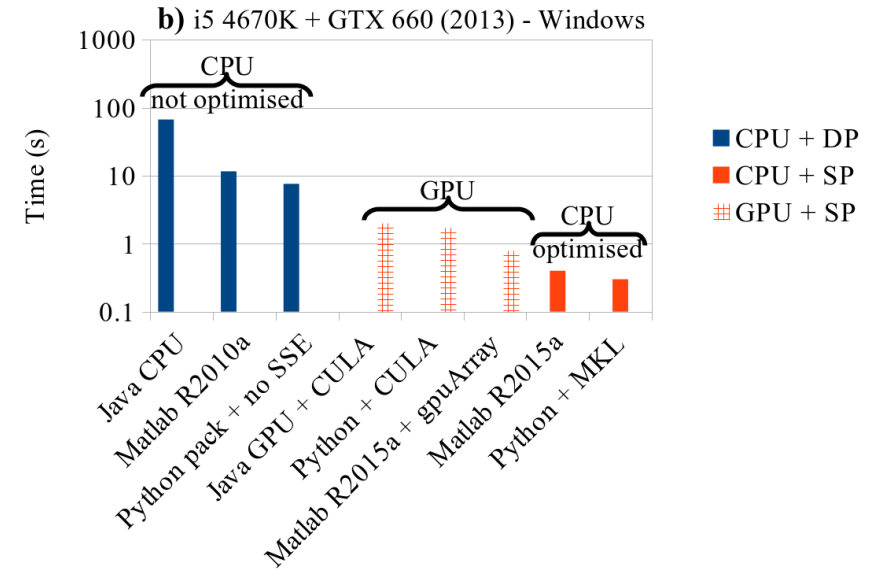
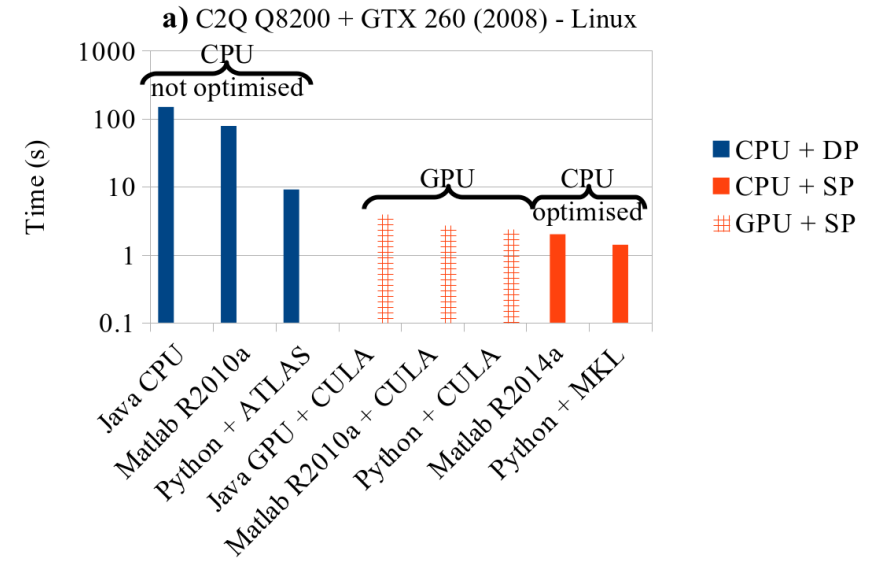
