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Demo 02: 3D ME Phantom data

data download and setup

add paths and set up data paths. Download phantom data (1.82 GB "phantom-DMI.tar.gz") from zenodo.org (DOI: 10.5281/zenodo.14652737).

```
% add all dependencies
addpath(genpath('/ptmp/pvalsala/Packages/mapVBVD'))
addpath(genpath('/ptmp/pvalsala/Packages/DeuteMetCon'))


% data path
sn='/ptmp/pvalsala/deuterium/dataForPublication/phantom-DMI';
dirst_me=dir(fullfile(sn,"*trufi_5E*.dat"));
dirst_noise=dir(fullfile(sn,"*trufi*noise*.dat"));
```

load metabolite structure

The chemical shifts, measured relaxation times and labels of all four metabolites in phantom is organised in a array of struct

```
% second argument is the frequency offset of water in Hz
metabolites=getMetaboliteStruct('phantom',0);
```

Inputs and flags for metabolite mapping

All functions and data required for all data processing steps like image reconstruciton, coil combination and spectral seperation were encapsualted in a single class `MetCon_CSI.m`. All inputs and flags except the raw data file is a name-value pair as described below.

```
% | name                       | description                                                  | default   | possible options                                                  |
% |----------------------------|--------------------------------------------------------------|-----------|-------------------------------------------------------------------|
% | metabolites                | struct array with definition of metabolites                  | []        | see getMetaboliteStruct.m function                                |
% | fm                         | 1H fieldmap in rad/s                                         | []        | 3D numeric matrix or 'IDEAL'                                      |
% | csm                        | coil maps                                                    | []        | 3D numeric matrix                                                 |
% | mask                       | mask for spectral separation                                 | []        | 3D logical matrix , scalar percentile (1-100) threshold           |
% | doDenosing                 | SVD denoising                                                | 0         | scalar No of components, -1 for debug                             |
% | Solver                     | spectral separation method                                   | 'IDEAL'   | {'phaseonly','pinv','IDEAL','IDEAL-modes','AMARES','LorentzFit'} |
% |                            |                                                              |           | 'phaseonly'- linear method with only phase evolution              |
% |                            |                                                              |           | 'pinv'- linear method with full signal model                      |
% |                            |                                                              |           | 'IDEAL'- iterative IDEAL algorithm                                |
% |                            |                                                              |           | 'IDEAL-modes'-IDEAL algorithm for phase cycled data               |
% |                            |                                                              |           | 'AMARES'- AMARES spectral fitting                                 |
% |                            |                                                              |           | 'LorentzFit'- lorentzian spectral fitting                         |
% | parfor                     | flag to use parfor                                           | true      | boolean                                                           |
% | doZeroPad                  | zero pad factor                                              | [1 1 1 0] | positive scalar array [3 physical axis x 1 time]                  |
% | 'doSmoothFM','maxit'       | IDEAL flags: fieldmap smooth factor and maximum iterations   | 1,10      | scalar(+ve: gaussian, -ve: median),postive scalar                 |
% | doPhaseCorr                | phase correction mode                                        | 'none'    | {'none','Manual','Burg'}                                          |
% | 'CoilSel','PCSel','EchoSel' | arrays to picks some of coils, time points and phasecyles.  | 1:max()   | positive integer array                                            |
% | doNoiseDecorr              | flag to perform noise decorrelation                          | true      | boolean                                                           |
```

Get noise decoorelation matrix

trufi sequence acquire noise data only when parallel imaging is enabled. Therefore, we acquire noise scan with 0 flip angle seperately.

```
twix_noise=mapVBVD(fullfile(sn,dirst_noise(1).name),'rmos');
```

```
Software version: VD (!?)
Reader version: 1660732089 (UTC: 17-Aug-2022 10:28:09)
Scan 1/1, read all mdhs:
Warning: MATLAB has disabled some advanced graphics rendering features by switching to software OpenGL. For more information, click here.
    40.4 MB read in    8 s
```

```
[D_noise,D_image,noise_info]=CalcNoiseDecorrMat(twix_noise);
%D_image is the noise correlation from image data measured with 0 FA
```

assemble inputs and processing flags

```
ME_setting={'NoiseDecorr',D_image,'mask',[],'metabolites',metabolites,...
            'doPhaseCorr',true,'doZeropad',[1 1 1]*0.5,'parfor',true,'fm','IDEAL','Solver','pinv'};
%
%'fm','IDEAL' : estimate field map from the averaged phasecycle volume using IDEAL algorithm
% 'Solver','pinv' : linear fit (least square fit of full signal model)
```

Process data

```
ME_filename=fullfile(sn,dirst_me(end).name);
mcobj_me=MetCon_ME(ME_filename,ME_setting{:});
```

