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# **pynibs Documentation**

***Release 0.1***

**Konstantin Weise**

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**pyNIBS** is a Python package to work with non-invasive brain stimulation (NIBS) data, foremost from transcranial magnetic stimulation (TMS) experiments.

We created this package to allow the mapping of causal structure-function relationships with TMS. A lot of analyses is based on calculations of the induced electric fields (e-fields) – for this we rely on [SimNIBS](#).

Install **pyNIBS** via pip:

```
pip install pynibs
```

or directly grab from our repository at [gitlab.gwdg.de/tms-localization/pynibs](https://gitlab.gwdg.de/tms-localization/pynibs)



## CONTENTS.

## 1.1 pynibs package

### 1.1.1 Subpackages

#### pynibs.congruence package

`pynibs.congruence` holds the initial congruence factor implementation as described in Weise, Numssen, et al., 2020 [1]. This code is mainly stored here for reproducibility reasons. The current approach (Numssen et al., 2021; [2]) uses the `pynibs.regression` methods.

#### References

#### Submodules

##### pynibs.congruence.congruence module

`pynibs.congruence.congruence.cf_curveshift_kernel(e_curve, mep_curve)`

Curve congruence (overlap) measure for multiple MEP curves per element. Determines the average displacement between the MEP curves. The congruence factor is weighted by `median(E)` and summed up. This favors elements which have greater E, as these are more likely to produce MEPs.

$$dE = \begin{bmatrix} dE_{11} & dE_{12} & \dots & dE_{1n} \\ dE_{21} & dE_{22} & \dots & dE_{2n} \\ \dots & \dots & \dots & \dots \\ dE_{n1} & dE_{n2} & \dots & dE_{nn} \end{bmatrix}$$

-> `congruence_factor ~ np.linalg.norm(dE)/median(E)/n_cond/2`

#### Parameters

- `e_curve` (*list of np.ndarray of float*) – (n\_cond) List over all conditions of electric field values corresponding to the mep amplitudes.
- `mep_curve` (*list of np.ndarray of float*) – (n\_cond) List over all conditions of mep values corresponding to the electric field.

#### Returns

`congruence_factor` – Congruence factor for the n\_cond electric field and MEP curves.

#### Return type

`float`

`pynibs.congruence.congruence.cf_curveshift_workhorse(elm_idx_list, mep, mep_params, e, n_samples=100)`

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`). `n_samples` are taken from `fitted_mep`, within the range of the `Mep`.

#### Parameters

- `elm_idx_list (np.ndarray)` – (chunksize) List of element indices, the congruence factor is computed for.
- `mep (list of Mep)` – (`n_cond`) List of fitted Mep object instances for all conditions.
- `mep_params (np.ndarray of float)` – (`n_mep_params_total`) List of all mep parameters of curve fits used to calculate the MEP, accumulated into one array.
  - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- `e (list of list of np.ndarray of float)` – [`n_cond`][`n_datasets`][`n_elm`] Tuple of `n_datasets` of the electric field to compute the congruence factor for, e.g. (`e_mag`, `e_norm`, `e_tan`). Each dataset is a list over all conditions containing the electric field component of interest.
  - `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g: `e_mag = e[0]`)
- `n_samples (int, default=100)` – Number of data points to generate discrete mep and e curves.

#### Returns

`congruence_factor` – (`n_roi, n_datasets`) Congruence factor in each element specified in `elm_idx_list` and for each input dataset.

#### Return type

`np.ndarray of float`

```
pynibs.congruence.congruence.cf_curveshift_workhorse_stretch_correction(elm_idx_list, mep,
                                                               mep_params, e,
                                                               n_samples=100)
```

Worker function for congruence factor computation - call from `multiprocessing.pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`). `n_samples` are taken from `fitted_mep`, within the range of the `Mep`.

#### Parameters

- `elm_idx_list (np.ndarray)` – (chunksize) List of element indices, the congruence factor is computed for
- `mep (list of Mep)` – (`n_cond`) List of fitted Mep object instances for all conditions.
- `mep_params (np.ndarray of float)` – (`n_mep_params_total`) List of all mep parameters of curve fits used to calculate the MEP, accumulated into one array.
  - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- `e (list of list of np.ndarray of float)` – [`n_cond`][`n_datasets`][`n_elm`] Tuple of `n_datasets` of the electric field to compute the congruence factor for, e.g. (`e_mag`, `e_norm`, `e_tan`). Each dataset is a list over all conditions containing the electric field component of interest
  - e.g.: `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g: `e_mag = e[0]`)

- **n\_samples** (`int`, `default=100`) – Number of data points to generate discrete mep and e curves.

**Returns**

**congruence\_factor** – (`n_roi`, `n_datasets`) Congruence factor in each element specified in `elm_idx_list` and for each input dataset.

**Return type**

`np.ndarray` of `float`

```
pynibs.congruence.congruence.cf_curveshift_workhorse_stretch_correction_new(mep,
                                                                           mep_params,
                                                                           e,
                                                                           n_samples=100,
                                                                           ref_idx=0)
```

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`). `n_samples` are taken from `fitted_mep`, within the range of the [Mep](#).

**Parameters**

- **mep** (list of [Mep](#)) – (`n_cond`) List of fitted Mep object instances for all conditions.
- **mep\_params** (`np.ndarray` of `float` [`n_mep_params_total`]) – List of all mep parameters of curve fits used to calculate the MEP (accumulated into one array)
  - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- **e** (`np.ndarray` of `float`) – (`n_elm, n_cond`) Electric field in elements.
- **n\_samples** (`int`, `default=100`) – Number of data points to generate discrete mep and e curves.

**Returns**

**congruence\_factor** – (`n_elm`) Congruence factor in each element specified in `elm_idx_list` and for each input dataset.

**Return type**

`np.ndarray` of `float`

```
pynibs.congruence.congruence.cf_curveshift_workhorse_stretch_correction_sign_new(mep,
                                                                           mep_params,
                                                                           e,
                                                                           n_samples=100,
                                                                           ref_idx=0)
```

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`). ```n_sample```s are taken from `fitted_mep`, within the range of the [Mep](#).

**Parameters**

- **mep** (list of [Mep](#)) – (`n_cond`) List of fitted Mep object instances for all conditions.
- **mep\_params** (`np.ndarray` of `float`) – (`n_mep_params_total`) List of all mep parameters of curve fits used to calculate the MEP, accumulated into one array.
  - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- **e** (`np.ndarray` of `float`) – (`n_elm, n_cond`) Electric field in elements.
- **n\_samples** (`int`, `default=100`) – Number of data points to generate discrete mep and e curves.

### Returns

**congruence\_factor** – (n\_elm, 1) Congruence factor in each element specified in elm\_idx\_list and for each input dataset.

### Return type

np.ndarray of float

```
pynibs.congruence.congruence.cf_curveshift_workhorse_stretch_correction_variance(elm_idx_list,
                                                               mep,
                                                               mep_params,
                                                               e,
                                                               n_samples=100)
```

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`). `n_samples` are taken from `fitted_mep`, within the range of the `Mep`.

### Parameters

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for.
- **mep** (list of `Mep`) – (n\_cond) List of fitted Mep object instances for all conditions
- **mep\_params** (`np.ndarray of float [n_mep_params_total]`) – List of all mep parameters of curve fits used to calculate the MEP (accumulated into one array)
  - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. (`e_mag, e_norm, e_tan`). Each dataset is a list over all conditions containing the electric field component of interest
  - e.g.: `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g. `e_mag = e[0]`)
- **n\_samples** (`int, default=100`) – Number of data points to generate discrete mep and e curves

### Returns

**congruence\_factor** – Congruence factor in each element specified in elm\_idx\_list and for each input dataset

### Return type

np.ndarray of float [n\_roi, n\_datasets]

```
pynibs.congruence.congruence.cf_variance_sign_workhorse(elm_idx_list, mep, mep_params, e)
```

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements.

### Parameters

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for.
- **mep** (list of `Mep`) – (n\_cond) List of fitted Mep object instances for all conditions.
- **mep\_params** (`np.ndarray of float`) – (n\_mep\_params\_total) List of all mep parameters of curve fits used to calculate the MEP, accumulated into one array), e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
- **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g.

(`e_mag`, `e_norm`, `e_tan`). Each dataset is a list over all conditions containing the electric field component of interest

- `len(e)` = `n_cond`
  - `len(e[0])` = `n_comp` (e.g: `e_mag = e[0]`))

## Returns

**congruence\_factor** – (n\_roi, n\_datasets) Congruence factor in each element specified in elm\_idx\_list and for each input dataset.

## Return type

np.ndarray of float

```
pynibs.congruence.congruence.cf_variance_workhorse(elm_idx_list, mep, mep_params, e,  
old_style=True)
```

Worker function for congruence factor computation - call from `multiprocessing.Pool`. Calculates congruence factor for  $e = (\mathbf{E}_{\text{mag}}, \mathbf{E}_{\text{norm}} \text{ and/or } \mathbf{E}_{\text{tan}})$  for given zaps and elements.

## Parameters

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for.
  - **mep** (list of `Mep`) – (n\_cond) List of fitted Mep object instances for all conditions.
  - **mep\_params** (`np.ndarray of float`) – (n\_mep\_params\_total) List of all mep parameters used to calculate the MEP, accumulated into one array).
    - e.g. `[mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...]`
  - **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. (`e_mag`, `e_norm`, `e_tan`). Each dataset is a list over all conditions containing the electric field component of interest
    - `len(e)` = n\_cond
    - `len(e[0])` = n\_comp (e.g: `e_mag = e[0]`)
  - **old\_style** (`boolean (default: True)`) – True: Weight `var(x_0_prime(r))` with `mean(e(r)) * mean(Stimulator Intensity)`, taken from `mep` False: Weight `var(x_0_prime(r))` with `mean(E(r))`, taken from `e`

## Returns

**congruence\_factor** – (n\_roi, n\_datasets) Congruence factor in each element specified in elm\_idx\_list and for each input dataset

## Return type

np.ndarray of float

```
pynibs.congruence.congruence.extract_condition_combination(fn_config_cfg, fn_results_hdf5,  
cond, fn_out_prefix)
```

Extract and plot congruence factor results for specific condition combinations from permutation analysis.

## Parameters

- **fn\_config\_cfg** (*str*) – Filename of .cfg file the permutation study was conducted with
  - **fn\_results\_hdf5** (*str*) – Filename of .hdf5 results file generated by `00_run_c_standard_compute_all_permutations.py` containing congruence factors and condition combinations.
  - **conds** (*list of str*) – (n\_cond) List containing condition combinations to extract and plot, e.g. `['P_0', 'I_225', 'M1_0', 'I_675', 'P_225']`.

- **fn\_out\_prefix** (*str*) – Prefix of output filenames of \*\_data.xdmf, \*\_data.hdf5 and \*\_geo.hdf5.

**Returns**

- <fn\_out\_prefix\_data.xdmf> (*.xdmf file*) – Output file linking \*\_data.hdf5 and \*\_geo.hdf5 file to plot in paraview.
- <fn\_out\_prefix\_data.hdf5> (*.hdf5 file*) – Output .hdf5 file containing the data.
- <fn\_out\_prefix\_geo.xdmf> (*.hdf5 file*) – Output .hdf5 file containing the geometry information.

## **pynibs.congruence.ext\_metrics module**

```
pynibs.congruence.ext_metrics.dvs_likelihood(params, x, y, verbose=True, normalize=False,  
bounds=[(1, 2), (1, 2)])
```

```
pynibs.congruence.ext_metrics.e_cog_workhorse(elm_idx_list, mep, mep_params, e)
```

Worker function for electric field center of gravity (e\_cog) computation after Opitz et al. (2013) [1] - call from `multiprocessing.Pool`. Calculates the e\_cog for `e = (E_mag, E_norm and/or E_tan)` for given zaps and elements. The electric field is weighted by the mean MEP amplitude (turning point of the sigmoid) and summed up. The computations are parallelized in terms of element indices (`elm_idx_list`).

**Parameters**

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for.
- **mep** (list of `Mep`) – (n\_cond) List of fitted Mep object instances for all conditions.
- **mep\_params** (`np.ndarray of float`) – (n\_mep\_params\_total) List of all mep parameters of curve fits used to calculate the MEP, accumulated into one array.
  - e.g. [`mep_#1_para_#1, mep_#1_para_#2, mep_#1_para_#3, mep_#2_para_#1, mep_#2_para_#1, ...`]
- **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. (`e_mag, e_norm, e_tan`). Each dataset is a list over all conditions containing the electric field component of interest
  - e.g.: `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g: `e_mag = e[0]`)

**Returns**

`e_cog` – (n\_roi, n\_datasets) RSD inverse in each element specified in `elm_idx_list` and for each input dataset.

**Return type**

`np.ndarray of float`

## Notes

`pynibs.congruence.ext_metrics.e_focal_workhorse(elm_idx_list, e)`

Worker function to determine the site of stimulation after Aonuma et al. (2018) [1], call from `multiprocessing.Pool`. Calculates the site of stimulation for  $e = (E_{mag}, E_{norm}$  and/or  $E_{tan})$  for given zaps and elements by multiplying the electric fields with each other. The computations are parallelized in terms of element indices (`elm_idx_list`).

### Parameters

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for
- **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. ( $e_{mag}$ ,  $e_{norm}$ ,  $e_{tan}$ ). Each dataset is a list over all conditions containing the electric field component of interest
  - `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g:  $e_{mag} = e[0]$ )

### Returns

**e\_focal** – (n\_roi, n\_datasets) Focal electric field in each element specified in `elm_idx_list` and for each input.

### Return type

`np.ndarray` of `float`

## Notes

`pynibs.congruence.ext_metrics.rsd_inverse_workhorse(elm_idx_list, mep, e)`

Worker function for RSD inverse computation after Bungert et al. (2017) [1], call from `multiprocessing.Pool`. Calculates the RSD inverse for  $e = (E_{mag}, E_{norm}$  and/or  $E_{tan})$  for given zaps and elements. The computations are parallelized in terms of element indices (`elm_idx_list`).

### Parameters

- **elm\_idx\_list** (`np.ndarray`) – (chunksize) List of element indices, the congruence factor is computed for
- **mep** (`list of Mep`) – (n\_cond) List of fitted Mep object instances for all conditions.
- **e** (`list of list of np.ndarray of float`) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. ( $e_{mag}$ ,  $e_{norm}$ ,  $e_{tan}$ ). Each dataset is a list over all conditions containing the electric field component of interest
  - `len(e) = n_cond`
  - `len(e[0]) = n_comp` (e.g:  $e_{mag} = e[0]$ )

### Returns

**rsd\_inv** – (n\_roi, n\_datasets) RSD inverse in each element specified in `elm_idx_list` and for each input dataset.

### Return type

`np.ndarray` of `float`

## Notes

### pynibs.congruence.stimulation\_threshold module

```
pynibs.congruence.stimulation_threshold.intensity_thresh(mep_curve, intensities,  
mep_threshold)
```

Determines the stimulation threshold of one particular condition (usually the most sensitive e.g. M1-45). The stimulation threshold is the stimulator intensity value in [A/us] where the mep curves exceed the value of mep\_threshold (in [mV]).

#### Parameters

- **mep\_curve** (*list [1] of np.ndarray of float [n\_samples]*) – MEP curve values for every conditions
- **intensities** (*list [1] of np.ndarray of float [n\_samples]*) – To the MEP values corresponding stimulator intensities in [A/us]
- **mep\_threshold** (*float*) – MEP value in [mV], which has to be exceeded for threshold definition

#### Returns

**stim\_threshold\_avg** – Average stimulation threshold in [V/m] where c\_factor is greater than c\_factor\_percentile

#### Return type

*float*

```
pynibs.congruence.stimulation_threshold.mean_mep_threshold(elm_idx, mep_curve, intensities, e,  
mep_threshold)
```

Determines the stimulation threshold by calculating the average electric field over all conditions, where the mep curves exceed the value of mep\_threshold (in [mV]).

#### Parameters

- **elm\_idx** (*list of np.ndarray of int*) – [n\_datasets](n\_elements) Element indices where the congruence factor exceeds a certain percentile, defined during the call of *stimulation\_threshold()*.
- **mep\_curve** (*list of np.ndarray of float*) – [n\_conditions](n\_samples) MEP curve values for every condition.
- **intensities** (*list of np.ndarray of float*) – [n\_conditions](n\_samples) To the MEP values corresponding stimulator intensities in [A/us].
- **e** (*list of list of np.ndarray of float*) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. (e\_mag, e\_norm, e\_tan). Each dataset is a list over all conditions containing the electric field component of interest
  - e.g.: len(e) = n\_cond
  - len(e[0]) = n\_comp (e.g: e\_mag = e[0]))
- **mep\_threshold** (*float*) – MEP value in [mV], which has to be exceeded for threshold definition.

#### Returns

**stim\_threshold\_avg** – Average stimulation threshold in [V/m] where c\_factor is greater than c\_factor\_percentile

#### Return type

*float*

---

```
pynibs.congruence.stimulation_threshold.sigmoid_thresh(elm_idx, mep_curve, intensities, e,
                                                       mep_threshold)
```

Determines the stimulation threshold by calculating an equivalent [pynibs.expio.Mep.sigmoid](#) over all conditions. The stimulation threshold is the electric field value where the mep curves exceed the value of mep\_threshold (in [mV]).

#### Parameters

- **elm\_idx** (*list of np.ndarray of int*) – [n\_datasets](n\_elements) Element indices where the congruence factor exceeds a certain percentile, defined during the call of [stimulation\\_threshold\(\)](#).
- **mep\_curve** (*list of np.ndarray of float*) – [n\_conditions](n\_samples) MEP curve values for every condition.
- **intensities** (*list of np.ndarray of float*) – [n\_conditions](n\_samples) To the MEP values corresponding stimulator intensities in [A/us].
- **e** (*list of list of np.ndarray of float*) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g. (e\_mag, e\_norm, e\_tan). Each dataset is a list over all conditions containing the electric field component of interest
  - e.g.: len(e) = n\_cond
  - len(e[0]) = n\_comp (e.g: e\_mag = e[0])
- **mep\_threshold** (*float*) – MEP value in [mV], which has to be exceeded for threshold definition

#### Returns

**stim\_threshold\_avg** – Average stimulation threshold in [V/m] where c\_factor is greater than c\_factor\_percentile

#### Return type

*float*

```
pynibs.congruence.stimulation_threshold.stimulation_threshold(elm_idx_list, mep,
                                                               mep_params, n_samples, e,
                                                               c_factor_percentile=95,
                                                               mep_threshold=0.5,
                                                               c_factor=None,
                                                               c_function=None,
                                                               t_function=None)
```

Computes the stimulation threshold in terms of the electric field in [V/m]. The threshold is defined as the electric field value where the mep exceeds mep\_threshold. The average value is taken over all mep curves in each condition and over an area where the congruence factor exceeds c\_factor\_percentile.

#### Parameters

- **elm\_idx\_list** (*np.ndarray*) – (chunksize) List of element indices, the congruence factor is computed for.
- **mep** (*list of Mep object instances*) – (n\_cond) List of fitted [Mep](#) object instances for all conditions.
- **mep\_params** (*np.ndarray of float [n\_mep\_params\_total]*) – List of all mep parameters of curve fits used to calculate the MEP (accumulated into one array)
  - e.g. [mep\_#1\_para\_#1, mep\_#1\_para\_#2, mep\_#1\_para\_#3, mep\_#2\_para\_#1, mep\_#2\_para\_#1, ...]
- **n\_samples** (*int*) – Number of data points to generate discrete mep and e curves.
- **e** (*list of list of np.ndarray of float*) – [n\_cond][n\_datasets][n\_elm] Tuple of n\_datasets of the electric field to compute the congruence factor for, e.g.

(e\_mag, e\_norm, e\_tan). Each dataset is a list over all conditions containing the electric field component of interest

- e.g.: len(e) = n\_cond
- len(e[0]) = n\_comp (e.g: e\_mag = e[0]))
- **c\_factor\_percentile** (*float*) – Percentile of the c\_factor taken into account for the threshold evaluation. Only c\_factors are considered exceeding this.
- **mep\_threshold** (*float*) – MEP value in [mV], which has to be exceeded for threshold definition.
- **c\_factor** (*np.ndarray of float*) –
- **(n\_roi** –
- **dataset**. (*n\_datasets*) Congruence factor in each element specified in elm\_idx\_list and for each input) –
- **c\_function** (*function*) – Defines the function to use during c\_gpc to calculate the congruence factor.
  - congruence\_factor\_curveshift\_workhorse: determines the average curve shift
  - congruence\_factor\_curveshift\_workhorse\_stretch\_correction: determines the average curve shift
  - congruence\_factor\_curveshift\_workhorse\_stretch\_correction\_variance: determines the average curve shift
  - congruence\_factor\_variance\_workhorse: evaluates the variance of the shifting and stretching parameters
- **t\_function** (*function*) – Defines the function to determine the stimulation\_threshold.
  - stimulation\_threshold\_mean\_mep\_threshold: uses mep\_threshold to determine the corresponding e\_threshold over all conditions and takes the average values as the stimulation threshold
  - stimulation\_threshold\_pynibs.sigmoid: Fits a new pynibs.sigmoid using all data-points in the mep-vs-E space and evaluates the threshold from the turning point or the intersection of the derivative in the crossing point with the e-axis

**Returns**

**stim\_threshold\_avg** – Average stimulation threshold in [V/m] where c\_factor is greater than c\_factor\_percentile.

**Return type**

*float*

## **pynibs.expio package**

### **Submodules**

#### **pynibs.expio.Mep module**

**class pynibs.expio.Mep(intensities, mep, intensity\_min\_threshold=None, mep\_min\_threshold=None)**

Bases: *object*

Mep object.

**fun**

Function type to fit data with (pynibs.sigmoid / pynibs.exp / pynibs.linear).

**Type**  
function

**fun\_sig**  
Best fitting equivalent sigmoidal function (added by `self.add_sigmoidal_bestfit()`).

**Type**  
function

**popt**  
(N\_para), Fitted optimal function parameters.

**Type**  
`np.ndarray of float`

**popt\_sig**  
(3), Best fitting parameters `x0`, `r`, and `amp` of equivalent sigmoidal function.

**Type**  
`np.ndarray of float`

**covt**  
(N\_para, N\_para), covariance matrix of fitted parameters.

**Type**  
`np.ndarray of float`

**pstd**  
(N\_para), Standard deviation of fitted parameters.

**Type**  
`np.ndarray of float`

**fit**  
Gmodel object instance of parameter fit.

**Type**  
object instance

**x\_limits**  
(2), Minimal and maximal value of intensity data.

**Type**  
`np.ndarray of float`

**y\_limits**  
(2), Minimal and maximal value of mep data.

**Type**  
`np.ndarray of float`

**mt**  
Motor threshold (MEP > 50 uV), evaluated from fitted curve, added after fitting.

**Type**  
`float`

**calc\_motor\_threshold(*threshold*)**  
Determine motor threshold of stimulator depending on MEP threshold given in [mV].

**Parameters**  
**threshold** (`float`) – Threshold of MEP amplitude in [mV].

## Notes

Add Attributes:

### Mep.mt

[float] Motor threshold for given MEP threshold.

### eval(x, p)

Evaluating fitted function with optimal parameters in points x.

#### Parameters

- **x** (*np.ndarray of float*) – (N\_x) Function arguments.
- **p** (*tuple of float*) – Function parameters.

#### Returns

y – (N\_x) Function values.

#### Return type

np.ndarray of float

### eval\_fun\_sig(x, p)

Evaluating optimally fitted sigmoidal function with optimal parameters in points x.

#### Parameters

- **x** (*np.ndarray of float*) – (N\_x) Function arguments.
- **p** (*tuple of float*) – Function parameters

#### Returns

y – (N\_x) Function values.

#### Return type

np.ndarray of float

### eval\_opt(x)

Evaluating fitted function with optimal parameters in points x.

#### Parameters

**x** (*np.ndarray of float*) – (N\_x) Function arguments.

#### Returns

y – (N\_x) Function values.

#### Return type

np.ndarray of float

### eval\_uncertainties(x, sigma=1)

Evaluating approximated uncertainty interval around fitted distribution.

#### Parameters

- **x** (*np.ndarray of float*) – (N\_x) Function values where uncertainty is evaluated.
- **sigma** (*float*) – Standard deviation of parameters taken into account when evaluating uncertainty interval.

#### Returns

- **y\_min** (*np.ndarray of float*) – (N\_x) Lower bounds of y-values.
- **y\_max** (*np.ndarray of float*) – (N\_x) Upper bounds of y-values.

### fit\_mep\_to\_function(p0=None)

Fits MEP data to function. The algorithm tries to fit the function first to a sigmoid, then to an exponential and finally to a linear function.

**Parameters**

**p0** (*np.ndarray of float*) – Initial guess of parameter values.

**Notes**

Add Attributes:

**Mep.popt**

[*np.ndarray of float*] (*N\_para*) Fitted optimal function parameters.

**Mep.copt**

[*np.ndarray of float*] (*N\_para, N\_para*) Covariance matrix of fitted parameters.

**Mep.pstd**

[*np.ndarray of float*] (*N\_para*) Standard deviation of fitted parameters.

**Mep.fun**

[function] Function mep data was fitted with.

**Mep.fit**

[object instance] Gmodel object instance of parameter fit.

**Mep.mt**

[float] Motor threshold (MEP > 50 uV).

**fit\_mep\_to\_function\_multistart(*p0=None, constraints=None, fun=None*)**

Fits MEP data to function.

**Parameters**

- **p0** (*np.ndarray of float*) – Initial guess of parameter values.
- **constraints** (*dict*) – Dictionary with parameter names as keys and [min, max] values as constraints.
- **fun** (*list of functions*) – Functions to incorporate in the multistart fit (e.g. [*pynibs.sigmoid*, *pynibs.exp0*, *pynibs.linear*]).

**Notes**

Add Attributes:

**Mep.popt**

[*np.ndarray of float*] (*N\_para*) Best fitted optimal function parameters.

**Mep.copt**

[*np.ndarray of float*] (*N\_para, N\_para*) Covariance matrix of best fitted parameters.

**Mep.pstd**

[*np.ndarray of float*] (*N\_para*) Standard deviation of best fitted parameters.

**Mep.fun**

[function] Function of best fit mep data was fitted with.

**Mep.fit**

[list of fit object instances] Gmodel object instances of parameter fits.

**Mep.best\_fit\_idx**

[int] Index of best function fit (*fit[best\_fit\_idx]*).

**Mep.constraints**

[dict] Dictionary with parameter names as keys and [min, max] values as constraints.

```
plot(label, sigma=3, plot_samples=True, show_plot=False, fname_plot='', ylim=None, ylabel=None, fontsize_axis=10, fontsize_legend=10, fontsize_label=10, fontsize_title=10, fun=None)
```

Plotting mep data and fitted curve together with uncertainties. If ``fun == None``, the optimal function is plotted.

#### Parameters

- **label** (*str*) – Plot title.
- **sigma** (*float*) – Factor of standard deviations the uncertainty of the fit is plotted with.
- **plot\_samples** (*boolean*) – Plot sampling curves of the fit in the uncertainty interval.
- **show\_plot** (*boolean*) – Show or hide plot window (TRUE / FALSE).
- **fname\_plot** (*str*) – Filename of plot showing fitted data (with .png extension).
- **ylim** (*list of float [2]*) – Min and max values of y-axis.
- **fontsize\_axis** (*int*) – Fontsize of axis numbers.
- **fontsize\_legend** (*int*) – Fontsize of Legend labels.
- **fontsize\_label** (*int*) – Fontsize of axis labels.
- **fontsize\_title** (*int*) – Fontsize of title.
- **fun** (*str or None (None, sigmoid, exp, linear)*) – Which function to plot.

#### Returns

**<File>** – Plot of Mep data and fit (format: png).

#### Return type

.png file

```
run_fit_multistart(fun, x, y, p0, constraints=None, verbose=False, n_multistart=100)
```

Run multistart approach to fit data to function. **n\_multistart** optimizations are performed based on random variations of the initial guess parameters **p0**. The fit with the lowest AIC (Akaike information criterion), i.e. best fit is returned as gmodel fit instance.

#### Parameters

- **fun** (*function*) – Function mep data has to be fitted with
- **x** (*np.ndarray of float*) – (N\_data), Independent variable the data is fitted on.
- **y** (*np.ndarray of float*) – (N\_data), Dependent data the curve is fitted through.
- **p0** (*np.ndarray of float or list of float*) – Initial guess of parameter values.
- **constraints** (*dict, optional*) – Dictionary with parameter names as keys and [min, max] values as constraints.
- **verbose** (*bool, default: False*) – Show output messages.
- **n\_multistart** (*int*) – Number of repeated optimizations with different starting points to perform.

#### Returns

**fit** – Gmodel object instance of best parameter fit with lowest parameter variance.

#### Return type

object instance

```
pynibs.expio.Mep.butter_lowpass(cutoff, fs, order=5)
```

Setup Butter low-pass filter and return filter parameters.

#### Parameters

- **cutoff** (*float*) – Cutoff frequency in [Hz].

- **fs** (*float*) – Sampling frequency in [Hz].
- **order** (*int*, *default*: 5) – Filter order.

**Returns**

**b, a** – Numerator (b) and denominator (a) polynomials of the IIR filter.

**Return type**

np.ndarray, np.ndarray

`pynibs.expio.Mep.butter_lowpass_filter(data, cutoff, fs, order=5)`

Applies Butterworth lowpass filter

**Parameters**

- **data** (*np.ndarray of float [N\_samples]*) – Input of the digital filter
- **cutoff** (*float*) – Cutoff frequency in [Hz]
- **fs** (*float*) – Sampling frequency in [Hz]
- **order** (*int*) – Filter order

**Returns**

**y** – Output of the digital filter

**Return type**

np.ndarray [N\_samples]

`pynibs.expio.Mep.calc_p2p(sweep, tms_pulse_time=0.2, start_mep=20, end_mep=35, measurement_start_time=0, sampling_rate=4000, cutoff_freq=500, fn_plot=None)`

Calc peak-to-peak values of and mep sweep.

**Parameters**

- **sweep** (*np.ndarray of float [Nx1]*) – Input curve
- **tms\_pulse\_time** (*float (Default: .2)*) – onset time of TMS pulse trigger in [s]
- **start\_mep** (*int (Default: 18)*) – start of p2p search window after TMS pulse. In [ms].
- **end\_mep** (*int (Default: 35)*) – end of p2p search window after TMS pulse. In [ms].
- **measurement\_start\_time** (*float (Default: 0)*) – start time of the EMG measurement. In [ms].
- **sampling\_rate** (*int (Default: 2000)*) – Sampling rate in Hz
- **cutoff\_freq** (*int (Default: 500)*) – Desired cutoff frequency of the filter, Hz
- **fn\_plot** (*str, default: None*) – Filename of sweep to plot (.png). If None, plot is omitted.

**Returns**

- **p2p** (*float*) – Peak-to-peak value of input curve
- **sweep\_filt** (*np.ndarray of float*) – Filtered input curve (Butter lowpass filter with specified cutoff\_freq)
- **onset** (*float*) – MEP onset after tms\_pulse\_time

`pynibs.expio.Mep.calc_p2p_old_exp0(sweep, start_mep=None, end_mep=None, tms_pulse_time=None, sampling_rate=None)`

Calc peak-to-peak values of an mep sweep. This version was probably used in the ancient times of experiment 0.

**Parameters**

- **sweep** (*np.ndarray of float*) – (Nx1) Input curve.
- **start\_mep** (*None*) – Not used.
- **end\_mep** (*None*) – Not used.
- **tms\_pulse\_time** (*None*) – Not used.
- **sampling\_rate** (*int (Default: 2000)*) – Sampling rate in Hz.

**Returns**

**p2p** – Peak-to-peak value of input curve

**Return type**

*float*

```
pynibs.expio.Mep.calc_p2p_old_exp1(sweep, start_mep=18, end_mep=35, tms_pulse_time=None,
                                     sampling_rate=2000)
```

Calc peak-to-peak values of an mep sweep. This version was probably used for the first fits of experiment 1.

**Parameters**

- **sweep** (*np.ndarray of float [Nx1]*) – Input curve
- **start\_mep: Int or Float (Default: 18)**  
Starttime in [ms] after TMS for MEP seach window.
- **end\_mep: Int or Float (Default: 35)**  
Endtime in [ms] after TMS for MEP seach window.
- **tms\_pulse\_time** (*None*) – Not used.
- **sampling\_rate** (*int (Default: 2000)*) – Sampling rate in Hz

**Returns**

**p2p** – Peak-to-peak value of input curve

**Return type**

*float*

```
pynibs.expio.Mep.dummy_fun(x, a)
```

Dummy function for congruence factor calculation.

```
pynibs.expio.Mep.exp(x, x0, r, y0)
```

Parametrized exponential function.

$$y = y_0 + e^{r(x-x_0)}$$

**Parameters**

- **x** (*np.ndarray of float*) – (N\_x) X-values the function is evaluated in.
- **x0** (*float*) – Horizontal shift along the abscissa.
- **r** (*float*) – Slope parameter.
- **y0** (*float*) – Offset parameter.

**Returns**

**y** – Function value at x

**Return type**

*np.ndarray of float [N\_x]*

```
pynibs.expio.Mep.exp0(x, x0, r)
```

Parametrized exponential function w/o offset.

$$y = e^{r(x-x_0)}$$

**Parameters**

- **x** (`np.ndarray of float`) – (N\_x) X-values the function is evaluated in.
- **x0** (`float`) – Horizontal shift along the abscissa.
- **r** (`float`) – Slope parameter.

**Returns**

`y` – (N\_x) Function value at x.

**Return type**

`np.ndarray of float`

`pynibs.expio.Mep.exp0_log(x, x0, r)`

Parametrized exponential function w/o offset.

$$y = e^{r(x-x_0)}$$

**Parameters**

- **x** (`np.ndarray of float`) – (N\_x) X-values the function is evaluated in.
- **x0** (`float`) – Horizontal shift along the abscissa.
- **r** (`float`) – Slope parameter.

**Returns**

`y` – (N\_x) Function value at x.

**Return type**

`np.ndarray of float`

`pynibs.expio.Mep.exp_log(x, x0, r, y0)`

Parametrized exponential function (log)

$$y = y_0 + e^{r(x-x_0)}$$

**Parameters**

- **x** (`np.ndarray of float`) – (N\_x) X-values the function is evaluated in.
- **x0** (`float`) – Horizontal shift along the abscissa.
- **r** (`float`) – Slope parameter.
- **y0** (`float`) – y-offset parameter.

**Returns**

`y` – (N\_x) Function value at x.

**Return type**

`np.ndarray of float`

`pynibs.expio.Mep.get_mep_elements(mep_fn, tms_pulse_time, drop_mep_idx=None, cfs_data_column=0, channels=None, time_format='delta', plot=False, start_mep=18, end_mep=35)`

Read EMG data from CED .cfs or .txt file and returns MEP amplitudes.

**Parameters**

- **mep\_fn** (`string`) – path to .cfs-file or .txt file (Signal export).
- **tms\_pulse\_time** (`float`) – Time in [s] of TMS pulse as specified in signal.
- **drop\_mep\_idx** (`List of int or None, default: None`) – Which MEPs to remove before matching.
- **cfs\_data\_column** (`int or list of int`) – Column(s) of dataset in cfs file. +1 for .txt.
- **channels** (`list of str, default: None`) – Channel names.

- **time\_format** (*str*, *default*: "delta") – Format of mep time stamps in time\_mep\_lst to return.
  - "delta" returns list of datetime.timedelta in seconds
  - "hms" returns datetime.datetime(year, month, day, hour, minute, second, microsecond)
- **plot** (*bool*, *default*: False) – Plot MEPs.
- **start\_mep** (*float*, *default*: 18) – Start of time frame after TMS pulse where p2p value is evaluated (in ms).
- **end\_mep** (*float*, *default*: 35) – End of time frame after TMS pulse where p2p value is evaluated (in ms).

#### Returns

- **p2p\_array** (*np.ndarray of float*) – (N\_stim) Peak to peak values of N sweeps.
- **time\_mep\_lst** (*list of datetime.timedelta*) – MEP-timestamps
- **mep\_raw\_data** (*np.ndarray of float*) – (N\_channel, N\_stim, N\_samples) Raw (unfiltered) MEP data.
- **mep\_filt\_data** (*np.ndarray of float*) – (N\_channel, N\_stim, N\_samples) Filtered MEP data (Butterworth lowpass filter).
- **time** (*np.ndarray of float*) – (N\_samples) Time axis corresponding to MEP data.
- **mep\_onset\_array** (*np.ndarray of float*) – (S\_samples) MEP onset after TMS pulse.

`pynibs.expio.Mep.get_mep_sampling_rate(cfs_path)`

Returns sampling rate [Hz] for CED Signal EMG data in .cfs, .mat or .txt file.

The sampling rate is saved in the cfs header like this: .. code-block:: sh

```
``Samplingrate": 3999.999810,
```

#### Parameters

##### **cfs\_path**

[str] Path to .cfs file or .txt file.

#### Returns

##### **float**

[sampling rate]

`pynibs.expio.Mep.get_mep_virtual_subject_DVS(x, x0=0.5, r=10, amp=1, sigma_x=0, sigma_y=0, y0=0.01, seed=None)`

Creates random mep data using the 2 variability source model from Goetz et al. 2014 [1] together with a standard 3 parametric sigmoid function.

## References

#### Parameters

- **x** (*np.ndarray of float*) – (n\_x) Normalized stimulator intensities [0 ... 1].
- **x0** (*float*, *default*: 0.5) – Location of turning point sigmoidal function.
- **r** (*float*, *default*: 0.25) – Steepness of sigmoidal function.
- **amp** (*float*, *default*: 1.0) – Saturation amplitude of sigmoidal function.

- **sigma\_x** (`float`, `default: 0.1`) – Standard deviation of additive x variability source.
- **sigma\_y** (`float`, `default: 0.1`) – Standard deviation of additive y variability source.
- **y0** (`float`, `default: 1e-2`) – y-offset.
- **seed** (`int`, `default: None`) – Seed to use.

