

RE: CoMP-MRS - Bruker loader progress

From Thanh Phong Lê <thanh.le@epfl.ch>

Date Fri 2025-01-24 4:46 AM

To Georg Oeltzschner <goeltzs1@jhmi.edu>; Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>

Cc Diana Georgiana Rotaru <dr3309@columbia.edu>; Jamie Near <jamie.near@utoronto.ca>

External Email - Use Caution

Hello Georg,

With pleasure!

- 1. Indeed, the value of *PVM_EncChanScaling* is copied into *RecoScaleChan* so you can use either. Is this parameter available in PV5 as well?. These coefficients are not calculated from the data you are processing: the values are purely obtained from hardware calibration. It is the product of a correction factor for each element sensitivity (defined in its coil file) and a correction factor for each receive channel (normally calibrated by Bruker service). Don't be surprised if they are set to one in some datasets, such as Cristina's 14.1T scans: it just means that no one ever bothered to do the calibrations:)
- 2. Okay, in my previous email I was only looking at Paravision 360 (v3.x). Looking between versions for STEAM and PRESS (the only Bruker stock MRS sequences that were available in all versions), it looks like the EDC, RFL, scaling of the channels, averaging of transients seem similar. At least the same arguments are given to the same functions in the reconstruction network. However, I noticed a difference in how the channels are combined (for both the main scan and the reference scan): In PV 6.0 and 7.0 the channels are summed, while in PV 360 V1.0 and onwards the channels are averaged. This global scaling should not affect the further steps, but it is useful to take into account to compare between Bruker's processing and your own processing. For differences in Paravision 5, I don't know, because I have not yet been able to get my hands on the installation disk or a copy of the source sequence files. If you happen to have a PV 5 reco file with the parameter *RecoStageNodes* saved, I will be happy to have a look!

Best,

Thanh

De: Georg Oeltzschner <goeltzs1@jhmi.edu>

Envoyé: jeudi, 23 janvier 2025 20:01

À: Thanh Phong Lê <thanh.le@epfl.ch>; Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch> Cc: Diana Georgiana Rotaru <dr3309@columbia.edu>; Jamie Near <jamie.near@utoronto.ca>

Objet: Re: CoMP-MRS - Bruker loader progress

Dear Thanh.

Thank you so much for this very detailed explanation - I think I'm seeing a little clearer, but not perfectly clear yet.

Please allow me two follow-up questions:

- 1) Not all of the datasets that I am trying to process have a "reco" file (some only have the "rawdata.job0"). Are the values for RecoScaleChan stored somewhere else? (I have found the array "PVM_EncChanScaling" that has as many elements as there are channels, does that array contain the same information?) If not, can you share how the software estimates the RecoScaleChan coefficients from the raw data?
- 2) Are there any differences in the data processing scripts between PV versions? I have a PV5 "reco" file that does not have the RecoScaleChan field at all (although that might be because there's only one channel).

Thanks again for any pointers you can offer,

Georg

From: Thanh Phong Lê < thanh.le@epfl.ch>
Sent: Wednesday, January 22, 2025 5:47 PM

To: Cristina Ramona Cudalbu < cristina.cudalbu@epfl.ch; Georg Oeltzschner < goeltzs1@jhmi.edu cc: Diana Georgiana Rotaru < dr3309@columbia.edu; Jamie Near < jamie.near@utoronto.ca cristina.cudalbu@epfl.ch; Georg Oeltzschner < goeltzs1@jhmi.edu cc Diana Georgiana Rotaru < <a href="mailto:driventa-bulba:driv

Subject: RE: CoMP-MRS - Bruker loader progress

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Hello everyone,

I'm very happy to help! If I understand correctly, the issue is to figure out exactly how Bruker goes from "rawdata.job0" to "fid_proc.64".

