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Spectra Denoising using Graphic Cards

Guillaume Laurent, Pascal Ping Man, Christian Bonhomme

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Context

CSPTC

TEOS

PVDF-HFP

Electrospinning → membrane

MAS 7 mm

MAS 4 mm

4 days
Maximum reasonable experiment time
Signal / Noise too low

V. Maneeratana et al, *Adv. Funct. Mater.* **2013**, *23*, 2872–2880

Tools

CPMG Echoes

repeat n times

4 times signal increase

T₂ distortions

H. Y. Carr and E. M. Purcell, *Phys. Rev.*, **1954**, *94*, 3, 630–638
 S. Meiboom and D. Gill, *Rev. Sci. Instrum.*, **1958**, *29*, 8, 688–691
 W. J. Malfait and W. E. Halter, *J. of Non-Cryst. Solids*, **2008**, *354*, 34, 4107–4114

SVD denoising

Temporal signal = before Fourier Transform

Matrice de Hankel

J.A. Cadzow, *IEEE Trans. Acoust. Speech Signal Process*, **1988**, *36*, 49–62
 P. Man, C. Bonhomme, F. Babonneau, *Solid State Nucl. Mag.*, **2014**, *61*-62, 28-34

Results

CPU vs GPU

CPU : Central Processing Unit
GPU : Graphics Processing Unit

CPU : 60-474 s / GPU : 3-20 s
20 times speedier

S. Lahabar, and P. J. Narayanan, *IEEE International Symposium on Parallel Distributed Processing, IPDPS*, 2009, 1-10

SVD Parameters

MTEOS/TEOS 50/50
29Si, CPMG, 4028 points, 22 SVD points

2014 columns
512 columns
128 columns
32 columns
no SVD

29Si CPMG, 4028 points, 2014 columns

75 SVD values
50 SVD values
47 SVD values
25 SVD values
no SVD

Square matrix, manual number of values
Minimum signal / noise = 2

Real samples

CSPTC/TEOS/PVDF-HFP
29Si, Hpdcc 4 days, 956 points, 478 columns

29Si, CPMG 4 days, 956 points, 478 columns

Improved results with preprocessing

Highlights

- Possible analysis of highly noisy spectra
- Short denoising time with GPU
- Easy to use
- Low cost (Nvidia GTX 750 = 120 €)

Future work

- Automatic number of SVD values
- NMRLab with Matlab
- Sparse matrix
- T₂ corrections

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