**Returns**

`mep` – (`n_x`) Motor evoked potential values

**Return type**

`np.ndarray` of `float`

```
pynibs.expio.Mep.get_mep_virtual_subject_TVS(x, p1=-5.0818, p2=-2.4677, p3=3.6466, p4=0.42639,
                                              p5=1.6665, mu_y_add=8.283235329759169e-06,
                                              mu_y_mult=-0.9645334, mu_x_add=0.68827324,
                                              sigma_y_add=1.4739e-06, k=0.39316,
                                              sigma2_y_mult=0.022759, sigma2_x_add=0.023671,
                                              subject_variability=False, trial_variability=True)
```

Creates random mep data using the 3 variability source model from [1]. There are typos in the paper but the code seems to be correct. Originally from S. Goetz: <https://github.com/sgoetzduke/Statistical-MEP-Model>. Rewritten from MATLAB to Python by Konstantin Weise.

**Parameters**

- **x** (`np.ndarray` of `float`) – (`n_x`) Normalized stimulator intensities [0 … 1],
- **p1** (`float`, `default: -5.0818`) – First parameter of sigmoidal hilltype function.
- **p2** (`float`, `default: 4.5323`) – Second parameter of sigmoidal hilltype function.
- **p3** (`float`, `default: 3.6466`) – Third parameter of sigmoidal hilltype function.
- **p4** (`float`, `default: 0.42639`) – Fourth parameter of sigmoidal hilltype function.
- **p5** (`float`, `default: 1.6665`) – Fifth parameter of sigmoidal hilltype function.
- **mu\_y\_add** (`float`, `default: 10**-5.0818`) – Mean value of additive y variability source.
- **mu\_y\_mult** (`float`, `default: -0.9645334`) – Mean value of multiplicative y variability source.
- **mu\_x\_add** (`float`, `default: -0.68827324`) – Mean value of additive x variability source.
- **sigma\_y\_add** (`float`, `default: 1.4739*1e-6`) – Standard deviation of additive y variability source.
- **k** (`float`, `default: 0.39316`) – Shape parameter of generalized extreme value distribution.
- **sigma2\_y\_mult** (`float`, `default: 2.2759*1e-2`) – Standard deviation of multiplicative y variability source.
- **sigma2\_x\_add** (`float`, `default: 2.3671*1e-2`) – Standard deviation of additive x variability source.
- **subject\_variability** (`bool`, `default: False`) – Choose if shape parameters from IO curve are sampled from random distributions to model subject variability. This does not influence the trial-to-trial variability.
- **trial\_variability** (`bool`, `default: True`) – Enable or disable trial-to-trial variability. Disabling it will result in ideal IO curves w/o noise.

**Returns**

**mep** – (N\_x) Motor evoked potential values in mV

**Return type**

np.ndarray of float

**References**

`pynibs.expio.Mep.get_time_date(cfs_paths)`

Get time and date of the start of the recording out of .cfs file.

**Parameters**

**cfs\_paths** (str) – Path to .cfs mep file.

**Returns**

**time\_date** – Date and time.

**Return type**

str

`pynibs.expio.Mep.linear(x, m, n)`

Parametrized linear function.

$$y = mx + n$$

**Parameters**

- **x** (np.ndarray of float) – (N\_x) X-values the function is evaluated in.
- **m** (float) – Slope parameter.
- **n** (float) – y-offset.

**Returns**

**y** – (N\_x) Function value at argument x.

**Return type**

np.ndarray of float

`pynibs.expio.Mep.linear_log(x, m, n)`

Parametrized log linear function

$$y = mx + n$$

**Parameters**

- **x** (np.ndarray of float) – (N\_x) X-values the function is evaluated in.
- **m** (float) – Slope.
- **n** (float) – Y-offset.

**Returns**

**y** – (N\_x) Function value at x.

**Return type**

np.ndarray of float

`pynibs.expio.Mep.read_biosig_emg_data(fn_data, include_first_trigger=False, type='cfs')`

`pynibs.expio.Mep.sigmoid(x, x0, r, amp)`

Parametrized sigmoid function.

$$y = \frac{amp}{1 + e^{-r(x-x_0)}}$$

**Parameters**

- **x** (*np.ndarray of float*) – (N\_x) X-values the function is evaluated in.
- **x0** (*float*) – Horizontal shift along the abscissa.
- **r** (*float*) – Slope parameter (steepness).
- **amp** (*float*) – Maximum value the sigmoid converges to.

**Returns**

**y** – (N\_x) Function value at argument x

**Return type**

*np.ndarray of float*

`pynibs.expio.Mep.sigmoid4(x, x0, r, amp, y0)`

Parametrized sigmoid function with 4 parameters.

$$y = y_0 + \frac{amp - y_0}{1 + e^{-r(x-x_0)}}$$

**Parameters**

- **x** (*np.ndarray of float*) – (N\_x) x-values the function is evaluated in.
- **x0** (*float*) – Horizontal shift along the abscissa.
- **r** (*float*) – Slope parameter (steepness).
- **amp** (*float*) – Maximum value the sigmoid converges to.
- **y0** (*float*) – Offset value of the sigmoid.

**Returns**

**y** – (N\_x) Function value at argument x.

**Return type**

*np.ndarray of float*

`pynibs.expio.Mep.sigmoid4_log(x, x0, r, amp, y0)`

Parametrized log transformed sigmoid function with 4 parameters.

$$y = \log \left( y_0 + \frac{amp - y_0}{1 + e^{-r(x-x_0)}} \right)$$

**Parameters**

- **x** (*np.ndarray of float*) – (N\_x) X-values the function is evaluated in.
- **x0** (*float*) – Horizontal shift along the abscissa.
- **r** (*float*) – Slope parameter (steepness).
- **amp** (*float*) – Maximum value the sigmoid converges to (upper saturation).
- **y0** (*float*) – Y-offset value of the sigmoid.

**Returns**

**y** – (N\_x) Function value at argument x.

**Return type**

*np.ndarray of float*

`pynibs.expio.Mep.sigmoid_log(x, x0, r, amp)`

Parametrized log transformed sigmoid function.

$$y = \log \left( \frac{amp}{1 + e^{-r(x-x_0)}} \right)$$

**Parameters**

- **x** (*np.ndarray of float*) – (N\_x) x-values the function is evaluated in.

- **x0** (*float*) – Horizontal shift along the abscissa.
- **r** (*float*) – Slope parameter (steepness).
- **amp** (*float*) – Maximum value the sigmoid converges to.

**Returns**

**y** – (N\_x) Function value at argument x

**Return type**

np.ndarray of *float*

## **pynibs.expio.brainsight module**

```
class pynibs.expio.brainsight.BrainSightCSVParser
```

Bases: *object*

```
class State
```

Bases: *object*

**DATA** = 3

**DATA\_HEADER** = 2

**FILE\_HEADER** = 0

**FIN** = 4

**SKIPPING** = 1

```
check_state_transition(line)
```

```
parse_line(line)
```

```
pynibs.expio.brainsight.create_merged_nnav_emg_file_brainsight(fn_brainsight_nnav_info,  
                                                               fn_emg_info, fn_out,  
                                                               p2p_window_start=18,  
                                                               p2p_window_end=35)
```

```
pynibs.expio.brainsight.merge_exp_data_brainsight(subject, exp_idx, mesh_idx,  
                                                 coil_outlier_corr_cond=False,  
                                                 remove_coil_skin_distance_outlier=True,  
                                                 coil_distance_corr=True, verbose=False,  
                                                 plot=False, start_mep=18, end_mep=35)
```

Merge the TMS coil positions and the mep data into an experiment.hdf5 file.

**Parameters**

- **subject** (*pynibs.Subject*) – Subject object
- **exp\_idx** (*str*) – Experiment ID
- **mesh\_idx** (*str*) – Mesh ID
- **coil\_outlier\_corr\_cond** (*bool*) – Correct outlier of coil position and orientation (+-2 mm, +-3 deg) in case of conditions
- **remove\_coil\_skin\_distance\_outlier** (*bool*) – Remove outlier of coil position lying too far away from the skin surface (+- 5 mm)
- **coil\_distance\_corr** (*bool*) – Perform coil <-> head distance correction (coil is moved towards head surface until coil touches scalp)
- **verbose** (*bool*) – Plot output messages
- **plot** (*bool*, optional, default: *False*) – Plot MEPs and p2p evaluation

- **start\_mep** (*float*, optional, default: 18) – Start of time frame after TMS pulse where p2p value is evaluated (in ms)
- **end\_mep** (*float*, optional, default: 35) – End of time frame after TMS pulse where p2p value is evaluated (in ms)

### pynibs.expio.brainsight.read\_targets\_brainsight(*fn*)

Reads target coil position and orientations from .txt file and returns it as 4 x 4 x N\_targets numpy array.

#### Parameters

**fn** (*str*) – Filename of output file.

#### Returns

**m\_nnav** – Tensor containing the 4x4 matrices with coil orientation and position.

#### Return type

ndarray of *float* [4 x 4 x N\_targets]

### pynibs.expio.brainsight.write\_targets\_brainsight(*targets*, *fn\_out*, *names=None*, *overwrite=True*)

Writes coil position and orientations in .txt file for import into Brainsight.

#### Parameters

- **targets** (*ndarray of float* [4 x 4 x N\_targets]) – Tensor containing the 4x4 matrices with coil orientation and position
- **fn\_out** (*str*) – Filename of output file
- **names** (*list of str*, optional, default: None) – Target names (If nothing is provided they will be numbered by their order)
- **overwrite** (*bool*, optional, default: True) – Overwrite existing .txt file

#### Return type

<file> .txt file containing the targets for import into Brainsight

## pynibs.expio.brainvis module

### pynibs.expio.brainvis.read\_channel\_names(*fname*)

Reads the channel names from .vhdr (info) file, which is recorded during EEG.

#### Parameters

**fname** (*str*) – Filename of .vhdr info file.

#### Returns

**channel\_names** – List containing the channel names.

#### Return type

*list of str*

### pynibs.expio.brainvis.read\_sampling\_frequency(*fname*)

Reads the sampling frequency from .vhdr (info) file, which is recorded during EEG.

#### Parameters

**fname** (*str*) – Filename of .vhdr info file.

#### Returns

**sampling\_frequency** – Sampling frequency.

#### Return type

*float*

## **pynibs.expio.cobot module**

```
pynibs.expio.cobot.merge_exp_data_cobot(subject, exp_idx, mesh_idx, coil_outlier_corr_cond=False,  
                                         remove_coil_skin_distance_outlier=True,  
                                         coil_distance_corr=True, verbose=False, plot=False)
```

Merge the TMS coil positions and the mep data into an experiment.hdf5 file.

### **Parameters**

- **subject** (*pyfempp.subject*) – Subject object
- **exp\_idx** (*str*) – Experiment ID
- **mesh\_idx** (*str*) – Mesh ID
- **coil\_outlier\_corr\_cond** (*bool*) – Correct outlier of coil position and orientation (+-2 mm, +-3 deg) in case of conditions
- **remove\_coil\_skin\_distance\_outlier** (*bool*) – Remove outlier of coil position lying too far away from the skin surface (+- 5 mm)
- **coil\_distance\_corr** (*bool*) – Perform coil <-> head distance correction (coil is moved towards head surface until coil touches scalp)
- **verbose** (*bool*) – Plot output messages
- **plot** (*bool, optional, default: False*) – Plot MEPs and p2p evaluation

## **pynibs.expio.exp module**

```
pynibs.expio.exp.add_sigmoidal_bestfit(mep, p0, constraints=None)
```

Add best fitting sigmoidal function to instance (determined by multistart approach)

### **Parameters**

- **mep** (*pynibs.Mep*) – Mep object class instance
- **p0** (*float*) –
- **constraints** (*dict*) – Dictionary with parameter names as keys and [min, max] values as constraints

### **Returns**

**mep** – Updated Mep object class instance with the following attributes

### **Return type**

*object*

## **Notes**

Adds Attributes

### **Mep.fun\_sig**

[function] Sigmoid function

### **Mep.popt\_sig**

[np.ndarray of float [3]] Parameters of sigmoid function

```
pynibs.expio.exp.calc_outlier(coords, dev_location, dev_radius, target=None, fn_out=None,  
                               print_msg=True)
```

Computes median coil position and angle, identifies outliers, plots neat figure. Returns a list of idx that are not outliers

### **Parameters**

- **coords** (*4 x 4 x n\_zaps np.ndarray*) –
- **dev\_location** (*float*) –
- **dev\_radis** (*flat*) –
- **target** (*np.ndarray*) – 4\*4 matrix with target coordinates. Optional.
- **fn\_out** (*string, optional*) –

**Returns****list of int, list of int, list of int****Return type**

idx\_keep, idx\_zero, idx\_outlier

**pynibs.expio.exp.cfs2hdf5(*fn\_cfs, fn\_hdf5=None*)**

Converts EMG data included in .cfs file to .hdf5 format.

**Parameters**

- **fn\_cfs** (*str*) – Filename of .cfs file
- **fn\_hdf5** (*str, optional, default: None*) – Filename of .hdf5 file (if not provided, a file with same name as fn\_cfs will be created with .hdf5 extension)

**Returns**

&lt;file&gt; – File containing: - EMG data in f[“emg”][:] - Time axis in f[“time”][:]

**Return type**

.hdf5 File

**pynibs.expio.exp.coil\_distance\_correction(*exp=None, fn\_exp=None, fn\_exp\_out=None, fn\_geo\_hdf5=None, remove\_coil\_skin\_distance\_outlier=False, fn\_plot=None, min\_dist=-5, max\_dist=2*)**

Corrects the distance between the coil and the head assuming that the coil is touching the head surface during the experiments. This is done since the different coil tracker result in different coil head distances due to tracking inaccuracies. Also averages positions and orientations over the respective condition and writes both mean position and orientation for every condition in fn\_exp\_out.

Depending on if exp (dict containing lists) or fn\_exp (csv file) is provided it returns the outlier corrected dict or writes a new &lt;fn\_exp\_out&gt;.csv file.

**Parameters**

- **exp** (*list of dict or dict of list, optional, default: None*) – List of dictionaries containing the experimental data
- **fn\_exp** (*str*) – Filename (incl. path) of experimental .csv file
- **fn\_exp\_out** (*str*) – Filename (incl. path) of distance corrected experimental .csv file
- **fn\_geo\_hdf5** (*str*) – Filename (incl. path) of geometry mesh file (.hdf5)
- **remove\_coil\_skin\_distance\_outlier** (*bool*) – Remove coil positions, which are more than +- 2 mm located from the zero mean skin surface.
- **fn\_plot** (*str, default: None (fn\_geo\_hdf5 folder)*) – Folder where plots will be saved in.
- **min\_dist** (*int*) – Ignored.
- **max\_dist** (*int*) – Ignored.

**Returns**

- <File> (.csv file) – experimental\_dc.csv file with distance corrected coil positions
- or

- **exp** (*dict*) – Dictionary containing the outlier corrected experimental data

```
pynibs.expio.exp.coil_distance_correction_matsimnibs(matsimnibs,fn_mesh_hdf5,distance=0,  
remove_coil_skin_distance_outlier=False)
```

Corrects the distance between the coil and the head assuming that the coil is located at a distance “d” with respect to the head surface during the experiments. This is done since the different coil tracker result in different coil head distances due to tracking inaccuracies.

#### Parameters

- **matsimnibs** (*ndarray of float [4 x 4] or [4 x 4 x n\_mat]*) – Tensor containing matsimnibs matrices
- **fn\_mesh\_hdf5** (*str*) – .hdf5 file containing the head mesh
- **distance** (*float*) – Target distance in (mm) between coil and head due to hair layer.  
All coil positions are moved to this distance.
- **remove\_coil\_skin\_distance\_outlier** (*bool*) – Remove coil positions, which are more than +- 6 mm located from the skin surface.

#### Returns

**matsimnibs** – Tensor containing matsimnibs matrices with distance corrected coil positions

#### Return type

*ndarray of float [4 x 4 x n\_mat]*

```
pynibs.expio.exp.coil_outlier_correction_cond(exp=None,fn_exp=None,fn_exp_out=None,  
outlier_angle=5.0,outlier_loc=3.0)
```

Searches and removes outliers of coil orientation and location w.r.t. the average orientation and location from all zaps. It generates plots of the individual conditions showing the outliers in the folder of fn\_exp\_out. Depending on if exp (dict containing lists) or fn\_exp (csv file) is provided it returns the outlier corrected dict or writes a new <fn\_exp\_out>.csv file. If \_exp\_ is provided, all keys are kept.

#### Parameters

- **exp** (*list of dict, optional, default: None*) – List of dictionaries containing the experimental data
- **fn\_exp** (*str, optional, default: None*) – Filename (incl. path) of experimental .csv file
- **fn\_exp\_out** (*str, optional, default: None*) – Filename (incl. path) of corrected experimental .csv file
- **outlier\_angle** (*float, optional, default: 5.*) – Coil orientation outlier “cone” around axes in +- deg. All zaps with coil orientations outside of this cone are removed.
- **outlier\_loc** (*float, optional, default: 3.*) – Coil position outlier “sphere” in +- mm. All zaps with coil locations outside of this sphere are removed.

#### Returns

- <File> (.csv file) – experimental\_oc.csv file with outlier corrected coil positions
- <Files> (.png files) – Plot showing the coil orientations and locations (folder\_of\_fn\_exp\_out/COND\_X\_coil\_position.png)
- or
- **exp** (*dict*) – Dictionary containing the outlier corrected experimental data

```
pynibs.expio.exp.combine_nnav_mep(xml_paths,cfs_paths,im,coil_sn,nii_exp_path,nii_conform_path,  
patient_id,tms_pulse_time,drop_mep_idx,mep_onsets,  
nnav_system,mesh_approach='headreco',temp_dir=None,  
cfs_data_column=0,channels=None,plot=False,start_mep=18,  
end_mep=35)
```

Creates dictionary containing all experimental data.

#### Parameters

- **xml\_paths** (*list of str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **cfs\_paths** (*list of str*) – Paths to .cfs mep file
- **im** (*list of str*) – List of path to the instrument-marker-file or list of strings containing the instrument marker
- **coil\_sn** (*str*) – Coil-serial-number
- **nii\_exp\_path** (*str*) – Path to the .nii file that was used in the experiment
- **nii\_conform\_path** (*str*) – Path to the conform\*.nii file used to calculate the E-fields with SimNIBS
- **patient\_id** (*str*) – Patient id
- **tms\_pulse\_time** (*float*) – Time in [s] of TMS pulse as specified in signal
- **drop\_mep\_idx** (*List of int or None*) – Which MEPs to remove before matching.
- **mep\_onsets** (*List of int or None (Default: None)*) – If there are multiple .cfs per TMS Navigator sessions, onsets in [ms] of .cfs. E.g.: [0, 71186].
- **temp\_dir** (*str, optional, default: None (fn\_exp\_mri\_nii folder)*) – Directory to save temporary files (transformation .nii and .mat files)
- **cfs\_data\_column** (*int or list of int*) – Column(s) of dataset in .cfs file.
- **channels** (*list of str, optional, default: None*) – Channel names
- **nnav\_system** (*str*) – Type of neuronavigation system (“Localite”, “Visor”)
- **mesh\_approach** (*str, optional, default: "headreco"*) – Approach the mesh is generated with (“headreco” or “mri2mesh”)
- **plot** (*bool, optional, default: False*) – Plot MEPs and p2p evaluation
- **start\_mep** (*float, optional, default: 18*) – Start of time frame after TMS pulse where p2p value is evaluated (in ms)
- **end\_mep** (*float, optional, default: 35*) – End of time frame after TMS pulse where p2p value is evaluated (in ms)

#### Returns

`dict_lst` – ‘number’ ‘condition’ ‘current’ ‘mep\_raw\_data’ ‘mep’ ‘mep\_latency’ ‘mep\_filt\_data’ ‘mep\_raw\_data\_time’ ‘time\_tms’ ‘ts\_tms’ ‘time\_mep’ ‘date’ ‘coil\_sn’ ‘patient\_id’

#### Return type

`list` of dicts, one dict for each zap

```
pynibs.expio.exp.combine_nnav_rt(xml_paths, behavior_paths, im, coil_sn, nii_exp_path,
                                    nii_conform_path, patient_id, drop_trial_idx, nnav_system, cond,
                                    mesh_approach='headreco', temp_dir=None, plot=False)
```

Creates dictionary containing all experimental data.

#### Parameters

- **xml\_paths** (*list of str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **behavior\_paths** (*list of str*) – Paths to .cfs mep file
- **im** (*list of str*) – List of path to the instrument-marker-file or list of strings containing the instrument marker

- **coil\_sn** (*str*) – Coil-serial-number
- **nii\_exp\_path** (*str*) – Path to the .nii file that was used in the experiment
- **nii\_conform\_path** (*str*) – Path to the conform\*.nii file used to calculate the E-fields with SimNIBS
- **patient\_id** (*str*) – Patient id
- **drop\_trial\_idx** (*List of int or None*) – Which MEPs to remove before matching.
- **temp\_dir** (*str, optional, default: None (fn\_exp\_mri\_nii folder)*) – Directory to save temporary files (transformation .nii and .mat files)
- **nnav\_system** (*str*) – Type of neuronavigation system (“Localite”, “Visor”)
- **cond** (*str*) – Condition name in data\_path
- **mesh\_approach** (*str, optional, default: "headreco"*) – Approach the mesh is generated with (“headreco” or “mri2mesh”)
- **plot** (*bool, optional, default: False*) – Plot MEPs and p2p evaluation

#### Returns

```
dict_lst = {'number': 'condition': 'current': 'mep_raw_data': 'mep': 'mep_latency': 'mep_filt_data': 'mep_raw_data_time': 'time_tms': 'ts_tms': 'time_mep': 'date': 'coil_sn': 'patient_id'}
```

#### Return type

*list* of dicts, one dict for each zap

`pynibs.expio.exp.convert_csv_to_hdf5(fn_csv, fn_hdf5, overwrite_arr=True, verbose=False)`

Wrapper from experiment.csv to experiment.hdf5

Saves all relevant columns from the (old) experiment.csv file to an .hdf5 file. fn\_hdf5:/stim\_data/

```
|--coil_sn |--current |--date |--time_diff |--time_mep |--time_tms |--ts_tms |--coil0 # <- all coil0_**  
columns |--coil1 # <- all coil1_** columns |--coil_mean # <- all coil_mean_** columns
```

All columns not found in experiment.csv are ignored (and a warning is thrown).

#### Parameters

- **fn\_csv** (*str*) – experiment.csv filename
- **fn\_hdf5** (*str*) – experiment.hdf5 filename. File is created if not existing.
- **overwrite\_arr** (*bool*) – Overwrite existing arrays. Otherwise: fail. Default: True.
- **verbose** (*bool*) – Print some information (default: false).

`pynibs.expio.exp.get_cnt_infos(fn_cnt)`

Read some meta information from .cnt file

#### Return type

*dict d*

`pynibs.expio.exp.get_coil_flip_m(source_system='simnibs', target_system=None)`

Returns a flimp matrix 4x4 to flip coil axis from one system to another.

#### Parameters

- **source\_system** (*str*) – Atm only possible source: ‘simnibs’
- **target\_system** – tmsnavigator, visor, brainsight

#### Returns

*flip\_m* – shape: 4x4

**Return type**`np.ndarray``pynibs.expio.exp.get_coil_sn_lst(fn_coil)``pynibs.expio.exp.get_csv_matrix(dictionary)``pynibs.expio.exp.get_intensity_e(e1, e2, target1, target2, radius1, radius2, headmesh, rmt=1, roi='midlayer_lh_rh', verbose=False)`

Computes the stimulator intensity adjustment factor based on the electric field

**Parameters**

- **e1** (`str`) – .hdf5 e field with midlayer
- **e2** (`str`) – .hdf5 e field with midlayer
- **target1** (`np.ndarray (3,)`) – Coordinates of cortical site of MT
- **target2** (`np.ndarray (3,)`) – Coordinates of cortical target site
- **radius1** (`float`) – Electric field of field1 is averaged over elements inside this radius around target1
- **radius2** (`float`) – Electric field of field2 is averaged over elements inside this radius around target2
- **headmesh** (`str`) – .hdf5 headmesh
- **rmt** (`float, optional, default=0`) – Resting motor threshold to be corrected
- **roi** (`str, optional, default='midlayer_lh_rh'`) – Name of roi. Expected to sit in mesh['/data/midlayer/roi\_surface/']
- **verbose** (`bool, optional, Default: False`) – Print verbosity information.

**Returns**`rmt_e_corr` – Adjusted stimulation intensity for target2**Return type**`float``pynibs.expio.exp.get_intensity_e_old(mesh1, mesh2, target1, target2, radius1, radius2, rmt=1, verbose=False)`

Computes the stimulator intensity adjustment factor based on the electric field

Something weird is going on here - check simnibs coordinates of midlayer before usage.

**Parameters**

- **mesh1** (`str or simnibs.msh.mesh_io.Msh`) – Midlayer mesh containing results of the optimal coil position of MT in the midlayer (e.g.: .../subject\_overlays/00001.hd\_fixed\_TMS\_1-0001\_MagVenture\_MCF\_B65\_REF\_highres.ccd\_scalar\_central.msh)
- **mesh2** (`str or simnibs.msh.mesh_io.Msh`) – Midlayer mesh containing results of the optimal coil position of the target in the midlayer (e.g.: .../subject\_overlays/00001.hd\_fixed\_TMS\_1-0001\_MagVenture\_MCF\_B65\_REF\_highres.ccd\_scalar\_central.msh)
- **target1** (`np.ndarray (3,)`) – Coordinates of cortical site of MT
- **target2** (`np.ndarray (3,)`) – Coordinates of cortical target site
- **radius1** (`float`) – Electric field in target 1 is averaged over elements inside this radius
- **radius2** (`float`) – Electric field in target 2 is averaged over elements inside this radius
- **rmt** (`float, optional, default=0`) – Resting motor threshold, which will be corrected

- **verbose** (*bool*, optional, Default: *false*) – Print verbosity information.

**Returns**

**rmt\_e\_corr** – Adjusted stimulation intensity for target2

**Return type**

*float*

```
pynibs.expio.exp.get_intensity_stokes(mesh, target1, target2, spat_grad=3, rmt=0, verbose=False,  
scalp_tag=1005, roi=None)
```

Computes the stimulator intensity adjustment factor according to Stokes et al. 2005 (doi:10.1152/jn.00067.2005). Adjustment is based on target-scalp distance differences: adj = (Dist2-Dist1)\*spat\_grad

**Parameters**

- **mesh** (*str* or *simnibs.msh.mesh\_io.Msh*) – Mesh of the head model
- **target1** (*np.ndarray* (3,)) – Coordinates of cortical site of MT
- **target2** (*np.ndarray* (3,)) – Coordinates of cortical target site
- **spat\_grad** (*float*) – Spatial gradient. Default: 3
- **rmt** (*float*, optional, default=0) – Resting motor threshold, which will be corrected
- **scalp\_tag** (*int*, optional, default: 1005) – Tag in the mesh where the scalp is to be set. Default: 1005
- **verbose** (*bool*, optional, Default: *false*) – Print verbosity information.
- **roi** (*np.ndarray* (3,N)) – Array of nodes to project targets onto

**Returns**

**rmt\_stokes** – Adjusted stimulation intensity for target2

**Return type**

*float*

```
pynibs.expio.exp.get_patient_id(xml_path)
```

Read patient-ID.

**Parameters**

**xml\_path** (*str*) – Path to coil0-file

**Returns**

**xml\_pd.find('patientID').text** – ID of patient

**Return type**

*str*

```
pynibs.expio.exp.get_trial_data_from_csv(behavior_fn, cond, drop_trial_idx=None, only_corr=True,  
startatzero=True)
```

Reads trial data from csv file. Reaction time is in [0.1ms]

**Parameters**

**behavior\_fn** (*str*) – Filename with columns: ‘trialtype’, ‘onset\_time’, ‘rt’

**cond**

[str] Which condition to choose from .csv file

**drop\_trial\_idx**

[list of int, optional] ‘trialnum’ to remove

**only\_corr**

[bool, default: True] Only return trials with correct responses

**startatzero**

[bool, default: True] Shift onset\_time axis to zero

**Returns**

- **rt** (*list of float*)
- **onsets** (*list of float*)
- **mean\_isi** (*tuple of int*) – in [s]

`pynibs.expio.exp.load_matsimnibs_txt(fn_matsimnibs)`

Loading matsimnibs matrices from .txt file.

**Parameters**

**fn\_matsimnibs** (*str*) – Filename of .txt file the matsimnibs matrices are stored in

**Returns**

**matsimnibs** – Tensor containing matsimnibs matrices

**Return type**

ndarray of *float* [4 x 4] or [4 x 4 x n\_mat]

`pynibs.expio.exp.match_behavior_and_triggermarker(mep_time_lst, xml_paths, bnd_factor=0.495, isi=None)`

Sort out timestamps of mep and tms files that do not match.

**Parameters**

- **mep\_time\_lst** (*list of datetime.timedelta*) – timedeltas of MEP recordings.
- **xml\_paths** (*list of str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **bnd\_factor** (*float, optional, default: 0.99/2*) – Bound factor relative to interstimulus interval in which +- interval to match neuronavigation and mep data from their timestamps. (0 means perfect matching, 0.5 means +- half interstimulus interval)
- **isi** (*float, optional*) – Interstimulus intervals. If not provided it's estimated from the first trial.

**Returns**

- **tms\_index\_lst** (*list of int*) – Indices of tms-timestamps that match
- **mep\_index\_lst** (*list of int*) – Indices of mep-timestamps that match
- **tms\_time\_lst** (*list of datetime*) – TMS timestamps

`pynibs.expio.exp.nnav2simnibs(fn_exp_nii, fn_conform_nii, m_nnav, nnav_system, mesh_approach='headreco', fiducials=None, orientation='RAS', fsl_cmd=None, target='simnibs', temp_dir=None, rem_tmp=False, verbose=True)`

Transforming TMS coil positions from neuronavigation to simnibs space

**Parameters**

- **fn\_exp\_nii** (*str*) – Filename of .nii file the experiments were conducted with
- **fn\_conform\_nii** (*str*) – Filename of .nii file from SimNIBS mri2msh function (e.g.: .../fs\_subjectID/subjectID\_T1fs\_conform.nii.gz)
- **m\_nnav** (*np.ndarray [4 x 4 x N]*) – Position matrices from neuronavigation
- **nnav\_system** (*str*) – Neuronavigation system: - “Localite” ... Localite neuronavigation system - “Visor” ... Visor neuronavigation system from ANT - “Brainsight” ... Brainsight neuronavigation system from Rougue Research

- **mesh\_approach** (*str*, optional, default: "headreco") – Approach the mesh is generated with ("headreco" or "mri2mesh")
- **fiducials** (*np.array of float [3 x 3]*) – Fiducial points in ANT nifti space from file (e.g.: /data/pt\_01756/probands/33791.b8/exp/1/33791.b8\_recording/MRI/33791.b8\_recording.mri) (x frontal-occipital, y right-left, z inferior-superior) VoxelOnPositiveXAxis (Nasion, first row) 221 131 127 VoxelOnPositiveYAxis (left ear, second row) 121 203 105 VoxelOnNegativeYAxis (right ear, third row) 121 57 105
- **orientation** (*str*) – Orientation convention ('RAS' or 'LPS') (can be read from neuronavigation .xml file under coordinateSpace="RAS")
- **fsl\_cmd** (*str*, optional) – bash command to start FSL environment (Default: None)
- **target** (*str*, optional, default: 'simnibs') – Either transform to 'simnibs' or to 'nnav' space
- **temp\_dir** (*str*, optional, default: None (*fn\_exp\_mri\_nii folder*)) – Directory to save temporary files (transformation .nii and .mat files)
- **rem\_tmp** (*bool*, optional, default: False) – Remove temporary files from registration
- **verbose** (*boolean*) – Print output (True / False)

**Returns**

**m\_simnibs**

**Return type**

*np.ndarray of float [4 x 4 x N]*

`pynibs.expio.exp.outliers_mask(data, m=2.0)`

`pynibs.expio.exp.print_time(relation, tms_time, tms_time_index, mep_time, mep_time_index, time_bnd_l, time_bnd_h)`

Print timestamps that do not match.

**Parameters**

- **relation** (*str*) – 'bigger' or 'smaller'
- **tms\_time** (*datetime.timedelta*) – TMS timestamps
- **tms\_time\_index** (*int*) – Index of tms timestamp
- **mep\_time** (*datetime.timedelta*) – Mep timestamps
- **mep\_time\_index** (*int*) – Index of mep timestamps
- **time\_bnd\_l** (*datetime.timedelta*) – Lowest datetime timestamp for matching
- **time\_bnd\_h** (*datetime.timedelta*) – Highest datetime timestamp for matching

`pynibs.expio.exp.read_csv(csv_path)`

Read dictionary from .csv-file.

**Parameters**

**csv\_path** (*str*) – Path to .csv-file

**Returns**

**dict\_lst** – Field name of the .csv-file as the key

**Return type**

*dict of list*

`pynibs.expio.exp.read_exp_stimulations(fname_results_conditions, fname_simpos, filter_bad_trials=False, drop_idx=None)`

Reads results\_conditions.csv and simPos.csv and returns data.

**Parameters**

- **fname\_results\_conditions** (*str*) – Filename of results\_conditions.csv file
- **fname\_simpos** (*str*) – Filename of simPos.csv file
- **filter\_bad\_trials** (*bool*, *False*) – If true, some filtering will be done to exclude erroneous data
- **drop\_idx** (*list*, *empty*) – Indices of trials to drop

**Returns**

- **positions\_all** (*list of np.ndarrays of float [N\_zaps x [4 x 4]]*) – List of position matrices of TMS coil, formatted in simnibs style

$$\begin{bmatrix} | & | & | & | \\ x & y & z & pos \\ | & | & | & | \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- **conditions** (*list of str [N\_zaps]*) – Str labels of the condition corresponding to each zap
- **position\_list** (*list of float and str [N\_zaps x 55]*) – List of data stored in results\_conditions.csv (condition, MEP amplitude, locations of neuronavigation trackers)
- **mep\_amp** (*np.array of float [N\_zaps]*) – MEP amplitude in [V] corresponding to each zap
- **intensities** (*np.array of float [N\_zaps]*) – Stimulator intensities corresponding to each zap
- **fails\_idx** (*np.array(N\_fails\_idx x 1)* (*only if filter\_bad\_trials*)) – Which trials were dropped through filtering?

`pynibs.expio.exp.save_matsimnibs_txt(fn_matsimnibs, matsimnibs)`

Saving matsimnibs matrices in .txt file.

**Parameters**

- **fn\_matsimnibs** (*str*) – Filename of .txt file the matsimnibs matrices are stored in
- **matsimnibs** (*ndarray of float [4 x 4] or [4 x 4 x n\_mat]*) – Tensor containing matsimnibs matrices

**Returns**

**<File>** – Textfile containing the matsimnibs matrices

**Return type**

.txt file

`pynibs.expio.exp.sort_by_condition(exp, conditions_selected=None)`

Sort experimental dictionary from experimental.csv into list by conditions.

**Parameters**

- **exp** (*dict or list of dict*) – Dictionary containing the experimental data information
- **conditions\_selected** (*str or list of str, Default=None*) – List of conditions returned by the function (in this order), the others are omitted, If None, all conditions are returned

**Returns**

**exp\_cond** – List of dictionaries containing the experimental data information sorted by condition

**Return type**

*list of dict*

`pynibs.expio.exp.sort_data_by_condition(conditions, return_alph_sorted=True, conditions_selected=None, *data)`

Sorts data by condition and returns tuples of data with corresponding labels.

#### Parameters

- **conditions** (*list of str [N\_zaps]*) – Str labels of the condition corresponding to each data
- **return\_alph\_sorted** (*Boolean, Default True*) – Shall returns be in alphabetically or original order
- **conditions\_selected** (*list of str or None*) – List of conditions returned by the function (in this order), the others are omitted
- **data** (*tuple of data indexed by condition [N\_data x N\_zaps x m]*) – Data to sort

#### Returns

- **cond\_labels** (*list of str [N\_cond]*) – Labels of conditions
- **data\_sorted** (*tuple of sorted data [N\_cond x N\_data x N\_zaps x m]*) – Sorted data by condition

`pynibs.expio.exp.splitext_niigz(fn)`

Splitting extension(s) from .nii or .nii.gz file

#### Parameters

- **fn** (*str*) – Filename of input image .nii or .nii.gz file

#### Returns

- **path** (*str*) – Path and filename without extension(s)
- **ext** (*str*) – Extension, either .nii or .nii.gz

`pynibs.expio.exp.square(x, a, b, c)`

Parametrized quadratic function

$$y = ax^2 + bx + c$$

#### Parameters

- **x** (*np.ndarray of float [N\_x]*) – X-values the function is evaluated in
- **a** (*float*) – Slope parameter of  $x^2$
- **b** (*float*) – Slope parameter of x
- **c** (*float*) – Offset parameter

#### Returns

y – Function value at argument x

#### Return type

np.ndarray of *float* [N\_x]

`pynibs.expio.exp.toRAS(fn_in, fn_out)`

Transforming MRI .nii image to RAS space.

#### Parameters

- **fn\_in** (*str*) – Filename of input image .nii file
- **fn\_out** (*str*) – Filename of output image .nii file in RAS space

#### Returns

<File> – .nii image in RAS space (fn\_out)

**Return type**

.nii file

`pynibs.expio.exp.write_csv(csv_output_path, dict_lst)`

Write dictionary into .csv-file.

**Parameters**

- `csv_output_path (str)` – Path to output-file
- `dict_lst (list of dict)` – Fields of the .csv-file

`pynibs.expio.exp.write_triggermarker_stats(tm_array, idx_keep, idx_outlier, idx_zero, fn, **kwargs)`

Write some stats about the triggermarker analyses to a .csv . Use kwargs to add some more information, like subject id, experiment, conditions, etc

## pynibs.expio.localite module

Functions to import data from Localite TMS Navigator

`pynibs.expio.localite.arrays_similar(tm_matrix, tm_matrix_post, pos_rtol=0, pos_atol=3.6, ang_rtol=0.1, ang_atol=0.1)`

C.compares angles and position for similarity.

Splitting the comparison into angles and position is angebracht, as the absolute tolereance (atol) should be different for angles (degree) and position (millimeter) comparisons.

**Parameters**

- `tm_matrix (array-like, shape = (4, 4))` – TMS Navigator triggermarker or instrument marker array
- `tm_matrix_post (array-like, shape = (4, 4))` – TMS Navigator triggermarker or instrument marker array
- `tm_mean_last (array-like, shape = (4, 4), optional)` – Mean TMS Navigator triggermarker or instrument marker array for n zaps

`pynibs.expio.localite.get_instrument_marker(im_path)`

`pynibs.expio.localite.get_marker(im_path, markertype)`

Read instrument-marker and conditions from Neuronavigator .xml-file.

