KUPROV I.

От: Stefan Stoll [sstoll@ucdavis.edu]
Отправлено: 10 October 2008 19:26
Кому: KUPROV I.
Тема: Re: SSR2

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

Dear Ilya,

things I would love to have in a GUI are:
- visual display of pulse sequence, with delays editable
- ability to edit pulse lengths
If you are also planning to add data browsing and editing functionality, the list would be very long, but most of it is probably identical to NMR requirements.

For EasySpin, the pulse interface documentation will come out with the next release. You are welcome to include an EasySpin export function.

Best
Stefan

KUPROV I. schrieb:
> Dear Stefan,
>
> we are thinking about creating a graphical user interface for the
> state space restriction program. The current plan is to make a
> standalone GUI that would be able to produce text inputs for a variety
> of existing simulation packages. Two questions in connection to that:
>
> 1. Do you have a 'wish list' of what features a 'good' GUI should have?
> Any comments or suggestions would be much appreciated.
>
> 2. May we include 'EasySpin input' into Save As menu? Essentially, the
> program would save a Matlab script prepared as the user manual
> prescribes.
>
> Best wishes,
> Ilya.
>
> -----Original Message-----
> From: Stefan Stoll [mailto:sstoll@ucdavis.edu]
> Sent: Tuesday, September 30, 2008 12:59 AM
> To: KUPROV I.
> Subject: Re: SSR2
>
> Dear Ilya,
>
> congratulations on getting money for your research.
> Have you been in contact with Veshtort from MIT and Nielsen from Arhus
> about their programs? It seems they are widely used in the community.
> Are you planning to render their efforts obsolete?
>
> Concerning EasySpin, I hope I can find some time to look where your
> ideas might be helpful. Then it would be great if we could show
> together that your ideas work well in some situations in EPR/EasySpin.
>

> Best
> Stefan
>
> KUPROV I. schrieb:
>> Dear Stefan,
>>
>> It's got an acknowledgement to you at the end. :)
>>
>> The ZTE/Lanczos procedure described there is much more
>> straightforward to implement for any matrix solver (spin-space as
>> well as spin) than
> SSR
>> - literally five lines in Matlab. It can be used by itself, although
> it
>> works best on top of SSR. Well-commented source code is in the
>> supplementary information.
>>
>> I've just got a three-year grant from UK's EPSRC to push ahead with
> this
>> research, so two more people will now be working on it with a view of
>> producing a powerful and user-friendly (i.e. GUI + kernel) NMR
>> simulation package. I will shortly be collecting "wish lists" from
>> the community for what needs to be included. I am very anxious at the
>> same time not to trespass on the EPR territory, where EasySpin
>> currently seems to be a standard -- it would be best to incorporate
>> (whenever
>> reasonable) these technologies directly into EasySpin instead.
>>
>> Best wishes,
>> Ilya.
>>
>>
>> -----Original Message-----
>> From: Stefan Stoll [mailto:sstoll@ucdavis.edu]
>> Sent: Thursday, September 25, 2008 10:05 PM
>> To: KUPROV I.
>> Subject: SSR2
>>
>> Hi Ilya,
>> just saw your next paper about state space reductions.
>> Looksg reat! Goes onto my reading stack.
>> Cheers
>> Stefan
>>
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