11th CONFERENCE ON FAST FIELD CYCLING NMR RELAXOMETRY

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Extra Byte snc

FIELD CYCLING RELAXOMETRY OF POLYDISPERSED SAMPLES: SOME SPECIAL ASPECTS

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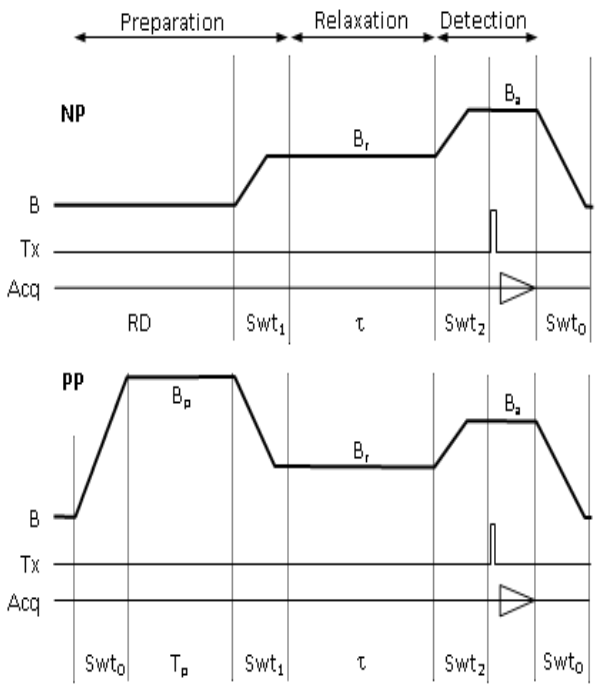
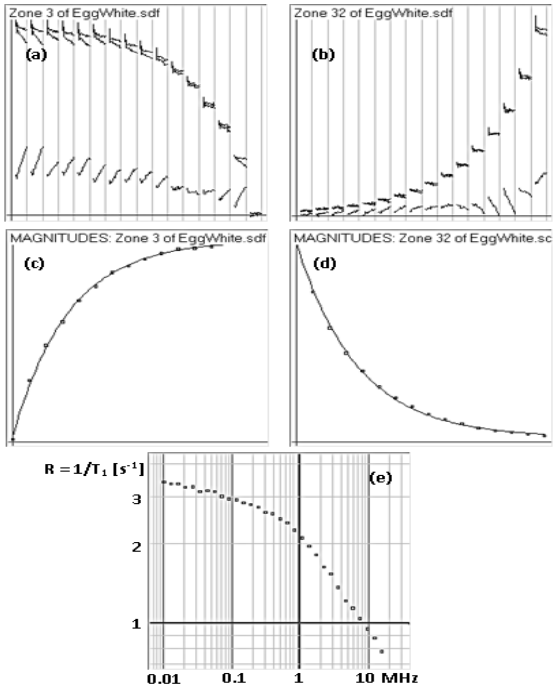
Field-Cycling NMR (**FFC** or **sample-shuffling**)

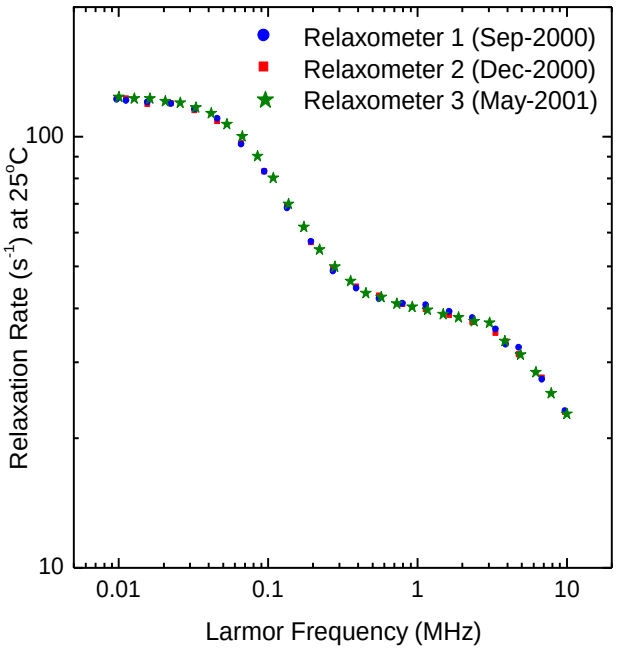
is great at measuring NMRD profiles of **single-component** samples

