Supplementary Materials II – Example Data and Code for QSM Reconstruction

3 Version, v0.2.0

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6 Full datasets, results and processing scripts are available on Zenodo:
7 https://doi.org/10.5281/zenodo.7410455

Data availability

9 Data are available from three vendors: GE, SIEMENS and PHILIPS, using the
10 recommended acquisition in the main text. For each vendor, both monopolar and
11 bipolar readout strategies were used to acquire the data. The data from GE and
12 SIEMENS are not pre-scan normalized, while the PHILIPS data have two normalization
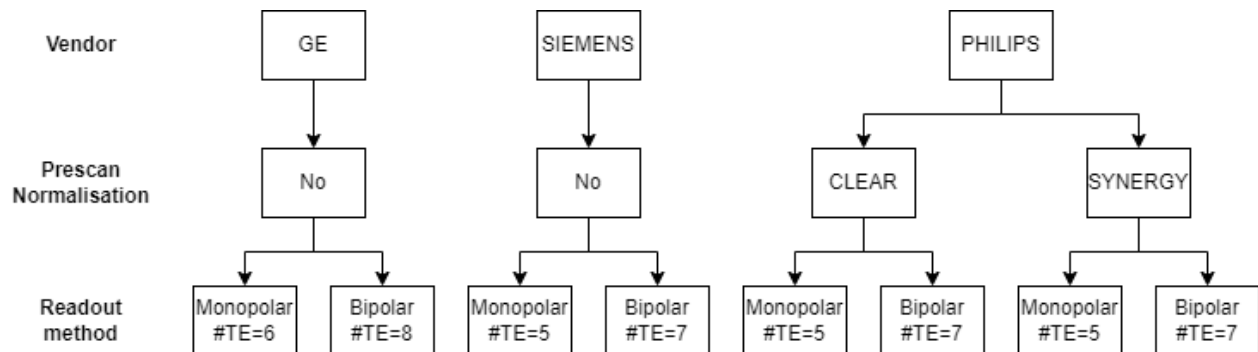13 methods applied.
14

16 Figure S1: An illustration of data availability.

Data preparation and organization

Data preparation

19 **Remark: The following steps for Data preparation are only required if you want to**
20 **start the processing using the 'QSM_CONSENSUS_DATA.zip' file from a clean**
21 **directory.**
22
23 **Step 1: Unzip the received data and reformat the directory structure**
24 Scripts:
25 • Preparation_01_rename_received_data.sh
26
27 **Step 2: Convert DICOM images into NIfTI format**

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Dependency: dcm2niix (version 1.0.20220720)
Scripts:
- Preparation_02_convert_dicom2nii.sh

Step 3: Rename the files according to the BIDS format
Dependency: Matlab R2016b onwards
The naming strategy as follows:
- Vendors are identified using the session tag: **ses-<GE|PHILIPS|SIEMENS>**
- For **GE** and **SIEMENS**, different readout methods are identified using the acquisition tag: **acq-<Bipolar|Monopolar>**;
- For **PHILIPS**, the normalisation method is also printed on the acquisition tag, i.e., **acq-<BipolarCLEAR|BipolarSYNERGY|MonopolarCLEAR|MonopolarSYNERGY>**

Script:
1. Preparation_03_rename_to_bids_format.m

Step 4: Prepare NIFTI data for SEPIA
Dependency: (1) Matlab R2016b onwards, (2) SEPIA v1.2.2.2
Involves the following operation:
- Combining individual multi-echo 3D volumes into a single 4D volume with TE in the 4th dimension;
- Obtaining header info (e.g., B_0 direction and TE) from NIfTI header and JSON sidecar files and saving as SEPIA's header format;
- (GE only) Correcting inter-slice opposite polarity on real and imaginary images and exporting phase images from the corrected real/imaginary data

