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Demo 04: 3D ME invivo data data

data download and setup

add paths and set up data paths. Download in invivo data (3.8 GB "sub-01-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'))


% setup data folder
sn='/ptmp/pvalsala/deuterium/dataForPublication/sub-01-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('invivo',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:
    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',[],'Solver','IDEAL-modes'};
%
%'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

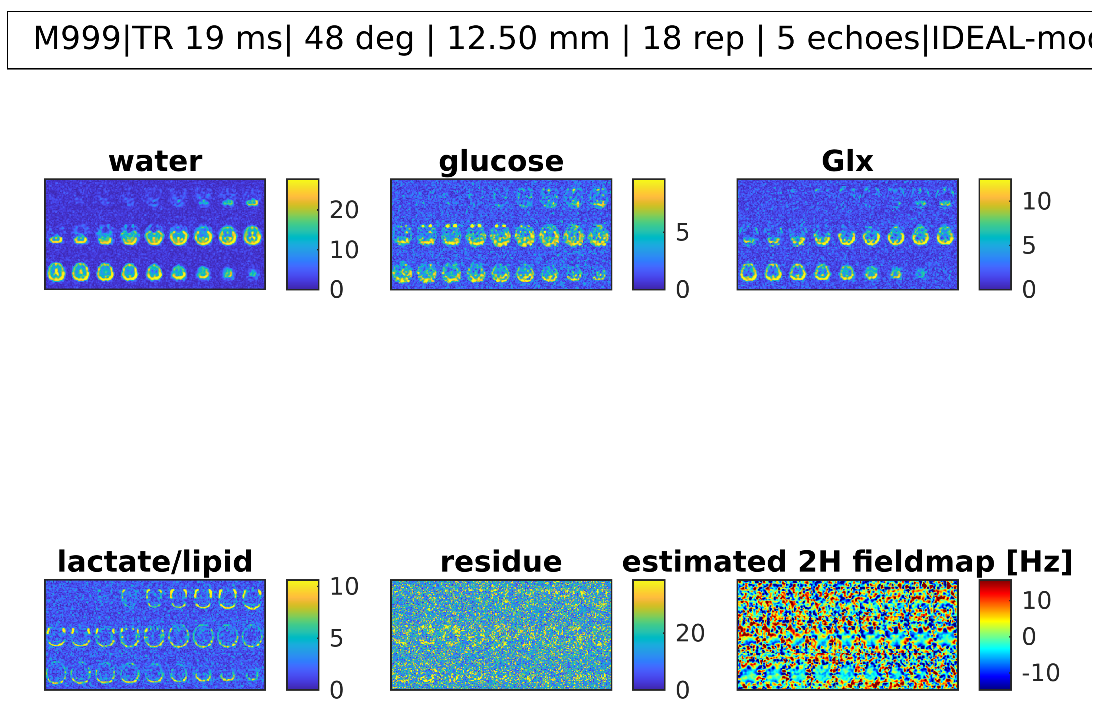
```
ME_filename=fullfile(sn,dirst_me(end).name);
mcobj_me=MetCon_ME(ME_filename,ME_setting{:});
```

```
Software version: VD (!?)
Reader version: 1660732089 (UTC: 17-Aug-2022 10:28:09)
Scan 1/1, read all mdhs:
   856.4 MB read in    9 s
starting reco
reco  time =    25.0 s
estimating field map(1/2)
estimating metabolities(2/2)
Performed pixel shift along read: (0.0,-1.9,-4.9 ,-6.9) mm
Metabolite mapping time =    31.5 s
```