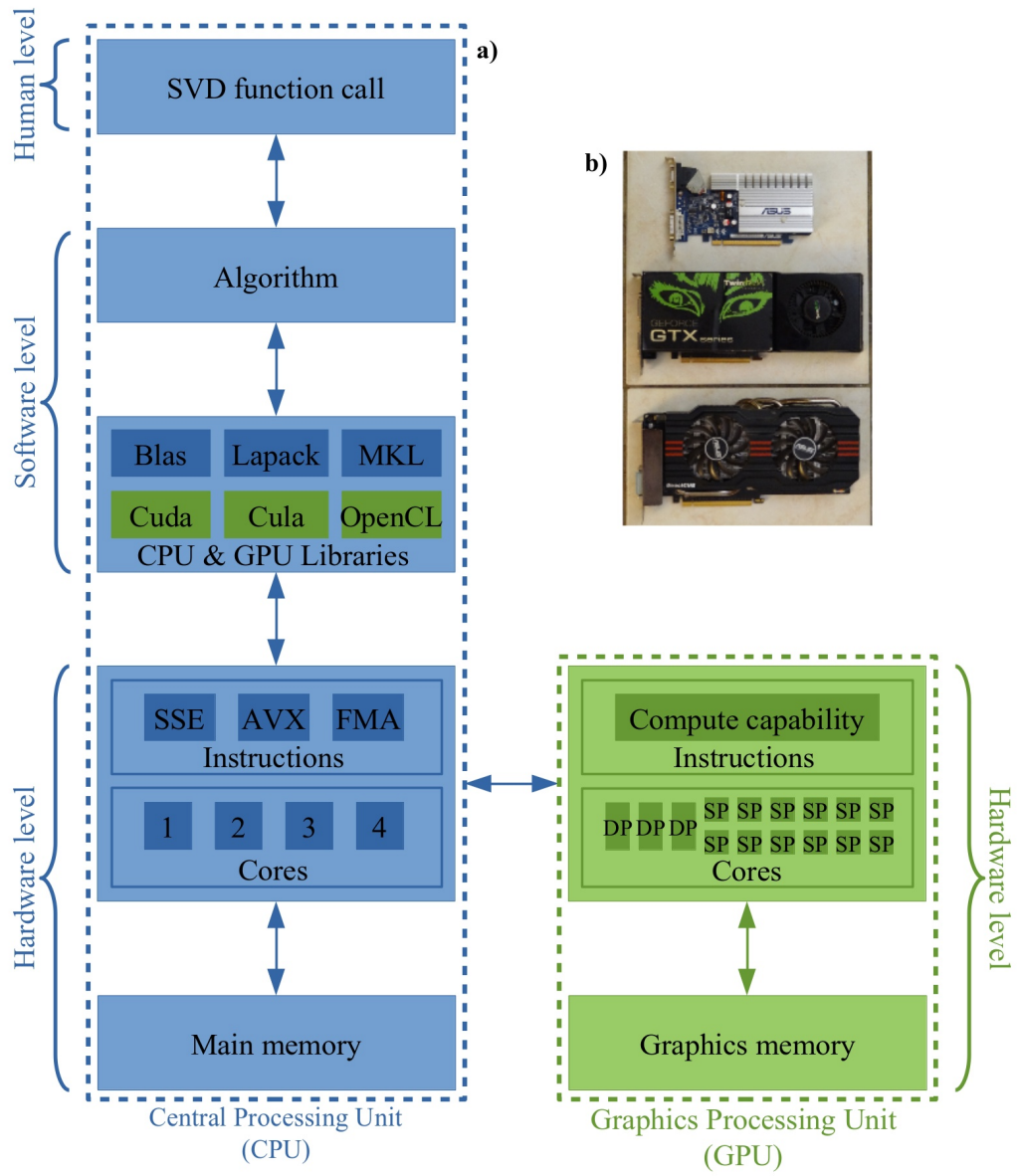
G. Laurent *et al.*, *Appl. Spectrosc. Rev.*, 54, 602–630 (2019).