**Parameters**

`im_path (str or list of str)` – Path to instrument-marker-file

**Returns**

- `im_array (np.array of float [Mx4x4])` – Instrument-marker-matrices
- `im_cond_lst (list of str)` – Labels of the instrument-marker-conditions
- `im_marker_times (list of float)` – Onset times

`pynibs.expio.localite.get_single_marker_file(im_path, markertype)`

Read instrument-marker and conditions from Neuronavigator .xml-file.

**Parameters**

`im_path (str or list of str)` – Path to instrument-marker-file

**Returns**

- `im_array (np.array of float [Mx4x4])` – Instrument-marker-matrices
- `im_cond_lst (list of str)` – Labels of the instrument-marker-conditions

`pynibs.expio.localite.get_tms_elements(xml_paths, verbose=False)`

Read needed elements out of the tms-xml-file.

**Parameters**

- **xml\_paths** (*list of str or str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **verbose** (*bool, optional, default: False*) – Print output messages

**Returns**

- **coils\_array** (*ndarray of float [3xNx4x4]*) – Coil0, coil1 and mean-value of N 4x4 coil-arrays
- **ts\_tms\_lst** (*list of int [N]*) – Timestamps of valid tms-measurements
- **current\_lst** (*list of int [N]*) – Measured currents
- **idx\_invalid** (*list of int*) – List of indices of invalid coil positions (w.r.t. all timestamps incl invalid)

`pynibs.expio.localite.marker_is_empty(arr)`

`pynibs.expio.localite.markers_are_empty(arr)`

`pynibs.expio.localite.match_instrument_marker_file(xml_paths, im_path)`

Assign right instrument marker condition to every triggermarker (get instrument marker out of file).

**Parameters**

- **xml\_paths** (*list of str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **im\_path** (*str*) – Path to instrument-marker-file

**Returns**

**coil\_cond\_lst** – Right conditions

**Return type**

*list of str*

`pynibs.expio.localite.match_instrument_marker_string(xml_paths, condition_order)`

Assign right instrument marker condition to every triggermarker (get instrument marker out of list of strings).

**Parameters**

- **xml\_paths** (*list of str*) – Paths to coil0-file and optionally coil1-file if there is no coil1-file, use empty string
- **condition\_order** (*list of str*) – Conditions in the right order

**Returns**

**coil\_cond\_lst**

**Return type**

*list of strings containing the right conditions*

`pynibs.expio.localite.match_tm_to_im(tm_array, im_array, tms_time_arr, tms_cur_arr)`

Match triggermarker with instrumentmarker and get index of best fitting instrumentmarker.

**Parameters**

- **tm\_array** (*ndarray of float [Nx4x4]*) – Mean-value of Nx4x4 coil matrices
- **im\_array** (*ndarray of float [Mx4x4]*) – Instrument-marker-matrices

**Returns**

**im\_index\_lst** – Indices of best fitting instrumentmarkers

**Return type**

list of int

```
pynibs.expio.localite.merge_exp_data_localite(subject, coil_outlier_corr_cond,
                                              remove_coil_skin_distance_outlier,
                                              coil_distance_corr, exp_idx=0, mesh_idx=0,
                                              drop_mep_idx=None, mep_onsets=None,
                                              cfs_data_column=None, channels=None,
                                              verbose=False, plot=False, start_mep=18,
                                              end_mep=35)
```

Merge the TMS coil positions (TriggerMarker) and the mep data into an experiment.hdf5 file.

**Parameters**

- **subject** (`pyfempp.subject`) – Subject object
- **exp\_idx** (`str`) – Experiment ID
- **mesh\_idx** (`str`) – Mesh ID
- **coil\_outlier\_corr\_cond** (`bool`) – Correct outlier of coil position and orientation (+-2 mm, +-3 deg) in case of conditions
- **remove\_coil\_skin\_distance\_outlier** (`bool`) – Remove outlier of coil position lying too far away from the skin surface (+- 5 mm)
- **coil\_distance\_corr** (`bool`) – Perform coil <-> head distance correction (coil is moved towards head surface until coil touches scalp)
- **drop\_mep\_idx** (`List of int or None`) – Which MEPs to remove before matching.
- **mep\_onsets** (`List of int or None (Default: None)`) – If there are multiple .cfs per TMS Navigator sessions, onsets in [ms] of .cfs. E.g.: [0, 71186].
- **cfs\_data\_column** (`int or list of int`) – Column(s) of dataset in .cfs file.
- **channels** (`list of str`) – List of channel names
- **verbose** (`bool`) – Plot output messages
- **plot** (`bool, optional, default: False`) – Plot MEPs and p2p evaluation
- **start\_mep** (`float, optional, default: 18`) – Start of time frame after TMS pulse where p2p value is evaluated (in ms)
- **end\_mep** (`float, optional, default: 35`) – End of time frame after TMS pulse where p2p value is evaluated (in ms)

```
pynibs.expio.localite.merge_exp_data_rt(subject, coil_outlier_corr_cond,
                                         remove_coil_skin_distance_outlier, coil_distance_corr,
                                         cond=None, exp_idx=0, mesh_idx=0, drop_trial_idx=None,
                                         verbose=False, plot=False)
```

Merge the TMS coil positions (TriggerMarker) and the mep data into an experiment.hdf5 file.

**Parameters**

- **subject** (`pynibs.subject`) – Subject object
- **exp\_idx** (`str`) – Experiment ID
- **mesh\_idx** (`str`) – Mesh ID
- **coil\_outlier\_corr\_cond** (`bool`) – Correct outlier of coil position and orientation (+-2 mm, +-3 deg) in case of conditions
- **cond** (`string`) – Which condition to analyse
- **remove\_coil\_skin\_distance\_outlier** (`bool`) – Remove outlier of coil position lying too far away from the skin surface (+- 5 mm)

- **coil\_distance\_corr** (`bool`) – Perform coil <-> head distance correction (coil is moved towards head surface until coil touches scalp)
- **drop\_trial\_idx** (*List of int or None*) – Which MEPs to remove before matching.
- **verbose** (`bool`) – Plot output messages
- **plot** (`bool, optional, default: False`) – Plot MEPs and p2p evaluation

`pynibs.expio.localite.read_coil(xml_ma)`

Read coil-data from xml element.

**Parameters**

`xml_ma` (*xml-element*) – Coil data

**Returns**

`coil` – Coil elements

**Return type**

nparray of `float` [4x4]

`pynibs.expio.localite.read_triggermarker_localite(fn_xml)`

Read instrument-marker and conditions from neuronavigator .xml-file.

**Parameters**

`fn_xml` (`str`) – Path to TriggerMarker.xml file (e.g. Subject\_0/Sessions/Session\_YYYYMMDDHHMMSS/TMSTrigger/TriggerMarkers\_Coil1\_YYYYMMDDHHMMSS

**Returns**

`m_nnav`

[ndarray of float [4x4xN]] Neuronavigation coordinates of N stimuli (4x4 matrices)

`didt`

[ndarray of float [N]] Rate of change of coil current in (A/us)

`stim_int`

[ndarray of float [N]] Stimulator intensity in (%)

`descr`

[list of str [N]] Labels of the instrument-marker-conditions

`rec_time`

[list of str [N]] Recording time in ms

**Return type**

list of

## **pynibs.expio.visor module**

Functions to import data from ANT Visor 2 / ANT EEG software go here

`pynibs.expio.visor.filter_emg(emg, fs)`

Filter emg signals

**Parameters**

- **emg** (*list of np.array [n\_stimuli]*) – Raw EMG data. Each list entry contains a np.ndarray of size [n\_samples x n\_channel] Each channel is filtered in the same way.
- **fs** (`float`) – Sampling frequency

**Returns**

`emg_filt` – Filtered EMG data

**Return type**`list of np.ndarray [n_stimuli]`

```
pynibs.expio.visor.get_cnt_data(fn, channels='all', trigger_val='I', max_duration=10, fn_hdf5=None,
                                 path_hdf5=None, verbose=False, return_data=False)
```

Reads ANT .cnt EMG/EEG data file and chunks timeseries into triggerN - triggerN+1 Can directly write the zaps into hdf5 if argument is provided. Starting with the first trigger and ending with get\_sample\_count()-1

**Parameters**

- **fn** (`str`) – .cnt Filename
- **channels** (`str` / `int` / `list of int` / `list of str`) – Which channel(s) to return. Default: all. Can be channel number(s) or channel name(s).
- **trigger\_val** (`str`) – Trigger value to read as zap trigger. Default: ‘I’
- **max\_duration** (`int`) – Maximum duration in [s] per chunk. Rest is dropped.
- **fn\_hdf5** (`str, optional, default: None`) – If given, cnt data is written into hdf5 file under “path\_hdf5” as pandas dataframe with column name “qoi\_name” and nothing is returned. Default: None
- **path\_hdf5** (`str, optional, default: None`) – If fn\_hdf5, path of pandas dataframe where the data is saved (e.g. “/phys\_data/raw/EEG”)
- **verbose** (`bool`) – Some verbosity messages (default: False)
- **return\_data** (`bool`) – Return data as list of np.array

**Returns**`data_lst` – List of EEG/EMG data. Only returned if fn\_hdf5 is not None**Return type**`list of np.ndarray with shape=(samples,channels), optional`

```
pynibs.expio.visor.get_instrument_marker(im_path, verbose=False)
```

Return all instrument markers from visor .cnt file Coordinate system in raw ANT space (NLR) defined as:

origin: intersection between line of ear fiducials and nasion x-axis: origin -> nasion y-axis: origin -> left ear z-axis: origin -> superior

**Parameters**

- **im\_path** (`str`) – Path to instrument-marker-file .cnt file
- **verbose** (`bool`) – Some verbosity messages (default: False)

**Returns**`im_list` – List containing stimulation parameters: - coil\_mean\_raw [4 x 4 matrix] - StimulusID - etc...**Return type**`list of dict`

```
pynibs.expio.visor.merge_exp_data_visor(subject, exp_id=0, mesh_idx=0, verbose=False,
                                         start_mep=18, end_mep=35)
```

Merges all experimental data from visor experiment into one .hdf5 file

**Parameters**

- **subject** (`Subject object`) – Subject object
- **exp\_id** (`int`) – Experiment index
- **mesh\_idx** (`int`) – Mesh index
- **verbose** (`bool`) – Print output

- **start\_mep** (*float*, *optional*, *default*: 18) – Start of time frame after TMS pulse where p2p value is evaluated (in ms)
- **end\_mep** (*float*, *optional*, *default*: 35) – End of time frame after TMS pulse where p2p value is evaluated (in ms)

**Returns**

**<File>** – File containing the stimulation and physiological data as pandas dataframes: - “stim\_data”: Stimulation parameters (e.g. coil positions, etc.) - “phys\_data/info/EMG”: Information about EMG data recordings (e.g. sampling frequency, etc.) - “phys\_data/info/EEG”: Information about EEG data recordings (e.g. sampling frequency, etc.) - “phys\_data/raw/EMG”: Raw EMG data - “phys\_data/raw/EEG”: Raw EEG data - “phys\_data/postproc/EMG”: Post-processed EMG data (e.g. filtered, p2p, etc.) - “phys\_data/postproc/EEG”: Post-processed EEG data (e.g. filtered, p2p, etc.)

**Return type**

.hdf5 file

**pynibs.expio.visor.read\_nlr(*fname*)**

Reads NLR coordinates from \*\_recording.mri file

**Parameters**

***fname*** –

**Returns**

**fiducials** – The rows contain the fiducial points in ANT nifit space (nasion, left ear, right ear)

**Return type**

np.array of **float** [3 x 3]

**pynibs.mesh package**

**Submodules**

**pynibs.mesh.mesh\_struct module**

**class pynibs.mesh.mesh\_struct.Mesh(*mesh\_name*, *subject\_id*, *subject\_folder*)**

Bases: **object**

” Mesh class to initialize default attributes.

**fill\_defaults(*approach*)**

Initializes attributes for a headreco mesh.

**Parameters**

**approach** (*str*) – ‘headreco’ ‘mri2mesh’ ‘charm’

**print()**

Print self information.

**write\_to\_hdf5(*fn\_hdf5*, *check\_file\_exist=False*, *verbose=False*)**

Write this mesh’ attributes to .hdf5 file.

**Parameters**

- **fn\_hdf5** (*str*) –
- **check\_file\_exist** (*bool*) – Check if provided filenames exist, warn if not.
- **verbose** (*bool*) – Print self information

---

```
class pynibs.mesh.mesh_struct.ROI(subject_id, roi_name, mesh_name)
```

Bases: `object`

” Region of interest class to initialize default attributes.

`print()`

Print self information.

`write_to_hdf5(fn_hdf5, check_file_exist=False, verbose=False)`

Write this mesh’ attributes to .hdf5 file.

#### Parameters

- `fn_hdf5 (str)` –
- `check_file_exist (bool)` – Check if provided filenames exist, warn if not.
- `verbose (bool)` – Print self information

```
class pynibs.mesh.mesh_struct.TetrahedraLinear(points, triangles, triangles_regions, tetrahedra,  
  tetrahedra_regions)
```

Bases: `object`

Mesh, consisting of linear tetrahedra.

#### Parameters

- `points (array of float [N_points x 3])` – Vertices of FE mesh
- `triangles (np.ndarray of int [N_tri x 3])` – Connectivity of points forming triangles
- `triangles_regions (np.ndarray of int [N_tri x 1])` – Region identifiers of triangles
- `tetrahedra (np.ndarray of int [N_tet x 4])` – Connectivity of points forming tetrahedra
- `tetrahedra_regions (np.ndarray of int [N_tet x 1])` – Region identifiers of tetrahedra

#### N\_points

Number of vertices

##### Type

`int`

#### N\_tet

Number of tetrahedra

##### Type

`int`

#### N\_tri

Number of triangles

##### Type

`int`

#### N\_region

Number of regions

##### Type

`int`

## **region**

Region labels

### **Type**

np.ndarray of int

## **tetrahedra\_volume**

Volumes of tetrahedra

### **Type**

np.ndarray of float [N\_tet x 1]

## **tetrahedra\_center**

Center of tetrahedra

### **Type**

np.ndarray of float [N\_tet x 1]

## **triangles\_center**

Center of triangles

### **Type**

np.ndarray of float [N\_tri x 1]

## **triangles\_normal**

Normal components of triangles pointing outwards

### **Type**

np.ndarray of float [N\_tri x 3]

## **calc\_E(*grad\_phi*, *omegaA*)**

Calculate electric field with gradient of electric potential and omega-scaled magnetic vector potential A.

$$\mathbf{E} = -\nabla\varphi - \omega\mathbf{A}$$

### **Parameters**

- **grad\_phi** (np.ndarray of float [N\_tet x 3]) – Gradient of Scalar DOF in tetrahedra center
- **omegaA** (np.ndarray of float [N\_tet x 3]) – Magnetic vector potential in tetrahedra center (scaled with angular frequency omega)

### **Returns**

E – Electric field in tetrahedra center

### **Return type**

np.ndarray of float [N\_tet x 3]

## **calc\_E\_normal\_tangential\_surface(*E*, *fname*)**

Calculate normal and tangential component of electric field on given surfaces of mesh instance.

### **Parameters**

- **E** (np.ndarray of float [N\_tri x 3]) – Electric field data on surfaces
- **fname** (str) – Filename of the .txt file containing the tetrahedra indices, which are adjacent to the surface triangles generated by the method “calc\_surface\_adjacent\_tetrahedra\_idx\_list(self, fname)”

### **Returns**

- **En\_pos** (np.ndarray of float [N\_tri x 3]) – Normal component of electric field of top side (outside) of surface
- **En\_neg** (np.ndarray of float [N\_tri x 3]) – Normal component of electric field of bottom side (inside) of surface

- **n** (*np.ndarray of float [N\_tri x 3]*) – Normal vector
- **Et** (*np.ndarray of float [N\_tri x 3]*) – Tangential component of electric field lying in surface
- **t** (*np.ndarray of float [N\_tri x 3]*) – Tangential vector

**calc\_E\_on\_GM\_WM\_surface(*E, roi*)**

Determines the normal and tangential component of the induced electric field on a GM-WM surface using nearest neighbour principle.

**Parameters**

- **E** (*np.ndarray of float [N\_tri x 3]*) – Induced electric field given in the tetrahedra centre of the mesh instance
- **roi** (*pynibs.roi.RegionOfInterestSurface*) – RegionOfInterestSurface object class instance

**Returns**

- **E\_normal** (*np.ndarray of float [N\_points x 3]*) – Normal vector of electric field on GM-WM surface
- **E\_tangential** (*np.ndarray of float [N\_points x 3]*) – Tangential vector of electric field on GM-WM surface

**calc\_E\_on\_GM\_WM\_surface3(*phi, dAdt, roi, verbose=True, mode='components'*)**

Determines the normal and tangential component of the induced electric field on a GM-WM surface by recalculating phi and dA/dt in an epsilon environment around the GM/WM surface (upper and lower GM-WM surface).

**Parameters**

- **phi** (*np.ndarray of float [N\_nodes x 1]*) – Scalar electric potential given in the nodes of the mesh
- **dAdt** (*np.ndarray of float [N\_nodes x 3]*) – Magnetic vector potential given in the nodes of the mesh
- **roi** (*object instance*) – RegionOfInterestSurface object class instance
- **verbose** (*boolean*) – Print information to stdout
- **mode** (*str*) – Select mode of output: - “components” : return x, y, and z component of tangential and normal components - “magnitude” : return magnitude of tangential and normal component (normal with sign for direction)

**Returns**

- **E\_normal** (*np.ndarray of float [N\_points x 3]*) – Normal vector of electric field on GM-WM surface
- **E\_tangential** (*np.ndarray of float [N\_points x 3]*) – Tangential vector of electric field on GM-WM surface

**calc\_E\_on\_GM\_WM\_surface\_simnibs(*phi, dAdt, roi, subject, verbose=False, mesh\_idx=0*)**

Determines the normal and tangential component of the induced electric field on a GM-WM surface by recalculating phi and dA/dt in an epsilon environment around the GM/WM surface (upper and lower GM-WM surface) or by using the Simnibs interpolation function.

**Parameters**

- **phi** (*np.ndarray of float [N\_nodes x 1]*) – Scalar electric potential given in the nodes of the mesh
- **dAdt** (*np.ndarray of float [N\_nodes x 3]*) – Magnetic vector potential given in the nodes of the mesh

- **roi** (*object instance*) – RegionOfInterestSurface object class instance
- **subject** (*Subject object*) – Subject object loaded from .hdf5 file
- **verbose** (*boolean*) – Print information to stdout
- **mesh\_idx** (*int*) – Mesh index

#### Returns

- **E\_normal** (*np.ndarray of float [N\_points x 3]*) – Normal vector of electric field on GM-WM surface
- **E\_tangential** (*np.ndarray of float [N\_points x 3]*) – Tangential vector of electric field on GM-WM surface

**calc\_E\_on\_GM\_WM\_surface\_simnibs\_KW**(*phi, dAdt, roi, subject, verbose=False, mesh\_idx=0*)

Determines the normal and tangential component of the induced electric field on a GM-WM surface by recalculating phi and dA/dt in an epsilon environment around the GM/WM surface (upper and lower GM-WM surface) or by using the Simnibs interpolation function.

#### Parameters

- **phi** (*np.ndarray of float [N\_nodes x 1]*) – Scalar electric potential given in the nodes of the mesh
- **dAdt** (*np.ndarray of float [N\_nodes x 3]*) – Magnetic vector potential given in the nodes of the mesh
- **roi** (*object instance*) – RegionOfInterestSurface object class instance
- **subject** (*Subject object*) – Subject object loaded from .hdf5 file
- **verbose** (*boolean*) – Print information to stdout
- **mesh\_idx** (*int*) – Mesh index

#### Returns

- **E\_normal** (*np.ndarray of float [N\_points x 3]*) – Normal vector of electric field on GM-WM surface
- **E\_tangential** (*np.ndarray of float [N\_points x 3]*) – Tangential vector of electric field on GM-WM surface

**calc\_J**(*E, sigma*)

Calculate current density J. The conductivity sigma is a list of np.arrays containing conductivities of regions (scalar and/or tensor).

$$\mathbf{J} = [\sigma] \mathbf{E}$$

#### Parameters

- **E** (*np.ndarray of float [N\_tet x 3]*) – Electric field in tetrahedra center
- **sigma** (*list of np.ndarray of float [N\_regions][3 x 3]*) – Conductivities of regions (scalar and/or tensor).

#### Returns

**E** – Electric field in tetrahedra center

#### Return type

*np.ndarray of float [N\_tet x 3]*

**calc\_QOI\_in\_points**(*qoi, points\_out*)

Calculate QOI\_out in points\_out using the mesh instance and the quantity of interest (QOI).

#### Parameters

- **qoi** (*np.ndarray of float*) – Quantity of interest in nodes of tetrahedra mesh instance
- **points\_out** (*np.ndarray of float*) – Point coordinates (x, y, z) where the qoi is going to be interpolated by linear basis functions

**Returns****qoi\_out** – Quantity of interest in points\_out**Return type***np.ndarray of float***calc\_QOI\_in\_points\_tet\_idx**(*qoi, points\_out, tet\_idx*)

Calculate QOI\_out in points\_out sitting in tet\_idx using the mesh instance and the quantity of interest (QOI).

**Parameters**

- **qoi** (*np.ndarray of float*) – Quantity of interest in nodes of tetrahedra mesh instance
- **points\_out** (*np.ndarray of float*) – Point coordinates (x, y, z) where the qoi is going to be interpolated by linear basis functions
- **tet\_idx** (*np.ndarray of int*) – Element indices where the points\_out are sitting

**Returns****qoi\_out** – Quantity of interest in points\_out**Return type***np.ndarray of float***calc\_gradient**(*phi*)

Calculate gradient of scalar DOF in tetrahedra center.

**Parameters****phi** (*np.ndarray of float [N\_nodes]*) – Scalar DOF the gradient is calculated for**Returns****grad\_phi** – Gradient of Scalar DOF in tetrahedra center**Return type***np.ndarray of float [N\_tet x 3]***calc\_surface\_adjacent\_tetrahedra\_idx\_list**(*fname*)

Determine the indices of the tetrahedra touching the surfaces and save the indices into a .txt file specified with fname.

**Parameters****fname** (*str*) – Filename of output .txt file**Returns**

&lt;File&gt; – Element indices of the tetrahedra touching the surfaces (outer-most elements)

**Return type***.txt file***data\_elements2nodes**(*data*)

Transforms an data in tetrahedra into the nodes after Zienkiewicz et al. (1992) [1]. Can only transform volume data, i.e. needs the data in the surrounding tetrahedra to average it to the nodes. Will not work well for discontinuous fields (like E, if several tissues are used).

**Parameters****data** (*np.ndarray [N\_elements x N\_data]*) – Data in tetrahedra**Returns****data\_nodes** – Data in nodes

**Return type**

np.ndarray [N\_nodes x N\_data]

**Notes**

**data\_nodes2elements(*data*)**

Interpolate data given in the nodes to the tetrahedra center.

**Parameters**

**data** (*np.ndarray [N\_nodes x N\_data]*) – Data in nodes

**Returns**

**data\_elements** – Data in elements

**Return type**

np.ndarray [N\_elements x N\_data]

**get\_faces(*tetrahedra\_indexes=None*)**

Creates a list of nodes in each face and a list of faces in each tetrahedra.

**Parameters**

**tetrahedra\_indexes** (*np.ndarray*) – Indices of the tetrahedra where the faces are to be determined (default: all tetrahedra)

**Returns**

- **faces** (*np.ndarray*) – List of nodes in faces, in arbitrary order
- **th\_faces** (*np.ndarray*) – List of faces in each tetrahedra, starts at 0, order=((0, 2, 1), (0, 1, 3), (0, 3, 2), (1, 2, 3))
- **face\_adjacency\_list** (*np.ndarray*) – List of tetrahedron adjacent to each face, filled with -1 if a face is in a single tetrahedron. Not in the normal element ordering, but only in the order the tetrahedra are presented

**get\_outside\_faces(*tetrahedra\_indexes=None*)**

Creates a list of nodes in each face that are in the outer volume.

**Parameters**

**tetrahedra\_indices** (*np.ndarray*) – Indices of the tetrahedra where the outer volume is to be determined (default: all tetrahedra)

**Returns**

**faces** – List of nodes in faces in arbitrary order

**Return type**

np.ndarray

## pynibs.mesh.transformations module

**pynibs.mesh.transformations.cell\_data\_to\_point\_data(*tris, data\_tris, nodes, method='nearest'*)**

A wrapper for scipy.interpolate.griddata to interpolate cell data to node data.

**Parameters**

- **tris** (*np.ndarray*) – element number list, (n\_tri, 3)
- **data\_tris** (*np.ndarray*) – data in tris, (n\_tri x 3)
- **nodes** (*np.ndarray*) – nodes coordinates, (n\_nodes, 3)
- **method** (*str, default: 'nearest'*) – Which method to use for interpolation. Default uses NearestNDInterpolator

**Returns**

**data\_nodes** – Data in nodes

**Return type**

np.ndarray

pynibs.mesh.transformations.**data\_elements2nodes**(*data, con, precise=False*)

Transforms data in elements (triangles or tetrahedra) to nodes. Data can be list of multiple data arrays.

**Parameters**

- **data** (*np.ndarray of float or list of np.ndarray*) – (N\_elements, N\_data)  
Data given in the elements (multiple datasets who fit to con may be passed in a list)
- **con** (*np.ndarray of int*) – triangles: (N\_elements, 3) tetrahedra: (N\_elements, 4)  
Connectivity index list forming the elements
- **precise** (*bool*, default: *False*) – Compute data transformation precisely but slow. Better for near-0 values.

**Returns**

**out** – (N\_nodes, N\_data) Data in nodes

**Return type**

np.ndarray of float or list of np.ndarray

pynibs.mesh.transformations.**data\_nodes2elements**(*data, con*)

Transforms data in nodes to elements (triangles or tetrahedra)

**Parameters**

- **data** (*np.ndarray of float*) – (N\_nodes, N\_data) Data given in the nodes
- **con** (*np.ndarray of int*) – triangles: (N\_elements, 3) tetrahedra: (N\_elements, 4)  
Connectivity index list forming the elements

**Returns**

**out** – (N\_elements, N\_data) Data given in the element centers

**Return type**

np.ndarray of float

pynibs.mesh.transformations.**map\_data\_to\_surface**(*datasets, points\_datasets, con\_datasets, fname\_fsl\_gm, fname\_fsl\_wm, fname\_midlayer=None, delta=0.5, input\_data\_in\_center=True, return\_data\_in\_center=True, data\_substitute=-1*)

Maps data from ROI of fsl surface (wm, gm, or midlayer) to given Freesurfer brain surface (wm, gm, inflated).

**Parameters**

- **datasets** (*np.ndarray of float [N\_points x N\_data] or list of np.ndarray*) – Data in nodes or center of triangles in ROI (specify this in “data\_in\_center”)
- **points\_datasets** (*np.ndarray of float [N\_points x 3] or list of np.ndarray*) – Point coordinates (x,y,z) of ROI where data in datasets list is given, the points have to be a subset of the GM/WM surface (has to be provided for each dataset)
- **con\_datasets** (*np.ndarray of int [N\_tri x 3] or list of np.ndarray*) – Connectivity matrix of dataset points (has to be provided for each dataset)
- **fname\_fsl\_gm** (*str or list of str or list of None*) – Filename of pial surface fsl file(s) (one or two hemispheres) e.g. in mri2msh: .../fs\_ID/surf/lh.pial
- **fname\_fsl\_wm** (*str or list of str or list of None*) – Filename of wm surface fsl file(s) (one or two hemispheres) e.g. in mri2msh: .../fs\_ID/surf/lh.white

- **fname\_midlayer** (*str or list of str*) – Filename of midlayer surface fsl file(s) (one or two hemispheres) e.g. in headreco: .../fs\_ID/surf/lh.central
- **delta** (*float*) – Distance parameter where gm-wm surface was generated 0...1 (default: 0.5) 0 -> WM surface 1 -> GM surface
- **input\_data\_in\_center** (*bool*) – Flag if data in datasets in given in triangle centers or in points (Default: True)
- **return\_data\_in\_center** (*bool*) – Flag if data should be returned in nodes or in elements (Default: True)
- **data\_substitute** (*float*) – Data substitute with this number for all points in the inflated brain, which do not belong to the given data set

#### Returns

**data\_mapped** – Mapped data to target brain surface. In points or elements

#### Return type

`np.ndarray of float [N_points_inf x N_data]`

```
pynibs.mesh.transformations.midlayer_2_surf(midlayer_data, coords_target, coords_midlayer,
                                             midlayer_con=None, midlayer_data_in_nodes=False,
                                             max_dist=5, outside_roi_val=0, precise_map=True)
```

Convert midlayer data to whole-brain surface data, e.g. grey matter. Output is returned as data in nodes.

#### Parameters

- **midlayer\_data** (*np.ndarray of float*) – (n\_elm\_midlayer,) or (n\_nodes\_midlayer,), the data in the midlayer.
- **coords\_target** (*np.ndarray of float*) – (n\_nodes\_target, 3) Coordinates of the nodes of the target surface.
- **coords\_midlayer** (*np.ndarray of float*) – (n\_nodes\_midlayer, 3) Coordinates of the nodes of the midlayer surface.
- **midlayer\_con** (*np.ndarray of int, optional*) – (n\_elm\_midlayer, 3) Connectivity of the midlayer elements. Provide if data\_in\_points == True.
- **midlayer\_data\_in\_nodes** (*bool, default=False*) – If midlayer data is provided in nodes, set to True and provide midlayer\_con.
- **max\_dist** (*float, default=5*) – Maximum distance between target and midlayer nodes to pull data from midlayer\_data for.
- **outside\_roi\_val** (*float, default=0*) – Areas outside of max\_dist are filled with outside\_roi\_val.
- **precise\_map** (*bool, default=True*) – If elements to nodes mapping is done, perform this precise and slow or not.
- **Returns** –
- -----
- **data\_target** (*np.ndarray*) – (n\_nodes\_target, 1) The data in nodes of the target surface.

```
pynibs.mesh.transformations.project_on_scalp(coords, mesh, scalp_tag=1005)
```

Find the node in the scalp closest to each coordinate

#### Parameters

- **coords** (*nx3 np.ndarray*) – Vectors to be transformed
- **mesh** (*pynibs.TetrahedraLinear or simnibs.msh.mesh\_io.Msh*) – Mesh structure in simnibs or pynibs format

- **scalp\_tag** (*int*, *optional*, *default: 1005*) – Tag in the mesh where the scalp is to be set. Default: 1005

**Returns**

**points\_closest** – (n, 3) coordinates projected scalp (closest skin points)

**Return type**

np.ndarray

`pynibs.mesh.transformations.project_on_scalp_hdf5(coords, mesh, scalp_tag=1005)`

Find the node in the scalp closest to each coordinate

**Parameters**

- **coords** (*nx3 np.ndarray*) – Vectors to be transformed
- **mesh** (*str* or *pynibs.TetrahedraLinear*) – Filename of mesh in .hdf5 format or Mesh structure
- **scalp\_tag** (*int (optional)*) – Tag in the mesh where the scalp is to be set. Default: 1005

**Returns**

**points\_closest** – coordinates projected scalp (closest skin points)

**Return type**

nx3 np.ndarray

`pynibs.mesh.transformations.refine_surface(fn_surf, fn_surf_refined, center, radius, repair=True, remesh=True, verbose=True)`

Refines surface (.stl) in spherical ROI and saves as .stl file.

**Parameters**

- **fn\_surf** (*str*) – Input filename (.stl)
- **fn\_surf\_refined** (*str*) – Output filename (.stl)
- **center** (*np.ndarray of float (3)*) – Center of spherical ROI (x,y,z)
- **radius** (*float*) – Radius of ROI
- **repair** (*bool, optional, default: True*) – Repair surface mesh to ensure that it is watertight and forms a volume
- **remesh** (*bool, optional, default:False*) – Perform remeshing with meshfix (also removes possibly overlapping facets and intersections)
- **verbose** (*bool, optional, default: True*) – Print output messages

**Returns**

<file>

**Return type**

.stl file

## pynibs.mesh.utils module

`pynibs.mesh.utils.calc_gradient_surface(phi, points, triangles)`

Calculate gradient of potential phi on surface (i.e. tangential component) given in vertices of a triangular mesh forming a 2D surface.

**Parameters**

- **phi** (*np.ndarray of float [N\_points x 1]*) – Potential in nodes
- **points** (*np.ndarray of float [N\_points x 3]*) – Coordinates of nodes (x,y,z)

- **triangles** (*np.ndarray of int32 [N\_tri x 3]*) – Connectivity of triangular mesh

**Returns**

**grad\_phi** – Gradient of potential phi on surface

**Return type**

*np.ndarray of float [N\_tri x 3]*

`pynibs.mesh.utils.calc_tet_volume(points, abs=True)`

Calculate tetrahedra volumes.

**Parameters**

- **points** (*np.ndarray*) – shape: (n\_tets,4,3) [[[Ax, Ay, Az], [Bx, By, Bz], [Cx, Cy, Cz], [Dx, Dy, Dz]],

[[Ax, Ay, Az],  
[Bx, By, Bz], [Cx, Cy, Cz], [Dx, Dy, Dz]],

...

]

- **abs** (*bool*) – Return magnitude. Default: True.

**Returns**

**volume** – shape: (n\_tets)

**Return type**

*np.ndarray*

`pynibs.mesh.utils.calc_tetrahedra_volume_cross(P1, P2, P3, P4)`

Calculates volume of tetrahedra specified by the 4 points P1...P4 multiple tetrahedra can be defined by P1...P4 as 2-D np.arrays using the cross and vector dot product

$$P1 = \begin{bmatrix} x_{tet_1} & y_{tet_1} & z_{tet_1} \\ x_{tet_2} & y_{tet_2} & z_{tet_2} \\ \dots & \dots & \dots \\ x_{tet_N} & y_{tet_N} & z_{tet_N} \end{bmatrix}$$

**Parameters**

- **P1** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of first point of tetrahedra
- **P2** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of second point of tetrahedra
- **P3** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of third point of tetrahedra
- **P4** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of fourth point of tetrahedra

**Returns**

**tetrahedra\_volume** – Volumes of tetrahedra

**Return type**

*np.ndarray of float [N\_tet x 1]*

`pynibs.mesh.utils.calc_tetrahedra_volume_det(P1, P2, P3, P4)`

Calculate volume of tetrahedron specified by 4 points P1...P4 multiple tetrahedra can be defined by P1...P4 as 2-D np.arrays using the determinant.

$$P1 = \begin{bmatrix} x_{tet_1} & y_{tet_1} & z_{tet_1} \\ x_{tet_2} & y_{tet_2} & z_{tet_2} \\ \dots & \dots & \dots \\ x_{tet_N} & y_{tet_N} & z_{tet_N} \end{bmatrix}$$

**Parameters**

- **P1** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of first point of tetrahedra
- **P2** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of second point of tetrahedra
- **P3** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of third point of tetrahedra
- **P4** (*np.ndarray of float [N\_tet x 3]*) – Coordinates of fourth point of tetrahedra

**Returns**

**tetrahedra\_volume** – Volumes of tetrahedra

**Return type**

*np.ndarray of float [N\_tet x 1]*

`pynibs.mesh.utils.calc_tri_surface(points)`

Calculate triangle surface areas.

**Parameters**

**points** (*np.ndarray*) – (n\_triangles,3,3)

**Returns**

**triangle\_area**

**Return type**

*np.ndarray*

`pynibs.mesh.utils.check_islands_for_single_elm(source_elm, connectivity=None, adjacency=None, island_crit=1)`

This identifies islands in a mesh for a given element. An island is a set of elements, that is only connect via a single node to another set of elements. These islands usually crash the FEM solver and should be removed.

1. Find all elements connect to source\_elm via one node (1-node-neighbor)
2. Start with source\_elm and visit all 2-node-neighbors ('shared-edge')
3. Continue recursively with all 2-node-neighbors and visit their 2-node-neighbors
4. See if any 1-node-neighbors have not been visited with this strategy. If so, an island has been found

**Parameters**

- **source\_elm** (*int*) – The source element to check
- **connectivity** (*np.ndarray, optional*) – Connectivity ('node\_number\_list') starting with 0. Can be triangles or tetrahedra (n\_elms, 3) or (n\_elms\_4).
- **adjacency** (*np.ndarry, optional*) – Adjenceny matrix (n\_elm, n\_elm). Weights are supposed to be number of shared nodes. Computed from neighbors if not provided.
- **island\_crit** (*int, optional, default: 'any'*) – How many nodes to define islands? 'any' -> Elements connected via a single node or single edge are defined as an island. 'node' -> Elements connected via a single \_node\_ are defined as an island. 'edge' -> Elements connected via a single \_edge\_ are defined as an island.

**Returns**

- **n\_visited** (*int*)
- **n\_not\_visited** (*int*)
- **neighbors\_visited** (*dict, which neighbors have been visited and which have not*)

```
pynibs.mesh.utils.determine_e_midlayer(fn_e_results, fn_mesh_hdf5, subject, mesh_idx, roi_idx,
                                         n_cpu=4, midlayer_fun='simnibs', phi_scaling=1.0,
                                         verbose=False)
```

Parallel version to determine the midlayer e-fields from a list of .hdf5 results files

#### Parameters

- **fn\_e\_results** (*list of str*) – List of results filenames (.hdf5 format)
- **fn\_mesh\_hdf5** (*str*) – Filename of corresponding mesh file
- **subject** (*pynibs.Subject*) – Subject object
- **mesh\_idx** (*int*) – Mesh index
- **roi\_idx** (*int*) – ROI index
- **n\_cpu** (*int, optional, default: 4*) – Number of parallel computations
- **midlayer\_fun** (*str, optional, default: "simnibs"*) – Method to determine the midlayer e-fields (“pynibs” or “simnibs”)
- **phi\_scaling** (*float, optional, default: 1.0*) – Scaling factor of scalar potential to change between “m” and “mm”

#### Returns

Adds midlayer e-field results to ROI

#### Return type

<File> .hdf5 file

```
pynibs.mesh.utils.determine_e_midlayer_workhorse(fn_e_results, subject, mesh_idx, midlayer_fun,
                                                 fn_mesh_hdf5, roi_idx, phi_scaling=1.0,
                                                 verbose=False)
```

#### phi\_scaling: float

simnibs < 3.0 : 1000. simnibs >= 3.0 : 1. (Default)

```
pynibs.mesh.utils.find_element_idx_by_points(nodes, con, points)
```

Finds the tetrahedral element index of an arbitrary point in the FEM mesh.

