# **NIRFASTerUFF**

Release 1.0.0

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NIRFAST was originally developed in 2001 as a MATLAB-based package used to model near-infrared light propagation through tissue and reconstruct images of optical biomarkers. At its core, NIRFAST is tool that does finite element modeling of the medium in which the light progagates, and calculates the fluence field by solving the diffusion equation.

A fully overhauled version, titled NIRFASTer, was published in 2018, thanks to the work of Dr. Stanisław Wojtkiewicz. In the new version, GPU support was added to the key algorithms, giving the software a dramatic boost in performance. The CPU versions of the algorithms were re-implemented in C++ with multithreading enabled, and the performance was improved considerably.

In this version, now titled NIRFASTerFF (Fast and Furious), the entire toolbox is re-written with Python as its interfacing language, while fully inter-operatable with the original Matlab version. The algorithms, running on both GPU and CPU, are yet again improved for even better performance. This is the compact, aka micro version of the NIRFASTerFF package.

This manual is a detailed documentation of all APIs in the package. Please also refer to the demos to see how the package is used in difference applications.

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# **ONE**

# **SUMMARY OF THE FUNCTIONALITIES**

Mesh types supported: standard

FEM solver calculates: CW fluence, FD fluence

СНАРТ	ΓER
TW	VO

# LINK TO THE FULL VERSION

https://github.com/milabuob/nirfaster-FF

**THREE** 

# **LINK TO THE MATLAB VERSION**

The original Matlab-based NIRFAST and NIRFASTer are still available for download, but we will gradually drop our support for them.

https://github.com/nirfast-admin/NIRFAST

https://github.com/nirfaster/NIRFASTer

# **FOUR**

# **REFERENCES**

If you use our package, please cite,

H. Dehghani, M.E. Eames, P.K. Yalavarthy, S.C. Davis, S. Srinivasan, C.M. Carpenter, B.W. Pogue, and K.D. Paulsen, "Near infrared optical tomography using NIRFAST: Algorithm for numerical model and image reconstruction," Communications in Numerical Methods in Engineering, vol. 25, 711-732 (2009) doi:10.1002/cnm.1162

**FIVE** 

# **API DOCUMENTATION**

# 5.1 nirfasteruff

# Modules

nirfasteruff.nirfasteruff
nirfasteruff.nirfasteruff\_cpu
nirfasteruff.nirfasteruff\_cuda

# 5.1.1 nirfasteruff.nirfasteruff

# **Classes**

base()	Dummy class holding the core classes Dummy class used so the function hierarchy can be compatible with the full version
forward()	Dummy class holding the forward modeling functions.
io()	Dummy class holding some I/O functions Dummy class used so the function hierarchy can be compatible with the full version
math()	Dummy class holding some low-level functions.
meshing()	
utils()	Dummy class holding some helper functions and helper classes Dummy class used so the function hierarchy can be compatible with the full version

# nirfasteruff.nirfasteruff.base

#### class nirfasteruff.nirfasteruff.base

```
Bases: object
```

Dummy class holding the core classes Dummy class used so the function hierarchy can be compatible with the full version

```
__init__()
```

# **Methods**

```
__init__()
```

#### class FDdata

Bases: object

Class holding FD/CW data.

# phi

Fluence from each source. If mesh contains non-tempty field vol, this will be represented on the grid. Last dimension has the size of the number of sources

# **Type**

double Numpy array

# complex

Complex amplitude of each channel. Same as amplitude in case of CW data

# Type

double or complex double Numpy vector

# link

Defining all the channels (i.e. source-detector pairs). Copied from mesh.link

#### Type

int32 NumPy array

# amplitude

Absolute amplitude of each channel. I.e. amplitude=abs(complex)

#### Type

double Numpy vector

# phase

phase data of each channel. All zero in case of CW data

# Type

double Numpy vector

### vol

Information needed to convert between volumetric and mesh space. Copied from mesh.vol

#### Type

nirfaseterff.base.meshvol

#### isvol()

Checks if data is in volumetric space.

# Returns

True if data is in volumetric space, False if not.

# Return type

bool

#### togrid(mesh)

Convert data to volumetric space as is defined in mesh.vol. If it is empty, the function does nothing.

If data is already in volumetric space, function casts data to the new volumetric space

```
CAUTION: This OVERRIDES the field phi
```

#### **Parameters**

**mesh** (nirfasteruff.base.stndmesh) — mesh whose .vol attribute is used to do the conversion.

#### Return type

None.

# tomesh(mesh)

Convert data back to mesh space using information defined in mesh.vol. If data.vol is empty, the function does nothing.