1a. The coefficients for the coil combination are found under the parameter "RecoScaleChan", which is saved in the "reco" file. The coefficient takes into account the differences between the channels of the coil, as well as the differences of sensitivity between the coil socket to the electronics cabinet. Under Bruker's implementation, the signal from each channel is multiplied by its coefficient, then signals from all channels are summed together, then the result is divided by the number of receiver channels ("to avoid integer overflow after channel summation")

Phase: In Bruker's implementation, the Eddy current compensation somehow integrates the receiver phase correction such that the parameter "RecoPhaseChan" is zero for all channels if EDC is ON. Specifically, I think that the phase difference between receivers is already corrected in the file "fid_refscan.64".

1b. Average or sum: It might depend on the sequence. We need to look at the argument of "RecoAverageFilter". In the "reco" file from a STEAM acquisition we did on the 9.4T, I see:

```
(<compute>, 0, <RecoAverageFilter AVE0{avList=\<AverageList\>;avListSize=1;nObj=1;newSize=\<RECO_inp_size\>;}>)
```

The fifth argument inside the {} is a flag for whether the data have to be accumulated or not. It is an optional argument. Here there is nothing and the default argument is false. Therefore, the data are averaged in this case.

1.b. receiver gain: My understanding is that the receiver gain (PVM_RgValue or PVM_RefScanRG) is a parameter of the acquisition and is not considered in the reconstruction, at least I can't find it in the reconstruction network.

By the way, here is how fid_refscan.64 is generated from the reference scan stored in the method file (under ##\$PVM_RefScan):

```
void writeRefFile(void)
{
    DB_MSG(("--> writeRefFile"));
    const int npoints=RECO_inp_size[0]*2; //real+imag pairs
    const int nchan= RecoNumInputChan;
```

```
if (PVM_RefScanYN == Yes && ParxRelsParHasValue("PVM_RefScan") == Yes &&
      ParxRelsParGetDim("PVM_RefScan",1)==nchan && ParxRelsParGetDim("PVM_RefScan",2)==npoints)
{
   FILE *fp=NULL;
   double *phase = PVM_ArrayPhase;
   double *scale= RecoScaleChan;
   char fname[PATH_MAX];
   PvOvIUtilGetProcnoPath(fname, PATH_MAX, "fid_refscan.64");
   fp=fopen(fname,"w");
   if(fp!=NULL)
   {
      double sumRe, sumIm;
      double re, im;
      for(int i=0;i<npoints;i+=2)
          sumRe=0; sumIm=0;
          for (int k=0;k<nchan;k++)
         {
             //phase shift and scaling before channel combination
             re = (PVM_RefScan[k][i] * cos(phase[k]/180.0*M_Pl) - PVM_RefScan[k][i+1] * sin(phase[k]/180.0*M_Pl)) * scale[k]; * line (PVM_RefScan[k][i+1] * sin(phase[k]/180.0*M_Pl)) * line (PVM_RefScan[k][i+1] * line (PVM_RefScan[k]/180.0*M_Pl)) * line (PVM_RefScan[k]/180.0*M_Pl) * line (PVM_RefScan[k]/
             im = (PVM_RefScan[k][i]*sin(phase[k]/180.0*M_Pl) + PVM_RefScan[k][i+1] * cos(phase[k]/180.0*M_Pl))*scale[k];
             sumRe+=re/nchan; //divide by number of channels to avoid integer overflow
             sumIm+=im/nchan;
          fwrite(&sumRe, sizeof(double),1,fp);
          fwrite(&sumIm, sizeof(double),1,fp);
      }
      fclose(fp);
   }
DB_MSG(("<-- writeRefFile"));
```

}

- 1.c. If I did not miss anything, the steps seem to be:
 - 1. For each channel, apply EDC+RFL correction
 - 2. For each channel, Average (or sum) the averages
 - 3. For each channel, scale the data according to RecoScaleChan and apply RecoPhaseChan.
 - 4. Sum all channels then divide the result by the number of channels.
 - 5. This gives the fid_proc.64 file.

I did not see any additional scaling factors, and no receiver gain.

Don't look at the 2dseq file, I think there are some additional steps.