#### Parameters

- **nodes** (*np.ndarray [N\_nodes x 3]*) – Coordinates (x, y, z) of the nodes
- **con** (*np.ndarray [N\_tet x 4]*) – Connectivity matrix
- **points** (*np.ndarray [N\_points x 3]*) – Points for which the element indices are found.

#### Returns

**ele\_idx** – Element indices of tetrahedra where corresponding ‘points’ are lying in

#### Return type

*np.ndarray [N\_points]*

```
pynibs.mesh.utils.find_island_elms(connectivity=None, adjacency=None, verbose=False,
                                     island_crit='edge', decision='cumulative')
```

Searches for islands in a mesh and returns element indices of the smallest island. Island is defines as a set of elements, which share a single node and/or single edge with the rest of the mesh.

#### Parameters

- **connectivity** (*np.ndarray, optional*) – Connectivity (‘node\_number\_list’) starting with 0. Can be triangles or tetrahedra (n\_elms, 3) or (n\_elms\_4).
- **adjacency** (*np.ndarry, optional*) – Adjenceny matrix (n\_elm, n\_elm). Weights are supposed to be number of shared nodes. Computed from neighbors if not provided.

- **island\_crit** (*int*, *optional*, *default*: ‘edge’) – How many nodes to define islands? ‘node’ -> Elements connected via a single *\_node\_* are defined as an island. ‘edge’ -> Elements connected via a single *\_edge\_* are defined as an island.
- **decision** (*string*, *optional*, *default*: ‘cumulative’) – ‘cumulative’ -> Return all element indices that are not visited any times ‘smallest’ -> Return smallest island.
- **verbose** (*bool*, *optional*) – Print some verbosity information. Default: False

**Returns****island****Return type****list** of island-elsms

```
pynibs.mesh.utils.find_islands(connectivity=None, adjacency=None, island_crit='any', verbose=False,
largest=False)
```

This identifies islands in a mesh. An island is a set of elements, that is only connect via a single node to another set of elements. These islands usually crash the FEM solver and should be removed.

**For each element:**

1. Find all elements connect to source\_elm via one node (1-node-neighbor)
2. Start with source\_elm and visit all 2-node-neighbors ('shared-edge')
3. Continue recursively with all 2-node-neighbors and visit their 2-node-neighbors
4. See if any 1-node-neighbors have not been visited with this strategy. If so, an island has been found

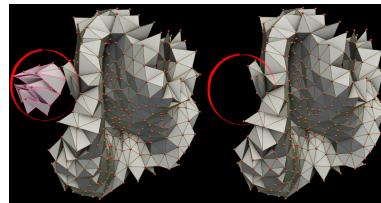


Fig. 1: Islands are groups of elements that are only connected via a single node/edge to another group.

**Parameters**

- **connectivity** (*np.ndarray*, *optional*) – Connectivity (‘node\_number\_list’) starting with 0. Can be triangles or tetrahedra (n\_elms, 3) or (n\_elms\_4).
- **adjacency** (*np.ndarray*, *optional*) – Adjenceny matrix (n\_elm, n\_elm). Weights are supposed to be number of shared nodes. Computed from neighbors if not provided.
- **island\_crit** (*int*, *optional*, *default*: ‘any’) – How many nodes to define islands? ‘any’ -> Elements connected via a single node or single edge are defined as an island. ‘node’ -> Elements connected via a single *\_node\_* are defined as an island. ‘edge’ -> Elements connected via a single *\_edge\_* are defined as an island.
- **largest** (*book*, *default*: *False*) – Only return largest island, speeds up computation quite a bit if only one large, and many small islands exist.
- **verbose** (*bool*, *optional*) – Print some verbosity information. Default: False

**Returns**

- **elms\_with\_island** (*list*) – Elements with neighboring islands
- **counter\_visited** (*np.ndarray*) – shape = (n\_elms). How often as each element been visited.
- **counter\_not\_visited** (*np.ndarray*) – shape = (n\_elms). How often as each element not been visited.

`pynibs.mesh.utils.find_nearest(array, value)`

Given an “array”, and given a “value”, returns an index  $j$  such that “value” is between  $\text{array}[j]$  and  $\text{array}[j+1]$ . “array” must be monotonic increasing.  $j=-1$  or  $j=\text{len}(\text{array})$  is returned to indicate that “value” is out of range below and above respectively.

#### Parameters

- **array** (`np.ndarray of float`) – Monotonic increasing array
- **value** (`float`) – Target value the nearest neighbor index in “array” is computed for

#### Returns

`idx` – Index  $j$  such that “value” is between  $\text{array}[j]$  and  $\text{array}[j+1]$

#### Return type

`int`

`pynibs.mesh.utils.get_indices_discontinuous_data(data, con, neighbor=False, deviation_factor=2, min_val=None, not_fitted_elms=None, crit='median', neigh_style='point')`

Get element indices (and the best neighbor index), where the data is discontinuous

#### Parameters

- **data** (`np.ndarray of float [n_data]`) – Data array to analyze given in the element center
- **con** (`np.ndarray of float [n_data, 3 or 4]`) – Connectivity matrix
- **neighbor** (`boolean, optional, default=False`) – Return also the element index of the “best” neighbor (w.r.t. median of data)
- **deviation\_factor** (`float`) – Allows data deviation from  $1/\text{deviation\_factor} < \text{data}[i]/\text{median} < \text{deviation\_factor}$
- **min\_val** (`float, optional`) – If given, only return elements which have a neighbor with data higher than `min_val`.
- **not\_fitted\_elms** (`np.ndarray`) – If given, these elements are not used as neighbors
- **crit** (`str, default: median`) – Criterium for best neighbor. Either median or max value
- **neigh\_style** (`str, default: 'point'`) – Should neighbors share point or ‘edge’

#### Returns

- **idx\_disc** (`list of int [n_disc]`) – Index list containing the indices of the discontinuous elements
- **idx\_neighbor** (`list of int [n_disc]`) – Index list containing the indices of the “best” neighbors of the discontinuous elements

`pynibs.mesh.utils.get_sphere(mesh=None, mesh_fn=None, target=None, radius=None, roi_idx=None, roi=None, elmttype='tris')`

Return element idx of elements within a certain distance to provided target. Element indices are 0-based (tris and tets start at 0, ‘pynibs’ style) Elements might be ‘tris’ (default) or ‘tets’

If roi object / idx and mesh fn is provided, the roi is expected to have midlayer information and the roi geometry is used.

#### Parameters

- **mesh** (`pynibs.mesh.TetrahedraLinear, optional`) –
- **mesh\_fn** (`str, optional`) – Filename to SimNIBS .msh or pyNIBS .hdf5 mesh file
- **target** (`np.ndarray of float, optional`) – (3,) X, Y, Z coordinates of target
- **radius** (`float, optional`) – Sphere radius im mm

- **roi\_idx** (*str or int*) – ROI name
- **elmtype** (*str, optional*) – Return triangles or tetrahedra in sphere around target. One of ('tris', 'tets')

**Returns****elms\_in\_sphere** – (n\_elements): Indices of elements found in ROI**Return type**

np.ndarray

**pynibs.mesh.utils.in\_hull**(*points, hull*)

Test if points in *points* are in *hull*. *points* should be a [N x K] coordinates of N points in K dimensions. *hull* is either a `scipy.spatial.Delaunay` object or the [M x K] array of the coordinates of M points in K dimensions for which Delaunay triangulation will be computed.

**Parameters**

- **points** (*np.ndarray*) – (N\_points x 3) Set of floating point data to test whether they are lying inside the hull or not
- **hull** (*scipy.spatial.Delaunay or np.ndarray*) – (M x K) Surface data

**Returns****inside** – TRUE: point inside the hull FALSE: point outside the hull**Return type**np.ndarray of `bool`**pynibs.mesh.utils.sample\_sphere**(*n\_points, r*)

Creates n\_points evenly spread in a sphere of radius r.

**Parameters**

- **n\_points** (*int*) – Number of points to be spread, must be odd
- **r** (*float*) – Radius of sphere

**Returns****points** – Evenly spread points in a unit sphere**Return type**np.ndarray of `float` [N x 3]**pynibs.mesh.utils.tets\_in\_sphere**(*mesh, target, radius, roi*)

Worker function for `get_sphere()`

Returns element idx of elements within a certain distance to provided target. If roi object / idx and mesh fn is provided, the roi is expected to have midlayer information and the roi geometry is used.

**Parameters**

- **mesh** (*pynibs.TetrahedraLinear, optional*) –
- **target** (*np.ndarray of float, optional*) – (3,) X, Y, Z coordinates of target
- **radius** (*float, optional*) – Sphere radius in mm
- **roi** (*pynibs.mesh.ROI, optional*) – Region of interest

**Returns****tets\_in\_sphere** – (n\_tets): Indices of elements found in ROI**Return type**

np.ndarray

`pynibs.mesh.utils.tris_in_sphere(mesh, target, radius, roi)`

Worker function for `get_sphere()`.

Returns triangle idx of elements within a certain distance to provided target. If `roi` object / idx and mesh fn is provided, the `roi` is expected to have midlayer information and the `roi` geometry is used.

**Parameters**

- `mesh (pynibs.mesh.TetrahedraLinear, optional)` –
- `target (np.ndarray of float, optional)` – (3,) X, Y, Z coordinates of target
- `radius (float, optional)` – Sphere radius in mm
- `roi (pynibs.mesh.ROI, optional)` – ROI

**Returns**

`tris_in_sphere` – (n\_triangles): Indices of elements found in sphere

**Return type**

`np.ndarray`

**pynibs.models package**

**pynibs.neuron package**

**Submodules**

**pynibs.neuron.neuron\_regression module**

`pynibs.neuron.neuron_regression.calc_e_effective(e, layerid, theta, gradient=None, neuronmodel='threshold', mep=None, waveform='biphasic')`

Determines the effective electric field using a neuron mean field model. Transforms the electric field by subtracting the threshold map (in V/m) from the original electric field. The remaining field is the effective electric field (`e_eff`), generating the stimulation effect, i.e. behavioural effects start at  $e_{eff} > 0$  because lower fields were not able to stimulate neurons.

**Parameters**

- `e (np.ndarray)` – Electric field (matrix) [N\_stim x N\_ele]
- `layerid (str)` – Choose from the neocortical layers (e.g. “L1”, “L23”, “L4”, “L5”, “L6”)
- `theta (np.ndarray)` – Theta angle (matrix) [N\_stim x N\_ele] of electric field with respect to surface normal
- `gradient (np.ndarray, optional, default: None)` – Electric field gradient (matrix) [N\_stim x N\_ele] between layer 1 and layer 6. Optional, the neuron mean field model is more accurate when provided.
- `neuronmodel (str, optional, default: "threshold")` – Select neuron model to modify the electric field values - “threshold”: subtract mean threshold from electric field - “IOcurve”: subtract value read from precomputed neuron IO curve from electric field
- `mep (np.array of float [N_stim], optional, default: None)` – MEP data (required in case of “IOcurve” approach (neuronmodel))
- `waveform (str, optional, default: biphasic)` – Waveform of TMS pulse: - “monophasic” - “biphasic”

**Returns**

**e\_eff** – Effective electric field (matrix) [N\_stim x N\_ele] the regression analysis can be performed with.

**Return type**

np.ndarray

```
pynibs.neuron.neuron_regression.calc_e_threshold(layerid, theta, gradient=None, mep=None, neuronmodel='threshold', waveform='biphasic')
```

Determine sensitivity map of electric field

**Parameters**

- **layerid** (*str*) – Choose from the neocortical layers (e.g. “L1”, “L23”, “L4”, “L5”, “L6”). The respective threshold model will be loaded.
- **theta** (*np.ndarray*) – Theta angle (matrix) [N\_stim x N\_ele] of electric field with respect to surface normal. in degrees [0 .. 180]
- **gradient** (*np.ndarray, optional, default: None*) – Electric field gradient (matrix) [N\_stim x N\_ele] between layer 1 and layer 6. Optional, the neuron mean field model is more accurate when provided. Percent [-100 .. 100]
- **mep** (*np.array of float [N\_stim], optional, default: None*) – MEP data (required in case of “IOcurve” approach (neuronmodel)
- **neuronmodel** (*str, optional, default: "threshold"*) – Select neuron model to modify the electric field values - “threshold”: subtract mean threshold from electric field - “IOcurve”: subtract value read from precomputed neuron IO curve from electric field
- **waveform** (*str, optional, default: biphasic*) – Waveform of TMS pulse: - “monophasic” - “biphasic”

**Returns**

**e\_sens** – Electric field sensitivity maps [N\_stim x N\_ele]

**Return type**

np.ndarray

```
pynibs.neuron.neuron_regression.load_cell_model(fn_csv)
```

Load interpolation points of the mean field model from the specified CSV file.

**Parameters**

**fn\_csv** (*str*) – Fully qualified path to the CSV containing the interpolation points of the mean field model.

**Returns**

- - *scipy.interpolate.LinearNDInterpolator*
- - *interpolation points ‘theta’*
- - *interpolation points ‘gradient’*

```
pynibs.neuron.neuron_regression.workhorse_interp(idx_list, interp, params)
```

Single core workhorse to interpolate data.

**Parameters**

- **idx\_list** (*np.array or list of float [n\_interpolations]*) – Indices in params array where the interpolation has to be performed (subset of all indices in params array)
- **interp** (*scipy.interpolate instance*) – Interpolator instance
- **params** (*np.array of float [N\_interpolations x N\_params]*) – Array containing the parameters the function is evaluated (total array with all parameters)

**Returns**

`res` – Interpolation results (subset params[idx\_list, :])

**Return type**

np.array of `float` [n\_interpolations]

## **pynibs.neuron.util module**

`pynibs.neuron.util.DI_wave(t, intensity, t0=5, dt=1.4, width=0.25)`

Determines cortical DI waves from TMS

**Parameters**

- `t` (*ndarray of float [n\_t]*) – Time axis in ms
- `intensity` (*float*) – Stimulator intensity w.r.t resting motor threshold (typical range: [0 … 2])
- `t0` (*float*) – offset time
- `dt` (*float*) – Spacing of waves in ms
- `width` (*float*) – Width of waves

**Returns**

`y` – DI waves

**Return type**

*ndarray of float [n\_t]*

## **pynibs.pckg package**

### **Subpackages**

`pynibs.pckg.libeep package`

#### **Submodules**

##### **pynibs.pckg.libeep.pyeep module**

`pynibs.pckg.libeep.pyeep.add_channel()`

add channel to channel info handle

`pynibs.pckg.libeep.pyeep.add_samples()`

add samples

`pynibs.pckg.libeep.pyeep.close()`

close handle

`pynibs.pckg.libeep.pyeep.close_channel_info()`

close channel info handle

`pynibs.pckg.libeep.pyeep.create_channel_info()`

create channel info handle

`pynibs.pckg.libeep.pyeep.get_channel_count()`

get channel count

`pynibs.pckg.libeep.pyeep.get_channel_label()`

get channel label

```
pynibs.pckg.libeep.pyeep.get_channel_reference()
    get channel reference
pynibs.pckg.libeep.pyeep.get_channel_unit()
    get channel unit
pynibs.pckg.libeep.pyeep.get_sample_count()
    get sample count
pynibs.pckg.libeep.pyeep.get_sample_frequency()
    get sample frequency
pynibs.pckg.libeep.pyeep.get_samples()
    get samples
pynibs.pckg.libeep.pyeep.get_trigger()
    get samples
pynibs.pckg.libeep.pyeep.get_trigger_count()
    get trigger count
pynibs.pckg.libeep.pyeep.get_version()
    get libeep version
pynibs.pckg.libeep.pyeep.read()
    open libeep file for reading
pynibs.pckg.libeep.pyeep.write_cnt()
    open libeep cnt file for writing
```

## pynibs.regression package

This holds methods for the TMS-based cortical localization approach as published in [1]

### References

#### Submodules

##### pynibs.regression.regression module

```
class pynibs.regression.Element(x, y, ele_id, fun=<function sigmoid4>, score_type='R2',
                                 select_signed_data=False, constants=None, **kwargs)
Bases: object
Fit Element object class
calc_score()
    Determine goodness-of-fit score
run_fit(max_nfev=1000)
    Perform data fit with lmfit
run_select_signed_data()
    Selects positive or negative data by performing an initial linear fit by comparing the resulting p-values,
    slopes and R2 values. Either positive or negative data (w.r.t. x-axis) yielding a fit with a p-value < 0.05,
    a positive slope and the higher R2 value is used and the remaining data with the other sign is omitted
    from the analysis
```

```
set_constants(value)
    Sets constants in self.constants and gmodel instance

set_init_vals(value)
    Sets initial values in self.init_vals and gmodel instance

set_limits(value)
    Sets limits in self.limits and gmodel instance

Parameters
    value (dict) – Parameters (keys) to set in self as limits.

set_random_init_vals()
    Set random initial values

setup_model()
    Setup model parameters (limits, initial values, etc. ...)

pynibs.regression.regression.fit_elms(elm_idx_list, e_matrix, mep, zap_idx=None, fun=<function sigmoid4>, init_vals=None, limits=None, log_scale=False, constants=None, max_nfev=None, bad Elm_idx=None, score_type='R2', verbose=False)
Workhorse for Mass-univariate nonlinear regressions on raw MEP_{AMP} ~ E. That is, for each element in elm_idx_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise r2 score is returned.

Parameters

- elm_idx_list (list of int or np.ndarray) – List containing the element indices the fit is performed for
- e_matrix (np.ndarray of float [n_zaps x n_ele]) – Electric field matrix
- mep (np.ndarray of float [n_zaps]) – Motor evoked potentials for every stimulation
- zap_idx (np.ndarray [n_zaps], optional, default: None) – Indices of zaps the congruence factor is calculated with (default: all)
- fun (str) – A function name of pynibs.exp.Mep (exp0, sigmoid)
- init_vals (np.ndarray of dict) – Dictionary containing the initial values for each element as np.ndarray [len(elm_idx_list)]. The keys are the free parameters of fun, e.g. “x0”, “amp”, etc
- limits (pd.DataFrame) – Dictionary containing the limits of each parameter for each element e.g.: limits[“x0”][elm_idx] = [min, max]
- log_scale (bool, optional, default: False) – Log-transform data before fit (necessary for functions defined in the log domain)
- constants (dict of <string>:<num>, optional, default: None) – key:value pair of model parameters not to optimize.
- max_nfev (int, default: None) – Max fits, passed to model.fit() as max_nfev=max_nfev*len(x).
- bad Elm_idx (np.ndarray) – Indices of elements not to fit, with indices corresponding to indices (not values) of elm_idx_list
- score_type (str, optional, default: "R2") – Goodness of fit measure; Choose SR for nonlinear fits and R2 or SR for linear fits: - “R2”: R2 score (Model variance / Total variance) [0, 1] for linear models; 0: bad fit; 1: perfect fit - “SR”: Relative standard error of regression (1 - Error 2-norm / Data 2-norm) [-inf, 1]; 1: perfect fit

```

- **mask\_e\_field** (*np.ndarray of bool [n\_zaps x n\_ele]*, optional, default: *None*) – Mask indicating for which e-field (and mep) values the fit is performed for. Changes for normal component in each element because of the sign and p-values. If None, all data is used in each element.
- **verbose** (*bool*, optional, default: *False*) – Print verbosity information

**Returns**

- **r2** (*np.ndarray of float [n\_roi, 1]*) – R2 for each element in elm\_idx\_list
- **best\_values** (*np.ndarray of object*) – Fit parameters returned from the optimizer

`pynibs.regression.regression.get_bad_elms(x, y, method='lstsq', verbose=False)`

This does an element-wise fast linear regression fit to identify bad elements. Bad is defined here as a negative slope.

**x**

[*np.ndarray of float [n\_zaps x n\_ele]*] Electric field matrix

**y**

[*np.ndarray of float [n\_zaps]*] Motor evoked potentials for every stimulation

**method**

[str, default: “lstsq”] Which method to use. (`numpy.linalg.lstsq`, `scipy.stats.linregress`, or `pinv`)

**verbose**

[*bool*, optional, default: *False*] Print verbosity information

**Returns****idx: np.ndarray**

Indices of bad elements

`pynibs.regression.regression.get_model_init_values(fun, elm_idx_list, e_matrix, mep, mask_e_field=None, rem_empty_hints=True)`

Calc appropriate init, limit, and max values for models fits depending on the data. If negative and positive x-data is present in case of e.g. normal component values are set according to the side (positive or negative) where more values are present. When more positive x-axis values are present, negative x-axis values will be ignored. When more negative x-axis values are present, the absolute values will be taken and the positive values are ignored.

Only parameters for sigmoid\* are optimized.

**Parameters**

- **fun** (*pyfempp.exp.Mep*) – IO curve function object
- **elm\_idx\_list** (*np.ndarray of int*) – Array containing the element indices the fit is performed for
- **e\_matrix** (*np.ndarray of float [n\_zaps x n\_ele]*) – Electric field matrix
- **mep** (*np.ndarray of float [n\_zaps]*) – Motor evoked potentials for every stimulation
- **mask\_e\_field** (*np.ndarray of bool [n\_zaps x n\_ele]*, optional, default: *None*) – Mask indicating for which e-field (and mep) values the fit is performed for. Changes for normal component in each element because of the sign and p-values. If None, all data is used in each element.
- **rem\_empty\_hints** (*bool*, default: *True*) – Remove any non-filled param hints from limits dict.

**Returns**

- **log\_scale** (*bool*) – Log scale

- **limits** (*dict of list [n elm\_index\_list]*) – Element-wise limit values for function fitting.
- **init\_vals** (*dict of list [n elm\_index\_list]*) – Element-wise init values for function fitting.
- **max\_vals\_refit** (*dict of list [n elm\_index\_list]*) – Element-wise perturbation range for refitting function.

`pynibs.regression.regression.init(l, zap_lists, res_fn)`

Pool init function to use with regression\_nl\_hdf5\_single\_core\_write

#### Parameters

- **l** (*multiprocessing.Lock()*) –
- **zap\_lists** (*list of list of int*) – Which zaps to compute.
- **res\_fn** (*str*) – .hdf5 fn

`pynibs.regression.regression.logistic_regression()`

Some ideas on how to improve regression approach

1. De-log data

Data range has to be transformed to a reasonable range. For a full sigmoid, -10:10 looks ok

```
sig <- function(z) {
  return( 1 / (1 + exp(-z)))
}

desig <- function(x) {
  return(- log((1/x) - 1))
}
```

This might be a reasonable fast approach, but the parameter range has to be estimated. Maybe remove some outliers?

2. fit logistic regression to raw data scipy.optimize provides `fit_curve()`, which does OLS-ish fitting to a given function <https://stackoverflow.com/questions/54376900/fit-sigmoid-curve-in-python>

I expect this to be rather slow.

3. Use the sklearn logistic\_regression classifier and access raw fit data. The logistic\_regression is implemented as a classifier, maybe it's possible to use its regression fit results. Implementation should be pretty fast.

`pynibs.regression.regression.nl_hdf5(elm_idx_list=None, fn_reg_hdf5=None, qoi_path_hdf5=None, e_matrix=None, mep=None, fun=<function sigmoid4>, zap_idx=None, n_cpu=4, con=None, n_refit=50, return_fits=False, score_type='R2', verbose=False, pool=None, refit_discontinuities=True)`

Mass-univariate nonlinear regressions on raw MEP\_{AMP} ~ E. That is, for each element in `elm_idx_list`, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise r2 score is returned. The function reads the precomputed array of E-MEP data from an .hdf5 file.

#### Parameters

- **elm\_idx\_list** (*np.ndarray of int*) – List containing the element indices the fit is performed for
- **fn\_reg\_hdf5** (*str*) – Filename (incl. path) containing the precomputed E-MEP dataframes
- **qoi\_path\_hdf5** (*Union[str, list[str]]*) – Path in .hdf5 file to dataset of electric field qoi e.g.: ["E", "E\_norm", "E\_tan"]
- **e\_matrix** (*np.ndarray of float [n\_zaps x n\_ele]*) – Electric field matrix

- **mep** (*np.ndarray of float [n\_zaps]*) – Motor evoked potentials for every stimulation
- **zap\_idx** (*np.array [n\_zaps]*, optional, default: *None*) – Indices of zaps the congruence factor is calculated with (default: all)
- **fun** (*pynibs.exp.Mep function*) – A function of pynibs.exp.Mep (exp0, sigmoid)
- **n\_cpu** (*int*) – Number of threads
- **con** (*np.ndarray of float [n\_roi, 3 or 4]*, optional, default: *None*) – Connectivity matrix of ROI (needed in case of refit because of discontinuity check)
- **n\_refit** (*int*, optional, default: 50) – Maximum number of refits of zero elements. No refit is applied in case of n\_refit = 0.
- **return\_fits** (*bool*, optional, default: *False*) – Return fit objects containing the parameter estimates
- **score\_type** (*str*, optional, default: "R2") – Error measure of fit: - "R2": R2 score (Model variance / Total variance); linear fits: [0, 1], 1 ... perfect fit - "SR": Relative standard error of regression (1 - Error 2-norm / Data 2-norm); [-Inf, 1], 1 ... perfect fit
- **verbose** (*bool*, optional, default: *False*) – Plot output messages
- **pool** (*multiprocessing.Pool()*) – pool instance to use.
- **refit\_discontinuities** (*bool*, optional, default: *True*) – Run refit for discontinuous elements at the end

### Returns

**r2** – R2 for each element in elm\_idx\_list

### Return type

*np.ndarray of float [n\_roi, n\_qoi]*

```
pynibs.regression.regression.nl_hdf5_single_core(zap_idx, elm_idx_list, fn_reg_hdf5=None,
                                                qoi_path_hdf5=None, e_matrix=None,
                                                mep=None, fun=<function sigmoid4>,
                                                con=None, n_refit=50, return_fits=False,
                                                constants=None, verbose=False, seed=None,
                                                rem_bad_elms=True,
                                                return_e_field_stats=True)
```

Mass-univariate nonlinear regressions on raw MEP\_{AMP} ~ E. That is, for each element in elm\_idx\_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise r2 score is returned. The function reads the precomputed array of E-MEP data from an .hdf5 file.

### Parameters

- **elm\_idx\_list** (*np.ndarray of int*) – List containing the element indices the fit is performed for
- **fn\_reg\_hdf5** (*str*) – Filename (incl. path) containing the precomputed E-MEP dataframes
- **qoi\_path\_hdf5** (*str or list of str*) – Path in .hdf5 file to dataset of electric field qoi e.g.: ["E", "E\_norm", "E\_tan"]
- **e\_matrix** (*np.ndarray of float [n\_zaps x n\_ele]*) – Electric field matrix
- **mep** (*np.ndarray of float [n\_zaps]*) – Motor evoked potentials for every stimulation
- **zap\_idx** (*np.array [n\_zaps]*, optional, default: *None*) – Indices of zaps the congruence factor is calculated with (default: all)

- **fun** (*function object*) – A function of pynibs.exp.Mep (exp0, sigmoid)
- **con** (*np.ndarray of float [n\_roi, 3 or 4], optional, default: None*) – Connectivity matrix of ROI (needed in case of refit because of discontinuity check)
- **n\_refit** (*int, optional, default: 50*) – Maximum number of refits of zero elements. No refit is applied in case of n\_refit = 0.
- **return\_fits** (*bool, optional, default: False*) – Return fit objects containing the parameter estimates
- **constants** (*dict of <string>:<num>, optional, default: None*) – key:value pair of model parameters not to optimize.
- **verbose** (*bool, optional, default: False*) – Plot output messages
- **seed** (*int, optional, default: None*) – Seed to use.
- **rem\_bad\_elms** (*bool, default: True*) – Remove elements based on a fast linear regression slope estimation
- **return\_e\_field\_stats** (*bool, default: True*) – Return some stats on the efield variance

#### Returns

**r2** – R2 for each element in elm\_idx\_list

#### Return type

np.ndarray of float [n\_roi, n\_qoi]

```
pynibs.regression.regression.nl_hdf5_single_core_write(i, elm_idx_list, fn_reg_hdf5=None,
                                                       qoi_path_hdf5=None, e_matrix=None,
                                                       mep=None, fun=<function sigmoid4>,
                                                       con=None, n_refit=50,
                                                       return_fits=False, constants=None,
                                                       verbose=False, seed=None,
                                                       stepdown=False, score_type='R2',
                                                       return_progress=False, geo=None)
```

```
pynibs.regression.regression.regress_data(e_matrix, mep, elm_idx_list=None, element_list=None,
                                           fun=<function sigmoid4>, n_cpu=4, con=None,
                                           n_refit=50, zap_idx=None, return_fits=False,
                                           score_type='R2', verbose=False, pool=None,
                                           refit_discontinuities=True, select_signed_data=False,
                                           **kwargs)
```

Mass-univariate nonlinear regressions on raw MEP\_{AMP} ~ E. That is, for each element in elm\_idx\_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise R2 score is returned. The function reads the precomputed array of E-MEP data from an .hdf5 file.

#### Parameters

- **e\_matrix** (*np.ndarray of float*) – (n\_zaps, n\_ele) Electric field matrix
- **mep** (*np.ndarray of float*) – (n\_zaps,) Motor evoked potential for each stimulation
- **elm\_idx\_list** (*np.ndarray of int or list of int*) – (n\_zaps,) List containing the element indices the fit is performed for
- **element\_list** (*list of Element object instances, optional*) – [n\_ele] pynibs.Element objects ot skip initialization here.
- **fun** (*pynibs.exp.Mep, default: pynibs.sigmoid4*) – A pynibs.exp.Mep function (exp0, sigmoid, sigmoid4, ...)
- **n\_cpu** (*int*) – Number of threads, if n\_cpu=1 no parallel pool will be opened and all calculations are done in serial

- **con** (*np.ndarray of float, optional*) – (n\_ele, 3 or 4) Connectivity matrix of ROI. Needed in case of refit for discontinuity checks
- **n\_refit** (*int, default: 50*) – Maximum number of refits of zero elements. No refit is applied in case of n\_refit = 0.
- **zap\_idx** (*np.ndarray of int or list of int, optional*) – Which e/mep pairs to use.
- **return\_fits** (*bool, optional*) – Return fit objects containing the parameter estimates
- **score\_type** (*str, default: "R2"*) – Error measure of fit: - “R2”: R2 score (Model variance / Total variance); linear fits: [0, 1], 1 … perfect fit - “SR”: Relative standard error of regression (1 - Error 2-norm / Data 2-norm); [-Inf, 1], 1 … perfect fit - “rho”: Spearman correlation coefficient [-1, 1]; finds any monotonous correlation (0 means no correlation)
- **verbose** (*bool, default: False*) – Plot output messages
- **pool** (*multiprocessing.Pool()*) – pool instance to use
- **refit\_discontinuities** (*bool, default: True*) – Refit discontinuous elements. If True, provide \_con\_
- **\*\*kwargs** – Passed on to pynibs.Element() to set fit parameters.

#### Returns

- **score** (*np.ndarray of float (n\_roi, n\_qoi)*) – Score for each element
- **best\_values** (*list of dict (n\_ele)*) – List of parameter fits

`pynibs.regression.regression.ridge_from_hdf5(elm_idx_list, fn_reg_hdf5, qoi_path_hdf5, zap_idx=None)`

Mass-univariate ridge regressions on raw MEP\_{AMP} ~ E. That is, for each element in elm\_idx\_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise sklearn.metrics.regression.r2\_score is returned. The function reads the precomputed array of E-MEP data from an .hdf5 file. Always uses all cores of a machine!

#### elm\_idx\_list

[list of int] List containing the element indices the fit is performed for

#### fn\_hdf5

[str] Filename (incl. path) containing the precomputed E-MEP dataframes

#### qoi\_path\_hdf5

[str] Path in .hdf5 file to dataset of electric field qoi

#### zap\_idx

[np.ndarray [n\_zaps], optional, default: None] Indices of zaps the congruence factor is calculated with (default: all)

#### Returns

**r2** – R^2 for each element in elm\_idx\_list

#### Return type

ndarray of float [n\_roi, n\_datasets]

`pynibs.regression.regression.sing_elm_fitted(elm_idx_list, mep_lst, mep_params, e, alpha=1000, n_samples=100)`

Mass-univariate ridge regressions on fitted MEP\_{AMP} ~ E. That is, for each element in elm\_idx\_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise sklearn.metrics.regression.r2\_score is returned.

**elm\_idx\_list: ndarray [chunksize]**

List of element indices, the congruence factor is computed for

**mep\_lst: list of Mep object instances [n\_cond]**

List of fitted Mep object instances for all conditions (see exp.py for more information of Mep class)

**mep\_params: ndarray of float [n\_mep\_params\_total]**

List of all mep parameters of curve fits used to calculate the MEP (accumulated into one array) (e.g.:

[mep\_#1\_para\_#1, mep\_#1\_para\_#2, mep\_#1\_para\_#3, mep\_#2\_para\_#1, mep\_#2\_para\_#1, ...])

**e: ndarray of float with e.shape == (n\_elm, n\_cond, n\_qoi)**

array of the electric field to compute the r2 factor for, e.g. (e\_mag, e\_norm, e\_tan)

**n\_samples**

[int, default=100] Number of data points to generate discrete mep and e curves

**Returns**

**r2** – R^2 for each element in elm\_idx\_list

**Return type**

ndarray of float [n\_roi, n\_datasets]

`pynibs.regression.regression.sing_elm_raw(elm_idx_list, mep_lst, mep_params, e, alpha=1000)`

Mass-univariate ridge regressions on raw MEP\_{AMP} ~ E. That is, for each element in elm\_idx\_list, it's E (mag | norm | tan) for each zap regressed on the raw MEP amplitude. An element wise sklearn.metrics.regression.r2\_score is returned.

**elm\_idx\_list: ndarray [chunksize]**

List of element indices, the congruence factor is computed for

**mep: list of Mep object instances [n\_cond]**

List of fitted Mep object instances for all conditions (see exp.py for more information of Mep class)

**mep\_params: ndarray of float [n\_mep\_params\_total]**

List of all mep parameters of curve fits used to calculate the MEP (accumulated into one array) (e.g.:

[mep\_#1\_para\_#1, mep\_#1\_para\_#2, mep\_#1\_para\_#3, mep\_#2\_para\_#1, mep\_#2\_para\_#1, ...])

**e: ndarray of float with e.shape == (n\_elm, n\_cond, n\_qoi)**

array of the electric field to compute the r2 factor for, e.g. (e\_mag, e\_norm, e\_tan)

**Returns**

**r2** – R^2 for each element in elm\_idx\_list

**Return type**

ndarray of float [n\_roi, n\_datasets]

`pynibs.regression.regression.single_fit(x, y, fun)`

Performs a single fit and returns fit object

**Parameters**

- **x** (ndarray of float) – x-values
- **y** (ndarray of float) – y-values
- **fun** (function) – Function for fitting

**Returns**

**fit** – Fit object

**Return type**

gmodel fit object

---

```
pynibs.regression.regression.stepdown_approach(zap_idx, elm_idx_list, fn_reg_hdf5=None,
                                                qoi_path_hdf5=None, e_matrix=None, mep=None,
                                                fun=<function sigmoid4>, con=None, n_refit=50,
                                                return_fits=False, constants=None, verbose=False,
                                                seed=None, rem_bad_elms=True,
                                                return_e_field_stats=True, score_type='R2',
                                                return_progress=False, smooth_data=True,
                                                geo=None)
```

Mass-univariate nonlinear regressions on raw MEP\_{AMP} ~ E in a stepdown manner to speed up computation.

**Initially, one set of fits is done for the complete dataset. Afterwards, the best 1% of the elements are used**

as initial fitting parameters for their neighboring elements. Then, neighboring elements are fitted accordingly and iteratively. Finally, discontinuous elements are refitted until a smooth map is found or n\_refit is hit.

Can be sped up with rem\_bad\_elms that computes a fast linear fit to identify elements with a negative slope.

The function reads the precomputed array of E-MEP data from an .hdf5 file.

#### Parameters

- **elm\_idx\_list** (*np.ndarray of int*) – List containing the element indices the fit is performed for
- **fn\_reg\_hdf5** (*str*) – Filename (incl. path) containing the precomputed E-MEP dataframes
- **qoi\_path\_hdf5** (*str or list of str*) – Path in .hdf5 file to dataset of electric field qoi e.g.: [“E”, “E\_norm”, “E\_tan”]
- **e\_matrix** (*np.ndarray of float [n\_zaps x n\_ele] / [n\_zapidx x n\_ele]*) – Electric field matrix
- **mep** (*np.ndarray of float [n\_zaps]*) – Motor evoked potentials for every stimulation
- **zap\_idx** (*np.array [n\_zaps], optional, default: None*) – Indices of zaps the congruence factor is calculated with (default: all)
- **fun** (*function object*) – A function of pynibs.exp.Mep (exp0, sigmoid)
- **con** (*np.ndarray of float [n\_elm\_roi, 3 or 4], optional, default: None*) – Connectivity matrix of ROI (needed in case of refit because of discontinuity check)
- **n\_refit** (*int, optional, default: 50*) – Maximum number of refits of zero elements. No refit is applied in case of n\_refit = 0.
- **return\_fits** (*bool, optional, default: False*) – Return fit objects containing the parameter estimates
- **constants** (*dict of <string>:<num>, optional, default: None*) – key:value pair of model parameters not to optimize.
- **verbose** (*bool, optional, default: False*) – Plot output messages
- **seed** (*int, optional, default: None*) – Seed to use.
- **rem\_bad\_elms** (*bool, default: True*) – Remove elements based on a fast linear regression slope estimation
- **return\_e\_field\_stats** (*bool, default: True*) – Return some stats on the efield variance

#### Returns

**r2**

[np.ndarray of float [n\_roi, n\_qoi]] R2 for each element in elm\_idx\_list

**best\_values: list of dict, optional**

fit information

**stats**

[dict, optional]

**'mc': float, optional**

Mutual coherence for e fields

**'sv\_rat'**

[float, optional] SVD singular value ratio

progress : cmaps for each step

**Return type**

dict

`pynibs.regression.regression.workhorse_element_init(ele_id, e_matrix, mep, fun, score_type, select_signed_data, constants, **kwargs)`

Workhorse to initialize Elements.