CAUTION: This OVERRIDES the field phi

#### **Parameters**

**mesh** (nirfasteruff.base.stndmesh) — mesh whose .vol attribute is used to do the conversion.

# Return type

None.

#### class meshvol

Bases: object

Small class holding the information needed for converting between mesh and volumetric space. Values calculated by nirfasteruff.base.\*mesh.gen\_intmat

Note that the volumetric space, defined by xgrid, ygrid, and zgrid (empty for 2D mesh), must be uniform

# xgrid

```
x grid of the volumetric space. In mm

Type

double Numpy array
```

# ygrid

```
y grid of the volumetric space. In mm
Type
double Numpy array
```

#### zgrid

```
z grid of the volumetric space. In mm. Empty for 2D meshes

Type

double Numpy array
```

# mesh2grid

matrix converting a vector in mesh space to volumetric space, done by mesh2grid.dot(data)

The result is vectorized in 'F' (Matlab) order

Size: (len(xgrid)\*len(ygrid)\*len(zgrid), NNodes)

# Type

double CSR sparse matrix

```
gridinmesh
         indices (one-based) of data points in the volumetric space that are within the mesh space, vectorized
         in 'F' order.
              Type
                int32 NumPy array
     res
         resolution in x, y, z (if 3D) direction, in mm. Size (2,) or (3,)
              Type
                double NumPy array
     grid2mesh
         matrix converting volumetric data, vectorized in 'F' order, to mesh space.
                                                                                                  Done by
         grid2mesh.dot(data)
         Size (Nnodes, len(xgrid)*len(ygrid)*len(ygrid))
                double CSR sparse matrix
     meshingrid
         indices (one-based) of data points in the mesh space that are within the volumetric space
              Type
                int32 NumPy array
class optode(coord=[])
     Bases: object
     Class for NIRFASTer optodes, which can be either a group of sources or a group of detectors.
     Note: The field fwhm for sources in the Matlab version has been dropped.
     fixed
         whether an optode is fixed.
         If not, it will be moved to one scattering length inside the surface (source) or on the surface (detector).
         Default: 0
              Type
                bool like
     num
         indexing of the optodes, starting from one (1,2,3,...)
              Type
                double NumPy vector
     coord
         each row is the location of an optode. Unit: mm
              Type
                double NumPy array
     int_func
         First column is the index (one-based) of the element each optode is in.
         The subsequent columns are the barycentric coordinates (i.e. integration function) in the correponding
         elements. Size (N, dim+2).
              Type
                double NumPy array
```

#### move\_detectors(mesh)

Moves detector to the appropriate locations in the mesh.

For each detector, first move it to the closest point on the surface of the mesh.

Integration functions are NOT calculated after moving, to be consistent with the Matlab version.

# **Parameters**

**mesh** (NIRFASTer mesh type) – The mesh on which the detectors are installed. Should be a 'stndmesh', either 2D or 3D

#### Raises

**ValueError** – If mesh.elements does not have 3 or 4 columns, or mesh.dimension is not 2 or 3.

#### Return type

None.

#### move\_sources(mesh)

Moves sources to the appropriate locations in the mesh.

For each source, first move it to the closest point on the surface of the mesh, and then move inside by one scattering length along surface normal.

where scattering length is  $1/\mu_s'$ 

Integration functions are also calculated after moving.

#### **Parameters**

**mesh** (NIRFASTer mesh type) – The mesh on which the sources are installed. Should be a 'stndmesh', either 2D or 3D

#### Raises

- **TypeError** If mesh type is not recognized.
- **ValueError** If mesh.elements does not have 3 or 4 columns, or mesh.dimension is not 2 or 3.

# Return type

None.

#### touch\_detectors(mesh)

Recalculate/fill in all other fields based on 'fixed' and 'coord'.

This is useful when a set of detectors are manually added and only the locations are specified.

For non-fixed detectors, function 'move\_detectors' is first called, and integration functions are calculated subsequentely.

For fixed detectors, recalculates integration functions directly.

If no detector locations are specified, the function does nothing

#### **Parameters**

**mesh** (*NIRFASTer mesh type*) – The mesh on which the sources are installed. Should be a 'stndmesh', either 2D or 3D

# Return type

None.

#### touch\_sources(mesh)

Recalculate/fill in all other fields based on 'fixed' and 'coord'.

This is useful when a set of sources are manually added and only the locations are specified.