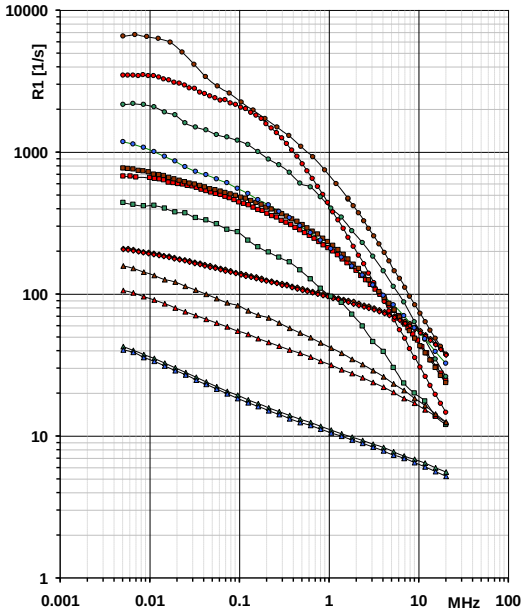




By single-component I will mean that the $S(\tau, B_{rlx})$ are, within experimental errors, **mono-exponential**

FC-NMR is also great at measuring **single-component samples** whose NMRD profiles are composite (**multiple relaxation paths**)

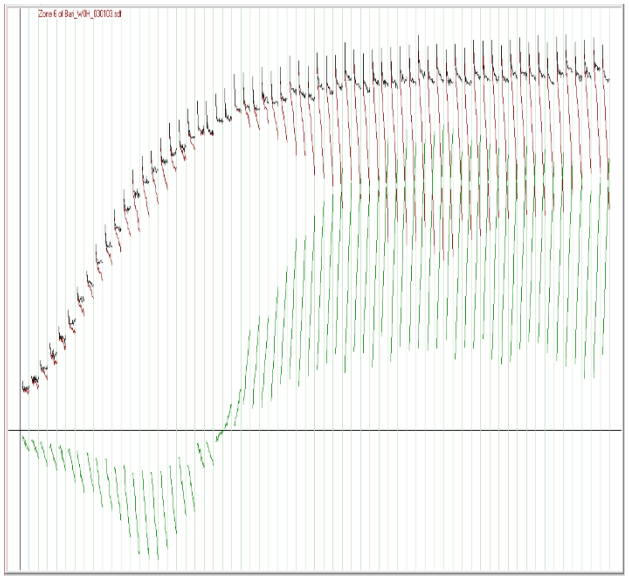


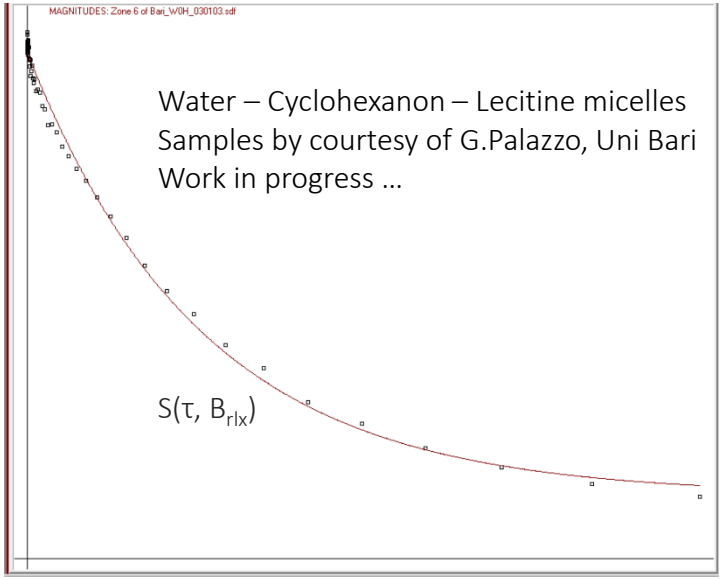


What about FC of multi-component samples?

When we intend only a **small number k of discrete components** that are distinguishable in the decays $S(\tau, B_{rlx})$, then this is not really a new idea.

Yet it is **a bit problematic** and quite **time consuming**, so it is **rarely done**.

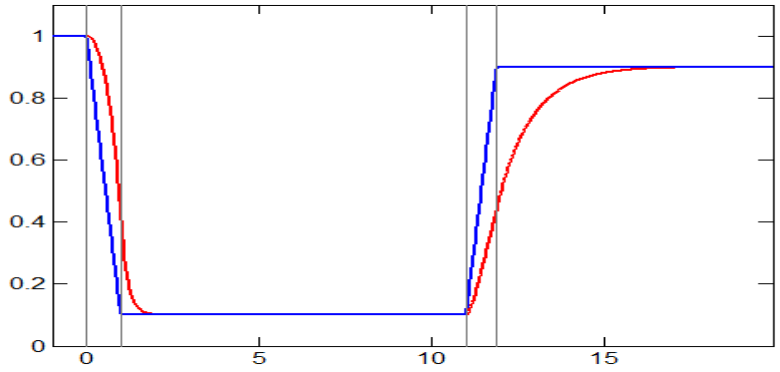




Why is it problematic (pardon, … challenging)? Part I

First, a doubt:

During the FC experiment, the sample is subject to crazy magnetic field rides. Can we be **really sure** that the measured relaxation rates are the correct ones, corresponding just to the specified relaxation field B_{rlx}?