`pynibs.regression.regression.workhorse_element_run_fit(element, max_nfev=10)`

Workhorse to run single Element fit. If status is False, the element will not be fitted.

`pynibs.regression.regression.write_regression_hdf5(fn_exp_hdf5, fn_reg_hdf5, qoi_path_hdf5, qoi_phys, e_results_folder, qoi_e, roi_idx, cond_exclude)`

Reads the stimulation intensities from the experiment.hdf5 file. Reads the qoi from the experiment.hdf5 file. Reads the electric fields from the electric field folder. Weights the electric field voxel wise with the respective intensities and writes an .hdf5 file containing the preprocessed data (pandas dataframe).

**fn\_exp\_hdf5: str**

Filename of the experiment.hdf5 file

**fn\_reg\_hdf5: str**

Filename of output regression.hdf5 file

**qoi\_path\_hdf5: str**

Path in experiment.hdf5 file pointing to the pandas dataframe containing the qoi (e.g.: “phys\_data/postproc/EMG”)

**qoi: str**

Name of QOI the congruence factor is calculated with (e.g.: “p2p”)

**fn\_e\_results: str**

Folder containing the electric fields (e.g.: “/data/pt\_01756/probands/13061.30/results/electric\_field/1”)

**qoi\_e: str or list of str**

Quantities of the electric field used to calculate the congruence factor (e.g. [“E”, “E\_norm”, “E\_tan”]  
Has to be included in e.hdf5 -> e.g.: “data/midlayer/roi\_surface/1/E”

**roi\_idx: int**

ROI index

**conds\_exclude: str or list of str**

Conditions to exclude

**Returns**

**<File>** – File containing the intensity (current) scaled E-fields of the conditions in the ROI.

Saved in datasets with the same name as qoi\_e [“E”, “E\_norm”, “E\_tan”]

**Return type**

.hdf5 file

## pynibs.regression.score\_types module

### pynibs.util package

#### Submodules

##### pynibs.util.plot module

`pynibs.util.plot.plot_surface(data, con, points)`

Plots data in triangle center

##### Parameters

- `data` (`np.array of float [n_tris]`) – Data in triangular center
- `con` (`np.array of float [n_tris x 3]`) – Connectivity list of triangles
- `points` (`np.array of float [n_points x 3]`) – Points (vertices) of surface mesh

##### pynibs.util.quality\_measures module

`pynibs.util.quality_measures.c_map_comparison(c1, c2, t1, t2, nodes, tris)`

Compares two c-maps in terms of NRMSD and calculates the geodesic distance between the hotspots.

##### Parameters

- `c1` (`np.ndarray of float [n_ele]`) – First c-map
- `c2` (`np.ndarray of float [n_ele]`) – Second c-map (reference)
- `t1` (`np.ndarray of float [3]`) – Coordinates of the hotspot in the first c-map
- `t2` (`np.ndarray of float [3]`) – Coordinates of the hotspot in the second c-map
- `nodes` (`np.ndarray of float [n_nodes x 3]`) – Node coordinates
- `tris` (`np.ndarray of float [n_tris x 3]`) – Connectivity of ROI elements

##### Returns

- `nrmsd` (`float`) – Normalized root-mean-square deviation between the two c-maps in (%)
- `gdist` (`float`) – Geodesic distance between the two hotspots in (mm)

`pynibs.util.quality_measures.euclidean_dist(nodes, tris, source, source_is_node=True)`

Returns euclidean\_dist distance of all nodes to source node (tria).

This is just a wrapper for the gdist package.

### Example

```
with h5py.File(fn,'r') as f:
    tris = f['mesh/elm/triangle_number_list'][:]
    nodes = f['mesh/nodes/node_coord'][:]
    nodes_dist_euc, tris_dist_euc = euclidean_dist(nodes, tris, 3017)

pynibs.write_data_hdf5(data_fn,
                       data=[tris_dist_euc, nodes_dist_euc],
                       data_names=["tris_dist_euc", "nodes_dist_euc", ""])
pynibs.write_xdmf(data_fn,hdfs_geo_fn=fn)
```

##### Parameters

- `nodes` (`np.ndarray(n_nodes, 3)`) –
- `tris` (`np.ndarray(n_tris, 3)`) –

- **source** (`np.ndarray(int)` or `int`) – geodesic distances of all nodes to this will be computed
- **source\_is\_node** (`bool`) – Is source a node idx or a tr idx

#### Returns

- **nodes\_dist** (`np.ndarray(n_nodes,)`)
- **tris\_dist** (`np.ndarray(n_tris,)`)

`pynibs.util.quality_measures.geodesic_dist(nodes, tris, source, source_is_node=True)`

Returns geodesic distance of all nodes to source node (or tri).

This is just a wrapper for the gdist package.

### Example

```
with h5py.File(fn,'r') as f:
    tris = f['mesh/elm/triangle_number_list'][:]
    nodes = f['mesh/nodes/node_coord'][:]
    nodes_dist_ged, tris_dist_ged = geodesic_dist(nodes, tris, 3017)

pynibs.write_data_hdf5(data_fn,
                       data=[tris_dist_ged, nodes_dist_ged],
                       data_names=['tris_dist_ged', 'nodes_dist_ged'])

pynibs.write_xdmf(data_fn,hdf5_geo_fn=fn)
```

#### Parameters

- **nodes** (`np.ndarray(n_nodes, 3)`) –
- **tris** (`np.ndarray(n_tris, 3)`) –
- **source** (`np.ndarray(int)` or `int`) – Geodesic distances of all nodes (or tri) to this will be computed
- **source\_is\_node** (`bool`) – Is source a node idx or a tr idx

#### Returns

- **nodes\_dist** (`np.ndarray(n_nodes,)`)
- **tris\_dist** (`np.ndarray(n_tris,)`)

`pynibs.util.quality_measures.nrmsd(array, array_ref, error_norm='relative', x_axis=False)`

Determine the normalized root-mean-square deviation between input data and reference data.

#### Parameters

- **array** (`np.ndarray`) – input data [ (x), y0, y1, y2 ... ]
- **array\_ref** (`np.ndarray`) – reference data [ (x\_ref), y0\_ref, y1\_ref, y2\_ref ... ] if array\_ref is 1D, all sizes have to match
- **error\_norm** (`str, optional, default="relative"`) – Decide if error is determined “relative” or “absolute”
- **x\_axis** (`boolean, optional, default=False`) – If True, the first column of array and array\_ref is interpreted as the x-axis, where the data points are evaluated. If False, the data points are assumed to be at the same location.

#### Returns

**normalized\_rms** – Normalized root-mean-square deviation between the columns of array and array\_ref

#### Return type

`np.ndarray of float [array.shape[1]]`

## pynibs.util.simnibs module

```
pynibs.util.simnibs.calc_e_in_midlayer_roi(phi_dadt, roi, subject, phi_scaling=1.0, mesh_idx=0,
                                             mesh=None, roi_hem='lh', depth=0.5, qoi=None,
                                             layer_gm_wm_info=None)
```

This is to be called by Simnibs as postprocessing function per FEM solve.

### Parameters

- **phi\_dadt** (*array-like, elmdata*) –
- **roi** ([pynibs.roi.RegionOfInterestSurface\(\)](#)) –
- **subject** ([pynibs.subject.Subject\(\)](#)) –
- **phi\_scaling** (*float*) –
- **mesh\_idx** (*int*) –
- **mesh** ([simnibs.msh.Mesh\(\)](#)) –
- **roi\_hem** ('lh') –
- **depth** (*float*) –
- **qoi** (*list of str*) – List of identifiers of the to-be calculated quantities of interest.
- **layer\_gm\_wm\_info** (*dict[str, dict[str,np.ndarray]]*) – For each layer defined in the mesh (outer dict key: layer\_id), provide pre-computed geometrical information as a dictionary (outer dict value): - key: gm\_nodes

For each layer node, the corresponding point on the GM surface.

- key: wm\_nodes For each layer node, the corresponding point on the WM surface.
- key: gm\_center\_distance The distance between the layer nodes and the corresponding points on the GM.
- key: wm\_center\_distance The distance between the layer nodes and the corresponding points on the WM.

### Returns

- **(roi.n\_tris,4)** (*np.vstack((e\_mag, e\_norm, e\_tan, e\_angle)).transpose()* for the midlayer)
- **(len(roi.layers)xroi.layers[idx].surface.n\_tris,4)** (*np.vstack((e\_mag, e\_norm, e\_tan, e\_angle)).transpose()*)

`pynibs.util.simnibs.check_mesh(mesh, verbose=False)`

### Check a simmibs.Mesh for degenerated elements:

- zero surface triangles
- zerso volume tetrahedra
- negative volume tetrahedra

### Parameters

- **mesh** (*str or simmibs.Mesh*) –
- **verbose** (*book, default: False*) – Print some verbosity messages.

### Returns

- **zero\_tris** (*np.ndarray*) – Element indices for zero surface tris (0-indexed)
- **zero\_tets** (*np.ndarray*) – Element indices for zero volume tets (0-indexed)
- **neg\_tets** (*np.ndarray*) – Element indicies for negative volume tets (0-indexed)

`pynibs.util.simnibs.e_field_angle_theta(surface, mesh)`

Compute angle between local the E-field vector and surface vector at the ROI nodes.

**Parameters**

- **surface** (`simnibs.Msh`) – The surface object representing the ROI.
- **mesh** (`simnibs.Msh`) – The (volumetric) head mesh.

**Returns**

**theta** – The angle between local the E-field vector and surface vector for each surface element of the ROI.

**Return type**

`simnibs.mesh.mesh_io.ElementData`

`pynibs.util.simnibs.e_field_gradient_between_wm_gm(roi_surf, mesh, gm_nodes, wm_nodes, gm_center_distance, wm_center_distance)`

Compute local the E-field gradient at the ROI nodes between the gray and white matter boundary surfaces.  
Adapted from neuronibis/cortical\_layer.py/add\_e\_field\_gradient\_between\_wm\_gm\_field

**Parameters**

- **roi\_surf** (`simnibs.Msh`) – The surface object representing the ROI.
- **volumetric\_mesh** (`simnibs.Msh`) – The (volumetric) head mesh.

**Returns**

**e\_field\_gradient\_per\_mm** – The E-field gradient from the GM to the WM surface normalized to 1 mm with respect to the gray matter thickness. per ROI node

**Return type**

`simnibs.mesh.mesh_io.ElementData`

`pynibs.util.simnibs.fix_mesh(mesh, verbose=False)`

Fixes simnibs.Mesh by removing any zero surface tris and zero volume tets and by fixing negative volume tets.

**Parameters**

- **mesh** (`str` or `simnibs.Mesh`) – Filename of mesh or mesh object.
- **verbose** (`bool`, default: `False`) – Print some verbosity messages.

**Returns**

`fixed_mesh`

**Return type**

`simnibs.Mesh`

`pynibs.util.simnibs.precompute_geo_info_for_layer_field_interpolation(simnibs_mesh, roi)`

Precomputes geometric properties of the corresponding GM and WM nodes in the ‘simnibs\_mesh’ of each node of each layer in ‘roi’. > The corresponding point on the GM and WM surface to each vertex of te ROI surface

are determined (by raycasting and nearest neighbour search as fallback) (interpolation will take place between these nodes)

- > **The nodes are moved inside the gray matter by 20 % of their total distance from the GM/WM boundary to the midlayer.**
- > **The distance of the relocated GM and WM nodes to the ROI nodes is determined (required to computed the gradient per mm).**

**Parameters**

`simnibs_mesh`

[simnibs.Msh] The head model volume mesh.

**roi: pynibs.roi.RegionOfInterestSurface**

The ROI object containing the layers.

**Returns****layer\_gm\_wm\_info**

[dict[str, dict[str,np.ndarray]]] For each layer defined in the mesh (outer dict key: layer\_id), provide pre-computed geometrical information as a dictionary (outer dict value): - key: gm\_nodes

For each layer node, the corresponding point on the GM surface.

- key: wm\_nodes For each layer node, the corresponding point on the WM surface.
- key: gm\_center\_distance The distance between the layer nodes and the corresponding points on the GM.
- key: wm\_center\_distance The distance between the layer nodes and the corresponding points on the WM.

**pynibs.util.simnibs.read\_coil\_geo(*fn\_coil\_geo*)**

Reads a coil .geo file.

**Parameters**

**fn\_coil\_geo (str)** – Filename of .geo file created from SimNIBS containing the dipole information

**Returns**

- **dipole\_pos (np.ndarray of float)**
- (n\_dip, 3) Dipole positions (x, y, z).
- **dipole\_mag (np.ndarray of float)**
- (n\_dip, 1) Dipole magnitude.

**pynibs.util.simnibs.smooth\_mesh(*mesh*, *output\_fn*, *smooth*=0.8, *approach*='taubin', *skin\_only\_output*=False, *smooth\_tissue*='skin')**

Smoothes the skin compartment of a simnibs mesh. Uses one of three trimesh.smoothing approaches. Because tetrahedra and triangle share the same nodes, this also smoothes the volume domain.

**Parameters**

- **mesh (str or simnibs.Mesh)** –
- **output\_fn (str)** –
- **smooth (float, default: 0.8)** – Smoothing aggressiveness. [0, ..., 1]
- **approach (str, default: 'taubin')** – Which smoothing approach to use. One of ('taubin', 'laplacian', 'humphrey')
- **smooth\_tissue (str or list of int, default: 'skin')** – Which tissue type to smooth. E.g. 'gm' or [2, 1002].
- **skin\_only\_output (bool, default: True)** – If true, a skin only mesh is written out instead of the full mesh.

**Returns**

<file>

**Return type**

The smoothed mesh.

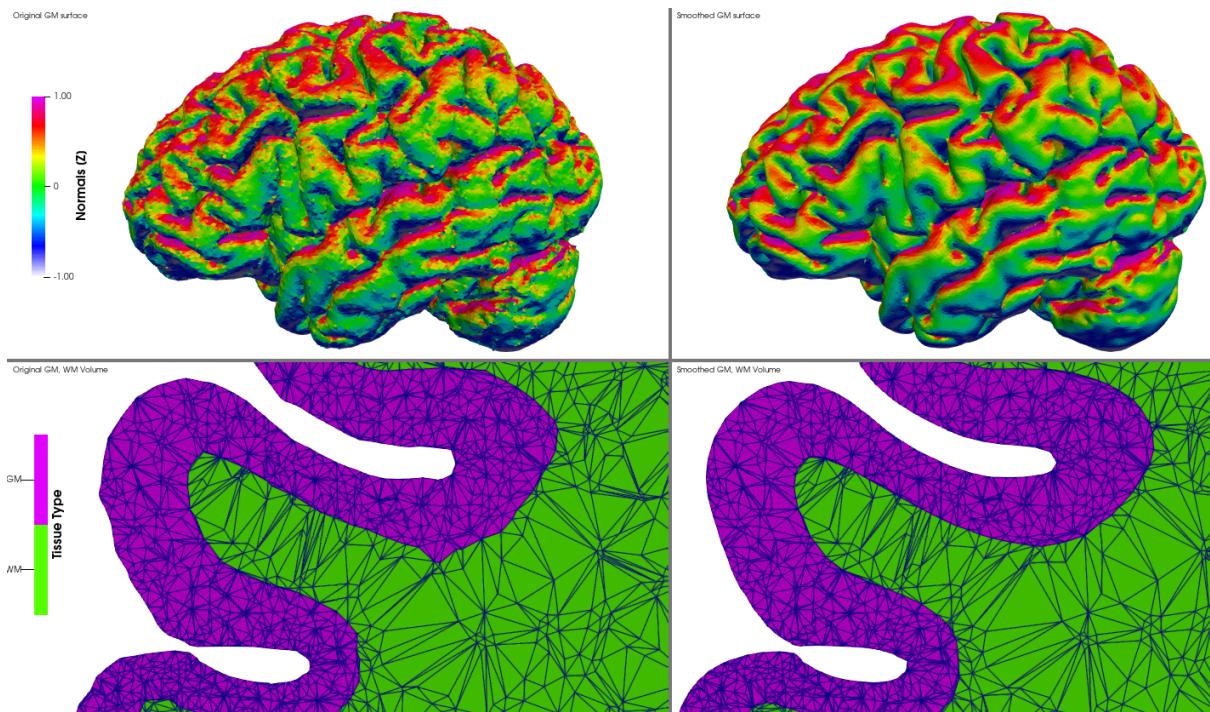


Fig. 2: Left: original, spiky mesh. Right: smoothed mesh.

## pynibs.util.util module

`pynibs.util.util.add_center(var)`

Adds center to argument list.

### Parameters

`var` (`list of float [2]`) – List containing two values [f1,f2]

### Returns

`out` – List containing the average value in the middle [f1, mean(f1,f2), f2]

### Return type

`list of float [3]`

`pynibs.util.util.bash(command)`

Executes bash command and returns output message in stdout (uses `os.popen`).

### Parameters

`command` (`str`) – Bash command

### Returns

- `output` (`str`) – Output from stdout
- `error` (`str`) – Error message from stdout

`pynibs.util.util.bash_call(command)`

Executes bash command and returns output message in stdout (uses `subprocess.Popen`).

### Parameters

`command` (`str`) – bash command

`pynibs.util.util.calc_n_network_combs(n_e, n_c, n_i)`

Determine number of combinations if all conditions may be replaced between N\_i elements (mixed interaction)

### Parameters

- **n\_e** (*int*) – Number of elements in the ROI
- **n\_c** (*int*) – Number of conditions (I/O curves)
- **n\_i** (*int*) – Number of maximum interactions

**Returns****n\_comb** – Number of combinations**Return type***int***pynibs.util.util.compute\_chunks**(*seq, num*)

Splits up a sequence *\_seq\_* into *\_num\_* chunks of similar size. If *len(seq) < num*, (*num-len(seq)*) empty chunks are returned so that *len(out) == num*

**Parameters**

- **seq** (*list of something [N\_ele]*) – List containing data or indices, which is divided into chunks
- **num** (*int*) – Number of chunks to generate

**Returns****out** – num sub-lists of seq with each of a similar number of elements (or empty).**Return type***list* of num sublists**pynibs.util.util.cross\_product**(*A, B*)

Evaluates the cross product between the vector pairs in a and b using pure Python.

**Parameters**

- **A** (*ndarray of float 2 x [N x 3]*) –
- **B** (*ndarray of float 2 x [N x 3]*) – Input vectors, the cross product is evaluated between

**Returns****c** – Cross product between vector pairs in a and b**Return type***ndarray of float* [N x 3]**pynibs.util.util.cross\_product\_einsum2**(*a, b*)

Evaluates the cross product between the vector pairs in a and b using the double Einstein sum.

**Parameters**

- **a** (*ndarray of float 2 x [N x 3]*) –
- **b** (*ndarray of float 2 x [N x 3]*) – Input vectors, the cross product is evaluated between

**Returns****c** – Cross product between vector pairs in a and b**Return type***ndarray of float* [N x 3]**pynibs.util.util.differential\_evolution**(*fobj, bounds, mut=0.8, crossp=0.7, popsize=20, its=1000, \*\*kwargs*)

Differential evolution optimization algorithm

**Parameters**

- **fobj** (*function object*) – Function to optimize
- **bounds** (*dict*) – Dictionary containing the bounds of the free variables to optimize

- **mut** (*float*) – Mutation factor
- **crossp** (*float*) – Cross population factor
- **popsize** (*int*) – Population size
- **its** (*int*) – Number of iterations
- **kwargs** (*dict*) – Arguments passed to fobj (constants etc...)

**Returns**

- **best** (*dict*) – Dictionary containing the best values
- **fitness** (*float*) – Fitness value of best solution

`pynibs.util.util.euler_angles_to_rotation_matrix(theta)`

Determines the rotation matrix from the three Euler angles theta = [Psi, Theta, Phi] (in rad), which rotate the coordinate system in the order z, y', x''.

**Parameters**

**theta** (*ndarray* [3]) – Euler angles in rad

**Returns**

**r** – Rotation matrix (z, y', x'')

**Return type**

*ndarray* [3 x 3]

`pynibs.util.util.generalized_extreme_value_distribution(x, mu, sigma, k)`

Generalized extreme value distribution

**Parameters**

- **x** (*ndarray of float* [n\_x]) – Events
- **mu** (*float*) – Mean value
- **sigma** (*float*) – Standard deviation
- **k** (*float*) – Shape parameter

**Returns**

**y** – Probability density of events

**Return type**

*ndarray* of *float* [n\_x]

`pynibs.util.util.get_cartesian_product(array_list)`

Generate a cartesian product of input arrays (all combinations).

`cartesian_product = get_cartesian_product(array_list)`

**Parameters**

**array\_list** (*list of 1D ndarray of float*) – Arrays to compute the cartesian product with

**Returns**

**cartesian\_product** – Array containing the cartesian products (all combinations of input vectors) (M, len(arrays))

**Return type**

*ndarray* of *float*

## Examples

```
>>> import pygpc
>>> out = pygpc.get_cartesian_product(([1, 2, 3], [4, 5], [6, 7]))
>>> out
```

`pynibs.util.util.invert(trans)`

Invert rotation matrix.

### Parameters

`trans (ndarray of float [3 x 3])` – Rotation matrix

### Returns

`rot_inv` – Inverse rotation matrix

### Return type

ndarray of `float` [3 x 3]

`pynibs.util.util.likelihood_posterior(x, y, fun, bounds=None, verbose=True, normalized_params=False, **params)`

Determines the likelihood of the data following the function “fun” assuming a two variability source of the data pairs (x, y) using the posterior distribution.

### Parameters

- `x (ndarray of float [n_points])` – x data
- `y (ndarray of float [n_points])` – y data
- `fun (function)` – Function to fit the data to (e.g. sigmoid)
- `bounds (dict, optional, default: None)` – Dictionary containing the bounds of “sigma\_x” and “sigma\_y” and the free parameters of fun
- `verbose (bool, optional, default: True)` – Print function output after every calculation
- `normalized_params (bool, optional, default: False)` – Are the parameters passed in normalized space between [0, 1]? If so, bounds are used to denormalize them before calculation
- `**params (dict)` – Free parameters to optimize. Contains “sigma\_x”, “sigma\_y”, and the free parameters of fun

### Returns

`l` – Negative likelihood

### Return type

`float`

`pynibs.util.util.list2dict(l)`

Transform list of dicts with same keys to dict of list

### Parameters

`l (list of dict)` – List containing dictionaries with same keys

### Returns

`d` – Dictionary containing the entries in a list

### Return type

`dict` of lists

`pynibs.util.util.load_muaps(fn_muaps, fs=1000000.0, fs_downsample=100000.0)`

`pynibs.util.util.mutual_coherence(array)`

Calculate the mutual coherence of a matrix A. It can also be referred as the cosine of the smallest angle between two columns.

```
mutual_coherence = mutual_coherence(array)
```

**Parameters**

**array** (*ndarray of float*) – Input matrix

**Returns**

**mutual\_coherence** – Mutual coherence

**Return type**

**float**

`pynibs.util.util.norm_percentile(data, percentile)`

Normalizes data to a given percentile.

**Parameters**

- **data** (*ndarray [n\_data, ]*) – Dataset to normalize

- **percentile** (*float*) – Percentile of normalization value [0 … 100]

**Returns**

**data\_norm** – Normalized dataset

**Return type**

*ndarray [n\_data, ]*

`pynibs.util.util.normalize_rot(rot)`

Normalize rotation matrix.

**Parameters**

**rot** (*ndarray of float [3 x 3]*) – Rotation matrix

**Returns**

**rot\_norm** – Normalized rotation matrix

**Return type**

*ndarray of float [3 x 3]*

`pynibs.util.util.quat_rotation_angle(q)`

Computes the rotation angle from the quaternion in rad.

**Parameters**

**q** (*ndarray of float*) – Quaternion, either only the imaginary part (length=3) [qx, qy, qz] or the full quaternion (length=4) [qw, qx, qy, qz]

**Returns**

**alpha** – Rotation angle of quaternion in rad

**Return type**

**float**

`pynibs.util.util.quat_to_rot(q)`

Computes the rotation matrix from quaternions.

**Parameters**

**q** (*ndarray of float*) – Quaternion, either only the imaginary part (length=3) or the full quaternion (length=4)

**Returns**

**rot** – Rotation matrix, containing the x, y, z axis in the columns

**Return type**

*ndarray of float [3 x 3]*

`pynibs.util.util.quaternion_conjugate(q)`

<https://stackoverflow.com/questions/15425313/inverse-quaternion>

**Parameters**

**q** –

**Returns****Return type**

pynibs.util.util.**quaternion\_diff**(*q1*, *q2*)

<https://math.stackexchange.com/questions/2581668/> error-measure-between-two-rotations-when-one-matrix-might-not-be-a-valid-rotation

**Parameters**

- **q1** –
- **q2** –

**Returns****Return type**

pynibs.util.util.**quaternion\_inverse**(*q*)

<https://stackoverflow.com/questions/15425313/inverse-quaternion>

**Parameters**

- **q** –

**Returns****Return type**

pynibs.util.util.**rd**(*array*, *array\_ref*)

Determine the relative difference between input data and reference data.

**Parameters**

- **array** (*np.ndarray*) – input data [ (x), y0, y1, y2 ... ]
- **array\_ref** (*np.ndarray*) – reference data [ (x\_ref), y0\_ref, y1\_ref, y2\_ref ... ] if array\_ref is 1D, all sizes have to match

**Returns**

**rd** – Relative difference between the columns of array and array\_ref

**Return type**

ndarray of **float** [array.shape[1]]

pynibs.util.util.**recursive\_len**(*item*)

Determine len of list of lists (recursively).

**Parameters**

- **item** (*list of list*) – List of list

**Returns**

**len** – Total length of list of lists

**Return type**

**int**

pynibs.util.util.**rot\_to\_quat**(*rot*)

Computes the quaternions from rotation matrix. (see e.g. <http://www.euclideanspace.com/mathematics/geometry/rotations/conversions/matrixToQuaternion/>)

**Parameters**

- **rot** (*nparray of float [3 x 3]*) – Rotation matrix, containing the x, y, z axis in the columns

**Returns**

**q** – Quaternion, full (length=4)

**Return type**

nparray of **float**

`pynibs.util.util.rotation_matrix_to_euler_angles(r)`

Calculates the euler angles theta = [Psi, Theta, Phi] (in rad) from the rotation matrix R which, rotate the coordinate system in the order z, y', x''. (<https://www.learnopencv.com/rotation-matrix-to-euler-angles/>)

**Parameters**

`r (np.array [3 x 3])` – Rotation matrix (z, y', x'')

**Returns**

`theta` – Euler angles in rad

**Return type**

`np.array [3]`

`pynibs.util.util.sigmoid_log_p(x, p)`

`pynibs.util.util.tal2mni(coords, direction='tal2mni', style='nonlinear')`

Transform Talairach coordinates into (SPM) MNI space and vice versa.

This is taken from <https://imaging.mrc-cbu.cam.ac.uk/imaging/MniTalairach> and <http://gibms.mc.ntu.edu.tw/bmlab/tools/data-analysis-codes/mni2tal-m/>

**Parameters**

- `coords (np.ndarray or list)` – x,y,z coordinates
- `direction (str, default: 'tal2mni')` – Transformation direction. One of ('tal2mni', 'mni2tal')
- `style(str, default: 'nonlinear')` – Transformation style. One of ('linear', 'non-linear')

**Returns**

`coords_trans`

**Return type**

`np.ndarray`

`pynibs.util.util.unique_rows(a)`

Returns the unique rows of np.array(a).

**Parameters**

`a (nparray of float [m x n])` – Array to search for double row entries

**Returns**

`a_unique` – array a with only unique rows

**Return type**

`np.array [k x n]`

## 1.1.2 Submodules

### 1.1.3 pynibs.coil module

`pynibs.coil.calc_coil_position_pdf(fn_rescon=None, fn_simpos=None, fn_exp=None, orientation='quaternions', folder_pdffplots=None)`

Determines the probability density functions of the transformed coil position (x', y', z') and quaternions of the coil orientations (x'', y'', z'')

**Parameters**

- `fn_rescon (str)` – Filename of the results file from TMS experiments (results\_conditions.csv)
- `fn_simpos (str)` – Filename of the positions and orientation from TMS experiments (simPos.csv)

- **fn\_exp** (*str*) – Filename of experimental.csv file from experiments
- **orientation** (*str*) – Type of orientation estimation: ‘quaternions’ or ‘euler’
- **folder\_pdpplots** (*str*) – Folder, where the plots of the fitted pdfs are saved (omitted if not provided)

**Returns**

- **pdf\_paras\_location** (*list of list of np.ndarray [n\_conditions]*) –  
Pdf parameters (limits and shape) of the coil position for x’, y’, and z’ for each:  
  - beta\_paras ... [p, q, a, b] (2 shape parameters and limits)
  - moments ... [data\_mean, data\_std, beta\_mean, beta\_std]
  - p\_value ... p-value of the Kolmogorov Smirnov test
  - uni\_paras ... [a, b] (limits)
- **pdf\_paras\_orientation\_euler** (*list of np.ndarray [n\_conditions]*) –  
Pdf parameters (limits and shape) of the coil orientation Psi, Theta, and Phi for each:  
  - beta\_paras ... [p, q, a, b] (2 shape parameters and limits)
  - moments ... [data\_mean, data\_std, beta\_mean, beta\_std]
  - p\_value ... p-value of the Kolmogorov Smirnov test
  - uni\_paras ... [a, b] (limits)
- **OP\_mean** (*List of [3 x 4] np.ndarray [n\_conditions]*) – List of mean coil position and orientation for different conditions (global coordinate system)

$$\begin{bmatrix} | & | & | & | \\ ori_x & ori_y & ori_z & pos \\ | & | & | & | \end{bmatrix}$$

- **OP\_zeromean** (*list of [3 x 4 x n\_con\_each] np.ndarray [n\_conditions]*) – List over conditions containing zero-mean coil orientations and positions
- **V** (*list of [3 x 3] np.ndarrays [n\_conditions]*) – Transformation matrix of coil positions from global coordinate system to transformed coordinate system
- **P\_transform** (*list of np.ndarray [n\_conditions]*) – List over conditions containing transformed coil positions [x’, y’, z’] of all stimulations (zero-mean, rotated by SVD)
- **quaternions** (*list of np.ndarray [n\_conditions]*) – List over conditions containing imaginary part of quaternions [x”, y”, z”] of all stimulations

`pynibs.coil.calc_coil_transformation_matrix(LOC_mean, ORI_mean, LOC_var, ORI_var, V)`

Calculate the modified coil transformation matrix needed for simnibs based on location and orientation variations observed in the framework of uncertainty analysis

**Parameters**

- **LOC\_mean** (*np.ndarray of float*) – (3), Mean location of TMS coil
- **ORI\_mean** (*np.ndarray of float*) – (3 x 3) Mean orientations of TMS coil

$$\begin{bmatrix} | & | & | \\ x & y & z \\ | & | & | \end{bmatrix}$$

- **LOC\_var** (*np.ndarray of float*) –  
(3) Location variation in normalized space (dx’, dy’, dz’), i.e. zero mean and projected on principal axes

- **ORI\_var** (*np.ndarray of float*) –  
(3) Orientation variation expressed in Euler angles [alpha, beta, gamma] in deg
- **V** (*np.ndarray of float*) – (3x3) V-matrix containing the eigenvectors from `_,_,V = numpy.linalg.svd`

#### Returns

- **mat** (*np.ndarray of float*)
- (4, 4) Transformation matrix containing 3 axis and 1 location vector –

$$\begin{bmatrix} | & | & | & | \\ x & y & z & pos \\ | & | & | & | \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

`pynibs.coil.check_coil_position(points, hull)`

Check if magnetic dipoles are lying inside head region

#### Parameters

- **points** (*np.ndarray of float*) – (N\_points, 3) Coordinates (x,y,z) of magnetic dipoles
- **hull** (*Delaunay object or np.ndarray of float*) – (N\_surface\_points, 3)  
Head surface data

#### Returns

**valid** – Validity of coil position: TRUE: valid FALSE: invalid

#### Return type

`bool`

`pynibs.coil.create_stimsite_from_exp_hdf5(fn_exp, fn_hdf, datanames=None, data=None, overwrite=False)`

This takes an experiment.hdf5 file and creates an .hdf5 + .xdmf tuple for all coil positions for visualization.

#### Parameters

- **fn\_exp** (*str*) – Path to experiment.hdf5
- **fn\_hdf** (*str*) – Filename for the resulting .hdf5 file. The .xdmf is saved with the same basename. Folder should already exist.
- **datanames** (*str or list of str*) – Dataset names for `_data_`. Default: None.
- **data** (*np.ndarray*) – Dataset array with (len(poslist.pos), len(datanames())). Default: None.
- **overwrite** (*boolean*) – Overwrite existing files. Default: False.

`pynibs.coil.create_stimsite_from_list(fn_hdf, poslist, datanames=None, data=None, overwrite=False)`

This takes a TMSLIST from simnibs and creates a .hdf5 + .xdmf tuple for all positions.

Centers and coil orientations are written so disk.

#### Parameters

- **fn\_hdf** (*str*) – Filename for the .hdf5 file. The .xdmf is saved with the same basename. Folder should already exist.
- **datanames** (*str or list of str*) – Dataset names for `_data_`. Default: None.
- **data** (*np.ndarray*) – Dataset array with (len(poslist.pos), len(datanames())). Default: None.

- **poslist** (*TMSLIST object (simnibs.simulation.simstruct.TMSLIST)*) – poslist.pos[\*].matsimnibs have to be set.
- **overwrite** (*boolean*) – Overwrite existing files. Default: False.

`pynibs.coil.create_stimsite_from_matsimnibs(fn_hdf, matsimnibs, datanames=None, data=None, overwrite=False)`

This takes a matsimnibs array and creates an .hdf5 + .xdmf tuple for all coil positions for visualization.

Centers and coil orientations are written disk.

#### Parameters

- **fn\_hdf** (*str*) – Filename for the .hdf5 file. The .xdmf is saved with the same basename. Folder should already exist.
- **matsimnibs** (*np.ndarray*) – (4, 4, n\_pos) Matsimnibs matrices containing the coil orientation (x,y,z) and position (p)

$$\begin{bmatrix} | & | & | & | \\ x & y & z & p \\ | & | & | & | \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- **datanames** (*str or list of str*) – Dataset names for \_data\_. Default: None.
- **data** (*np.ndarray, optional*) – (len(poslist.pos), len(datanames)).
- **overwrite** (*boolean, default: False*) – Overwrite existing files.

`pynibs.coil.create_stimsite_from_tmslist(fn_hdf, poslist, datanames=None, data=None, overwrite=False)`

This takes a TMSLIST from simnibs and creates a .hdf5 + .xdmf tuple for all positions.

Centers and coil orientations are written so disk.

#### Parameters

- **fn\_hdf** (*str*) – Filename for the .hdf5 file. The .xdmf is saved with the same basename. Folder should already exist.
- **datanames** (*str or list of str*) – Dataset names for \_data\_. Default: None.
- **data** (*np.ndarray*) – Dataset array with (len(poslist.pos), len(datanames())). Default: None.
- **poslist** (*TMSLIST object (simnibs.simulation.simstruct.TMSLIST)*) – poslist.pos[\*].matsimnibs have to be set.
- **overwrite** (*boolean*) – Overwrite existing files. Default: False.

`pynibs.coil.create_stimsite_hdf5(fn_exp, fn_hdf, conditions_selected=None, sep='_', merge_sites=False, fix_angles=False, data_dict=None, conditions_ignored=None)`

Reads results\_conditions and creates an hdf5/xdmf pair with condition-wise centers of stimulation sites and coil directions as data.

#### Parameters

- **fn\_exp** (*str*) – Path to results.csv
- **fn\_hdf** (*str*) – Path where to write file. Gets overridden if already existing
- **conditions\_selected** (*str or list of str, Default=None*) – List of conditions returned by the function, the others are omitted, If None, all conditions are returned
- **sep** (*str, Default: "\_"*) – Separator between condition label and angle (e.g. M1\_0, or M1-0)

- **merge\_sites** (*boolean*) – If true, only one coil center per site is generated.
- **fix\_angles** (*boolean*) – rename 22.5 -> 0, 0 -> -45, 67.5 -> 90, 90 -> 135
- **data\_dict** (*dict of np.ndarray of float [n\_stimsites] (optional), default: None*) – Dictionary containing data corresponding to the stimulation sites (keys)
- **conditions\_ignored** (*str or list of str, Default=None*) – Conditions, which are not going to be included in the plot

**Returns**

**<Files>** – Contains information about condition-wise stimulation sites and coil directions (fn\_hdf)

**Return type**

hdf5/xdmf file pair

**Example**

```
pynibs.create_stimsite_hdf5('/exp/1/experiment_corrected.csv',  
    '/stimsite', True, True)
```

**pynibs.coil.get\_coil\_dipole\_pos(coil\_fn, matsimnibs)**

Apply transformation to coil dipoles and return position.

**Parameters**

- **coil\_fn** (*str*) – Filename of coil .ccd file
- **matsimnibs** (*np.ndarray of float*) – Transformation matrix

**Returns**

- **dipoles\_pos** (*np.ndarray*)
- *(N, 3) Cartesian coordinates (x, y, z) of coil magnetic dipoles*

**pynibs.coil.get\_invalid\_coil\_parameters(param\_dict, coil\_position\_mean, svd\_v, del\_obj, fn\_coil, fn\_hdf5\_coilpos=None)**

Finds gpc parameter combinations, which place coil dipoles inside subjects head. Only endpoints (and midpoints) of the parameter ranges are examined.