Plotting

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

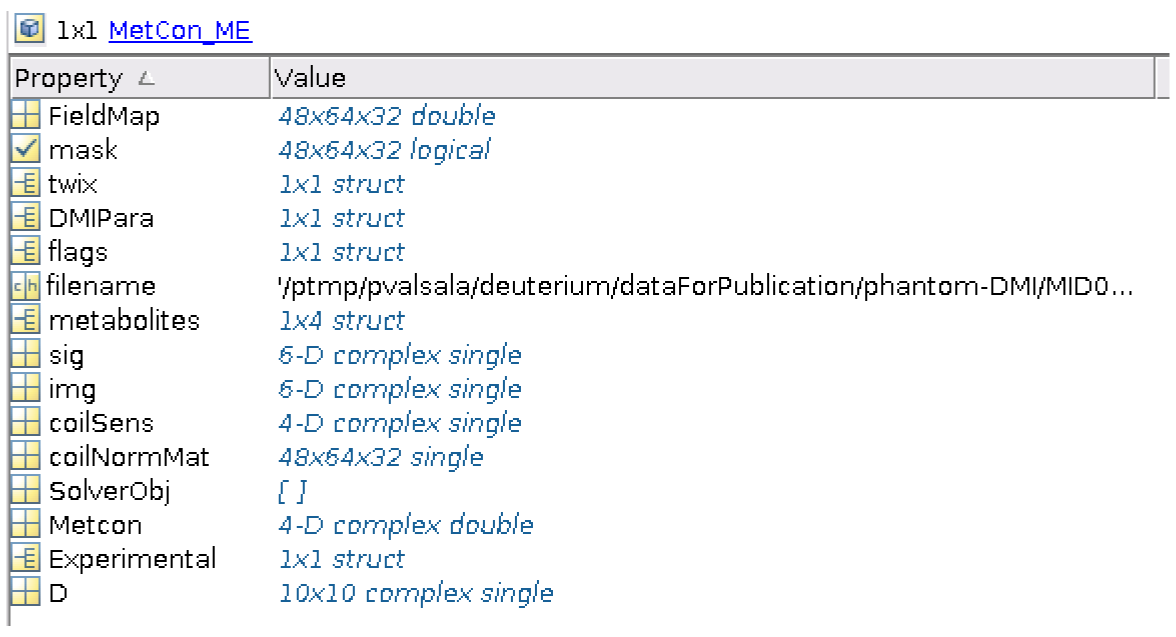
```
mcobj_me.PlotResults()
```



M999|TR 19 ms| 48 deg | 12.50 mm | 18 rep | 5 echoes|IDEAL-moc
water
20
10
0
glucose
5
0
Glx
10
5
0
lactate/lipid
10
5
0
residue
20
0
estimated 2H fieldmap [Hz]
10
0
-10

```
%if you have array show in path :
% as(mcobj_me.getNormalized)
```

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

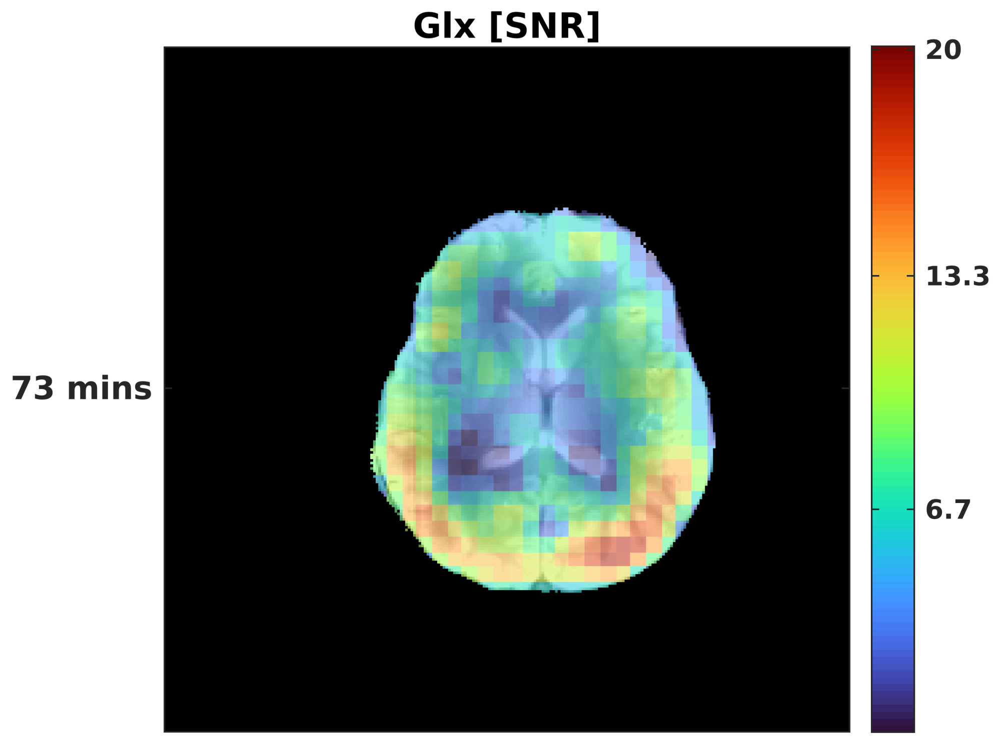
- DMIPara are the important sequence parameters parsed from twix with `getDMIPara.m` fucntion
- flags contains all the processing flags
- sig - averaged signal [CHA x LIN x COL x PAR x ECO x REP]
- img - reconstructed image [CHA x Phase x Read xSlice x echo x PC]
- Metcon - Metabolite amplitudes [CHA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

Overlay plot with anatomy

```
%add SPM12
addpath('/ptmp/pvalsala/Packages/spm12/')

anat_tra=fullfile(sn,'anat/brain_tra.nii');

% 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);cd(pn);
niiFileName=mcobj_me.WriteImages(pn);
% reslice the metabolite amplitude to anatomy!
resliced_metcon=myspm_reslice(anat_tra,dir(fullfile(pn,'Metcon_SNR_*trufi*.nii')),'nearest','rt');
```