- 1.d The repetitions (whose number are set by "PVM_NRepetitions") are appended in "fid_proc.64" so not averaged nor added (Or maybe I misunderstood your meaning of "repetitions".)
- 2. The programming manual says: *Eddy current compensation (EDC): A reference scan can be passed (as parameter) from which the waterline phase evolution is determined. This phase evolution is subtracted from each FID.* I attach a htm file where you can find what Bruker's function takes as arguments (look for "RecoSpectCorrFilter").
- 3. I think so but I'm not 100% sure.

Unfortunately, I do not have a working example to check right now, but I am happy to contribute in debugging! Let me know!

Best,

Thanh Phong Lê, PhD R&D Engineer, CIBM MRI EPFL



Animal Imaging and Technology

EPFL CIBM-AIT

CH F1 592, Station 6

1015 Lausanne

Switzerland

+41 21 693 05 85 // +41 76 458 78 61

cibm.ch



De: Cristina Ramona Cudalbu < cristina.cudalbu@epfl.ch >

Envoyé : mercredi, 22 janvier 2025 11:29 **À :** Thanh Phong Lê <<u>thanh.le@epfl.ch</u>>

Cc: Georg Oeltzschner <goeltzs1@jhmi.edu>; Diana Georgiana Rotaru <dra309@columbia.edu>; Jamie Near <jamie.near@utoronto.ca>

Objet: RE: CoMP-MRS - Bruker loader progress

Hi Thanh,

For the CoMP-MRS project (preclinical multi-site 1H MRS) Georg is preparing the loader of all data in Osprey for fitting.

And for Bruker data Georg has some questions. As you have a lot of experience with Bruker, I was wondering if you could help with some answers – please see email below in yellow .

Yesterday I forgot to check on the scanner for point 1, but I can do it tomorrow

Best

Cristina

Cristina Cudalbu, PhD

Research Staff Scientist, CIBM MRI EPFL Section

9.4T MRI Operational Manager, CIBM MRI EPFL Section

Maître d'enseignement et de recherche (MER), School of Basic Sciences, EPFL

Animal Imaging and Technology

CIBM Center for Biomedical Imaging Station 6 CH F0-628

EPFL AVP-CP CIBM-AIT

CH-1015 Lausanne, Switzerland

(+41) 21 693 76 85

cibm.ch



From: Georg Oeltzschner <goeltzs1@jhmi.edu>

Sent: Tuesday, 21 January 2025 18:37

To: Diana Georgiana Rotaru <drain diana di

Cc: Cristina Ramona Cudalbu <<u>cristina.cudalbu@epfl.ch</u>> **Subject:** Re: CoMP-MRS - Bruker loader progress

Hi all,

Thanks a lot - I think we should send the questions to all your Bruker contacts. The more, the merrier.

Here we go:

I am trying to re-construct the Bruker-processed spectra (in fid or proc64 files) from raw (coil-uncombined and un-averaged) data, but there are a couple of questions remaining that I cannot find answers in the manual for:

- 1) What are the procedures that Bruker processing on the scanner console applies for combining the coil channel signals and scaling the resulting spectrum?
 - 1. Specifically, what are the amplitude coefficients for the coil combination? The phases are stored in the PVM_ArrayPhase header fields, but the amplitudes are unclear. Are the channels summed up, averaged, or weighted? Can the coefficients be found anywhere?
 - 1. I understand that the averages are **summed**, not **averaged** to yield the processed spectrum. How are the various receiver gains applied? I understand there are separate gain fields in the header for the water-suppressed and reference scans.
 - 1. Are there any additional scaling factors besides the coil combination amplitude coefficients and the receiver gain?
 - 1. Are 'repetitions' also simply added or averaged?
- 2) What is the exact procedure for eddy-current correction? Is the phase of the reference signal simply subtracted from the water-suppressed signal or are there intermediate steps?
- 3) What happens to the points before the echo (stored in GRPDLY)? Are they simply chopped off (and zeros appended at the end of the FID)?

I think that should suffice for now.