`get_invalid_coil_parameters(param_dict, pos_mean, v, del_obj, fn_coil, fn_hdf5_coilpos=None)`

**Parameters**

- **param\_dict** (*dict*) – Dictionary containing dictionary with ‘limits’ and ‘pdfshape’ keys: ‘x’, ‘y’, ‘z’, ‘psi’, ‘theta’, ‘phi’
- **coil\_position\_mean** (*np.ndarray [3 x 4]*) – Mean coil positions and orientations
- **svd\_v** (*np.ndarray [3 x 3]*) – SVD matrix V
- **del\_obj** (*Delaunay object*) – Skin surface (created with `scipy.spatial.Delaunay`)
- **fn\_coil** (*str*) – Filename of coil .ccd file
- **fn\_hdf5\_coilpos** (*str*) – Filename of .hdf5 file to save coil\_pos in (incl. path and .hdf5 extension)

**Returns**

**fail\_params** – Index and combination of failed parameter

**Return type**

list of int

---

```
pynibs.coil.sort_opt_coil_positions(fn_coil_pos_opt, fn_coil_pos, fn_out_hdf5=None,
                                     root_path='/0/0/', verbose=False, print_output=False)
```

Sorts coil positions according to Traveling Salesman problem

#### Parameters

- **fn\_coil\_pos\_opt** (*str*) – Name of .hdf5 file containing the optimal coil position indices
- **fn\_coil\_pos** (*str*) – Name of .hdf5 file containing the matsimnibs matrices of all coil positions
- **fn\_out\_hdf5** (*str*) – Name of output .hdf5 file (will be saved in the same format as fn\_coil\_pos\_opt)
- **verbose** (*bool, optional, default: False*) – Print output messages
- **print\_output** (*bool or str, optional, default: False*) – Print output image as .png file showing optimal path

#### Return type

<file> .hdf5 file containing the sorted optimal coil position indices

```
pynibs.coil.test_coil_position_gpc(parameters)
```

Testing valid coil positions for gPC analysis

```
pynibs.coil.write_coil_pos_hdf5(fn_hdf, centers, m0, m1, m2, datanames=None, data=None,
                                  overwrite=False)
```

Creates a .hdf5 + .xdmf file for all coil positions.

Centers and coil orientations are written to disk.

#### Parameters

- **fn\_hdf** (*str*) – Filename for the .hdf5 file. The .xdmf is saved with the same basename. Folder should already exist.
- **centers** (*np.ndarray of float [n\_pos x 3]*) – Coil positions
- **m0** (*np.ndarray of float [n\_pos x 3]*) – Coil orientation x-axis (looking at the active (patient) side of the coil pointing to the right)
- **m1** (*np.ndarray of float [n\_pos x 3]*) – Coil orientation y-axis (looking at the active (patient) side of the coil pointing up away from the handle)
- **m2** (*np.ndarray of float [n\_pos x 3]*) – Coil orientation z-axis (looking at the active (patient) side of the coil pointing to the patient)
- **datanames** (*str or list of str [n\_data]*) – Dataset names for \_data\_. Default: None.
- **data** (*np.ndarray [n\_pos, n\_data]*) – Dataset array with (len(poslist.pos), len(datanames())). Default: None.
- **overwrite** (*boolean*) – Overwrite existing files. Default: False.

## 1.1.4 pynibs.freesurfer module

This holds methods to interact with FreeSurfer ([1]), for example to translate FreeSurfer files into Paraview readable .vtk files.

### References

```
pynibs.freesurfer.data_sub2avg(fn_subject_obj, fn_average_obj, hemisphere, fn_in_hdf5_data,
                                data_hdf5_path, data_label, fn_out_hdf5_geo, fn_out_hdf5_data,
                                mesh_idx=0, roi_idx=0, subject_data_in_center=True,
                                data_substitute=-1, verbose=True, replace=True, reg_fn='sphere.reg')
```

Maps the data from the subject space to the average template. If the data is given only in an ROI, the data is mapped to the whole brain surface.

#### Parameters

- **fn\_subject\_obj** (*str*) – Filename of subject object .hdf5 file (incl. path), e.g. .../probands/subjectID/subjectID.hdf5
- **fn\_average\_obj** (*str*) – Filename of average template object .pkl file (incl. path), e.g. .../probands/avg\_template/avg\_template.hdf5.
- **hemisphere** (*str*) – Define hemisphere to work on ('lh' or 'rh' for left or right hemisphere, respectively).
- **fn\_in\_hdf5\_data** (*str*) – Filename of .hdf5 data input file containing the subject data.
- **data\_hdf5\_path** (*str*) – Path in .hdf5 data file where data is stored (e.g. '/data/tris/').
- **data\_label** (*str* or *list of str*) – Label of datasets contained in hdf5 input file to map.
- **fn\_out\_hdf5\_geo** (*str*) – Filename of .hdf5 geo output file containing the geometry information.
- **fn\_out\_hdf5\_data** (*str*) – Filename of .hdf5 data output file containing the mapped data.
- **mesh\_idx** (*int*) – Index of mesh used in the simulations.
- **roi\_idx** (*int*) – Index of region of interest used in the simulations.
- **subject\_data\_in\_center** (*bool*, *default*: True) – Specify if the data is given in the center of the triangles or in the nodes.
- **data\_substitute** (*float*) – Data substitute with this number for all points outside the ROI mask
- **verbose** (*bool*) – Verbose output (Default: True)
- **replace** (*bool*) – Replace output files (Default: True)
- **reg\_fn** (*str*) – Sphere.reg fn

#### Returns

<Files> – Geometry and corresponding data files to plot with Paraview:

- fn\_out\_hdf5\_geo.hdf5: geometry file containing the geometry information of the average template
- fn\_out\_hdf5\_data.hdf5: geometry file containing the data

#### Return type

.hdf5 files

---

```
pynibs.freesurfer.freesurfer2vtk(in_fns, out_folder, hem='lh', surf='pial', prefix=None,  
                                fs_subject='fsaverage', fs_subjects_dir=None)
```

Transform multiple FreeSurfer .mgh files into one .vtk file. This can be read with Paraview and others.

#### Parameters

- ***in\_fns*** (*list of str or str*) – Input filenames.
- ***out\_folder*** (*str*) – Output folder.
- ***hem*** (*str, default: 'lh'*) – Which hemisphere: 'lh' or 'rh'.
- ***surf*** (*str, default: 'pial'*) – Which FreeSurfer surface: 'pial', 'inflated', ...
- ***prefix*** (*str, optional*) – Prefix to add to each filename.
- ***fs\_subject*** (*str, default: 'fsaverage'*) – FreeSurfer subject.
- ***fs\_subjects\_dir*** (*str, optional*) – FreeSurfer subjects directory. If not provided, read from environment.

#### Returns

**<File>** – One .vtk file with data as overlays from all .mgh files provided

#### Return type

*out\_folder*/*{prefix}\_{{hem}}\_{{surf}}*.vtk

```
pynibs.freesurfer.make_average_subject(subjects, subject_dir, average_dir, fn_reg='sphere.reg')
```

Generates the average template from a list of subjects using the FreeSurfer average.

#### Parameters

- ***subjects*** (*list of str*) – Paths of subjects directories, where the FreeSurfer files are located, e.g. for simnibs mri2mesh .../fs SUBJECT\_ID.
- ***subject\_dir*** (*str*) – Temporary subject directory of FreeSurfer (symlinks of subjects will be generated in there and average template will be temporarily stored before it is copied to *average\_dir*).
- ***average\_dir*** (*str*) – path to directory where average template will be stored, e.g. probands/avg\_template\_15/mesh/0/fs\_avg\_template\_15.
- ***fn\_reg*** (*str, default: 'sphere.reg' --> ?h.sphere.reg*) – Filename suffix of FreeSurfer registration file containing registration information to template.

#### Returns

**<Files>** – Average template in *average\_dir* and registered curvature files, ?h.sphere.reg in *subjects*/surf folders.

#### Return type

.tif and .reg files

```
pynibs.freesurfer.make_group_average(subjects=None, subject_dir=None, average=None, hemi='lh',  
                                    template='mytemplate', steps=3, n_cpu=2, average_dir=None)
```

Creates a group average from scratch, based on one subject. This prevents for example the fsaverage problems of large elements at M1, etc. This is an implementation of [2] ‘Creating a registration template from scratch (GW)’.

## References

### Parameters

- **subjects** (*list of str*) – List of FreeSurfer subjects names.
- **subject\_dir** (*str*) – Temporary subject directory of FreeSurfer (symlinks of subjects will be generated in there and average template will be temporarily stored before it is copied to `average_dir`).
- **average** (*str*, default: `subjects[0]`) – Which subject to base new average template on.
- **hemi** (*str*, default: 'lh') – Which hemisphere: lh or rh.  
Deprecated since version 0.0.1: Don't use any more.
- **template** (*str*, default: 'mytemplate') – Basename of new template.
- **steps** (*int*, default: 2) – Number of iterations.
- **n\_cpu** (*int*, default: 4) – How many cores for multithreading.
- **average\_dir** (*str*) – Path to directory where average template will be stored, e.g. `probands/avg_template_15/mesh/0/fs_avg_template_15`.

### Returns

- <File> (.tif file) – SUBJECT\_DIR/TEMPLATE\*.tif, TEMPLATE0.tif based on AVERAGE, rest on all subjects.
- <File> (.myreg file) – SUBJECT\_DIR/SUBJECT\*/surf/HEMI.sphere.myreg\*.
- <File> (.tif file) – Subject wise sphere registration based on TEMPLATE\*.tif.

`pynibs.freesurfer.read_curv_data(fname_curv, fname_inf, raw=False)`

Read curvature data provided by FreeSurfer with optional normalization.

### Parameters

- **fname\_curv** (*str*) – Filename of the FreeSurfer curvature file (e.g. ?h.curv), contains curvature data in nodes can be found in mri2mesh proband folder: proband\_ID/fs\_ID/surf/?h.curv.
- **fname\_inf** (*str*) – Filename of inflated brain surface (e.g. ?h.inflated), contains points and connectivity data of surface can be found in mri2mesh proband folder: proband\_ID/fs\_ID/surf/?h.inflated.
- **raw** (*bool*) – If raw-data is returned or if the data is normalized to -1 for neg. and +1 for pos. curvature.

### Returns

**curv** – Curvature data in element centers.

### Return type

np.ndarray of float or int

## 1.1.5 pynibs.hdf5\_io module

`pynibs.hdf5_io.create_fibre_hdf5(fn_fibres_hdf5, overwrite=True)`

Reformats geometrical fibre data and adds a /plot subfolder containing geometrical fibre data including connectivity

### Parameters

- `fn_fibres_hdf5 (str)` – Path to fibre.hdf5 file containing the original fibre data
- `overwrite (bool)` – Overwrites existing /plot subfolder in .hdf5 file

`pynibs.hdf5_io.create_fibre_xdmf(fn_fibre_geo_hdf5, fn_fibre_data_hdf5=None, overwrite=True, fibre_points_path='fibre_points', fibre_con_path='fibre_con', fibre_data_path='')`

Creates .xdmf file to plot fibres in Paraview

### Parameters

- `fn_fibre_geo_hdf5 (str)` – Path to fibre\_geo.hdf5 file containing the geometry (in /plot subfolder created with create\_fibre\_geo\_hdf5())
- `fn_fibre_data_hdf5 (str (optional) default: None)` – Path to fibre\_data.hdf5 file containing the data to plot (in parent folder)
- `fibre_points_path (str (optional) default: fibre_points)` – Path to fibre point array in .hdf5 file
- `fibre_con_path (str (optional) default: fibre_con)` – Path to fibre connectivity array in .hdf5 file
- `fibre_data_path (str (optional) default: "")` – Path to parent data folder in data.hdf5 file (Default: no parent folder)

### Returns

`<File>`

### Return type

.xdmf file for Paraview

`pynibs.hdf5_io.create_position_path_xdmf(sorted_fn, coil_pos_fn, output_xdmf, stim_intens=None, coil_sorted='/0/0/coil_seq')`

Creates one .xdmf file that allows paraview plottings of coil position paths.

### Parameters

- `sorted_fn (str)` – .hdf5 filename with position indices, values, intensities from pynibs.sort\_opt\_coil\_positions()
- `coil_pos_fn (str)` – .hdf5 filename with original set of coil positions. Indices from sorted\_fn are mapped to this. Either '/matsimnibs' or 'm1' and 'm2' datasets.
- `output_xdmf (str)` –
- `stim_intens (int, optional)` – Intensities are multiplied by this factor
- `coil_sorted (str)` – Path to coil positions in sorted\_fn

### Returns

`output_xdmf`

### Return type

`<file>`

`pynibs.hdf5_io.data_superimpose(fn_in_hdf5_data, fn_in_geo_hdf5, fn_out_hdf5_data, data_hdf5_path='/data/tris/', data_substitute=-1, normalize=False)`

Overlaying data stored in .hdf5 files except in regions where data\_substitute is found. These points are omitted in the analysis and will be replaced by data\_substitute instead.

### Parameters

- **fn\_in\_hdf5\_data** (*list of str*) – Filenames of .hdf5 data files with common geometry (e.g. generated by pynibs.data\_sub2avg(...))
- **fn\_in\_geo\_hdf5** (*str*) – Geometry .hdf5 file, which corresponds to the .hdf5 data files
- **fn\_out\_hdf5\_data** (*str*) – Filename of .hdf5 data output file containing the superimposed data
- **data\_hdf5\_path** (*str*) – Path in .hdf5 data file where data is stored (e.g. '/data/tris/')
- **data\_substitute** (*float or NaN*) – Data substitute with this number for all points in the inflated brain, which do not belong to the given data set (Default: -1)
- **normalize** (*boolean or str*) – Decide if individual datasets are normalized w.r.t. their maximum values before they are superimposed (Default: False)
  - 'global': global normalization w.r.t. maximum value over all datasets and subjects
  - 'dataset': dataset wise normalization w.r.t. maximum of each dataset individually (over subjects)
  - 'subject': subject wise normalization (over datasets)

### Returns

**<File>** – Overlayed data

### Return type

.hdf5 file

`pynibs.hdf5_io.hdf_2_ascii(hdf5_fn)`

Prints out structure of given .hdf5 file.

### Parameters

**hdf5\_fn** (*str*) – Filename of .hdf5 file.

### Returns

**h5** – Structure of .hdf5 file

### Return type

items

`pynibs.hdf5_io.load_mesh_hdf5(fname)`

Loading mesh from .hdf5 file and setting up *TetrahedraLinear* class.

### Parameters

**fname** (*str*) – Name of .hdf5 file (incl. path)

### Returns

**obj** – *TetrahedraLinear* object

### Return type

`pynibs.mesh.mesh_struct.TetrahedraLinear`

## Example

.hdf5 file format and contained groups. The content of .hdf5 files can be shown using the tool HDFView (<https://support.hdfgroup.org/products/java/hdfview/>)

```

mesh
I---/elm
I   I--/elm_number      [1,2,3,...,N_ele]           Running index over all elements starting at 1,
                                                triangles and tetrahedra
I   I--/elm_type        [2,2,2,...,4,4]           Element type: 2 triangles, 4 tetrahedra
I   I--/node_number_list [1,5,6,0;... ;1,4,8,9]       Connectivity of triangles [X, X, X, 0] and tetrahedra
                                                [X, X, X, X]
I   I--/tag1            [1001,1001, ..., 4,4,4]     Surface (100X) and domain (X) indices with 1000 offset
                                                for surfaces
I   I--/tag2            [ 1, 1, ..., 4,4,4]       Surface (X) and domain (X) indices w/o offset
I
I---/nodes

```

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```

I   I--/node_coord      [1.254, 1.762, 1.875;...] Node coordinates in (mm)
I   I--/node_number     [1,2,3,...,N_nodes] Running index over all points starting at 1
I   I--/units            ["mm"] .value is unit of geometry
I
I---/fields
I   I--/E/value          [E_x_1, E_y_1, E_z_1;...] Electric field in all elms, triangles and tetrahedra
I   I--/J/value           [J_x_1, J_y_1, J_z_1;...] Current density in all elms, triangles and tetrahedra
I   I--/normE/value      [normE_1,..., normE_N_ele] Magnitude of electric field in all elements,
I                                         triangles and tetrahedra
I   I--/normJ/value      [normJ_1,..., normJ_N_ele] Magnitude of current density in all elements,
I                                         triangles and tetrahedra

/data
I---/potential          [phi_1, ..., phi_N_nodes] Scalar electric potential in nodes (size N_nodes)
I---/dA/dt               [A_x_1, A_y_1, A_z_1,...] Magnetic vector potential (size 3xN_nodes)

```

**pynibs.hdf5\_io.load\_mesh\_msh(fname)**Loading mesh from .msh file and return *TetrahedraLinear* object.**Parameters****fname** (*str*) – .msh filename (incl. path)**Returns****obj****Return type***pynibs.mesh.mesh\_struct.TetrahedraLinear***pynibs.hdf5\_io.msh2hdf5(fn\_msh=None, skip\_roi=False, include\_data=False, approach='mri2mesh', subject=None, mesh\_idx=None)**

Transforms mesh from .msh to .hdf5 format. Mesh is read from subject object or from fn\_msh.

**Parameters**

- **fn\_msh** (*str*, optional, default: *None*) – Filename of .msh file
- **skip\_roi** (*bool*, optional, default: *False*) – Skip generating ROI in .hdf5
- **include\_data** (*bool*, optional, default: *False*) – Also convert data in .msh file to .hdf5 file
- **subject** (*Subject object*, optional, default: *None*) – Subject object
- **mesh\_idx** (*int* or *list of int*, optional, default: *None*) – Mesh index, the conversion from .msh to .hdf5 is conducted for
- **approach** (*str*) – Approach the headmodel was created with (“mri2mesh” or “head-reco”)

Deprecated since version 0.0.1: Not supported any more.

**Returns**

&lt;File&gt; – .hdf5 file with mesh information

**Return type**

.hdf5 file

**pynibs.hdf5\_io.print\_attrs(name, obj)**Helper function for *hdf2ascii()*. To be called from *h5py.Group.visititems()***Parameters**

- **name** (*str*) – Name of structural element
- **obj** (*object*) – Structural element

**Returns**

&lt;Print&gt;

**Return type**

Structure of .hdf5 file

`pynibs.hdf5_io.read_arr_from_hdf5(fn_hdf5, folder)`

Reads array from and .hdf5 files and returns as list: Strings are returned as `np.bytes_ to str` and ‘None’ to None

**Parameters**

- `fn_hdf5 (str)` – Filename of .hdf5 file
- `folder (str)` – Folder inside .hdf5 file to read

**Returns**

`data_from_hdf5` – List containing data from .hdf5 file

**Return type**

`list`

`pynibs.hdf5_io.read_data_hdf5(fname)`

Reads phi and dA/dt data from .hdf5 file (phi and dAdt are given in the nodes).

**Parameters**

`fname (str)` – Filename of .hdf5 data file

**Returns**

- `phi (np.ndarray of float [N_nodes])` – Electric potential in the nodes of the mesh
- `da_dt (np.ndarray of float [N_nodesx3])` – Magnetic vector potential in the nodes of the mesh

`pynibs.hdf5_io.read_dict_from_hdf5(fn_hdf5, folder)`

Read all arrays from from hdf5 file and return them as dict

**Parameters**

- `fn_hdf5 (str)` – Filename of .hdf5 file
- `folder (str)` – Folder inside .hdf5 file to read

**Returns**

`d` – Dictionary from .hdf5 file folder

**Return type**

`dict`

`pynibs.hdf5_io.simnibs_results_msh2hdf5(fn_msh, fn_hdf5, S, pos_tms_idx, pos_local_idx, subject, mesh_idx, mode_xdmf='r+', n_cpu=4, verbose=False, overwrite=False, mid2roi=False)`

Converts simnibs .msh results file(s) to .hdf5 / .xdmf tuple.

**Parameters**

- `fn_msh(str list of str)` – Filenames (incl. path) of .msh results files from simnibs
- `fn_hdf5 (str or list of str)` – Filenames (incl. path) of .hdf5 results files
- `S (Simnibs Session object)` – Simnibs Session object the simulations are conducted with
- `pos_tms_idx (list of int)` – Index of the simulation w.r.t. to the simnibs TMSList (inside Session object S) For every coil a separate TMSList exists, which contains multiple coil positions.
- `pos_local_idx (list of int)` – Index of the simulation w.r.t. to the simnibs POSlist in the TMSList (inside Session object S) For every coil a separate TMSList exists, which contains multiple coil positions.
- `subject (Subject object)` – Subject object loaded from .pkl file
- `mesh_idx (int)` – Mesh index

- **mode\_xdmf** (*str*, *optional*, *default*: "r+") – Mode to open hdf5\_geo file to write xdmf. If hdf5\_geo is already separated in tets and tris etc., the file is not changed, use "r" to avoid IOErrors in case of parallel computing.
- **n\_cpu** (*int*) – Number of processes
- **verbose** (*bool*, *optional*, *default*: *False*) – Print output messages
- **overwrite** (*bool*, *optional*, *default*: *False*) – Overwrite .hdf5 file if existing
- **mid2roi** (*bool or string*, *optional*, *default*: *False*) – If the mesh contains ROIs and the e-field was calculated in the midlayer using simnibs (S.map\_to\_surf = True), the midlayer results will be mapped from the simnibs midlayer to the ROIs (takes some time for large ROIs)

**Returns**

**<File>** – .hdf5 file containing the results. An .xdmf file is also created to link the results with the mesh .hdf5 file of the subject

**Return type**

.hdf5 file

```
pynibs.hdf5_io.simnibs_results_msh2hdf5_workhorse(fn_msh, fn_hdf5, S, pos_tms_idx,  

pos_local_idx, subject, mesh_idx,  

mode_xdmf='r+', verbose=False,  

overwrite=False, mid2roi=False)
```

Converts simnibs .msh results file to .hdf5 (including midlayer data if desired)

**Parameters**

- **fn\_msh** (*list of str*) – Filenames (incl. path) of .msh results files from simnibs
- **fn\_hdf5** (*str or list of str*) – Filenames (incl. path) of .hdf5 results files
- **S** (*Simnibs Session object*) – Simnibs Session object the simulations are conducted with
- **pos\_tms\_idx** (*list of int*) – Index of the simulation w.r.t. to the simnibs TMSList (inside Session object S) For every coil a separate TMSList exists, which contains multiple coil positions.
- **pos\_local\_idx** (*list of int*) – Index of the simulation w.r.t. to the simnibs POSlist in the TMSList (inside Session object S) For every coil a separate TMSList exists, which contains multiple coil positions.
- **subject** (*Subject object*) – Subject object loaded from .pkl file
- **mesh\_idx** (*int*) – Mesh index
- **mode\_xdmf** (*str, optional, default: "r+"*) – Mode to open hdf5\_geo file to write xdmf. If hdf5\_geo is already separated in tets and tris etc., the file is not changed, use "r" to avoid IOErrors in case of parallel computing.
- **verbose** (*bool, optional, default: False*) – Print output messages
- **overwrite** (*bool, optional, default: False*) – Overwrite .hdf5 file if existing
- **mid2roi** (*bool, list of string, or string, optional, default:False*) – If the mesh contains ROIs and the e-field was calculated in the midlayer using simnibs (S.map\_to\_surf = True), the midlayer results will be mapped from the simnibs midlayer to the ROIs (takes some time for large ROIs)

**Returns**

**<File>** – .hdf5 file containing the results. An .xdmf file is also created to link the results with the mesh .hdf5 file of the subject

**Return type**

.hdf5 file

`pynibs.hdf5_io.split_hdf5(hdf5_in_fn, hdf5_geo_out_fn='', hdf5_data_out_fn=None)`

Splits one hdf5 into one with spatial data and one with statistical data. If coil data is present in `hdf5_in`, it is saved in `hdf5Data_out`. If new spatial data is added to file (curve, inflated, whatever), add this to the `geogroups` variable.

#### Parameters

- `hdf5_in_fn (str)` – Filename of .hdf5 input file
- `hdf5_geo_out_fn (str)` – Filename of .hdf5 .geo output file
- `hdf5_data_out_fn (str)` – Filename of .hdf5 .data output file (if none, remove data from `hdf5_in`)

#### Returns

- `<File> (.hdf5 file)` – `hdf5Geo_out_fn` (spatial data)
- `<File> (.hdf5 file)` – `hdf5Data_out_fn` (data)

`pynibs.hdf5_io.write_arr_to_hdf5(fn_hdf5, arr_name, data, overwrite_arr=True, verbose=False, check_file_exist=False)`

Takes an array and adds it to an hdf5 file

If data is list of dict, `write_dict_to_hdf5()` is called for each dict with adapted hdf5-folder name Otherwise, data is casted to np.ndarray and dtype of unicode data casted to '|S'.

#### Parameters

- `fn_hdf5 (str)` – Filename of .hdf5 file
- `arr_name (str)` – Complete path in .hdf5 file with array name
- `data (ndarray, list or dict)` – Data to write
- `overwrite_arr (bool, optional, default: True)` – Overwrite existing array
- `verbose (bool, optional, default: False)` – Print information

`pynibs.hdf5_io.write_data_hdf5(out_fn, data, data_names, hdf5_path='/data', mode='a')`

Creates a .hdf5 file with data.

#### Parameters

- `out_fn (str)` – Filename of output .hdf5 file containing the geometry information
- `data (np.ndarray or list of nparrays of float)` – Data to save in hdf5 data file
- `data_names (str or list of str)` – Labels of data
- `hdf5_path (str)` – Folder in .hdf5 geometry file, where the data is saved in (Default: /data)
- `mode (str, optional, default: "a")` – Mode: "a" append, "w" write (overwrite)

#### Returns

`<File>` – File containing the stored data

#### Return type

.hdf5 file

## Example

File structure of .hdf5 data file

```
data
|---/data_names[0]      [data[0]]      First dataset
|---/ ...
|---/data_names[N-1]    [data[N-1]]    Last dataset
```

`pynibs.hdf5_io.write_data_hdf5_surf(data, data_names, data_hdf_fn_out, geo_hdf_fn, replace=False, replace_array_in_file=True)`

Saves surface data to .hdf5 data file and generates corresponding .xdmf file linking both. The directory of data\_hdf\_fn\_out and geo\_hdf\_fn should be the same, as only basenames of files are stored in the .xdmf file.

### Parameters

- **data** (`np.ndarray or list [N_points_ROI x N_components]`) – Data to map on surfaces
- **data\_names** (`str or list`) – Names for datasets
- **data\_hdf\_fn\_out** (`str`) – Filename of .hdf5 data file
- **geo\_hdf\_fn** (`str`) – Filename of .hdf5 geo file containing the geometry information (has to exist)
- **replace** (`boolean, optional, default: False`) – Replace existing .hdf5 and .xdmf file completely
- **replace\_array\_in\_file** (`boolean, optional, default: True`) – Replace existing array in file

### Returns

- `<File> (.hdf5 file)` – data\_hdf\_fn\_out.hdf5 containing data
- `<File> (.xdmf file)` – data\_hdf\_fn\_out.xdmf containing information about .hdf5 file structure for Paraview

## Example

File structure of .hdf5 data file

```
/data
|---/tris
|   |---dataset_0  [dataset_0]  (size: N_dataset_0 x M_dataset_0)
|   |---...
|   |---dataset_K  [dataset_K]  (size: N_dataset_K x M_dataset_K)
```

`pynibs.hdf5_io.write_dict_to_hdf5(fn_hdf5, data, folder, check_file_exist=False, verbose=False)`

Takes dict (from subject.py) and passes its keys to write\_arr\_to\_hdf5()

```
fn_hdf5:folder/
    |--key1
    |--key2
    |...
```

### Parameters

- **fn\_hdf5** (`str`) –
- **data** (`dict or pynibs.Mesh`) –
- **folder** (`str`) –
- **verbose** (`bool`) –
- **check\_file\_exist** (`bool`) –

`pynibs.hdf5_io.write_geo_hdf5(out_fn, msh, roi_dict=None, hdf5_path='/mesh')`

Creates a .hdf5 file with geometry data from mesh including region of interest(s).

#### Parameters

- **out\_fn** (`str`) – Output hdf5 filename for mesh' geometry information.
- **msh** (`pynibs.mesh.mesh_struct.TetrahedraLinear`) – Mesh to write to file.
- **roi\_dict** (dict of (`RegionOfInterestSurface` or `RegionOfInterestVolume`)) – Region of interest (surface and/or volume) information.
- **hdf5\_path** (`str`, `default: '/mesh'`) – Path in output file to store geometry information.

#### Returns

`<File>` – File containing the geometry information

#### Return type

.hdf5 file

### Example

File structure of .hdf5 geometry file

```

mesh
I---/elm
I   I--/elm_number          [1,2,3,...,N_ele]      Running index over all elements starting at 1
                                                (triangles and tetrahedra)
I   I--/elm_type            [2,2,2,...,4,4]      Element type: 2 triangles, 4 tetrahedra
I   I--/tag1                [1001,1001, ..., 4,4,4] Surface (100X) and domain (X) indices with 1000
                                                offset for surfaces
I   I--/tag2                [ 1, 1, ..., 4,4,4] Surface (X) and domain (X) indices w/o offset
I   I--/triangle_number_list [1,5,6,... ;1,4,8]   Connectivity of triangles [X, X, X]
I   I--/tri_tissue_type     [1,1, ..., 3,3,3]   Surface indices to differentiate between surfaces
I   I--/tetrahedra_number_list [1,5,6,7;... ;1,4,8,12] Connectivity of tetrahedra [X, X, X, X]
I   I--/tet_tissue_type     [1,1, ..., 3,3,3]   Volume indices to differentiate between volumes
I   I--/node_number_list    [1,5,6,0;... ;1,4,8,9] Connectivity of triangles [X, X, X, 0] and
                                                tetrahedra [X, X, X, X]
I
I---/nodes
I   I--/node_coord          [1.254, 1.762, 1.875;...] Node coordinates in (mm)
I   I--/node_number          [1,2,3,...,N_nodes]   Running index over all points starting at 1
I   I--/units                ['mm']                 .value is unit of geometry

roi_surface
I---/0
I   I--/node_coord_up       [1.254, 1.762, 1.875;...] Region of Interest number
I   I--/node_coord_mid      [1.254, 1.762, 1.875;...] Coordinates of upper surface points
I   I--/node_coord_low       [1.254, 1.762, 1.875;...] Coordinates of middle surface points
I   I--/node_coord_low       [1.254, 1.762, 1.875;...] Coordinates of lower surface points
I   I--/tri_center_coord_up [1.254, 1.762, 1.875;...] Coordinates of upper triangle centers
I   I--/tri_center_coord_mid [1.254, 1.762, 1.875;...] Coordinates of middle triangle centers
I   I--/tri_center_coord_low [1.254, 1.762, 1.875;...] Coordinates of lower triangle centers
I   I--/node_number_list     [1,5,6,0;... ;1,4,8,9] Connectivity of triangles [X, X, X]
I   I--/delta                0.5                   Distance parameter between GM and WM surface
I   I--/tet_idx_tri_center_up [183, 913, 56, ...] Tetrahedra indices where triangle center of
                                                upper surface are lying in
I   I--/tet_idx_tri_center_mid [185, 911, 58, ...] Tetrahedra indices where triangle center of
                                                middle surface are lying in
I   I--/tet_idx_tri_center_low [191, 912, 59, ...] Tetrahedra indices where triangle center of
                                                lower surface are lying in
I   I--/tet_idx_node_coord_mid [12, 15, 43, ...] Tetrahedra indices where the node_coords_mid
                                                are lying in
I   I--/gm_surf_fname        .../surf/lh.pial   Filename of GM surface from segmentation
I   I--/wm_surf_fname        .../surf/lh.white  Filename of WM surface from segmentation
I   I--/layer                 3                     Number of layers
I   I--/fn_mask               .../simnibs/mask.mgh  Filename of region of interest mask
I   I--/X_ROI                 [-10, 15]        X limits of region of interest box
I   I--/Y_ROI                 [-10, 15]        Y limits of region of interest box
I   I--/Z_ROI                 [-10, 15]        Z limits of region of interest box
I
I---/1
I   I ...

roi_volume
I---/0
I   I--/node_coord          [1.254, 1.762, 1.875;...] Region of Interest number
I   I--/tet_node_number_list [1,5,6,7;... ;1,4,8,9] Coordinates (x,y,z) of ROI nodes
I   I--/tri_node_number_list [1,5,6;... ;1,4,8]   Connectivity matrix of ROI tetrahedra
I   I--/tet_idx_node_coord  [183, 913, 56, ...] Connectivity matrix of ROI triangles
I   I--/tet_idx_tetrahedra_center [12, 15, 43, ...] Tetrahedra indices where ROI nodes are
                                                Tetrahedra indices where center points of
                                                ROI tetrahedra are
I   I--/tet_idx_triangle_center [12, 15, 43, ...] Tetrahedra indices where center points of
                                                ROI triangles are

I---/1
I   I ...

```

`pynibs.hdf5_io.write_geo_hdf5_surf(out_fn, points, con, replace=False, hdf5_path='/mesh')`

Creates a .hdf5 file with geometry data from midlayer.

#### Parameters

- **out\_fn** (`str`) – Filename of output .hdf5 file containing the geometry information
  - **points** (`np.ndarray [N_points x 3]`) – Coordinates of nodes (x,y,z)
  - **con** (`np.ndarray [N_tri x 3]`) – Connectivity list of triangles
  - **replace** (`boolean`) – Replace .hdf5 geometry file (True / False)
  - **hdf5\_path** (`str`) – Folder in .hdf5 geometry file, where the geometry information is saved in (Default: /mesh)

## Returns

**<File>** – File containing the geometry information.

## Return type

.hdf5 file

## Example

## File structure of .hdf5 geometry file:

```

mesh
|---/elm
|   |--triangle_number_list [1,5,6;... ;1,4,8] Connectivity of triangles [X, X, X]
|   |--tri_tissue_type [1,1, ..., 3,3,3] Surface indices to differentiate between surfaces
|
|---/nodes
|   |--node_coord [1.2, 1.7, 1.8; ...] Node coordinates in (mm)

```

```
pynibs.hdf5_io.write_temporal_xdmf(hdf5_fn, data_folder='c', coil_center_folder=None,  
                                   coil_ori_0_folder=None, coil_ori_1_folder=None,  
                                   coil_ori_2_folder=None, coil_current_folder=None,  
                                   hdf5_geo_fn=None, overwrite_xdmf=False, verbose=False)
```

Creates .xdmf markup file for given ROI hdf5 data file with 4D data. This was written to be able to visualize data from the permutation analysis of the regression approach It expects an .hdf5 with a data group with (many) subarrays. The N subarrays name should be named from 0 to N-1 Each subarray has shape (N\_elemons, 1)

Not tested for whole brain.