Script:
- Preparation_04_prepare_for_sepia.m

Data organization

```
QSM_Consensus_Paper_Example_DICOM_Code/
|-- QSM_CONSENSUS_DATA.zip                 % Zip file containing all DICOM images
|-- protocols                              % Protocol text files
|-- QSM_Consensus_Paper_Example_Code       % Containing all the scripts
|   |-- From_DICOM_zip_file_to_SEPIA_ready  % Scripts for preparing QSM_CONSENSUS_DATA.zip
|   |-- SEPIA_Standard_Pipeline            % SEPIA pipeline config files for Standard
|   |-- SEPIA_Alternative1_Pipeline  % SEPIA pipeline config files for Alternative 1 (MEDI)
|   `-- SEPIA_Alternative2_Pipeline  % SEPIA pipeline config files for Alternative 2 (FANSI)
|-- raw                                    % DICOM images
|-- converted                              % dcm2niix output
|   |-- GE
|   |   |-- Bipolar                        % Bipolar readout acquisition
|   |   `-- Monopolar                      % Monopolar readout acquisition
|   |-- PHILIPS
|   |   |-- Bipolar_CLEAR                  % with CLEAR normalisation
|   |   |-- Bipolar_SYNERGY                % with SYNERGY normalisation
|   |   |-- Monopolar_CLEAR
|   |   `-- Monopolar_SYNERGY
|   `-- SIEMENS
|       |-- Bipolar
|       `-- Monopolar
`-- derivatives                            % directory contains all derived output
    `-- SEPIA                              % SEPIA output
        |-- GE
        |   |-- Bipolar
```

```
|   |     `-- GRE
|   |         |-- Pipeline_Standard          % Standard reconstruction output
|   |         |-- Pipeline_Alternative1       % Dipole inversion Alternative 1 output
|   |         `-- Pipeline_Alternative2       % Dipole inversion Alternative 2 output
|   `-- Monopolar
|-- PHILIPS
`-- SIEMENS
```

QSM reconstruction pipeline

This section describes all the QSM reconstruction processing steps performed in SEPIA. All the processing steps are specified in the SEPIA pipeline configuration files, which are in the sub-directories of the script directory:
'*QSM_Consensus_Paper_Example_Code/SEPIA_Standard_Pipeline/*',
'QSM_Consensus_Paper_Example_Code/SEPIA_Alternative1_Pipeline/' and
'QSM_Consensus_Paper_Example_Code/SEPIA_Alternative2_pipeline/',
corresponding to the three processing pipelines demonstrated as follows.

Environment and dependencies

The data were processed using the following set-up

Operating system
- Linux CentOS 7

Environment
- Matlab R2021a (but the scripts are backwards compatible to earlier Matlab versions from R2016b to R2022a)

Dependencies
- SEPIA v1.2.2.2 [https://github.com/kschan0214/sepia/releases/tag/v1.2.2.2]
- MRITOOLS v3.5.6 [https://github.com/korbinian90/CompileMRI.jl/releases/tag/v3.5.6]
- MRI susceptibility calculation methods (accessed 12 September 2019) [https://xip.uclb.com/product/mri_qsm_tkd]
- MEDI toolbox (release: 15th January 2020) [http://pre.weill.cornell.edu/mri/pages/qsm.html]
- FANSI toolbox [v3] [https://gitlab.com/cmilovic/FANSI-toolbox]

Processing steps

Step 1: Preparation
- (GE only) Phase data is inverted before processing (i.e., phase = -phase), so that paramagnetic susceptibility gives a positive value while diamagnetic susceptibility gives a negative value, same as the data from other vendors
- Brain mask is obtained by using MEDI toolbox implementation of FSL's BET on the 1st echo magnitude image, using default setting -f 0.5 -g 0
- (Bipolar readout data only) Bipolar readout correction based on (Li et al., 2015) using the implementation provided with SEPIA.

Step 2: Total field estimation and echo combination

Table S1: Algorithm parameters for total field estimation and echo combination.

Parameters	Values	Remark

3

Echo phase combination	ROMEO total field calculation	(Dymerska et al., 2020)
MCPC-3D-S phase offset correction	On	
Mask for unwrapping	SEPIA mask	FSL's BET mask
Using ROMEO Mask in SEPIA	Off	
Exclude voxel using relative residual with threshold	0.3 (applied on weighting map)	See https://sepia-documentation.readthedocs.io/en/latest/method/weightings.html

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2 **Step 3: Background field removal**

3 Table S2: Algorithm parameters for background field removal.

Parameters	Values	Remark
Method	VSHARP	(Li et al., 2011)
Maximum spherical mean value filtering size	12	Unit: voxel
Minimum spherical mean value filtering size	1	Unit: voxel
Remove residual B1 field	No	
Erode brain mask before BFR	1	Unit: voxel
Erode brain mask after BFR	0	

4

5 **Step 4: Dipole inversion (corresponding to "Standard" pipeline)**

6 Table S3: Algorithm parameters for dipole field inversion using 'Standard' pipeline.

Parameters	Values	Remark
Method	Iterative Tikhonov	
Regularisation parameter (lambda)	0.1	(Karsa et al., 2020; Schweser et al., 2013)
Conjugate gradient tolerance	0.03	
Reference tissue	Brain mask	

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8 Alternative dipole inversion methods: (MEDI and FANSI)

9 **Step 4 (Alternative 1): Dipole inversion**

10 Table S4: Algorithm parameters for dipole field inversion using 'Alternative 1' pipeline.

Parameters	Values	Remark
Method	MEDI	(Liu et al., 2011)