The answer is affirmative: under relatively broad assumptions, the measured values of $R_k(B_{rlx})$ are correct, regardless of what happened to the field before and after the nominal relaxation period. Amazing.

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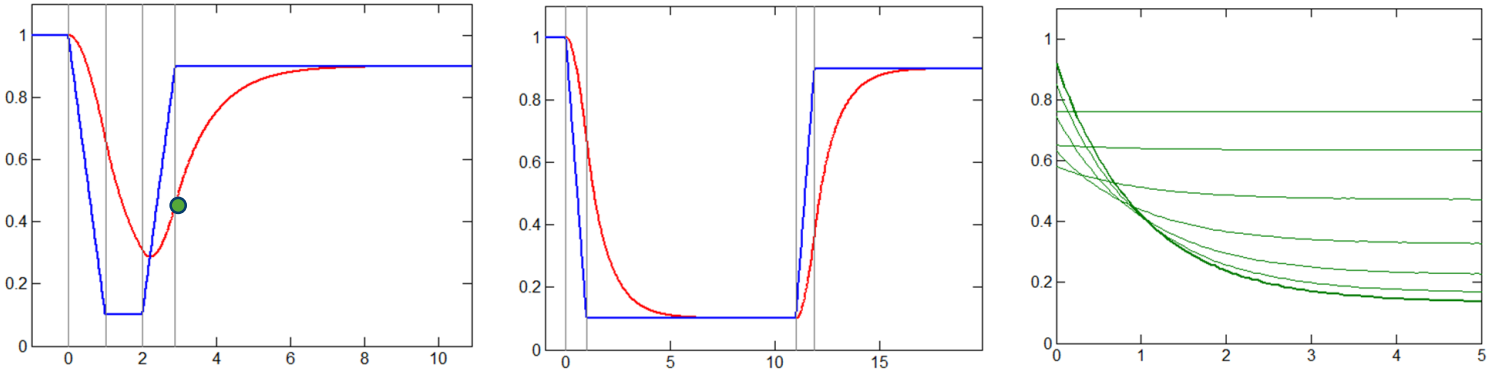
Why is it challenging? Part II

Second, a certainty:

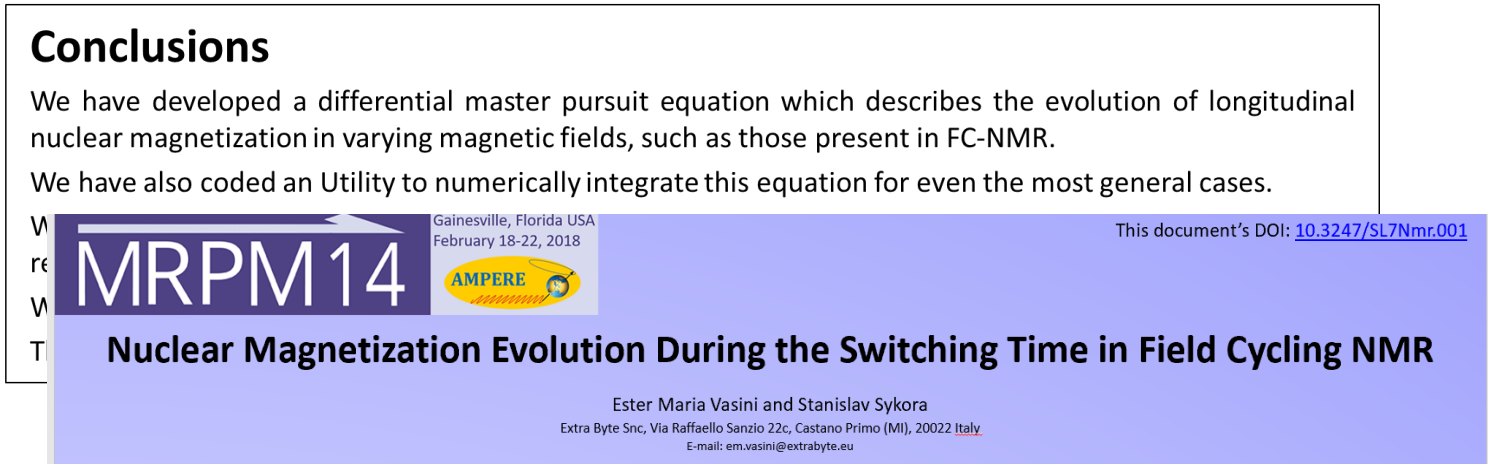
The magnetization of the k-th component $S_k(\tau, B_{rlx})$ evolves during acquisition of the signal $S(\tau, B_{rlx})$ in a way that **does depend** upon the magnetic field switching waveforms, as well as on the component's specific NMRD profile.



