%% jobfile.m

% This function describes an Osprey job defined in a MATLAB script.

%

% A valid Osprey job contains four distinct classes of items:

% 1. basic information on the MRS sequence used

% 2. several settings for data handling and modeling

% 3. a list of MRS (and, optionally, structural imaging) data files

% to be loaded

% 4. an output folder to store the results and exported files

%

% The list of MRS and structural imaging files is provided in the form of

% cell arrays. They can simply be provided explicitly, or from a more

% complex script that automatically determines file names from a given

% folder structure.

%

% Osprey distinguishes between four sets of data:

% - metabolite (water-suppressed) data

% (MANDATORY)

% Defined in cell array "files"

% - water reference data acquired with the SAME sequence as the

% metabolite data, just without water suppression RF pulses. This

% data is used to determine complex coil combination

% coefficients, and perform eddy current correction.

% (OPTIONAL)

% Defined in cell array "files\_ref"

% - additional water data used for water-scaled quantification,

% usually from short-TE acquisitions due to reduced T2-weighting

% (OPTIONAL)

% Defined in cell array "files\_w"

% - Structural image data used for co-registration and tissue class

% segmentation (usually a T1 MPRAGE). These files need to be

% provided in the NIfTI format (\*.nii) or, for GE data, as a

% folder containing DICOM Files (\*.dcm).

% (OPTIONAL)

% Defined in cell array "files\_nii"

% - External segmentation results. These files need to be

% provided in the NIfTI format (\*.nii or \*.nii.gz).

% (OPTIONAL)

% Defined in cell array "files\_seg" with 1 x 3 cell for each

% subject or 1 x 1 cell if a single 4D NIfTI is supplied.

%

% Files in the formats

% - .7 (GE)

% - .SDAT, .DATA/.LIST, .RAW/.SIN/.LAB (Philips)

% - .DAT (Siemens)

% - .nii, .nii.gz (NIfTI-MRS)

% usually contain all of the acquired data in a single file per scan. GE

% systems store water reference data in the same .7 file, so there is no

% need to specify it separately under files\_ref.

%

% Files in the formats

% - .DCM (any)

% - .IMA, .RDA (Siemens)

% may contain separate files for each average. Instead of providing

% individual file names, please specify folders. Metabolite data, water

% reference data, and water data need to be located in separate folders.

%

% In the example script at hand the MATLAB functions strrep and which are

% used to generate a relative path, which allows you to run the examples

% on your machine directly. To set up your own Osprey job supply the

% specific locations as described above.

%

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%

% HISTORY:

% 2019-07-15: First version of the code.

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%%% 1. SPECIFY SEQUENCE INFORMATION %%%

% Specify sequence type

seqType = 'unedited'; % OPTIONS: - 'unedited' (default)

% - 'MEGA'

% - 'HERMES'

% - 'HERCULES'

% Specify editing targets

editTarget = {'GABA'}; % OPTIONS: - {'none'} (default if 'unedited')

% - {'GABA'}, {'GSH'}, {'Lac'}, {'PE322'}, {'PE398'} (for 'MEGA')

% - {'GABA', 'GSH'}, {'GABA', 'Lac'}, {'NAA', 'NAAG'} (for 'HERMES'and 'HERCULES')

% Specify data scenario

dataScenario = 'invivo'; % OPTIONS: - 'invivo' (default)

% - 'phantom'

% - 'PRIAM'

% - 'MRSI'

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%%% 2. SPECIFY DATA HANDLING AND MODELING OPTIONS %%%

% Which spectral registration method should be used? Robust spectral

% registration is default, a frequency restricted spectral registration

% method is also availaible and is linked to the fit range.

opts.SpecReg = 'RobSpecReg'; % OPTIONS: - 'RobSpecReg' (default) Spectral aligment with Water/Lipid removal, using simialrity meric, and weighted averaging

% - 'ProbSpecReg' Probabilistic spectral aligment to median target and weighted averaging

% - 'RestrSpecReg' Frequency restricted (fit range) spectral aligment, using simialrity meric, and weighted averaging

% - 'none'

% Which algorithm do you want to align the sub spectra? L2 norm

% optimization is the default. This is only used for edited MRS!

% Which algorithm do you want to align the sub spectra? L2 norm

% optimization is the default. This is only used for edited MRS!