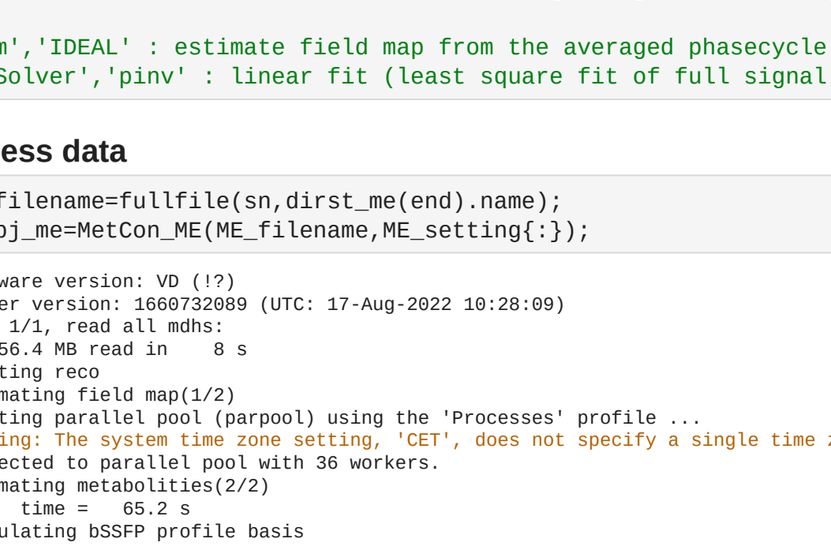
```
Software version: VD (!?)
Reader version: 1660732089 (UTC: 17-Aug-2022 10:28:09)
Scan 1/1, read all mdhs:
   856.4 MB read in    8 s
starting reco
estimating field map(1/2)
Starting parallel pool (parpool) using the 'Processes' profile ...
Warning: The system time zone setting, 'CET', does not specify a single time zone unambiguously. It will be treated as 'Europe/Zurich'. See the datetime.TimeZone property for details about specifying time zones.
Connected to parallel pool with 36 workers.
estimating metabolities(2/2)
reco  time =   65.2 s
Calculating bSSFP profile basis
done.....

 Metabolite fitting done in 5.2 s !
Performed pixel shift along read: (0.0,-2.2,-5.2 ,-7.2) mm
Metabolite mapping time =    5.3 s
```

Plotting

After image reconstruciton and spectral seperation, metbolite amplitudes are store in mcobj_csi.Metcon. The 4D Metcon matrix and 2H field map estimated by IDEAL algorithm can be quickly visualized with `PlotResults` method.

```
mcobj_me.PlotResults()
```



Data structure of Metcon_ME object

1x1 MetCon_ME

Property	Value
FieldMap	*48x64x32 double*
mask	*48x64x32 logical*
twix	*1x1 struct*
DMIPara	*1x1 struct*
flags	*1x1 struct*
filename	'/ptmp/pvalsala/deuterium/dataForPublication/phantom-DMI/MID0...
metabolites	*1x4 struct*
sig	*6-D complex single*
img	*6-D complex single*
coilSens	*4-D complex single*
coilNormMat	*48x64x32 single*
SolverObj	*[ ]*
Metcon	*4-D complex double*
Experimental	*1x1 struct*
D	*10x10 complex single*

Where

- DMIPara are the important sequence parameters parsed from twix with `getDMIPara.m` fucntion
- flags contains all the processing flags
- sig - averaged signal [CHA x LIN x COL x PAR x ECO x REP]
- img - reconstructed image [CHA x Phase x Read xSlice x echo x PC]
- Metcon - Metabolite amplitudes [CHA x 3 physical dimension x time]
- Experimental- contains all experimental outputs of processing (fieldmap, residue, other fit parameters, fit quality)
- D- noise decorrelation matrix.

Other miscallaneous methods which can be useful

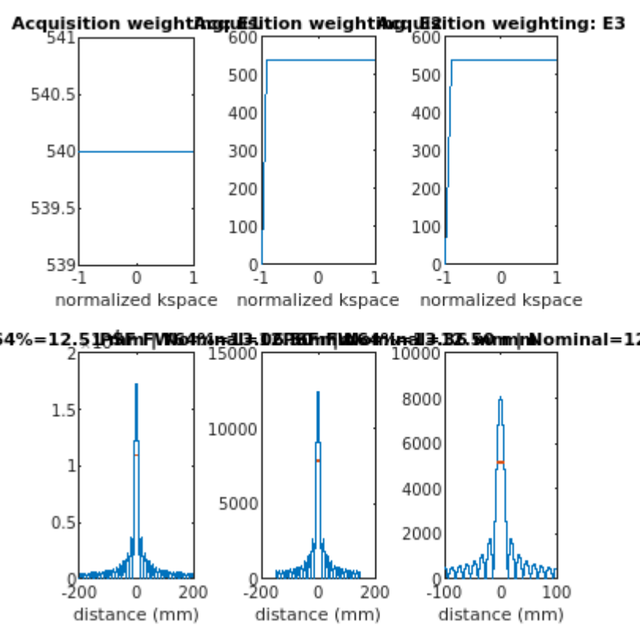
```
% The metabolite amplitudes can be normalized into SNR
metcon_SNR= mcobj_me.getNormalized();

% method and quantified into mM with 10 mM water reference using `getmM`
% fucntion.
metcon_mM= mcobj_me.getmM();

% caculate measurement time after glucose intake in mins
Intake_time_mins=mcobj_me.getMinutesAfterIntake('08:00');

% export NIFTI volumes of all outputs (average image, metabolite amplitude in SNR unit and mM)
pn=fullfile(sn,'proc',sprintf('ME_%s',datetime('today','Format','yyyyMMMdd')));
mkdir(pn);
niiFileName=mcobj_me.WriteImages(pn);

%plot the k-space weighting and PSF to get realistic voxel size (FW64%)
voxel_size_mm= getPSF_CSI(mcobj_me.twix)
```




```
voxel_size_mm = 4×1
   12.5122
   13.0642
   13.3602
         0
```

Debug (only for 'pinv' (linear) fit mode)

Useful for checking data at a particular voxel index. [24,33,27] is a lactate voxel.

```
%prints metabolite amplitudes and plot fit and basis functions
mcobj_me.demoFit([24,33,27])
```

```
   12.4828
    1.6200
    0.1262
   77.7509
```