```
hdf5:/data_folder/0  
    /1  
    /2  
    /3  
    /4  
    ...
```

## Parameters

- **hdf5\_fn** (*str*) – Filename of hdf5 file containing the data
  - **data\_folder** (*str*) – Path within hdf5 to group of dataframes
  - **hdf5\_geo\_fn** (*str optional*) – Filename of hdf5 file containing the geometry
  - **overwrite\_xdmf** (*boolean*) – Overwrite existing .xdmf file if present
  - **coil\_center\_folder** (*str*) –
  - **coil\_ori\_0\_folder** (*str*) –
  - **coil\_ori\_1\_folder** (*str*) –
  - **coil\_ori\_2\_folder** (*str*) –
  - **coil\_current\_folder** (*str*) –
  - **verbose** (*boolean*) – Print output or not

## Returns

<File> – hdf5\_fn[-4].xdmf

**Return type**

.xdmf file

```
pynibs.hdf5_io.write_xdmf(hdf5_fn, hdf5_geo_fn=None, overwrite_xdmf=False, overwrite_array=False,  
                           verbose=False, mode='r+')
```

Creates .xdmf markup file for given hdf5 file, mainly for paraview visualization. Checks if triangles and tetrahedra already exists as distinct arrays in hdf5\_fn. If not, these are added to the .hdf5 file and rebased to 0 (from 1). If only hdf5\_fn is provided, spatial information has to be present as arrays for tris and tets in this dataset.

**Parameters**

- **hdf5\_fn** (*str*) – Filename of hdf5 file containing the data
- **hdf5\_geo\_fn** (*str*) – Filename of hdf5 file containing the geometry. Optional.
- **overwrite\_xdmf** (*bool*) – Overwrite existing xdmf file if present. Default: False.
- **overwrite\_array** (*bool*) – Overwrite existing arrays if present. Default: False.
- **verbose** (*boolean*) – Print output or not
- **mode** (*str, optional, default: "r+"*) – Mode to open hdf5\_geo file. If hdf5\_geo is already separated in tets and tris etc., nothing has to be written, use “r” to avoid IOErrors in case of parallel computing.

**Returns**

- **fn\_xml** (*str*) – Filename of the created .xml file
- **<File> (.xdmf file)** – hdf5\_fn[-4].xdmf (only data if hdf5Geo\_fn provided)
- **<File> (.hdf5 file)** – hdf5\_fn changed if necessary
- **<File> (.hdf5 file)** – hdf5geo\_fn containing spatial data

## 1.1.6 pynibs.muap module

```
pynibs.muap.calc_mep_wilson(firing_rate_in, t, Qvmax=900, Qmmax=300, q=8, Tmin=14, N=100,  
                             M0=42, lam=0.002, tau0=0.006)
```

Determine motor evoked potential from incoming firing rate

**Parameters**

- **firing\_rate\_in** (*ndarray of float [n\_t]*) – Input firing rate from alpha motor neurons
- **t** (*ndarray of float [n\_t]*) – Time axis in s
- **Qvmax** (*float, optional, default: 900*) – Max of incoming firing rate [1/s]
- **Qmmax** (*float, optional, default: 300*) – Max of MU firing rate [1/s]
- **q** (*float, optional, default: 8*) – Min firing rate of MU [1/s]
- **Tmin** (*float, optional, default: 14*) – Min MU threshold [1/s]
- **N** (*float, optional, default: 100*) – Number of MU
- **M0** (*float, optional, default: 42*) – Scaling constant of MU amplitude [mV/s]
- **lam** (*float, optional, default: 0.002*) – MUAP timescale of first order Hermite Rodriguez function [s]
- **tau0** (*float, optional, default: 0.006*) – Standard shift of MUAP to ensure causality [s]

**Returns**

**mep** – Motor evoked potential at surface electrode

**Return type**

ndarray of `float` [n\_t]

`pynibs.muap.compute_signal(signal_matrix, sensor_matrix)`

Determine average signal from one single muscle fibre on all point electrodes

**Parameters**

- **signal\_matrix** (*ndarray of float [n\_time x n\_fibre]*) – Signal matrix containing the action potential values for each time step in the rows
- **sensor\_matrix** (*ndarray of float [n\_fibre x n\_ele]*) – Sensor matrix containing the inverse distances weighted with the anisotropy of muscle tissue

**Returns**

**signal** – Average signal detected all point electrodes

**Return type**

ndarray of `float` [n\_time]

`pynibs.muap.create_electrode(l_x, l_z, n_x, n_z)`

Creates electrode coordinates

**Parameters**

- **l\_x** (`float`) – X-extension of electrode in mm
- **l\_z** (`float`) – Z-extension of electrode in mm
- **n\_x** (`int`) – Number of point electrode in x-direction
- **n\_z** (`int`) – Number of point electrodes in z-direction

**Returns**

**electrode\_coords** – Coordinates of point electrodes (x, y, z)

**Return type**

ndarray of `float` [n\_ele x 3]

`pynibs.muap.create_muscle_coords(l_x, l_y, n_x, n_y, h)`

Create x and y coordinates of muscle fibres in muscle

**Parameters**

- **l\_x** (`float`) – X-extension of muscle in mm
- **l\_y** (`float`) – Y-extension of muscle in mm
- **n\_x** (`int`) – Number of muscle fibres in x-direction
- **n\_y** (`int`) – Number of muscle fibres in y-direction
- **h** (`float`) – Offset of muscle from electrode plane in mm

**Returns**

**muscle\_coords** – Coordinates of muscle fibres in x-y plane (x, y, z)

**Return type**

ndarray of `float` [n\_muscle x 3]

`pynibs.muap.create_muscle_fibre(x0, y0, L, n_fibre)`

Creates muscle fibre coordinates (in z-direction)

**Parameters**

- **x0** (`float`) – X-location of muscle fibre
- **y0** (`float`) – Y-location of muscle fibre

- **L** (*float*) – Length of muscle fibre
- **n\_fibre** (*float*) – Number of discrete fibre elements

**Returns**

**fibre\_coords** – Coordinates of muscle fibre in z-direction (x, y, z)

**Return type**

ndarray of *float* [n\_fibre x 3]

`pynibs.muap.create_sensor_matrix(electrode_coords, fibre_coords, sigma_r=1, sigma_z=1)`

Create sensor matrix containing the inverse distances from the point electrodes to the fibre elements weighted by the anisotropy factor of the muscle tissue.

**Parameters**

- **electrode\_coords** (ndarray of *float* [n\_ele x 3]) – Coordinates of point electrodes (x, y, z)
- **fibre\_coords** (ndarray of *float* [n\_fibre x 3]) – Coordinates of muscle fibre in z-direction (x, y, z)
- **sigma\_r** (*float*, optional, default: 1) – Radial conductivity of muscle
- **sigma\_z** (*float*, optional, default: 1) – Axial conductivity of muscle along fibre

**Returns**

**sensor\_matrix** – Sensor matrix containing the inverse distances weighted with the anisotropy of muscle tissue

**Return type**

ndarray of *float* [n\_fibre x n\_ele]

`pynibs.muap.create_signal_matrix(T, dt, fibre_coords, z_e, v)`

Create signal matrix containing the travelling action potential on the fibre

**Parameters**

- **T** (*float*) – Total time
- **dt** (*float*) – Time step
- **fibre\_coords** (ndarray of *float* [n\_fibre x 3]) – Coordinates of muscle fibre in z-direction (x, y, z)
- **z\_e** (*float*) – Location of action potential generation
- **v** (*float*) – Velocity of action potential

**Returns**

**signal\_matrix** – Signal matrix containing the action potential values for each time step in the rows

**Return type**

ndarray of *float* [n\_time x n\_fibre]

`pynibs.muap.dipole_potential(z, loc, response)`

Returns dipole potential at given coordinates z (interpolates given dipole potential)

`pynibs.muap.hermite_rodriguez_1st(t, tau0=0, tau=0, lam=0.002)`

First order Hermite Rodriguez function to model surface MUAPs

**Parameters**

- **t** (ndarray of *float* [n\_t]) – Time axis in s
- **tau0** (*float*, optional, default: 0) – initial shift to ensure causality in s
- **tau** (*float*, optional, default: 0) – shift (firing time) in s

- **lam** (*float*, optional, default: 2) – Timescale in s

**Returns**

**y** – Surface MUAP

**Return type**

ndarray of *float* [n\_t]

`pynibs.muap.sfap(z, sigma_i=1.01, d=5.499999999999995e-05, alpha=0.5)`

Single fibre propagating transmembrane current (second spatial derivative of transmembrane potential).

S. D. Nandedkar and E. V. Stalberg, “Simulation of single musclefiber action potentials” Med. Biol. Eng. Comput., vol. 21, pp. 158–165, Mar.1983.

J. Duchene and J.-Y. Hogrel, “A model of EMG generation,” IEEETrans. Biomed. Eng., vol. 47, no. 2, pp. 192–200, Feb. 2000

Hamilton-Wright, A., & Stashuk, D. W. (2005). Physiologically based simulation of clinical EMG signals. IEEE Transactions on biomedical engineering, 52(2), 171-183.

**Parameters**

- **t** (*ndarray of float* [n\_t]) – Time in (ms)
- **sigma\_i** (*float*, optional, default: 1.01) – Intracellular conductivity in (S/m)
- **d** (*float*, optional, default: 55\*1e-6) – Diameter of muscle fibre in (m)
- **v** (*float*, optional, default: 1) – Conduction velocity in (m/s)
- **alpha** (*float*, optional, default: 0.5) – Scaling factor to adjust length of AP

**Returns**

**i** – Transmembrane current of muscle fibre

**Return type**

ndarray of *float* [n\_t]

`pynibs.muap.sfap_dip(z)`

`pynibs.muap.weight_signal_matrix(signal_matrix, fn_imp, t, z)`

Weight signal matrix with impulse response from single dipole at every location

## 1.1.7 pynibs.opt module

`pynibs.opt.get_det_fim(x, fun, p, fim_matrix)`

Updates the Fisher Information Matrix and returns the negative determinant based on the sample x. It is a score how much information the additional sample yields.

**Parameters**

- **fun** (*function object*) – Function object defined in interval [0, 1].
- **x** (*float*) – Single sample location (interval [0, 1])
- **p** (*dict*) – Dictionary containing the parameter estimates. The keys are the parameter names of fun.
- **fim\_matrix** (*ndarray of float* [n\_params x n\_params]) – Fisher Information Matrix

**Returns**

**det** – Determinant of the Fisher Information Matrix after adding sample x

**Return type**

*float*

`pynibs.opt.get_fim_sample(fun, x, p)`

Get Fisher Information Matrix of one single sample.

#### Parameters

- **fun** (*function object*) – Function object the fisher information matrix is calculated for. The sample is passed as the first argument.
- **x** (*float*) – Sample passed to function
- **p** (*dict*) – Dictionary containing the parameter estimates. The keys are the parameter names of fun.

#### Returns

**fim\_matrix** – Fisher information matrix

#### Return type

ndarray of *float* [n\_params x n\_params]

`pynibs.opt.get_optimal_coil_positions(e_matrix, criterion, n_stim, ele_idx_1=None, ele_idx_2=None, fn_out_hdf5=None, n_cpu=4, zap_idx_opt=None, fun=None, p=None, c=None, weights=None, overwrite=True, verbose=True, fn_coilpos_hdf5=None, start_zap_idx=0)`

Determine set of optimal coil positions for TMS regression analysis.

#### Parameters

- **e\_matrix** (*ndarray of float [n\_stim, n\_ele]*) – Matrix containing the electric field values in the ROI
- **criterion** (*str*) – Optimization criterion: - “mc\_cols”: Minimization of mutual coherence between columns - “mc\_rows”: Minimization of mutual coherence between rows - “svd”: Minimization of condition number - “dist”: Equal distant sampling - “dist\_svd”: Minimization of condition number and equidistant sampling - “dist\_mc\_cols”: Minimization of mutual coherence between columns and equidistant sampling - “dist\_mc\_rows”: Minimization of mutual coherence between rows and equidistant sampling - “coverage”: Maximizes the electric field coverage - “variability”: Maximizes variability between elements
- **n\_stim** (*int*) – Maximum number of stimulations
- **ele\_idx\_1** (*ndarray of int, optional, default: None*) – Element indices the first optimization goal is performed for, If None, all elements are considered
- **ele\_idx\_2** (*ndarray of int, optional, default: None*) – Element indices the first optimization goal is performed for. If None, all elements are considered
- **n\_cpu** (*int*) – Number of threads
- **fn\_out\_hdf5** (*str, optional, default: None*) – Returns the list of optimal zap indices if fn\_out\_hdf5 is None, otherwise, save the results in .hdf5 file. Filename of output .hdf5 file where the zap index lists are saved in subfolder “zap\_index\_lists” - “zap\_index\_lists/0”: [213] - “zap\_index\_lists/1”: [213, 5] - etc
- **zap\_idx\_opt** (*list of int, optional, default: None*) – List of already selected optimal coil positions (those are ignored in the optimization and will not be picked again)
- **fun** (*function object*) – Function object defined in interval [0, 1]. (only needed for fim optimization)
- **p** (*list of dict [n\_ele], optional, default: None*) – List of dicts containing the parameter estimates (whole ROI). The keys are the parameter names of fun. (only needed for fim and dist optimization)

- **c** (*ndarray of float [n\_ele]*, *optional, default: None*) – Congruence factor in each ROI element. Used to weight fim and dist optimization. (only needed for fim and dist optimization)
- **weights** (*list of float [2]*, *optional, default: [0.5, 0.5]*) – Weights of optimization criteria in case of multiple goal functions (e.g. fim\_svd). Higher weight means higher importance for the respective criteria. By default both optimization criteria are weighted equally [0.5, 0.5].
- **overwrite** (*bool, optional, default: True*) – Overwrite existing solutions or read existing hdf5 file and continue optimization
- **verbose** (*bool, optional, default: True*) – Print output messages
- **fn\_coilpos\_hdf5** (*str*) – File containing the corresponding coil positions and orientations (centers, m0, m1, m2)
- **start\_zap\_idx** (*int, optional, default: 0*) – First zap index to start greedy search

**Returns**

- **zap\_idx\_e\_opt** (*list of int [n\_stim]*) – Optimal zap indices
- *<File>.hdf5 file* – Output file containing the zap index lists

**pynibs.opt.get\_optimal\_sample\_fim(fun, p, x=None)**

Determines optimal location of next sample by maximizing the determinant of the Fisher Information Matrix.

**Parameters**

- **fun** (*function object*) – Function object (interval [0, 1]).
- **x** (*ndarray of float, optional, default: None*) – Previous sample locations (interval [0, 1]).
- **p** (*dict*) – Dictionary containing the parameter estimates. The keys are the parameter names of fun.

**Returns****x\_opt** – Optimal location of next sample (interval [0, 1]).**Return type****float****pynibs.opt.init\_fim\_matrix(fun, x, p)**

Initializes the Fisher Information Matrix based on the samples given in x.

**Parameters**

- **fun** (*function object*) – Function object defined in interval [0, 1].
- **x** (*ndarray of float*) – Initial sample locations (interval [0, 1])
- **p** (*dict*) – Dictionary containing the parameter estimates. The keys are the parameter names of fun.

**Returns****fim\_matrix** – Fisher Information Matrix**Return type***ndarray of float [n\_params x n\_params]***pynibs.opt.online\_optimization(fn\_subject\_hdf5, fn\_roi\_ss\_indices\_hdf5, fn\_out\_hdf5, fn\_stimsites\_hdf5, e\_matrix, mep, mesh\_idx, roi\_idx, n\_zaps\_init=3, criterion\_init='mc\_rows', criterion='coverage', n\_cpu=4, threshold=0.8, weights=None, eps0=0.01, eps0\_dist=1, exponent=5, perc=99, n\_refit=0, fun=<function sigmoid>, verbose=True)**

Performs virtual online optimization to determine the congruence factor. After an initial set of coil positions, the algorithm iteratively optimizes the next coil position based on the virtually measured MEP data.

### Parameters

- **fn\_subject\_hdf5** (`str`) – Filename of subject .hdf5 file
- **fn\_roi\_ss\_indices\_hdf5** (`str`) – Filename of .hdf5 file containing the element indices of the subsampled ROI in f["roi\_indices"]
- **e\_matrix** (`ndarray of float [n_zaps x n_ele]`) – Electric field matrix
- **mep** (`ndarray of float [n_zaps]`) – Motor evoked potentials for every stimulation
- **fn\_out\_hdf5** (`str`) – Filename of .hdf5 output file containing the coil positions and the congruence factor maps for every iteration
- **fn\_stimsites\_hdf5** (`str`) – Filename of the .hdf5 file containing the stimulation sites in "centers", "m0", "m1", "m2"
- **mesh\_idx** (`int`) – Mesh index
- **roi\_idx** (`int`) – ROI index
- **n\_zaps\_init** (`int, optional, default: 3`) – Number of initial samples optimized using optimization criterion specified in "criterion\_init"
- **criterion\_init** (`str, optional, default: "mc_rows"`) – Optimization criterion for which the initial samples are optimized (e.g. "mc\_rows", "svd", ...)
- **criterion** (`str, optional, default: "coverage"`) – Optimization criterion for which the online optimization is performed (e.g. "coverage", "mc\_rows", "svd", ...)
- **n\_cpu** (`int, optional, default: 4`) – Number of CPU cores to use
- **threshold** (`float, optional, default: 0.1`) – Threshold between [0 ... 1] of the maximal congruence factor. Elements where c > threshold \* max(c) are included in the online optimization to select the next optimal coil position.
- **weights** (`list of float [2], optional, default: [0.5, 0.5]`) – Weights of optimization criteria in case of multiple goal functions (e.g. fim\_svd). Higher weight means higher importance for the respective criteria. By default both optimization criteria are weighted equally [0.5, 0.5].
- **eps0** (`float, optional, default: 0.01`) – First error threshold to terminate the online optimization. The normalized root mean square deviation is calculated between the current and the previous solution. If the error is lower than eps0 for 3 times in a row, the online optimization terminates and returns the results.
- **eps0\_dist** (`float, optional, default: 1`) – Second error threshold to terminate the online optimization. The geodesic distance in mm of the hotspot is calculated between the current and the previous solution. If the error is lower than eps0\_dist for 3 times in a row, the online optimization terminates and returns the results.
- **exponent** (`float, optional, default: 5`) – Exponent the congruence factor map is scaled  $c^{**}exponent$
- **perc** (`float, optional, default: 99`) – Percentile the congruence factor map is normalized (between 0 and 100)
- **n\_refit** (`int, optional, default: 0`) – Number of refit iterations. No refit is applied if n\_refit=0.
- **fun** (`function object, optional, default: pynibs.linear`) – Function to use to determine the congruence factor (e.g. pynibs.linear, pynibs.sigmoid, ...)
- **verbose** (`bool, optional, default: True`) – Plot output messages

**Returns**

Results output file containing the coil positions and the congruence factor maps for every iteration

**Return type**

<file> .hdf5 file

`pynibs.opt.workhorse_corr(idx_list, array, ele_idx_1)`

**Parameters**

- **idx\_list** –
- **array** –
- **ele\_idx\_1** –

**Returns**

`pynibs.opt.workhorse_coverage(idx_list, array, x, y, ele_idx_1)`

Determine coverage score (likelihood) for given zap indices in idx\_list

**Parameters**

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **x** (*ndarray of float [200 x n\_ele]*) – x-values of coverage distributions, defined in interval [0, 1] (element wise normalized electric field)
- **y** (*ndarray of float [200 x n\_ele]*) – y-values of coverage distributions (element wise probability of already included e-fields)
- **ele\_idx\_1** (*ndarray of float [n\_roi]*) – Element indices for which the coverage optimization is performed for

**Returns**

**res** – Coverage score (likelihood) for given electric field combinations. Lower values indicate that the new zap fills a gap which was not covered before.

**Return type**

*ndarray of float [n\_combs]*

`pynibs.opt.workhorse_coverage_prepare(idx_list, array, zap_idx)`

Prepares coverage calculation. Determines coverage distributions for elements in idx\_list given the zaps in zap\_idx

**Parameters**

- **idx\_list** (*list [n\_ele]*) – Index lists of elements.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **zap\_idx** (*ndarray of int*) – Included zaps in coverage distribution.

**Returns**

- **x** (*ndarray of float [200 x n\_ele]*) – x-values of coverage distributions, defined in interval [0, 1] (element wise normalized electric field)
- **y** (*ndarray of float [200 x n\_ele]*) – y-values of coverage distributions (element wise probability of already included e-fields)

`pynibs.opt.workhorse_dist(idx_list, array, ele_idx_1)`

Determines distance score for given zap indices in idx\_list.

#### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the optimization is performed

#### Returns

`res` – Distance based score. Lower values indicate more equidistant sampling (better)

#### Return type

`ndarray of float [n_combs]`

`pynibs.opt.workhorse_dist_mc(idx_list, array, ele_idx_1, ele_idx_2, mode='cols')`

Determines distance score and mutual coherence for given zap indices in idx\_list. If c\_max\_idx is given, the distance based score is calculated only for this element. The condition number however is optimized for all elements in array

#### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **mode** (*str, optional, default: "cols"*) – Set if the mutual coherence is calculated w.r.t. columns or rows (“cols”, “rows”)
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the dist optimization is performed for
- **ele\_idx\_2** (*ndarray of float [n\_ele]*) – Element indices for which the mc optimization is performed for

#### Returns

- **res\_dist** (*ndarray of float [n\_combs]*) – Distance based score. Lower values indicate more equidistant sampling (better)
- **res\_mc** (*ndarray of float [n\_combs]*) – Mutual coherence. Lower values indicate more orthogonal e-field combinations (better)

`pynibs.opt.workhorse_dist_svd(idx_list, array, ele_idx_1, ele_idx_2)`

Determines distance score and condition number for given zap indices in idx\_list. If c\_max\_idx is given, the distance based score is calculated only for this element. The condition number however is optimized for all elements in array

#### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the dist optimization is performed for
- **ele\_idx\_2** (*ndarray of float [n\_ele]*) – Element indices for which the svd optimization is performed for

**Returns**

- **res\_dist** (*ndarray of float [n\_combs]*) – Distance based score. Lower values indicate more equidistant sampling (better)
- **res\_svd** (*ndarray of float [n\_combs]*) – Condition number. Lower values indicate more orthogonal e-field combinations (better)

`pynibs.opt.workhorse_fim(idx_list, array, ele_idx_1, e_opt, c=None)`

Determine difference between e-fields and optimal e-field determined using the Fisher Information Matrix.

**Parameters**

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_roi]*) – Element indices for which the fim optimization is performed for
- **e\_opt** (*ndarray of float [n\_roi]*) – Optimal electric field value(s) (target) determined by FIM method
- **c** (*ndarray of float [n\_ele], optional, default: None*) – Congruence factor map normalized to 1 (whole ROI) used to weight the difference between the optimal e-field and the candidate e-field. If None, no weighting is applied.

**Returns**

**res** – Difference between e-fields and optimal e-field.

**Return type**

*ndarray of float [n\_combs]*

`pynibs.opt.workhorse_fim_mc(idx_list, array, ele_idx_1, ele_idx_2, e_opt, c=None, mode='rows')`

Determine difference between e-fields and optimal e-field determined using the Fisher Information Matrix and mutual coherence.

**Parameters**

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_roi\_1]*) – Element indices for which the fim optimization is performed for
- **ele\_idx\_2** (*ndarray of float [n\_roi\_2]*) – Element indices for which the mc optimization is performed for
- **e\_opt** (*float*) – Optimal electric field value (target) determined by FIM method
- **c** (*ndarray of float [n\_ele], optional, default: None*) – Congruence factor map normalized to 1 (whole ROI) used to weight the difference between the optimal e-field and the candidate e-field. If None, no weighting is applied.

**Returns**

- **res\_fim** (*ndarray of float [n\_combs]*) – Difference between e-fields and optimal e-field.
- **res\_mc** (*ndarray of float [n\_combs]*) – Mutual coherence. Lower values indicate more orthogonal e-field combinations (better)

`pynibs.opt.workhorse_fim_svd(idx_list, array, ele_idx_1, ele_idx_2, e_opt, c=None)`

Determine difference between e-fields and optimal e-field determined using the Fisher Information Matrix and condition number.

### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_roi\_1]*) – Element indices for which the fim optimization is performed for
- **ele\_idx\_2** (*ndarray of float [n\_roi\_2]*) – Element indices for which the svd optimization is performed for
- **e\_opt** (*float*) – Optimal electric field value (target) determined by FIM method
- **c** (*ndarray of float [n\_ele], optional, default: None*) – Congruence factor map normalized to 1 (whole ROI) used to weight the difference between the optimal e-field and the candidate e-field. If None, no weighting is applied.

### Returns

- **res\_fim** (*ndarray of float [n\_combs]*) – Difference between e-fields and optimal e-field.
- **res\_svd** (*ndarray of float [n\_combs]*) – Condition number. Lower values indicate more orthogonal e-field combinations (better)

`pynibs.opt.workhorse_mc(idx_list, array, ele_idx_1, mode='cols')`

Determines mutual coherence for given zap indices in idx\_list.

### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the optimization is performed
- **mode** (*str, optional, default: "cols"*) – Set if the mutual coherence is calculated w.r.t. columns or rows ("cols", "rows")

### Returns

**res** – Mutual coherence. Lower values indicate more orthogonal e-field combinations (better)

### Return type

*ndarray of float [n\_combs]*

`pynibs.opt.workhorse_smooth(idx_list, array, ele_idx_1)`

`pynibs.opt.workhorse_svd(idx_list, array, ele_idx_1)`

Determines condition number for given zap indices in idx\_list.

### Parameters

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the optimization is performed

### Returns

**res** – Condition number. Lower values indicate more orthogonal e-field combinations (better)

**Return type**

ndarray of float [n\_combs]

pynibs.opt.**workhorse\_var**(idx\_list, array, ele\_idx\_1)pynibs.opt.**workhorse\_variability**(idx\_list, array, ele\_idx\_1)

Determines variability score for given zap indices in idx\_list.

**Parameters**

- **idx\_list** (*list of lists [n\_combs][n\_zaps]*) – Index lists of zaps containing different possible combinations. Usually only the last index changes.
- **array** (*ndarray of float [n\_zaps x n\_ele]*) – Electric field for different coil positions and elements
- **ele\_idx\_1** (*ndarray of float [n\_ele]*) – Element indices for which the optimization is performed

**Returns****res** – Condition number. Lower values indicate more orthogonal e-field combinations (better)**Return type**

ndarray of float [n\_combs]

## 1.1.8 pynibs.para module

pynibs.para.**ResetSession**()

Resets Paraview session (needed if multiple plots are generated successively)

pynibs.para.**b2rcw**(cmin\_input, cmax\_input)

BLUEWHITERED Blue, white, and red color map. This function is designed to generate a blue to red colormap. The color of the colorbar is from blue to white and then to red, corresponding to the data values from negative to zero to positive, respectively. The color white always corresponds to value zero. The brightness of blue and red will change according to your setting, so that the brightness of the color corresponded to the color of his opposite number. e.g. b2rcw(-3,6) is from light blue to deep red e.g. b2rcw(-3,3) is from deep blue to deep red

**Parameters**

- **cmin\_input** (*float*) – Minimum value of data
- **cmax\_input** (*float*) – Maximum value of data

**Returns****newmap****Return type**

ndarray of float [N\_RGB x 3]

pynibs.para.**create\_plot\_settings\_dict**(plotfunction\_type)

Creates a dictionary with default plotsettings.

**Parameters****plotfunction\_type** (*str*) – Plot function the dictionary is generated for:

- 'surface\_vector\_plot'
- 'surface\_vector\_plot\_vtu'
- 'volume\_plot'
- 'volume\_plot\_vtu'

**Returns**

- **ps** (*dict*) – Dictionary containing the plotsettings:
- **axes** (*boolean*) – Show orientation axes (TRUE / FALSE)
- **background\_color** (*nparray [1 x 3]*) – Set background color of exported image RGB (0...1)
- **calculator** (*str*) – Format string with placeholder of the calculator expression the quantity to plot is modified with (e.g.: “{}^5”)
- **clip\_coords** (*nparray of float [N\_clips x 3]*) – Coordinates of clip surface origins (x,y,z)
- **clip\_normals** (*nparray of float [N\_clips x 3]*) – Surface normals of clip surfaces pointing in the direction where the volume is kept for **clip\_type** = ['clip' ...] (x,y,z)
- **clip\_type** (*list of str*) – Type of clipping:
  - 'clip': cut geometry but keep volume behind
  - 'slice': cut geometry and keep only the slice
- **coil\_dipole\_scaling** (*list [1 x 2]*) – Specify the scaling type of the dipoles (2 entries):
  - coil\_dipole\_scaling[0]**:
  - 'uniform': uniform scaling, i.e. all dipoles have the same size
  - 'scaled': size scaled according to dipole magnitude
  - coil\_dipole\_scaling[1]**:
  - scalar scale parameter of dipole size
- **coil\_dipole\_color** (*str or list*) – Color of the dipoles; either str to specify colormap (e.g. ‘jet’) or list of RGB values [1 x 3] (0...1)
- **coil\_axes** (*boolean*) – Plot coil axes visualizing the principle direction and orientation of the coil (Default: True)
- **colorbar\_label** (*str*) – Label of plotted data close to colorbar
- **colorbar\_position** (*list of float [1 x 2]*) – Position of colorbar (lower left corner) 0...1 [x\_pos, y\_pos]
- **colorbar\_orientation** (*str*) – Orientation of colorbar ('Vertical', 'Horizontal')
- **colorbar\_aspectratio** (*int*) – Aspectratio of colorbar (higher values make it thicker)
- **colorbar\_titlefontsize** (*float*) – Fontsize of colorbar title
- **colorbar\_labelfontsize** (*float*) – Fontsize of colorbar labels (numbers)
- **colorbar\_labelformat** (*str*) – Format of colorbar labels (e.g.: ‘%-#6.3g’)
- **colorbar\_numberoflabels** (*int*) – maximum number of colorbar labels
- **colorbar\_labelcolor** (*list of float [1 x 3]*) – Color of colorbar labels in RGB (0...1)
- **colormap** (*str or nparray*) – if nparray [1 x 4\*N]: custom colormap providing data and corresponding RGB values

$$\begin{bmatrix} data_1 & R_1 & G_1 & B_1 \\ data_2 & R_2 & G_2 & B_2 \\ \dots & \dots & \dots & \dots \\ data_N & R_N & G_N & B_N \end{bmatrix}$$

if str: colormap of plotted data chosen from included presets:

- 'Cool to Warm',
- 'Cool to Warm (Extended)',
- 'Blue to Red Rainbow',

- ‘X Ray’,
  - ‘Grayscale’,
  - ‘jet’,
  - ‘hsv’,
  - ‘erdc\_iceFire\_L’,
  - ‘Plasma (matplotlib)’,
  - ‘Viridis (matplotlib)’,
  - ‘gray\_Matlab’,
  - ‘Spectral\_lowBlue’,
  - ‘BuRd’
  - ‘Rainbow Blended White’
  - ‘b2rcw’
- **colormap\_categories** (*boolean*) – Use categorized (discrete) colormap
  - **datarange** (*list [1 x 2]*) – Minimum and Maximum of plotted datarange [MIN, MAX] (default: automatic)
  - **domain\_IDs** (*int or list of int*) – Domain IDs
    - surface plot: Index of surface where the data is plotted on (Default: 0)
    - volume plot: Specify the domains IDs to show in plot (default: all) Attention! Has to be included in the dataset under the name ‘tissue’! e.g. for SimNIBS:
      - 1 -> white matter (WM)
      - 2 -> grey matter (GM)
      - 3 -> cerebrospinal fluid (CSF)
      - 4 -> skull
      - 5 -> skin
  - **domain\_label** (*str*) – Label of the dataset which contains the domain IDs (default: ‘tissue\_type’)
  - **edges** (*boolean*) – Show edges of mesh (TRUE / FALSE)
  - **fname\_in** (*str or list of str*) – Filenames of input files, 2 possibilities:
    - .xdmf-file: filename of .xmdf (needs the corresponding .hdf5 file(s) in the same folder)
    - .hdf5-file(s): filename(s) of .hdf5 file(s) containing the data and the geometry. The data can be provided in the first hdf5 file and the geometry can be provided in the second file. However, both can be also provided in a single hdf5 file.
  - **fname\_png** (*str*) – Name of output .png file (incl. path)
  - **fname\_vtu\_volume** (*str*) – Name of .vtu volume file containing volume data (incl. path)
  - **fname\_vtu\_surface** (*str*) – Name of .vtu surface file containing surface data (incl. path) (to distinguish tissues)
  - **fname\_vtu\_coil** (*str*) – Name of coil .vtu file (incl. path) (optional)
  - **info** (*str*) – Information about the plot the settings are belonging to
  - **interpolate** (*boolean*) – Interpolate data for visual smoothness (TRUE / FALSE)
  - **NanColor** (*list of float [3]*) – RGB color values for “Not a Number” values (range 0 ... 1)

- **opacitymap** (*nparray*) – Points defining the piecewise linear opacity transfer function (transparency) (default: no transparency) connecting data values with opacity (alpha) values ranging from 0 (max. transparency) to 1 (no transparency)

$$\begin{bmatrix} data_1 & opac_1 & 0.5 & 0 \\ data_2 & opac_2 & 0.5 & 0 \\ \dots & \dots & \dots & \dots \\ data_N & opac_N & 0.5 & 0 \end{bmatrix}$$

- **plot\_function** (*str*) – Function the plot is generated with:
  - ‘surface\_vector\_plot’
  - ‘surface\_vector\_plot\_vtu’
  - ‘volume\_plot’
  - ‘volume\_plot\_vtu’
- **png\_resolution** (*float*) – Resolution parameter of output image (1...5)
- **quantity** (*str*) – Label of magnitude dataset to plot
- **surface\_color** (*nparray [1 x 3]*) – Color of brain surface in RGB (0...1) for better visibility of tissue borders
- **surface\_smoothing** (*bool*) – Smooth the plotted surface (True/False)
- **show\_coil** (*boolean*) – show coil if present in dataset as block termed ‘coil’ (Default: True)
- **vcolor** (*nparray of float [N\_vecs x 3]*) – Array containing the RGB values between 0...1 of the vector groups in dataset to plot
- **vector\_mode** (*dict*) – dict key determines the type how many vectors are shown: - ‘All Points’ - ‘Every Nth Point’ - ‘Uniform Spatial Distribution’  
dict value (int) is the corresponding number of vectors
  - ‘All Points’ (not set)
  - ‘Every Nth Point’ (every Nth vector is shown in the grid)
  - ‘Uniform Spatial Distribution’ (not set)
- **view** (*list*) – Camera position and angle [[3 x CameraPosition], [3 x CameraFocalPoint], [3 x CameraViewUp], 1 x CameraParallelScale]
- **viewsize** (*nparray [1 x 2]*) – Set size of exported image in pixel [width x height] will be extra scaled by parameter png\_resolution
- **vlabels** (*list of str*) – Labels of vector datasets to plot (other present datasets are ignored)
- **vscales** (*list of float*) – Scale parameters of vector groups to plot
- **vscale\_mode** (*list of str [N\_vecs x 1]*) – List containing the type of vector scaling:
  - ‘off’: all vectors are normalized
  - ‘vector’: vectors are scaled according to their magnitudeeee

### `pynibs.para.crop_data_hdf5_to_datarange(ps)`

Crops the data (quantity) in .hdf5 data file to datarange and overwrites the original .hdf5 data file pointed by the .xdmf file.

#### Parameters

**ps** (*dict*) – Plot settings dictionary created with `create_plotsettings_dict(plot_function)`

#### Returns

- **fn\_hdf5** (*str*) – Filename (incl. path) of data .hdf5 file (read from .xmdf file)

- <File> (.hdf5 file) – \*\_backup.hdf5 backup file of original .hdf5 data file
- <File> .hdf5 file – Cropped data

`pynibs.para.crop_image(fname_image, fname_image_cropped)`

Remove surrounding empty space around an image. This implementation assumes that the surrounding space has the same colour as the top leftmost pixel.

**Parameters**

`fname_image (str)` – Filename of image to be cropped

**Returns**

<File> – Cropped image file saved as “`fname_image_cropped`”

**Return type**

.png file

`pynibs.para.surface_vector_plot(ps)`

Generate plot with Paraview from data in .hdf5 file(s).

**Parameters**

`ps (dict)` – Plot settings dict initialized with create\_plot\_settings\_dict(plotfunction\_type='surface\_vector\_plot')

**Returns**

<File> – Generated plot

**Return type**

.png file

`pynibs.para.surface_vector_plot_vtu(ps)`

Generate plot with Paraview from data in .vtu file.

**Parameters**

`ps (dict)` – Plot settings dict initialized with create\_plot\_settings\_dict(plotfunction\_type='surface\_vector\_plot\_vtu')

**Returns**

<File> – Generated plot

**Return type**

.png file

`pynibs.para.volume_plot(ps)`

Generate plot with Paraview from data in .hdf5 file.

**Parameters**

`ps (dict)` – Plot settings dict initialized with create\_plot\_settings\_dict(plotfunction\_type='volume\_plot')

**Returns**

<File> – Generated plot

**Return type**

.png file

`pynibs.para.volume_plot_vtu(ps)`

Generate plot with Paraview from data in .vtu file.

**Parameters**

`ps (dict)` – Plot settings dict initialized with create\_plot\_settings\_dict(plotfunction\_type='volume\_plot\_vtu')

**Returns**

<File> – Generated plot

**Return type**

.png file

`pynibs.para.write_vtu(fname, data_labels, points, connectivity, idx_start, data)`

Writes data in tetrahedra centers into .vtu file, which can be loaded with Paraview.

**Parameters**

- **fname** (`str`) – Name of .vtu file (incl. path)
- **data\_labels** (`list with N_data str`) – Label of each dataset
- **points** (`array of float [N_points x 3]`) – Coordinates of vertices
- **connectivity** (`array of int [N_tet x 4]`) – Connectivity of points forming tetrahedra
- **idx\_start** (`int`) – Smallest index in connectivity matrix, defines offset w.r.t Python indexing, which starts at ‘0’
- **\*data** (`array(s) [N_tet x N_comp(N_data)]`) – Arrays containing data in tetrahedra center multiple components per dataset possible e.g. [Ex, Ey, Ez]

**Returns**

`<File>` – Geometry and data information

**Return type**

.vtu file

`pynibs.para.write_vtu_coilpos(fname_geo, fname_vtu)`

Read dipole data of coil (position and magnitude of each dipole) from geo file and store it as vtu file.

**Parameters**

- **fname\_geo** (`str`) – .geo file from SimNIBS.
- **fname\_vtu** (`str`) – .vtu output file. Nodes and nodedata.

**Returns**

`<File>` – Magnetic dipoles of the TMS coil

**Return type**

.vtu file

`pynibs.para.write_vtu_mult(fname, data_labels, points, triangles, tetrahedras, idx_start, *data)`

Writes data in triangles and tetrahedra centers into .vtu file, which can be loaded with Paraview.

**Parameters**

- **fname** (`str`) – Name of .vtu file (incl. path)
- **data\_labels** (`list of str [N_data]`) – Label of each dataset
- **points** (`nparray of float [N_points x 3]`) – Coordinates of vertices
- **triangles** (`nparray of int [N_tri x 3]`) – Connectivity of points forming triangles
- **tetrahedras** (`nparray of int [N_tri x 4]`) – Connectivity of points forming tetrahedra idx\_start: int smallest index in connectivity matrix, defines offset w.r.t python indexing, which starts at ‘0’
- **\*data** (`nparray(s) [N_tet x N_comp(N_data)]`) – Arrays containing data in tetrahedra center multiple components per dataset possible e.g. [Ex, Ey, Ez]

**Returns**

`<File>` – Geometry and data information

**Return type**

.vtu file

## 1.1.9 pynibs.roi module

```
class pynibs.roi.CorticalLayer(create_key, id, volumetric_mesh=None, roi=None, depth=None,
                                path=None, surface=None)

Bases: object

class Settings
    Bases: object

    GRID_POINTS_PER_MM = 1.5

    NUM_TRIANGLE_SMOOTHING_STEPS = 30

    ROI_SIZE_OFFSET = 5

    TAG_GRAY_MATTER_SURF = 1002

    TAG_GRAY_MATTER_VOL = 2

    TAG_WHITE_MATTER_SURF = 1001

    TAG_WHITE_MATTER_VOL = 1

classmethod create_in_bbox(id, bbox, depth, volmesh)
    Factory method for constructing a CorticalLayer-object within a region-of-interest and a specified cortical depth.

    Parameters
        • id (str) – Identifier of the layer.
        • bbox (List[float]) – List of bounding values around the ROI box: [x_min, x_max, y_min, y_max, z_min, z_max].
        • depth (float) – Normalized distance of the layer from gray matter surface. Provide values in the open interval (0,1)
        • volmesh (simnibs.Msh) – The tetrahedral volume mesh, in which the layer should be generated.

classmethod create_in_roi(id, roi, depth, volmesh)
    Factory method for constructing a CorticalLayer-object within a region-of-interest and a specified cortical depth.