It follows that the apparent **weights W_k of the individual components** of the $S(\tau, B_{rlx})$ curve **depend on the field-switching waveforms and thus on B_{rlx}**.

A little bit of luck

Fortunately, we were able to derive a closed formula which makes it possible to correct the component weights, provided that one knows their NMRD profiles $R_k(B_{rlx})$, and carries out a prior calibration of the field-switching waveforms.



Conclusions

We have developed a differential master pursuit equation which describes the evolution of longitudinal nuclear magnetization in varying magnetic fields, such as those present in FC-NMR.

We have also coded an Utility to numerically integrate this equation for even the most general cases.

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Nuclear Magnetization Evolution During the Switching Time in Field Cycling NMR

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Note: the corrections are not needed when, at any magnetic field value traversed during the switching intervals, the T_1 values of a component are a few times longer than the switching times.

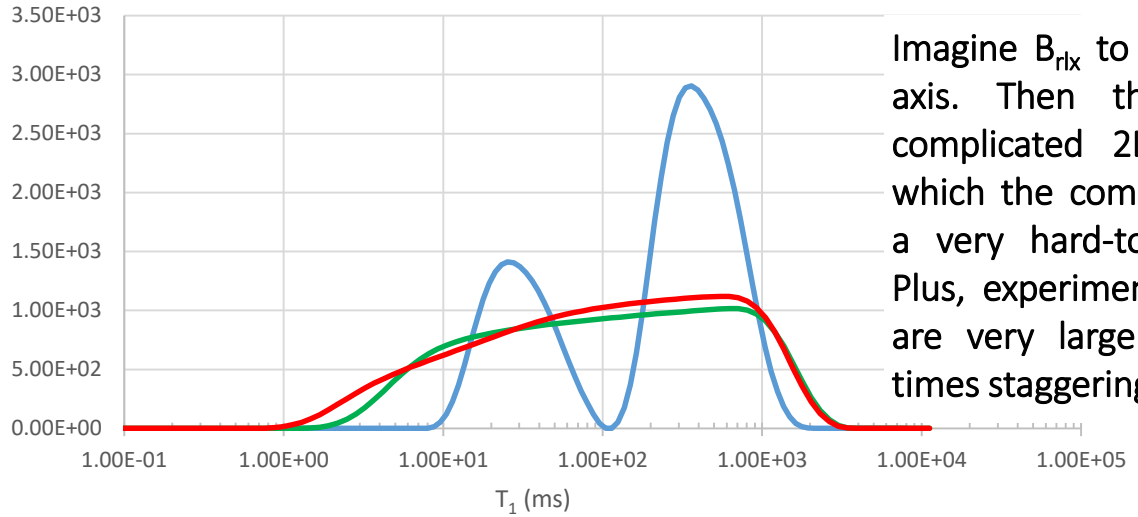
Workflow for FC of multi-component samples

- Pre-calibrate your magnetic field-switching waveforms for any field «jump» to be useed. Demanding, but yes, it can be done.
- Measure the experimental relaxation curve $S(\tau, B_{rlx})$ at a series of field values covering the full range of fields that will be traversed during field switching intervals.
- At each value of B_{rlx}, decompose the $S(\tau, B_{rlx})$ curve - by whatever means - into its discrete components, thus obtaining the separate NMRD profiles $R_k(B_{rlx})$.
- Correct the weight W_k of each component by applying the known formula.

The Next and Really Scary Thing!

What about samples exhibiting a **continuous distribution of R_1 rates**?

A micellar system evaluated by UPEN at 3 different values of B_{rlx}



Imagine B_{rlx} to be an additional axis. Then this leads to a complicated 2D surface along which the components move in a very hard-to-model manner. Plus, experimental uncertainties are very large and acquisition times staggering …

I do not think that we can crack such cases any soon!

Even if ILT were much better behaved than it is, the complexity intrinsic in a continuous distribution of components, each of them with a different NMRD profile, potentially with multiple and distinct relaxation paths, exeeds the information content of FC.

<u>Perhaps with new pulse sequences, acquisition techniques, … and much patience</u>

Thank you all for your attention!

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