%Perform correction on the metabolite data (raw) or metabolite

%-nulled data (mm).

opts.SubSpecAlignment.mets = 'L2Norm'; % OPTIONS: - 'L2Norm' (default)

% - 'L1Norm'

% - 'none'

%Perform eddy-current correction on the metabolite data (raw) or metabolite

%-nulled data (mm). This can either be done similar for all data sets by

%supplying a single value or specified for each dataset individually by supplying

% multiple entries (number has to match the number of datasets) e.g. to perform ECC

% for the second dataset only:

% opts.ECC.raw = [0 1];

% opts.ECC.mm = [0 1];

opts.ECC.raw = 1; % OPTIONS: - '1' (default)

opts.ECC.mm = 1; % - '0' (no)

% - [] array

% Save processed spectra in vendor-specific format (SDAT/SPAR, RDA, P)?

opts.saveVendor = 0; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save LCModel-exportable files for each spectrum?

opts.saveLCM = 1; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save jMRUI-exportable files for each spectrum?

opts.saveJMRUI = 1; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save processed spectra in NIfTI-MRS format?

opts.saveNII = 0; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Save PDF output for all Osprey modules and subjects?

opts.savePDF = 1; % OPTIONS: - 0 (no, default)

% - 1 (yes)

% Choose the fitting algorithm

opts.fit.method = 'Osprey'; % OPTIONS: - 'Osprey' (default)

% - 'LCModel'

% Select the metabolites to be included in the basis set as a cell array,

% with entries separates by commas.

% With default Osprey basis sets, you can select the following metabolites:

% Ala, Asc, Asp, bHB, bHG, Cit, Cr, Cystat, CrCH2, EtOH, GABA, GPC, GSH, Glc, Gln,

% Glu, Gly, H2O, mI, Lac, NAA, NAAG, PCh, PCr, PE, Phenyl, sI, Ser,

% Tau, Tyros, MM09, MM12, MM14, MM17, MM20, Lip09, Lip13, Lip20.

% If you enter 'default', the basis set will include all of the above

% except for Ala, bHB, bHG, Cit, Cystat, EtOH, Glc, Gly, Phenyl, Ser, and Tyros.

opts.fit.includeMetabs = {'default'}; % OPTIONS: - {'default'}

% - {'full'}

% - {custom}

% Choose the fitting algorithm

opts.fit.method = 'Osprey'; % OPTIONS: - 'Osprey' (default)

% - 'AQSES' (planned)

% - 'TARQUIN' (planned)

% Choose the fitting style for difference-edited datasets (MEGA, HERMES, HERCULES)

% (only available for the Osprey fitting method)

opts.fit.style = 'Separate'; % OPTIONS: - 'Concatenated' (default) - will fit DIFF and SUM simultaneously)

% - 'Separate' - will fit DIFF and OFF separately

% Determine fitting range (in ppm) for the metabolite and water spectra

opts.fit.range = [0.5 4]; % [ppm] Default: [0.5 4]

opts.fit.rangeWater = [2.0 7.4]; % [ppm] Default: [2.0 7.4]

% Determine the baseline knot spacing (in ppm) for the metabolite spectra

opts.fit.bLineKnotSpace = 0.4; % [ppm] Default: 0.4.

% Add macromolecule and lipid basis functions to the fit?

opts.fit.fitMM = 1; % OPTIONS: - 0 (no)

% - 1 (yes, default)

% Optional: In case the automatic basisset picker is not working you can manually

% select the path to the basis set in the osprey/fit/basis, i.e.:

% opts.fit.basisSetFile = 'osprey/fit/basis/3T/philips/mega/press/gaba68/basis\_philips\_megapress\_gaba68.mat';

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%%% 3. SPECIFY MRS DATA AND STRUCTURAL IMAGING FILES %%

% When using single-average Siemens RDA or DICOM files, specify their

% folders instead of single files!

% Clear existing files

clear files files\_ref files\_w files\_nii files\_mm

% Data folder in BIDS format

% The filparts(which()) comment is needed to find the data on your machine. If you set

% up the jobFile for your own data you can set a direct path to your data

% folder e.g., data\_folder = /Users/rhideetajalal/Osprey/'

data\_folder = fileparts(which(fullfile('data','twix','jobfile.m')));

% The following lines perform an automated set-up of the jobFile which

% takes advatage of the BIDS foramt. If you are not using BIDS (highly

% recommended) you can look at the definitions below the loop to see how to

% set up direct path links to your data.

subs = dir(data\_folder);

subs(1:3) = [];

subs = subs([subs.isdir]);

subs = subs(contains({subs.name},'sub'));

counter = 1;

for kk = 1:length(subs)

% Loop over sessions

sess = dir([subs(kk).folder filesep subs(kk).name]);

sess(1:2) = [];

sess = sess([sess.isdir]);

sess = sess(contains({sess.name},'ses'));

for ll = 1:length(sess)

% Specify metabolite data

% (MANDATORY)

dir\_metabolite = dir([sess(ll).folder filesep sess(ll).name filesep 'mrs' filesep subs(kk).name '\_' sess(ll).name '\_press' filesep '\*.dat']);

files(counter) = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/mrs/sub-18\_ses-01\_press/sub-18\_press.dat'};

% Specify water reference data for eddy-current correction (same sequence as metabolite data!)