    Parameters
        • id (str) – Identifier of the layer.
        • roi (RegionOfInterestSurface instance) – RegionOfInterestSurface
        • depth (float) – Normalized distance of the layer from gray matter surface. Provide values in the open interval (0,1)
        • volmesh (simnibs.Msh) – The tetrahedral volume mesh, in which the layer should be generated.

static crop_mesh_with_box(mesh, roi, keep_elements=False)
    Returns the cropped mesh with all points that are inside the region of interest

    Parameters
        • keep_elements (bool, default = False) – If True, keeps elements with at least one point in roi, else removes them.
        • mesh (simnibs.Msh) – The mesh that is supposed to be cropped.
        • roi (List[float]) – The bounding box of the region of interest which the mesh should be cropped to. [x-min, x-max, y-min, y-max, z-min, z-max]
```

**Returns**

**mesh\_cropped** – The cropped mesh.

**Return type**

simnibs.Msh

**static crop\_mesh\_with\_surface(mesh, roi, keep\_elements=False, radius=3)**

Returns the cropped mesh with all points that are close to the surface of interest

**Parameters**

- **keep\_elements** (*bool*, *default = False*) – If True, keeps elements with at least one point in roi, else removes them.
- **mesh** (*simnibs.Msh*) – The mesh that is supposed to be cropped.
- **roi** (*RegionOfInterestSurface instance*) – RegionOfInterestSurface
- **radius** (*float*, *default = 3*) – Search radius of mesh elements around ROI nodes

**Returns**

**mesh\_cropped** – The cropped mesh.

**Return type**

simnibs.Msh

**generate\_layer(depth, roi)**

Create the geometry of the layer at the specified depth using marching cubes.

**Parameters**

- **depth** (*float*) – The depth below the GM surface at which the layer should be generated; in [0,1].
- **roi** (*RegionOfInterestSurface instance*) – RegionOfInterestSurface

**get\_evenly\_spaced\_element\_subset(elements\_per\_square\_mm)**

Subsample the surface representation of the layer.

**Parameters**

**elements\_per\_square\_mm** (*float*) – Number of triangles per mm<sup>2</sup> in the layer.

**Returns**

**selected elements** – List of indices of selected elements as a result of the subsampling.

**Return type**

Typing.List[int]

**get\_smoothed\_normals()**

Computed the smoothed normals of the surface representation of this layer. Note: For the later stages, we don't want a smoothed surface, but smooth

normals in order to maintain the location of the cells, but orient them more smoothly. Therefore, we use smoothed normals, e.g. for the computation of the theta angle, but do not smooth the entire layer surface.

**Returns**

**normals** – The tetrahedral volume mesh, in which the layer should be generated.

**Return type**

np.ndarray

**classmethod init\_from\_file(id, fn)**

Factory method for constructing a CorticalLayer-object from a file.

**Parameters**

- **id** (*str*) – Identifier of the layer.

- **fn** (*str*) – File path to a region of interest surface (e.g. midlayer).

### **classmethod init\_from\_surface(id, surf)**

Factory method for constructing a CorticalLayer-object from a Simnibs-surface object.

#### Parameters

- **id** (*str*) – Identifier of the layer.
- **surf** (*simnibs.Msh*) – The surface representation of an already existing layer (e.g. midlayer).

### **remove\_unconnected\_surfaces()**

Remove elements small unconnected element-clusters from this layer.

### **static roi\_bbox\_from\_points(points, offset=0)**

Find the minimal bounding box around the provided points.

#### Parameters

- **points** (*simnibs.Msh*) – The tetrahedral volume mesh, in which the layer should be generated.
- **offset** (*float*) – Normalized distance of the layer from gray matter surface. Provide values in the open interval (0,1)

#### Returns

**bounding\_box** – List of bounding values around the provided points: [x\_min, x\_max, y\_min, y\_max, z\_min, z\_max].

#### Return type

*List[float]*

### **save(fn)**

Save the current surface representation of this CorticalLayer instance at the specified location.

#### Parameters

**fn** (*str*) – Target file name of the surface-file of this layer.

## **class pynibs.roi.RegionOfInterestSurface**

Bases: **object**

Region of interest (surface).

### **node\_coord\_up**

(N\_points, 3) Coordinates (x,y,z) of upper surface nodes

#### Type

*np.ndarray*

### **node\_coord\_mid**

(N\_points, 3) Coordinates (x,y,z) of middle surface nodes

#### Type

*np.ndarray*

### **node\_coord\_low**

(N\_points, 3) Coordinates (x,y,z) of lower surface nodes

#### Type

*np.ndarray*

### **node\_number\_list**

(N\_points, 3) Connectivity matrix of triangles

#### Type

*np.ndarray*

**delta**

Distance parameter between WM and GM (0 -> WM, 1 -> GM)

**Type**

float

**tet\_idx\_tri\_center\_up**

Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the upper surface are lying in

**Type**

np.ndarray [N\_points]

**tet\_idx\_tri\_center\_mid**

Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the middle surface are lying in

**Type**

np.ndarray [N\_points]

**tet\_idx\_tri\_center\_low**

Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the lower surface are lying in

**Type**

np.ndarray [N\_points]

**tet\_idx\_node\_coord\_mid**

(N\_tri,) Tetrahedra indices of TetrahedraLinear object instance where the nodes of the middle surface are lying in

**Type**

np.ndarray

**tri\_center\_coord\_up**

(N\_tri, 3) Coordinates of roi triangle center of upper surface

**Type**

np.ndarray

**tri\_center\_coord\_mid**

(N\_tri, 3) Coordinates of roi triangle center of middle surface

**Type**

np.ndarray

**tri\_center\_coord\_low**

(N\_tri, 3) Coordinates of roi triangle center of lower surface

**Type**

np.ndarray

**fn\_mask**

Filename for surface mask in subject space. .mgh file or freesurfer surface file.

**Type**

string

**fn\_mask\_avg**

Filename for .mgh mask in fsaverage space. Absolute path or relative to mesh folder.

**Type**

string

**fn\_mask\_nii**

Filename for .nii or .nii.gz mask. Absolute path or relative to mesh folder.

**Type**

string

**X\_ROI**

Region of interest [Xmin, Xmax], whole X range if empty [0,0] or None (left - right)

**Type**

list of float

**Y\_ROI**

Region of interest [Ymin, Ymax], whole Y range if empty [0,0] or None (anterior - posterior)

**Type**

list of float

**Z\_ROI**

Region of interest [Zmin, Zmax], whole Z range if empty [0,0] or None (inferior - superior)

**Type**

list of float

**template**

‘MNI’, ‘fsaverage’, ‘subject’

**Type**

str

**center**

Center coordinates for spherical ROI in self.template space

**Type**

list of float

**radius**

Radius in [mm] for spherical ROI

**Type**

float

**gm\_surf\_fname**

Filename(s) of GM surface generated by freesurfer (lh and/or rh) (e.g. in mri2msh: .../fs\_ID/surf/lh.pial)

**Type**

str or list of str

**wm\_surf\_fname**

Filename(s) of WM surface generated by freesurfer (lh and/or rh) (e.g. in mri2msh: .../fs\_ID/surf/lh.white)

**Type**

str or list of str

**layer**

Define the number of layers:

- 1: one layer
- 3: additionally upper and lower layers are generated around the central midlayer

**Type**

int

### `determine_element_idx_in_mesh(msh)`

Determines tetrahedra indices of msh where the triangle center points of upper, middle and lower surface and the nodes of middle surface are lying in.

#### Parameters

`msh (pynibs.TetrahedraLinear)` – Object instance of TetrahedraLinear class

#### Returns

- `RegionOfInterestSurface.tet_idx_tri_center_up (np.ndarray [N_points])` – Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the upper surface are lying in
- `RegionOfInterestSurface.tet_idx_tri_center_mid (np.ndarray [N_points])` – Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the middle surface are lying in
- `RegionOfInterestSurface.tet_idx_tri_center_low (np.ndarray [N_points])` – Tetrahedra indices of TetrahedraLinear object instance where the center points of the triangles of the lower surface are lying in
- `RegionOfInterestSurface.tet_idx_node_coord_mid (np.ndarray [N_tri])` – Tetrahedra indices of TetrahedraLinear object instance where the nodes of the middle surface are lying in

### `generate_cortical_laminae(head_model_mesh, bbox=None, laminae=(0.06, 0.4, 0.55, 0.65, 0.85), layer_ids=('L1', 'L23', 'L4', 'L5', 'L6'))`

Create the cortical layering with the provided laminar depths. Defaults to the standard depths of the laminae in the neo-cortex from layer I to VI

from “Simulation of transcranial magnetic stimulation in head model with morphologically-realistic cortical neurons”, Aberra et al., <https://doi.org/10.1016/j.brs.2019.10.002>

#### Parameters

- `head_model_mesh (simnibs.Msh)` – The head model volume mesh. Inside the GM compartment of this mesh, the layering will be generated.
- `bbox (np.ndarray (optional))` – Bounding coordinates of the region of interest. Optional, if the mid-layer surface is already existing (and can thus be used to determine the bounding coordinates).
- `laminae (Dict[str, float] / Tuple)` – List of depths of the individual to-be created lamiae.

### `make_GM_WM_surface(gm_surf_fname=None, wm_surf_fname=None, midlayer_surf_fname=None, mesh_folder=None, delta=0.5, x_roi=None, y_roi=None, z_roi=None, layer=1, fn_mask=None, refine=False)`

Generating a surface between WM and GM in a distance of delta 0...1 for ROI, given by Freesurfer mask or coordinates.

#### Parameters

- `gm_surf_fname (str or list of str)` – Filename(s) of GM FreeSurfer surface(s) (lh and/or rh). Either relative to mesh\_folder (fs\_ID/surf/lh.pial) or absolute (/full/path/to/lh.pial)
- `wm_surf_fname (str or list of str)` – Filename(s) of WM FreeSurfer surface(s) (lh and/or rh) Either relative to mesh\_folder (fs\_ID/surf/lh.white) or absolute (/full/path/to/lh.white)
- `midlayer_surf_fname (str or list of str)` – Filename(s) of midlayer surface (lh and/or rh) Either relative to mesh\_folder (fs\_ID/surf/lh.central) or absolute (/full/path/to/lh.central)

- **mesh\_folder** (*str*) – Root folder of mesh, Needed if paths above are given relative, or refine=True
- **m2m\_mat\_fname** (*[defunct]*) – Filename of mri2msh transformation matrix (e.g. in mri2msh: .../m2m\_ProbandID/MNI2conform\_6DOF.mat)
- **delta** (*float*) – Distance parameter where surface is generated 0...1 (default: 0.5)
  - 0 -> WM surface
  - 1 -> GM surface
- **x\_roi** (*list of float*) – Region of interest [Xmin, Xmax], whole X range if empty [0,0] or None (left - right)
- **y\_roi** (*list of float*) – Region of interest [Ymin, Ymax], whole Y range if empty [0,0] or None (anterior - posterior)
- **z\_roi** (*list of float*) – Region of interest [Zmin, Zmax], whole Z range if empty [0,0] or None (inferior - superior)
- **layer** (*int*) – Define the number of layers:
  - 1: one layer
  - 3: additionally upper and lower layers are generated around the central midlayer
- **fn\_mask** (*str*) – Filename for FreeSurfer .mgh mask.
- **refine** (*bool, optional, default: False*) – Refine ROI by splitting elements

#### Returns

- **node\_coord\_up** (*np.ndarray of float [N\_roi\_points x 3]*) – Node coordinates (x, y, z) of upper epsilon layer of ROI surface
- **node\_coord\_mid** (*np.ndarray of float [N\_roi\_points x 3]*) – Node coordinates (x, y, z) of ROI surface
- **node\_coord\_low** (*np.ndarray of float [N\_roi\_points x 3]*) – Node coordinates (x, y, z) of lower epsilon layer of ROI surface
- **node\_number\_list** (*np.ndarray of int [N\_roi\_tri x 3]*) – Connectivity matrix of intermediate surface layer triangles
- **delta** (*float*) – Distance parameter where surface is generated 0...1 (default: 0.5)
  - 0 -> WM surface
  - 1 -> GM surface
- **tri\_center\_coord\_up** (*np.ndarray of float [N\_roi\_tri x 3]*) – Coordinates (x, y, z) of triangle center of upper epsilon layer of ROI surface
- **tri\_center\_coord\_mid** (*np.ndarray of float [N\_roi\_tri x 3]*) – Coordinates (x, y, z) of triangle center of ROI surface
- **tri\_center\_coord\_low** (*np.ndarray of float [N\_roi\_tri x 3]*) – Coordinates (x, y, z) of triangle center of lower epsilon layer of ROI surface
- **fn\_mask** (*str*) – Filename for freesurfer mask. If given, this is used instead of \*\_ROIs
- **X\_ROI** (*list of float*) – Region of interest [Xmin, Xmax], whole X range if empty [0,0] or None (left - right)
- **Y\_ROI** (*list of float*) – Region of interest [Ymin, Ymax], whole Y range if empty [0,0] or None (anterior - posterior)
- **Z\_ROI** (*list of float*) – Region of interest [Zmin, Zmax], whole Z range if empty [0,0] or None (inferior - superior)

## Example

```
make_GM_WM_surface(self, gm_surf_fname, wm_surf_fname, delta, X_ROI, Y_ROI, Z_ROI)
make_GM_WM_surface(self, gm_surf_fname, wm_surf_fname, delta, mask_fn, layer=3)
```

### `project_on_midlayer(target, verbose=False)`

Project a coordinate on the nearest midlayer node

#### Parameters

- **target** (`np.ndarray`) – Coordinate to project as (3,) array
- **verbose** (`bool`) – Print some verbosity information. Default: False

#### Returns

**target\_proj** – Node coordinate of nearest midlayer node.

#### Return type

`np.ndarray`

### `subsample(dist=10, fn_sphere="")`

Subsample ROI surface and return element indices

#### Parameters

- **dist** (`float`) – Distance in mm the subsampled points lie apart
- **fn\_sphere** (`str`) – Name of ?.sphere file (freesurfer)

#### Returns

**ele\_idx** – Element indices of the subsampled surface

#### Return type

`ndarray of float [n_ele]`

## `class pynibs.roi.RegionOfInterestVolume`

Bases: `object`

Region of interest (volume) class

### `node_coord`

Coordinates (x,y,z) of ROI tetrahedra nodes

#### Type

`np.ndarray [N_points x 3]`

### `tet_node_number_list`

Connectivity matrix of ROI tetrahedra

#### Type

`np.ndarray [N_tet_roi x 3]`

### `tri_node_number_list`

Connectivity matrix of ROI tetrahedra

#### Type

`np.ndarray [N_tri_roi x 3]`

### `tet_idx_node_coord`

Tetrahedra indices of TetrahedraLinear object instance where the ROI nodes are lying in

#### Type

`np.ndarray [N_points]`

### `tet_idx_tetrahedra_center`

Tetrahedra indices of TetrahedraLinear object instance where the center points of the ROI tetrahedra are lying in

**Type**`np.ndarray [N_tet_roi]`**tet\_idx\_triangle\_center**

Tetrahedra indices of TetrahedraLinear object instance where the center points of the ROI triangle are lying in. If the ROI is directly generated from the msh instance using “make\_roi\_volume\_from\_msh”, these indices are the triangle indices of the head mesh since the ROI mesh and the head mesh are overlapping. If the ROI mesh is not the same as the head mesh, the triangle center of the ROI mesh are always lying in a tetrahedra of the head mesh (these indices are given in this case)

**Type**`np.ndarray [N_tri_roi]`**make\_roi\_volume\_from\_msh(msh, volume\_type='box', x\_roi=None, y\_roi=None, z\_roi=None)**

Generate region of interest (volume) and extract nodes, triangles and tetrahedra from msh instance.

**Parameters**

- **msh** (*pynibs.TetrahedraLinear*) – Mesh object instance of type TetrahedraLinear (see main.py)
- **volume\_type** (*str*) – Type of ROI ('box' or 'sphere')
- **x\_roi** (*list of float*) –
  - type = 'box': [Xmin, Xmax] (in mm), whole X range if empty [0,0] or None (left - right)
  - type = 'sphere': origin [x,y,z]
- **y\_roi** (*list of float*) –
  - type = 'box': [Ymin, Ymax] (in mm), whole Y range if empty [0,0] or None (anterior - posterior)
  - type = 'sphere': radius (in mm)
- **z\_roi** (*list of float*) –
  - type = 'box': [Zmin, Zmax] (in mm), whole Z range if empty [0,0] or None (inferior - superior)
  - type = 'sphere': None

**Returns**

- **RegionOfInterestVolume.node\_coord** (*np.ndarray [N\_points x 3]*) – Coordinates (x,y,z) of ROI tetrahedra nodes
- **RegionOfInterestVolume.tet\_node\_number\_list** (*np.ndarray [N\_tet\_roi x 3]*) – Connectivity matrix of ROI tetrahedra
- **RegionOfInterestVolume.tri\_node\_number\_list** (*np.ndarray [N\_tri\_roi x 3]*) – Connectivity matrix of ROI tetrahedra
- **RegionOfInterestVolume.tet\_idx\_node\_coord** (*np.ndarray [N\_points]*) – Tetrahedra indices of TetrahedraLinear object instance where the ROI nodes are lying in
- **RegionOfInterestVolume.tet\_idx\_tetrahedra\_center** (*np.ndarray [N\_tet\_roi]*) – Tetrahedra indices of TetrahedraLinear object instance where the center points of the ROI tetrahedra are lying in
- **RegionOfInterestVolume.tet\_idx\_triangle\_center** (*np.ndarray [N\_tri\_roi]*) – Tetrahedra indices of TetrahedraLinear object instance where the center points of the ROI triangle are lying in. If the ROI is directly generated from the msh instance using “make\_roi\_volume\_from\_msh”, these indices are the triangle indices of the head mesh since the ROI mesh and the head mesh are overlapping. If the ROI mesh is not the same as the head mesh, the triangle center of the ROI mesh are always lying in a tetrahedra of the head mesh (these indices are given in this case)

`pynibs.roi.clean_roi(img, vox_thres=0.5, fn_out=None)`

Remove values < vox thres from image.

#### Parameters

- `img (str or nibabel.nifti1.Nifti1Image)` –
- `vox_thres (float, optional)` –
- `fn_out (str)` –

#### Returns

- `img_thres (nibabel.nifti1.Nifti1Image)`
- `img_thres (<file>)` – If fn\_out is specified, thresholded image is saved here

`pynibs.roi.create_refine_spherical_roi(center, radius, final_tissues_nii, out_fn, target_size=0.5, outside_size=None, outside_factor=3, out_spher_fn=None, tissue_types=None, verbose=False)`

Create a spherical roi nifti for simnibs 4 refinement. Only tissue types accoring to \_tissue\_types will be refined.

Use the resulting output file as input for –sizing\_field in SimNIBS-4/simnibs/cli/meshmesh.py

#### Parameters

- `center (list of float)` – Center of spherical ROI in mm
- `radius (float)` – Radius of spherical ROI in mm
- `final_tissues_nii (string or nib.nifti1.Nifti1Image)` – final\_tissues.nii.gz to create roi for.
- `out_fn (str)` – Final output filename
- `target_size (float, default = 0.5)` – Target element size of refined areas in mm (?)
- `outside_size (float, default = None)` – Element size outside of target size.
- `outside_factor (float, default = None)` – Distance factor to define the ‘outside’ area: oudsiefactor \* radius -> outside
- `out_spher_fn (str, optional)` – Output filename of original, raw spherical ROI
- `tissue_types (list of float, default = [1,2,3])` – Which tissue types to refine. Defaults to WM, GM, CSF
- `verbose (bool, optional, default=False)` – Print additional information

`pynibs.roi.determine_element_idx_in_mesh(fname, msh, points, compute_baricentric=False)`

Finds the tetrahedron that contains each of the described points using a stochastic walk algorithm. Implemented from Devillers et al. (2002) [1]

#### Parameters

- `msh (pynibs.mesh.mesh_struct.TetrahedraLinear)` –
- `fname (str or None)` – Filename of saved .txt file containing the element indices (no data is saved when fname=None or fname="")
- `points (np.ndarray (N, 3) or list of np.ndarray)` – List of points to be queried
- `compute_baricentric (bool)` – Wether or not to compute baricentric coordinates of the points

#### Returns

- **th\_with\_points** (*np.ndarray*) – List with the tetrahedron that contains each point. If the point is outside the mesh, the value will be -1
- **baricentric** (*np.ndarray [n, 4]*(if *compute\_baricentric == True*)) – Baricentric coordinates of point. If the point is outside, a list of zeros

## Notes

`pynibs.roi.elem_workhorse(chunk, points_out, P1_all, P2_all, P3_all, P4_all, N_points_total, N_CPU)`

### Parameters

- **chunk** (*np.ndarray*) – Indices of points the CPU thread is computing the element indices for
- **points\_out** (*np.ndarray of float*) – (N\_points, 3) Coordinates of points, the tetrahedra indices are computed for
- **P1\_all** (*np.ndarray of float*) –
- **(N\_tet** –
- **tetrahedra** (3) *Coordinates of first point of* –
- **P2\_all** (*np.ndarray of float*) – (N\_tet, 3) Coordinates of second point of tetrahedra
- **P3\_all** (*np.ndarray of float*) – (N\_tet, 3) Coordinates of third point of tetrahedra
- **P4\_all** (*np.ndarray of float*) – (N\_tet, 3) Coordinates of fourth point of tetrahedra
- **N\_points\_total** (*int*) – Total number of points
- **N\_CPU** (*int*) – Number of CPU cores to use

### Returns

`tet_idx_local`

### Return type

`np.ndarray of int` (N\_points,)

`pynibs.roi.get_mask(areas, fn_annot, fn_inflated_fs, fn_out)`

Determine freesurfer average mask .overlay file, which is needed to generate subject specific ROIs.

### Parameters

- **areas** (*list of str*) – Brodmann areas (e.g. ['Brodmann.6', 'Brodmann.4', 'Brodmann.3', 'Brodmann.1'])
- **fn\_annot** (*str*) – Annotation file of freesurfer (e.g. 'FREESURFER\_DIR/fsaverage/label/lh.PALS\_B12\_Brodmann.annot')
- **fn\_inflated\_fs** (*str*) – Inflated surface of freesurfer average (e.g. 'FREESURFER\_DIR/fsaverage/surf/lh.inflated')
- **fn\_out** (*str*) – Filename of .overlay file of freesurfer mask

### Returns

`<File>` – fn\_out.overlay file of freesurfer mask

### Return type

.overlay file

`pynibs.roi.get_sphere_in_nii(center, radius, nii=None, out_fn=None, thresh_by_nii=True, val_in=1, val_out=0, outside_val=0, outside_radius=inf)`

Computes a spherical ROI for a given Nifti image (defaults to SimNIBS MNI T1 tissue). The ROI area is defined in nifti coordinates. By default, everything inside the ROI is set to 1, areas outside = 0. The ROI is further thresholded by the nifti. A nib.Nifti image is returned and optionally saved.

### Parameters

- **center** (*array-like*) – X, Y, Z coordinates in nifti space
- **radius** (*float*) – radius of sphere
- **nii** (*string or nib.nifti1.Nifti1Image, optional*) – The nifti image to work with.
- **out\_fn** (*string, optional*) – If provided, sphere ROI image is saved here
- **outside\_val** (*float, default = None*) – Value outside of outside\_radius.
- **outside\_radius** (*float, default = None*) – Distance factor to define the ‘outside’ area: outsidefactor \* radius -> outside
- **thresh\_by\_nii** (*bool, optional*) – Mask sphere by nii != 0
- **val\_in** (*float, optional*) – Value within ROI
- **val\_out** (*float, optional*) – Value outside ROI

### Returns

- **sphere\_img** (*nib.nifti1.Nifti1Image*)
- **sphere\_img** (*<file>, optional*)

### Raises

**ValueError** – If the final ROI is empty.

`pynibs.roi.load_roi_surface_obj_from_hdf5(fname)`

Loading and initializing RegionOfInterestSurface object/s from .hdf5 mesh file.

### Parameters

**fname** (*str*) – Filename (incl. path) of .hdf5 mesh file, e.g. from subject.fn\_mesh\_hdf5

### Returns

**RegionOfInterestSurface** – RegionOfInterestSurface

### Return type

*pynibs.roi.RegionOfInterestSurface* or list of *pynibs.roi.RegionOfInterestSurface*

`pynibs.roi.make_GM_WM_surface(gm_surf_fname, wm_surf_fname, mesh_folder,  
midlayer_surf_fname=None, delta=0.5, x_roi=None, y_roi=None,  
z_roi=None, layer=1, fn_mask=None, refine=False)`

Generating a surface between WM and GM in a distance of delta 0...1 for ROI, given by freesurfer mask or coordinates.

### Parameters

- **gm\_surf\_fname** (*str or list of str*) – Filename(s) of GM surface generated by freesurfer (lh and/or rh) (e.g. in mri2msh: fs\_ID/surf/lh.pial)
- **wm\_surf\_fname** (*str or list of str*) – Filename(s) of WM surface generated by freesurfer (lh and/or rh) (e.g. in mri2msh: fs\_ID/surf/lh.white)
- **mesh\_folder** (*str*) – Path of mesh (parent directory)
- **midlayer\_surf\_fname** (*str or list of str*) – filename(s) of midlayer surface generated by headreco (lh and/or rh) (e.g. in headreco: fs\_ID/surf/lh.central) (after conversion)
- **m2m\_mat\_fname** ([*defunct*]) – Filename of mri2msh transformation matrix (e.g. in mri2msh: m2m\_ProbandID/MNI2conform\_6DOF.mat)
- **delta** (*float*) – Distance parameter where surface is generated 0...1 (default: 0.5)
  - 0 -> WM surface
  - 1 -> GM surface

- **x\_roi** (*list of float or None*) – Region of interest [Xmin, Xmax], whole X range if empty [0,0] or None (left - right)
- **y\_roi** (*list of float or None*) – Region of interest [Ymin, Ymax], whole Y range if empty [0,0] or None (anterior - posterior)
- **z\_roi** (*list of float or None*) – Region of interest [Zmin, Zmax], whole Z range if empty [0,0] or None (inferior - superior)
- **layer** (*int*) – Define the number of layers:
  - 1: one layer
  - 3: additionally upper and lower layers are generated around the central midlayer
- **fn\_mask** (*string or None*) – Filename for freesurfer mask. If given, this is used instead of `*_ROIs`
- **refine** (*bool, optional, default: False*) – Refine ROI by splitting elements

**Returns**

- *if layer == 3*
- **surface\_points\_upper** (*np.ndarray of float*) – (N\_points, 3) Coordinates (x, y, z) of surface + epsilon (in GM surface direction)
- **surface\_points\_middle** (*np.ndarray of float*) – (N\_points, 3) Coordinates (x, y, z) of surface
- **surface\_points\_lower** (*np.ndarray of float*) – (N\_points, 3) Coordinates (x, y, z) of surface - epsilon (in WM surface direction)
- **connectivity** (*np.ndarray of int*) – (N\_tri x 3) Connectivity of triangles (indexation starts at 0!)
- *else*
- **surface\_points\_middle** (*np.ndarray of float*) – (N\_points, 3) Coordinates (x, y, z) of surface
- **connectivity** (*np.ndarray of int*) – (N\_tri x 3) Connectivity of triangles (indexation starts at 0!)

**Example**

```
make_GM_WM_surface(self, gm_surf_fname, wm_surf_fname, delta, X_ROI, Y_ROI, Z_ROI)
make_GM_WM_surface(self, gm_surf_fname, wm_surf_fname, delta, mask_fn, layer=3)
```

`pynibs.roi.nii2msh(mesh, m2m_dir, nii, out_folder, hem, out_fsaverage=False, roi_name='ROI')`

Transform a nifti ROI image to subject space .mgih file.

**Parameters**

- **mesh** (*simnibs.Mesh or str*) –
- **m2m\_dir** (*str*) –
- **nii** (*nibabel.nifti1.Nifti1Image or str*) –
- **out\_folder** (*str*) –
- **hem** (*str*) – ‘lh’ or ‘rh’
- **out\_fsaverage** (*bool*) –
- **roi\_name** (*str*) – How to name the ROI

**Returns**

`roi = f'{out_folder}/{hem}.mesh.central.{roi_name}'`

**Return type**  
file

## 1.1.10 pynibs.subject module

**class** pynibs.subject.**Subject**(*subject\_id*, *subject\_folder*)

Bases: **object**

Subject containing subject specific information, like mesh, roi, uncertainties, plot settings.

**self.id**

Subject id from MPI database

**Type**

str

### Notes

#### Initialization

sub = pynibs.subject(subject\_ID, mesh)

#### Parameters

**id**

[str] Subject id

**fn\_mesh**

[str] .msh or .hdf5 file containing the mesh information

#### Subject.seg, segmentation information dictionary

**fn\_lh\_wm**

[str] Filename of left hemisphere white matter surface

**fn\_rh\_wm**

[str] Filename of right hemisphere white matter surface

**fn\_lh\_gm**

[str] Filename of left hemisphere grey matter surface

**fn\_rh\_gm**

[str] Filename of right hemisphere grey matter surface

**fn\_lh\_curv**

[str] Filename of left hemisphere curvature data on grey matter surface

**fn\_rh\_curv**

[str] Filename of right hemisphere curvature data on grey matter surface

#### Subject.mri, mri information dictionary

**fn\_mri\_T1**

[str] Filename of T1 image

**fn\_mri\_T2**

[str] Filename of T2 image

**fn\_mri\_DTI**

[str] Filename of DTI dataset

**fn\_mri\_DTI\_bvec**

[str] Filename of DTI bvec file

**fn\_mri\_DTI\_bval**

[str] Filename of DTI bval file

**fn\_mri\_conform**

[str] Filename of conform T1 image resulting from SimNIBS mri2mesh function

**Subject.ps, plot settings dictionary**

see plot functions in para.py for more details

**Subject.exp, experiment dictionary****info**

[str] General information about the experiment

**date**

[str] Date of experiment (e.g. 01/01/2018)

**fn\_tms\_nav**

[str] Path to TMS navigator folder

**fn\_data**

[str] Path to data folder or files

**fn\_exp\_csv**

[str] Filename of experimental data .csv file containing the merged experimental data information

**fn\_coil**

[str] Filename of .ccd or .nii file of coil used in the experiment (contains ID)

**fn\_mri\_nii**

[str] Filename of MRI .nii file used during the experiment

**cond**

[str or list of str] Conditions in the experiment in the recorded order (e.g. ['PA-45', 'PP-00'])

**experimenter**

[str] Name of experimenter who conducted the experiment

**incidents**

[str] Description of special events occurred during the experiment

**Subject.mesh, mesh dictionary****info**

[str] Information about the mesh (e.g. discretization etc)

**fn\_mesh\_msh**

[str] Filename of the .msh file containing the FEM mesh

**fn\_mesh\_hdf5**

[str] Filename of the .hdf5 file containing the FEM mesh

**seg\_idx**

[int] Index indicating to which segmentation dictionary the mesh belongs

**Subject.roi region of interest dictionary****type**

[str] Specify type of ROI ('surface', 'volume')

**info**

[str] Info about the region of interest, e.g. "M1 midlayer from freesurfer mask xyz"

**region**

[list of str or float] Filename for freesurfer mask or [[X\_min, X\_max], [Y\_min, Y\_max], [Z\_min, Z\_max]]

**delta**

[float] Distance parameter between WM and GM (0 -> WM, 1 -> GM) (for surfaces only)

**add\_experiment\_info(exp\_dict)**

Adding information about a particular experiment.

**Parameters**

**exp\_dict** (*dict of dict or list of dict*) – Dictionary containing information about the experiment

**Notes**

**Adds Attributes**

**exp**

[list of dict] Dictionary containing information about the experiment

**add\_mesh\_info(mesh\_dict)**

Adding filename information of the mesh to the subject object (multiple filenames possible).

**Parameters**

**mesh\_dict** (*dictionary or list of dictionaries*) – Dictionary containing the mesh information

**Notes**

**Adds Attributes**

**Subject.mesh**

[list of dict] Dictionaries containing the mesh information

**add\_mri\_info(mri\_dict)**

Adding MRI information to the subject object (multiple MRIs possible).

**Parameters**

**mri\_dict** (*dictionary or list of dictionaries*) – Dictionary containing the MRI information of the subject

**Notes**

**Adds Attributes**

**Subject.mri**

[list of dict] Dictionary containing the MRI information of the subject

**add\_plotsettings(ps\_dict)**

Adding ROI information to the subject object (multiple ROIs possible).

**Parameters**

**ps\_dict** (*dictionary or list of dictionaries*) – Dictionary containing plot settings of the subject

**Notes**

**Adds Attributes**

**Subject.ps**

[list of dict] Dictionary containing plot settings of the subject

**add\_roi\_info(roi\_dict)**

Adding ROI (surface) information of the mesh with mesh\_index to the subject object (multiple ROIs possible).

**Parameters**

**roi\_dict** (*dict of dict or list of dictionaries*) – Dictionary containing the ROI information of the mesh with mesh\_index [mesh\_idx][roi\_idx]

**Notes****Adds Attributes**

**Subject.mesh[mesh\_index].roi**

[list of dict] Dictionaries containing ROI information

`pynibs.subject.check_file_and_format(fname)`

Checking existence of file and transforming to list if necessary.

**Parameters**

**fname** (*str or list of str*) – Filename(s) to check

**Returns**

**fname** – Checked filename(s) as list

**Return type**

*list of str*

`pynibs.subject.fill_from_dict(obj, d)`

Set all attributes from d in obj.

**Parameters**

- **obj** (*pynibs.Mesh or pynibs.ROI*) –
- **d** (*dict*) –

**Returns**

**obj**

**Return type**

*pynibs.Mesh or pynibs.ROI*

`pynibs.subject.load_subject(fname, filetype=None)`

Wrapper for pkl and hdf5 subject loader

**Parameters**

- **fname** (*str*) – endwith('.pkl') | endswith('.hdf5')
- **filetype** (*str*) – Explicitely set file version.

**Returns**

**subject**

**Return type**

*pynibs.subject.Subject*

`pynibs.subject.load_subject_hdf5(fname)`

Loading subject information from .hdf5 file and returning subject object.

**Parameters**

**fname** (*str*) – Filename with .hdf5 extension (incl. path)

**Returns**

**subject** – Loaded Subject object

**Return type**

*pynibs.subject.Subject*

`pynibs.subject.load_subject_pkl(fname)`

Loading subject object from .pkl file.

**Parameters**

`fname (str)` – Filename with .pkl extension

**Returns**

`subject` – Loaded Subject object

**Return type**

`pynibs.subject.Subject`

`pynibs.subject.save_subject(subject_id, subject_folder, fname, mri_dict=None, mesh_dict=None, roi_dict=None, exp_dict=None, ps_dict=None, **kwargs)`

Saves subject information in .pkl or .hdf5 format (preferred)

**Parameters**

- `subject_id (str)` – ID of subject
- `subject_folder (str)` – Subject folder
- `fname (str)` – Filename with .hdf5 or .pkl extension (incl. path)
- `mri_dict (list of dict, optional, default: None)` – MRI info
- `mesh_dict (list of dict, optional, default: None)` – Mesh info
- `roi_dict (list of list of dict, optional, default: None)` – Mesh info
- `exp_dict (list of dict, optional, default: None)` – Experiment info
- `ps_dict (list of dict, optional, default:None)` – Plot-settings info
- `kwargs (str or np.array)` – Additional information saved in the parent folder of the .hdf5 file

**Returns**

`<File>` – Subject information

**Return type**

.hdf5 file

`pynibs.subject.save_subject_hdf5(subject_id, subject_folder, fname, mri_dict=None, mesh_dict=None, roi_dict=None, exp_dict=None, ps_dict=None, overwrite=True, check_file_exist=False, verbose=False, **kwargs)`

Saving subject information in hdf5 file.

**Parameters**

- `subject_id (str)` – ID of subject
- `subject_folder (str)` – Subject folder
- `fname (str)` – Filename with .hdf5 extension (incl. path)
- `mri_dict (list of dict, optional, default: None)` – MRI info
- `mesh_dict (list of dict, optional, default: None)` – Mesh info
- `roi_dict (list of list of dict, optional, default: None)` – Mesh info
- `exp_dict (list of dict or dict of dict, optional, default: None)` – Experiment info
- `ps_dict (list of dict, optional, default:None)` – Plot-settings info
- `overwrite (bool)` – Overwrites existing .hdf5 file
- `check_file_exist (bool)` – Hide warnings.
- `verbose (bool)` – Print information about meshes and ROIs.

- **kwargs** (`str` or `np.ndarray`) – Additional information saved in the parent folder of the .hdf5 file

**Returns**

`<File>` – Subject information

**Return type**

.hdf5 file

`pynibs.subject.save_subject_pkl(sobj, fname)`

Saving subject object as pickle file.

**Parameters**

- **sobj** (`object`) – Subject object to save
- **fname** (`str`) – Filename with .pkl extension

**Returns**

`<File>` – Subject object instance

**Return type**

.pkl file

### 1.1.11 pynibs.tensor\_scaling module

`pynibs.tensor_scaling.ellipse_eccentricity(a, b)`

Calculates the eccentricity of an 2D ellipse with the semi axis a and b. An eccentricity of 0 corresponds to a sphere and an eccentricity of 1 means complete eccentric (line) with full restriction to the other axis

**Parameters**

- **a** (`float`) – First semi axis parameter
- **b** (`float`) – Second semi axis parameter

**Returns**

`e` – Eccentricity (0...1)

**Return type**

`float`

`pynibs.tensor_scaling.rescale_lambda_centerized(D, s, tsc=False)`

Rescales the eigenvalues of the matrix D according to their eccentricity. The scale factor is between 0...1 a scale factor of 0.5 would not alter the eigenvalues of the matrix D. A scale factor of 0 would unify all eigenvalues to one value such that it corresponds to a isotropic sphere. A scale factor of 1 alters the eigenvalues in such a way that the resulting ellipsoid is fully eccentric and anisotropic.

**Parameters**

- **D** (`ndarray of float [3 x 3]`) – Diffusion tensor
- **s** (`float`) – Scale parameter [0 (iso) ... 0.5 (unaltered)... 1 (aniso)]
- **tsc** (`boolean`) – Tensor singularity correction

**Returns**

`Ds` – Scaled diffusion tensor

**Return type**

`ndarray of float [3 x 3]`

`pynibs.tensor_scaling.rescale_lambda_centerized_workhorse(D, s, tsc=False)`

Rescales the eigenvalues of the matrix D according to their eccentricity. The scale factor is between 0...1 a scale factor of 0.5 would not alter the eigenvalues of the matrix D. A scale factor of 0 would unify all eigenvalues to one value such that it corresponds to a isotropic sphere. A scale factor of 1 alters the eigenvalues in such a way that the resulting ellipsoid is fully eccentric and anisotropic

### Parameters

- **D** (*ndarray of float [n x 9]*) – Diffusion tensor
- **s** (*float*) – Scale parameter [0 (iso) ... 0.5 (unaltered)... 1 (aniso)]
- **tsc** (*boolean*) – Tensor singularity correction

### Returns

**Ds** – Scaled diffusion tensor

### Return type

*list* of nparray of *float* [3 x 3]

## 1.1.12 pynibs.tms\_pulse module

`pynibs.tms_pulse.biphasic_pulse(t, R=0.0338, L=1.55e-05, C=0.0001936, alpha=1089.8, f=2900)`

Returns normalized single biphasic pulse waveform of electric field (first derivative of coil current)

### Parameters

- **t** (*ndarray of float [n\_t]*) – Time array in seconds
- **R** (*float, optional, default: 0.0338 Ohm*) – Resistance of coil in (Ohm)
- **L** (*float, optional, default: 15.5\*1e-6 H*) – Inductance of coil in (H)
- **C** (*float, optional, default: 193.6\*1e-6*) – Capacitance of coil in (F)
- **alpha** (*float, optional, default: 1089.8 1/s*) – Damping coefficient in (1/s)
- **f** (*float, optional, default: 2900 Hz*) – Frequency in (Hz)

### Returns

**e** – Normalized electric field time course (can be scaled with electric field)

### Return type

*ndarray of float [n\_t]*

- genindex
- modindex
- search

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**CHAPTER  
TWO**

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