KUPROV I.

От: Malcolm Levitt [malcolm.levitt@soton.ac.uk]
Отправлено: 15 October 2008 22:38
Кому: KUPROV I.
Тема: Re: Zero track elimination.

Отметка "К исполнению": К исполнению
Состояние отметки: Отмечено

Hi Ilya,

> On a different note, do you and your research group members have a "wish list" for what features you'd like to see implemented in NMR simulation software and (importantly) its graphical user interface? Our current plan is for the GUI to be compatible with most existing simulation suites (Save As... 'Simpson input' etc), but any specific wishes would be much appreciated.

I think it would be good to meet up and talk this through. I certainly have ideas but dont have time to put them down on a paper in a formal way. Its really important that a GUI starts off with the right concept. For me the main thing I would like to see happen would be to create an infinite hierarchical structure in which pulse sequences may be assembled from blocks which can inherit parameters from their parents but which can also have locally defined parameters. The overall parameters should include overall phases and frequencies. The pulse sequence blocks may have their internal protocols for how to respond to changes in control parameters (for example, internal handling of finite pulse lengths, etc.).

If this is done properly and demonstrates its power in a simulation context one may have some hope of a real hardware implementation happening as well for real spectrometer control.

best wishes and good luck
malcolm

From: Malcolm Levitt [mailto:malcolm.levitt@soton.ac.uk]
Sent: Friday, September 26, 2008 2:51 PM
To: KUPROV I.
Subject: Re: Zero track elimination.

Dear Ilya,
thanks for the beautiful article, which is extremely well-written, by the way.

I guess I retain a *little* scepticism about the usefulness of this in solids, where such algorithms are particularly badly needed. The J-coupling cases you choose for demonstration are a little "easy", since the relatively large chemical shift differences will (approximately) truncate the smaller couplings, giving rise a problem particularly well-adapted to this type of pruning. So I feel that some of your more general statements might be a bit optimistic, or at least not demonstrated to a level beyond criticism.
I really hope that you can apply this to some really hard solid-state NMR problems, for example the simulation of 13C lineshapes in MAS NMR where the 13C is coupled to many protons and subjected to a

multiple-pulse sequence as well as the MAS. There are quite a few methodological problems in solids crying out for this type of simulation. Another case is the simulation of 1H lineshapes in the presence of MAS and homonuclear decoupling. In addition there is the propagation of high spherical tensor ranks in networks of spins - here your restriction to 4-spin orders is clearly not suitable.

I'm sure you are thinking on these lines too, and I really hope you find a way to implement these things in SIMPSON or similar, so that the community can really run it through its paces. I've little doubt it will be a big advance in the field and lead in turn to even bigger advances and new experiments.

best wishes

malcolm

On 17 Sep 2008, at 11:09, KUPROV I. wrote:

Dear Malcolm,

section 3 of the enclosed paper answers your question. Counterintuitive as it is, if the magnitude of a given state is identically zero within the first step, it stays that way for the rest of the simulation. If it's small, but non-zero, the situation is more complicated, but still tractable.

Best wishes,

Ilya.

<Kuprov - JMR, in press.pdf>

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