# Supplementary Materials II – Example Data and Code for QSM Reconstruction

Version, v0.2.0

Full datasets, results and processing scripts are available on Zenodo:

https://doi.org/10.5281/zenodo.7410455

## Data availability

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

Diagram

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Figure S1: An illustration of data availability.

## Data preparation and organization

### Data preparation

**Remark: The following steps for Data preparation are only required if you want to start the processing using the ‘QSM\_CONSENSUS\_DATA.zip’ file from a clean directory.**

**Step 1: Unzip the received data and reformat the directory structure**

Scripts:

* Preparation\_01\_rename\_received\_data.sh

**Step 2: Convert DICOM images into NIfTI format**

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., B0 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](https://github.com/kschan0214/sepia/releases/tag/v1.1.0)]
* MRITOOLS v3.5.6 [[https://github.com/korbinian90/CompileMRI.jl/releases/tag/v3.5.6](https://github.com/korbinian90/CompileMRI.jl/releases/tag/v3.5.5)]
* 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** |
| **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 |

**Step 3: Background field removal**

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 |  |

**Step 4: Dipole inversion (corresponding to “Standard” pipeline)**

Table S3: Algorithm parameters for dipole field inversion using ‘Standard’ pipeline.

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

#### Alternative dipole inversion methods: (MEDI and FANSI)

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

Table S4: Algorithm parameters for dipole field inversion using ‘Alternative 1’ pipeline.

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

P.S. Output from the ‘Standard’ pipeline is required. The scripts are in ‘*QSM\_Consensus\_Paper\_Example\_Code/SEPIA\_Alternative1\_Pipeline/’*.

**Step 4 (Alternative 2): Dipole inversion**

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 |  |
| **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

Text

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Figure S2: Susceptibility maps derived using the ‘Standard’ processing pipeline.

Text

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Figure S3: Susceptibility maps derived using the ‘Alternative 1’ (MEDI) processing pipeline.

Text

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Figure S4: Susceptibility maps derived using the ‘Alternative 2’ (FANSI) processing pipeline.

## References

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