Automatic thresholding

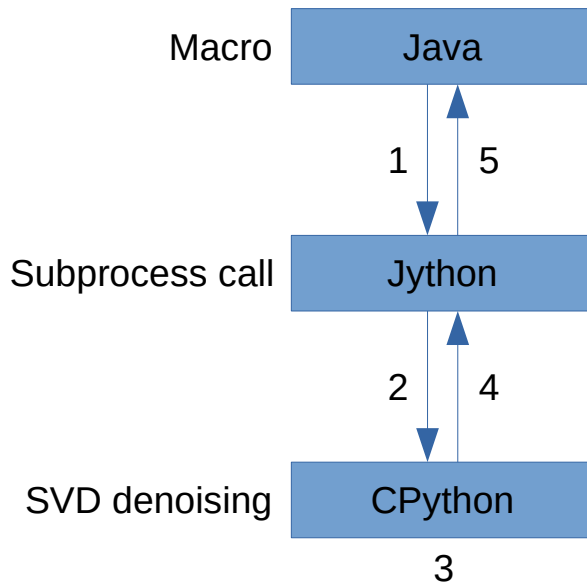
E. R. Malinowski, *Factor analysis in chemistry* (Wiley, 3rd ed., 2002).

Image compression, data mining
 (Principal Component Analysis, PCA)