% (OPTIONAL)

% Leave empty for GE P-files (.7) - these include water reference data by

% default.

dir\_ref = dir([sess(ll).folder filesep sess(ll).name filesep 'mrs' filesep subs(kk).name '\_' sess(ll).name '\_press-ref' filesep '\*.dat']);

files\_ref(counter) = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/mrs/sub-18\_ses-01\_press-ref/sub-18\_press\_ref.dat'};

% Specify water data for quantification (e.g. short-TE water scan)

% (OPTIONAL)

files\_w = {};

% Specify metabolite-nulled data for quantification

% (OPTIONAL)

files\_mm = {};

% Specify T1-weighted structural imaging data

% (OPTIONAL)

% Link to single NIfTI (\*.nii) files for Siemens and Philips data

% Link to DICOM (\*.dcm) folders for GE data

files\_nii(counter) = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/ses-01\_T1w.nii.gz'};

% External segmentation results

% (OPTIONAL)

% Link to NIfTI (\*.nii or \*.nii.gz) files with segmentation results

% Add supply gray matter, white matter, and CSF as 1 x 3 cell within a

% cell array or a single 4D file in the same order supplied as 1 x 1 cell;

% files\_seg(counter) = {{['/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c1T1w.nii.gz'],...

% ['/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c2T1w.nii.gz'],...

% ['/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c3T1w.nii.gz']}};

% files\_seg(counter) = {{['/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/4DT1w.nii.gz']}};

counter = counter + 1;

end

end

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% Definitions without using BIDS

% You can always supply direct path to each of the files within

% the cell array. For example:

% Specify metabolite data

% (MANDATORY)

% files(counter) = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/mrs/sub-18\_ses-01\_press/sub-18\_press.dat'};

% Specify water reference data for eddy-current correction (same sequence as metabolite data!)

% (OPTIONAL)

% Leave empty for GE P-files (.7) - these include water reference data by

% default.

% files\_ref(counter) = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/mrs/sub-18\_ses-01\_press-ref/sub-18\_press\_ref.dat'};

% Specify water data for quantification (e.g. short-TE water scan)

% (OPTIONAL)

% files\_w = {};

% Specify metabolite-nulled data for quantification

% (OPTIONAL)

% files\_mm = {};

% Specify T1-weighted structural imaging data

% (OPTIONAL)

% Link to single NIfTI (\*.nii.gz or #.nii) files for GE, Siemens and Philips data

% files\_nii = {'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/ses-01\_T1w.nii.gz'};

% External segmentation results

% (OPTIONAL)

% Link to NIfTI (\*.nii or \*.nii.gz) files with segmentation results

% Add supply gray matter, white matter, and CSF as 1 x 3 cell within a

% cell array or a single 4D file in the same order supplied as 1 x 1 cell;

% files\_seg(counter) = {{'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c1T1w.nii.gz',...

% '/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c2T1w.nii.gz',...

% '/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/c3T1w.nii.gz'}};

% files\_seg(counter) = {{'/Users/rhideetajalal/Osprey/data/twix/sub-18/ses-01/anat/sub-18/4DT1w.nii.gz'}};

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%%% 4. SPECIFY STAT FILE %%%

% Supply location of a csv file, which contains possible correlation

% measures and group variables. Each column must start with the name of the

% measure. For the grouping variable use 'group' and numbers between 1 and

% the number of included groups. If no group is supplied the data will be

% treated as one group. (You can always use the direct path)

file\_stat = fullfile(data\_folder, 'stat.csv');

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%%% 5. SPECIFY OUTPUT FOLDER %%

% The Osprey data container will be saved as a \*.mat file in the output

% folder that you specify below. In addition, any exported files (for use

% with jMRUI, TARQUIN, or LCModel) will be saved in sub-folders.

% Specify output folder (you can always use the direct path)

% (MANDATORY)

outputFolder = fullfile(data\_folder, 'derivatives');

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%