4

Regularisation parameter (lambda)	2000	
Method of data weighting	1	SNR weighting
Percentage of voxels considered to be edges	90	
Array size for zero padding	[0 0 0]	
Performing spherical mean value operator	On	
Radius of the spherical mean value operation	5	Unit: voxel
Performing modal error reduction through iterative tuning (MERIT)	On	
Performing automatic zero reference (MEDI+0)	Off	
Reference tissue	Brain mask	

1 P.S. Output from the 'Standard' pipeline is required. The scripts are in
2 '*QSM_Consensus_Paper_Example_Code/SEPIA_Alternative1_Pipeline/*'.
3
4 **Step 4 (Alternative 2): Dipole inversion**
5 Table S4: Algorithm parameters for dipole field inversion using 'Alternative 2' pipeline.

Parameters	Values	Remark
Method	FANSI	(Milovic et al., 2019, 2018)
Iteration tolerance	0.1	
Maximum number of iterations	400	
Gradient L1 penalty, regularisation weight	0.0005	
Gradient consistency weight	0.05	
Fidelity consistency weight	1	
Solver	Non-linear	
Constraint	TV	
Method for regularisation spatially variable weight	Vector field	
Using weak harmonic regularisation	On	
Harmonic constraint weight	150	

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Harmonic consistency weight	3	
Reference tissue	Brain mask	

P.S. Output from the 'Standard' pipeline is required. The scripts are in '*QSM_Consensus_Paper_Example_Code/SEPIA_Alternative2_Pipeline/'.*

Re-run the scripts

To re-run the processing scripts, including the preparation shell scripts and the SEPIA pipeline configuration scripts, you may need to adopt the file and/or directory paths on the scripts to the correct paths of the files/directories stored in your local computer.
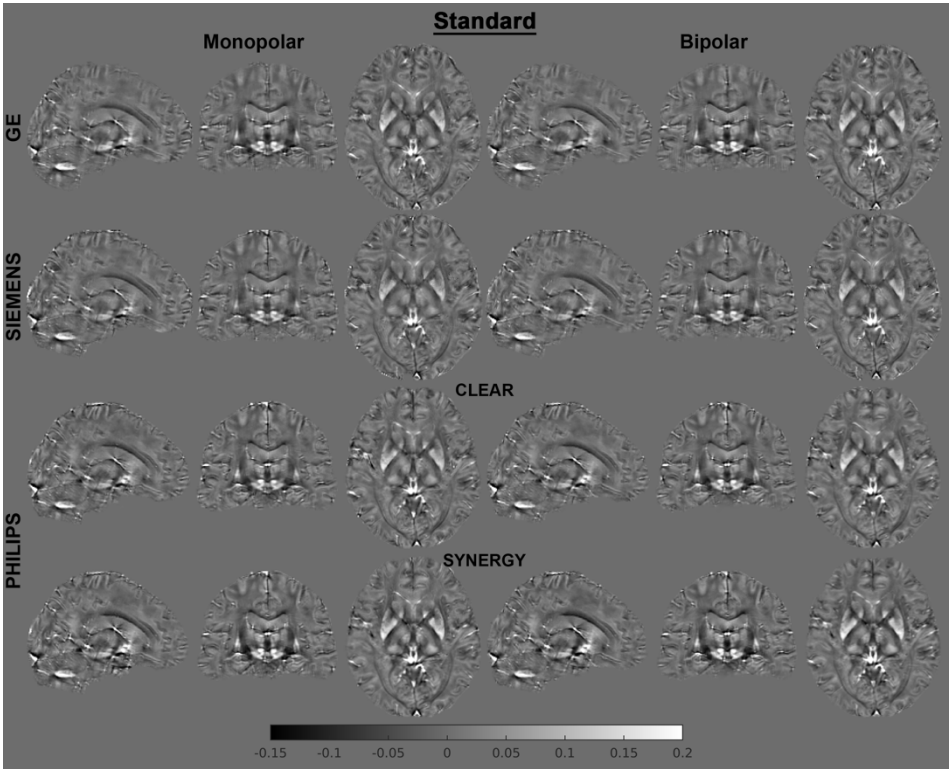
Example results