SVD computation time



SVD on NMR spectra

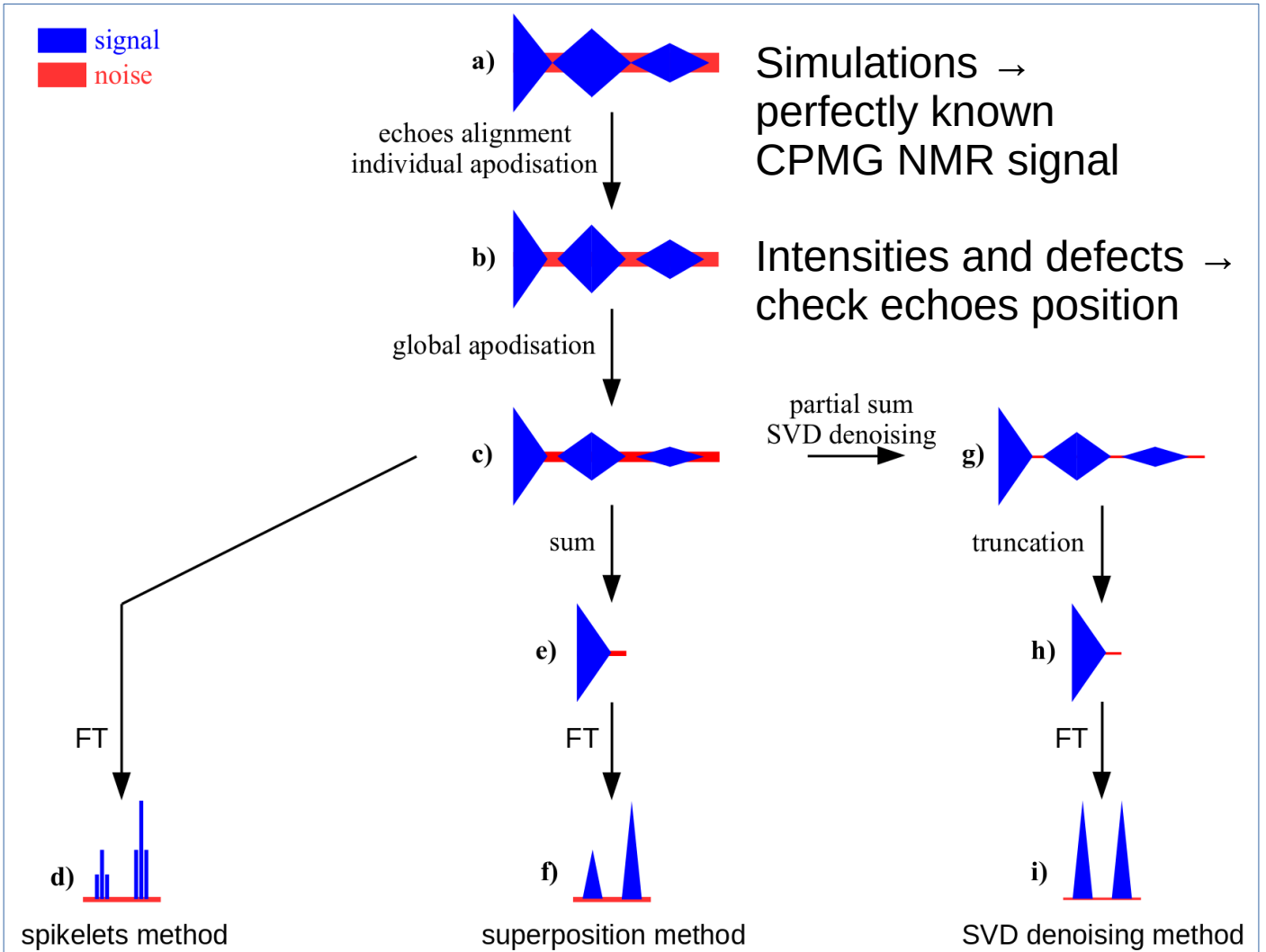


2

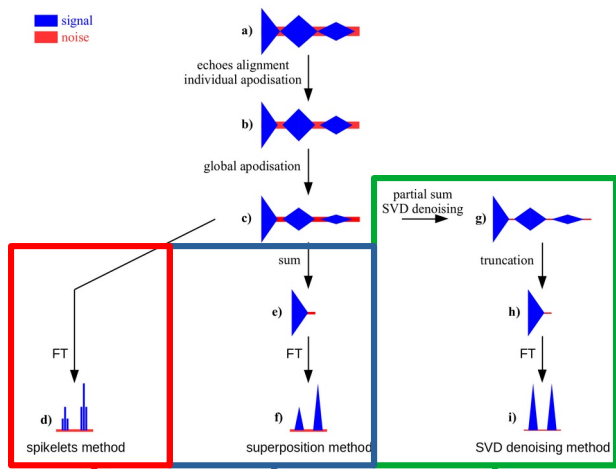
```
p = Popen(COMMAND_LINE,
          stdin=PIPE, stdout=PIPE, stderr=PIPE)
```

```
output, err = p.communicate()
```