Thanks,

Georg

From: Diana Georgiana Rotaru < dr3309@columbia.edu>

Sent: Monday, January 20, 2025 5:59 PM **To:** Jamie Near < jamie.near@utoronto.ca>

Cc: Georg Oeltzschner <goeltzs1@jhmi.edu>; Cristina Ramona Cudalbu <<u>cristina.cudalbu@epfl.ch</u>>

Subject: Re: CoMP-MRS - Bruker loader progress

External Email - Use Caution

Hi Georg, Jamie and Cristina,

Incredible work, Georg! Well done on putting it all together. I can also send the list of questions to another contact I know at Bruker, Kristin Granlund - she is an engineer if I remember well and she helped me a lot with the pulse sequence information. It might be worth sending the questions to all contacts, let me know if you want me to reach out to her too.

Regards,

Diana

Diana Rotaru, PhD

Postdoctoral Research Scientist

MR Scientific Engineering for Clinical Excellence (MR SCIENCE) Laboratory

Department of Biomedical Engineering

Fu Foundation School of Engineering and Applied Science

Columbia University in the City of New York

On Sat, Jan 18, 2025 at 8:00 AM Jamie Near < jamie.near@utoronto.ca > wrote:

This Message Is From an External Sender

Hi Georg, This message came from outside your organization.

Thank you so much for your efforts on this. I peeked in at the GitHub yesterday and I saw a bit of what you've done and it all looks really really fantastic!!!

Yes, I'm happy to send a list of questions to Bruker. I will probably send them to Saausan Madi, but I'll take any suggestions from Cristina and Diana about who else I should send them to. In the meantime, Georg, can you please send me the other questions you had about the eddy current correction?

Thanks a million! And have a great weekend.

-Jamie

On Jan 17, 2025, at 4:15 PM, Georg Oeltzschner <goeltzs1@jhmi.edu> wrote:

Hi everyone,

I've made a lot of progress since Christmas on the loader. It can now load Bruker-processed and raw data for all the datasets, and I'm retrieving the correct coil phases from the header.

In the past 2 days I've tried **a lot** of different things to reverse-engineer the Bruker on-scanner recon. I can get **very very close** except for a scaling factor that I can't seem to reliably determine for all datasets. There is an interplay between the receiver gain and, presumably, the way that the coil combination amplitudes are determined (are they simply summed? averaged? something else?), but I'm a stage where I'm getting diminishing returns for my time. The manuals are not sufficiently clear on what exactly is going on.

Can we reach out to Bruker to ask for help with this? I think the scaling is very important for subsequent quantification relative to the water reference data.

I have a few additional questions (e.g., about the eddy-current correction), but the scaling is the most pressing one. Happy to write out a list of Qs for you to forward to your Bruker contacts, Jamie.

Other than that, I'd say we're 95% there.

Cheers, and happy weekend everyone,

Georg

PS: We've also set up a protocol on the 11.7T at JHU, but we've had a bit of troubles getting the shimming to work properly (despite Dunja's formidable expertise).

From: Jamie Near < jamie.near@utoronto.ca>
Sent: Tuesday, December 10, 2024 12:04 PM

To: Diana Georgiana Rotaru < dr3309@columbia.edu>

Cc: Cristina Ramona Cudalbu < cristina.cudalbu@epfl.ch; Georg Oeltzschner < goeltzs1@jhmi.edu>

Subject: Re: CoMP-MRS meeting notes

External Email - Use Caution

Thank you Diana!	
-J	
	On Dec 10, 2024, at 11:14 AM, Diana Georgiana Rotaru < <u>dr3309@columbia.edu</u> > wrote:
	Dear all,
	Please find the link to the meeting notes below:
	CoMP-MRS meeting notes
	If I missed anything, please feel free to add or change as needed.
	The project Google Drive folder can be accessed using this link:
	CoMP-MRS project folder
	The data - using this link:
	CoMP-MRS_Hackathon2.0
	And the data info spreadsheet - using this other link:
	CoMP-MRS data spreadsheet
	Wish you all a productive week!
	Regards,
	Diana
	Diana Rotaru, PhD
	Postdoctoral Research Scientist
	MR Scientific Engineering for Clinical Excellence (MR SCIENCE) Laboratory
	Department of Biomedical Engineering
	Fu Foundation School of Engineering and Applied Science
	Columbia University in the City of New York