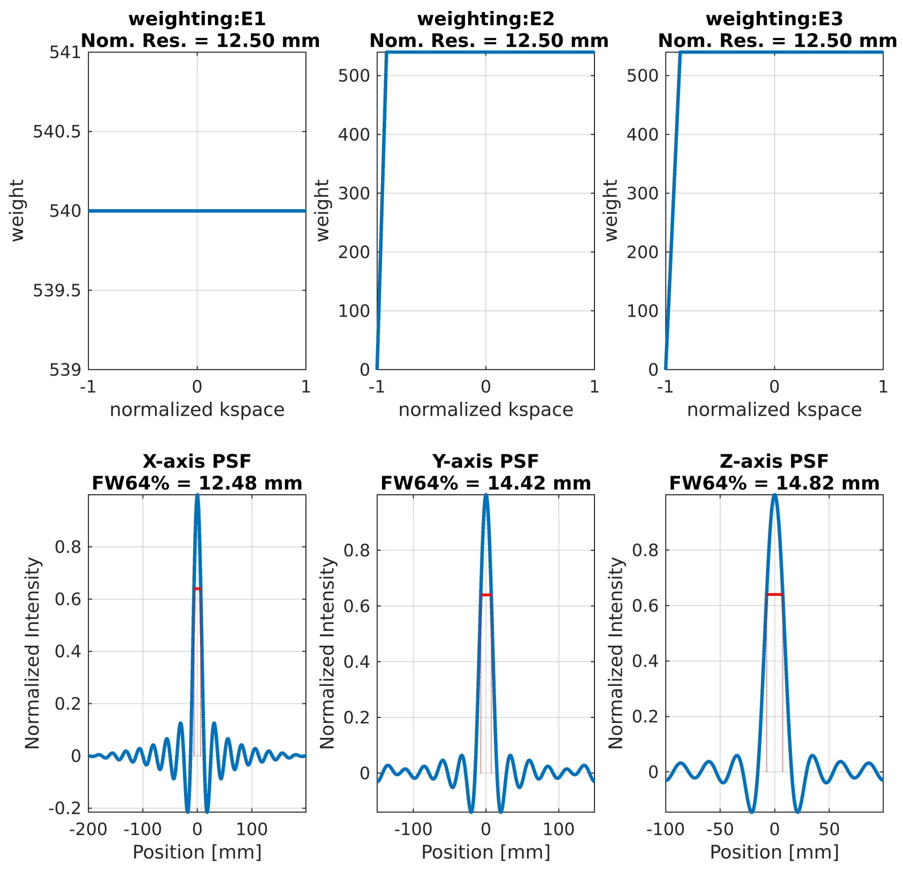
```
reslicing 1 volumes: Metcon_SNR_m00999_pvrh_trufi_5E_18PC_12P5mm_FA50_s4_r180_IDEAL-modes.nii


------------------------------------------------------------------------
14-Apr-2025 16:24:02 - Running job #1
------------------------------------------------------------------------
14-Apr-2025 16:24:02 - Running 'Coregister: Reslice'

SPM12: spm_reslice (v7141)                         16:24:02 - 14/04/2025
========================================================================
Completed                               :          16:24:03 - 14/04/2025
14-Apr-2025 16:24:03 - Done    'Coregister: Reslice'
14-Apr-2025 16:24:03 - Done
```

```

% Overlay plot
clim_glx=[0 20];
figure,
overlayplot(dir(anat_tra),dir(fullfile(pn,'rt*.nii')),'MetIdx',3,'SlcSel',15, ...
    'transform',@(x) flip(permute(x,[2 1 3 4 5]),1),...
   'cax',clim_glx,'cax_im',[0,0.9],'cmap',turbo,'alpha_overlay',0.5);
title([metabolites(3).name,' [SNR]']) % 'MetIdx',3
yticklabels(sprintf('%d mins',mcobj_me.getMinutesAfterIntake('08:36')));

%make your own colorbar
cb_handle=colorbar;
cb_handle.Visible='off';
ax2 = axes('Position',cb_handle.Position);
imagesc(linspace(0,1,100)'),colormap(ax2,'turbo')
set(ax2,'YAxisLocation','right','FontSize',10,'FontWeight','bold','YDir','normal')
yticks(round(linspace(0,100,4)))
yticklabels(round(linspace(0,1,4)*clim_glx(2),1))
xticks([])
```



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 (08:14) in mins
Intake_time_mins=mcobj_me.getMinutesAfterIntake('08:14');


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



```
voxel_size_mm = 4×1
   12.4793
   14.4160
   14.8232
         0
```

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

Useful for checking data at a particular voxel index.[34,38,22]is a gray matter voxel.

```
%prints metabolite amplitudes and plot fit and basis functions
 % mcobj_me.demoFit([34,38,22])
```