3



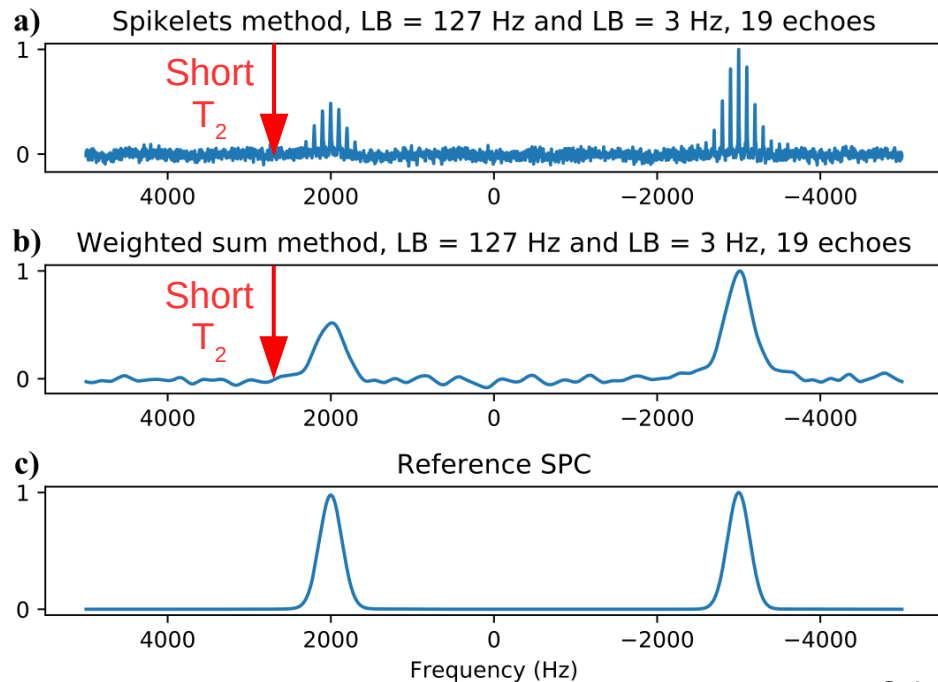
CPMG Methods comparison



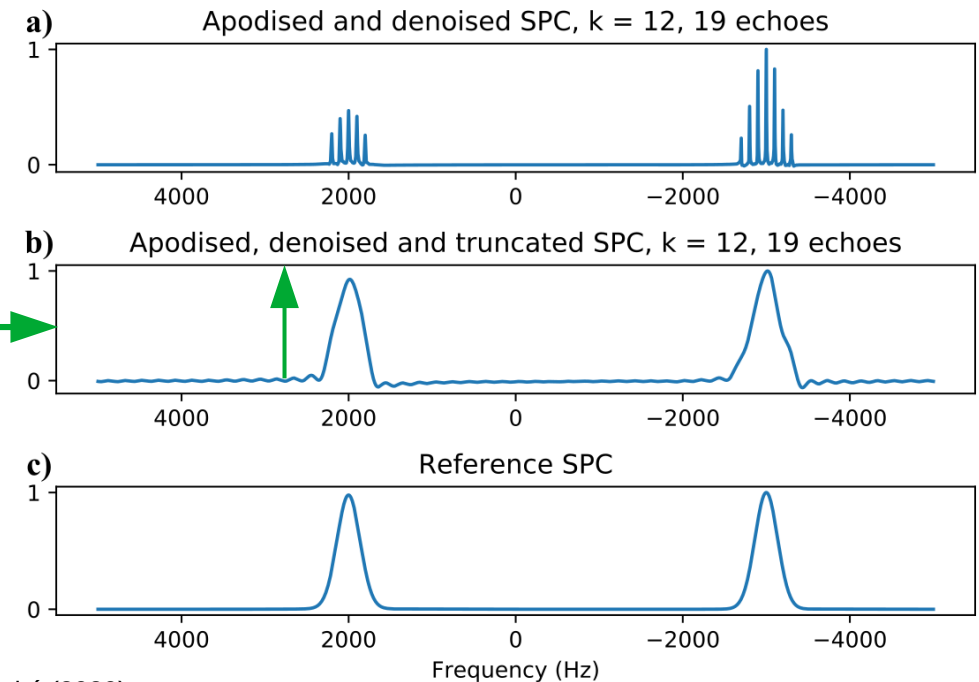
Relaxation → distortions

Corrected intensities

CPMG NMR signal processing - standard methods



CPMG NMR signal processing - denoising



SVD useful to denoise spectra

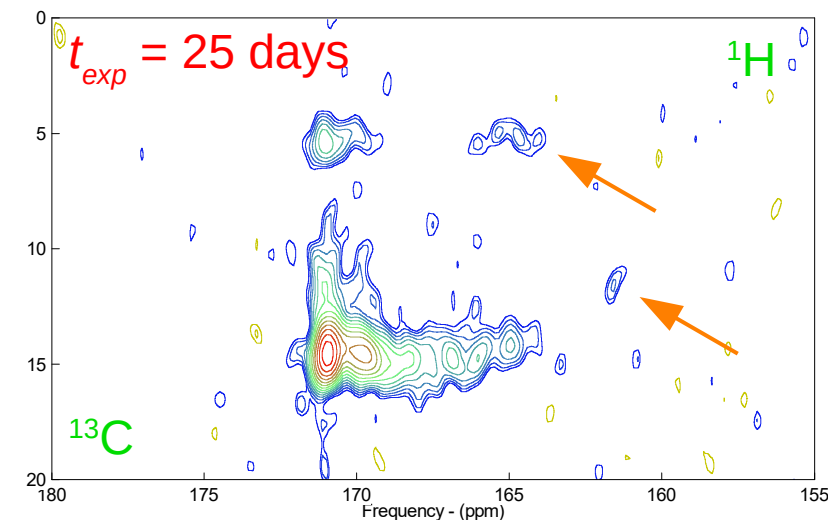
Integration to manufacturer software

Experiment time gain ~2.3

Computation time gain ~100

Improve 2D denoising

Sparse matrices



W. Ajili et al., *J. Phys. Chem. C*, in press, doi:10.1021/acs.jpcc.0c00280.

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- Pierre-Aymeric Gilles (2017)

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