Figure S2: Susceptibility maps derived using the 'Standard' processing pipeline.
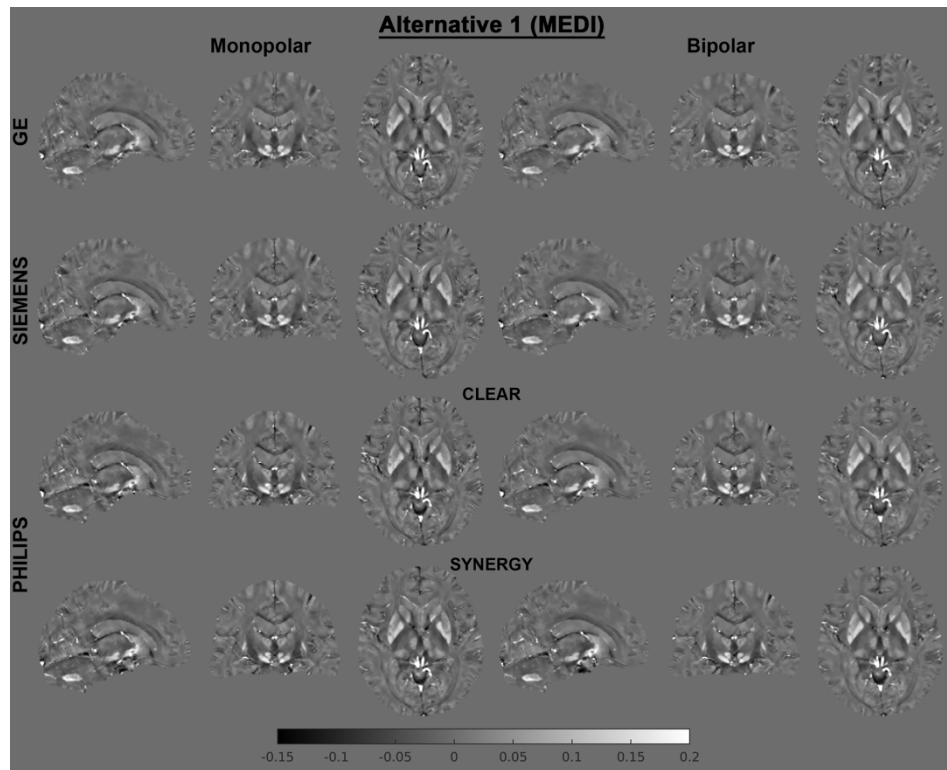
1

2 Figure S3: Susceptibility maps derived using the 'Alternative 1' (MEDI) processing
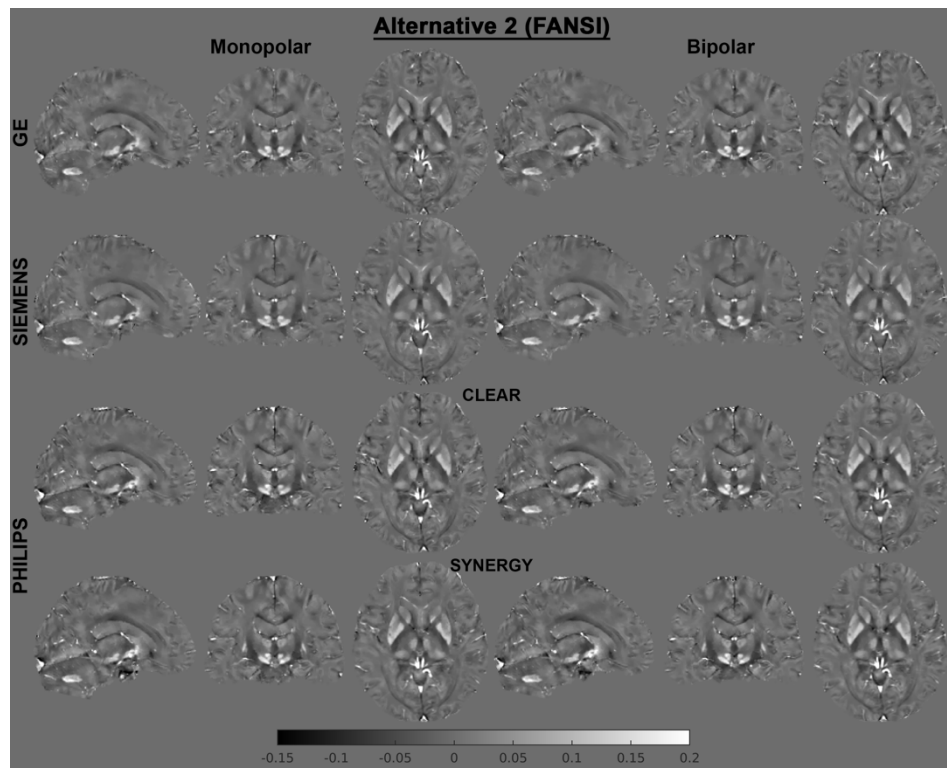
3 pipeline.

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5 Figure S4: Susceptibility maps derived using the 'Alternative 2' (FANSI) processing

6 pipeline.

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References

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