For non-fixed sources, function 'move\_sources' is called, otherwise recalculates integration functions directly

If no source locations are specified, the function does nothing

```
Parameters
                mesh (NIRFASTer mesh type) – The mesh on which the sources are installed. Should be
                a 'stndmesh', either 2D or 3D
             Return type
                None.
class stndmesh
     Bases: object
     Main class for standard mesh. The methods should cover most of the commonly-used functionalities
     name
         name of the mesh. Default: 'EmptyMesh'
             Type
                str
     nodes
         locations of nodes in the mesh. Unit: mm. Size (NNodes, dim)
             Type
                double NumPy array
     bndvtx
         indicator of whether a node is at boundary (1) or internal (0). Size (NNodes,)
                double NumPy array
     type
         type of the mesh. It is always 'stnd'.
             Type
                str
     mua
         absorption coefficient (mm^-1) at each node. Size (NNodes,)
             Type
                double NumPy array
     kappa
         diffusion coefficient (mm) at each node. Size (NNodes,). Defined as 1/(3*(mua + mus))
             Type
                double NumPy array
     ri
         refractive index at each node. Size (NNodes,)
             Type
                double NumPy array
     mus
         reduced scattering coefficient (mm^-1) at each node. Size (NNodes,)
                (double NumPy array
     elements
         triangulation (tetrahedrons or triangles) of the mesh, Size (NElements, dim+1)
         Row i contains the indices of the nodes that form tetrahedron/triangle i
         One-based indexing for direct interoperatability with the Matlab version
```

```
Type
          double NumPy array
region
    region labeling of each node. Starting from 1. Size (NNodes,)
          double NumPy array
source
    information about the sources
        Type
          nirfasteruff.base.optode
meas
    information about the the detectors
        Type
          nirfasteruff.base.optode
link
    list of source-detector pairs, i.e. channels. Size (NChannels,3)
    First column: source; Second column: detector; Third column: active (1) or not (0)
        Type
          int32 NumPy array
c
    light speed (mm/sec) at each node. Size (NNodes,). Defined as c0/ri, where c0 is the light speed in
    vacuum
        Type
          double NumPy array
ksi
    photon fluence rate scale factor on the mesh-outside_mesh boundary as derived from Fresenel's law.
    Size (NNodes,)
        Type
          double NumPy array
element_area
    volume/area (mm^3 or mm^2) of each element. Size (NElements,)
          double NumPy array
support
    total volume/area of all the elements each node belongs to. Size (NNodes,)
        Type
          double NumPy array
vol
    object holding information for converting between mesh and volumetric space.
        Type
          nirfasteruff.base.meshvol
change_prop(idx, prop)
    Change optical properties (mua, musp, and ri) at nodes specified in idx, and automatically change
    fields kappa, c, and ksi as well
        Parameters
```

- idx (1ist or NumPy array or -1) zero-based indices of nodes to change. If idx==-1, function changes all the nodes
- **prop** (*list or NumPy array of length 3*) new optical properties to be assigned to the specified nodes. [mua(mm-1) musp(mm-1) ri].

#### Return type

None.

**femdata**(freq, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates fluences for each source using a FEM solver, and then the boudary measurables for each channel

If mesh.vol is set, fluence data will be represented in volumetric space

See femdata\_stnd\_CW() and femdata\_stnd\_FD() for details

#### **Parameters**

- **freq** (*double*) modulation frequency in Hz. If CW, set to zero and a more efficient CW solver will be used.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasteruff.utils.SolverOptions, optional) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Returns

• **data** (*nirfasteruff.base.FDdata*) – fluence and boundary measurables given the mesh and optodes.

See FDdata() for details.

• **info** (*nirfasteruff.utils.ConvergenceInfo*) – convergence information of the solver.

See ConvergenceInfo() for details

# from\_copy(mesh)

Deep copy all fields from another mesh.

#### **Parameters**

mesh (nirfasteruff.base.stndmesh) - the mesh to copy from.

# **Return type**

None.

# from\_file(file)

Read from classic NIRFAST mesh (ASCII) format, not checking the correctness of the loaded integration functions.

All fields after loading should be directly compatible with Matlab version.

# Parameters

**file** (str) – name of the mesh. Any extension will be ignored.

# **Return type**

None.

# **Examples**

```
>>> mesh = nirfasteruff.base.stndmesh()
>>> mesh.from_file('meshname')
```

# from\_mat(matfile, varname=None)

Read from Matlab .mat file that contains a NIRFASTer mesh struct. All fields copied as is without error checking.

#### **Parameters**

- **matfile** (*str*) name of the .mat file to load. Use of extension is optional.
- **varname** (*str*, *optional*) if your .mat file contains multiple variables, use this argument to specify which one to load. The default is None.

When *varname==None*, *matfile* should contain exatly one structure, which is a NIR-FASTer mesh, or the function will do nothing

# **Return type**

None.

**from\_solid**(ele, nodes, prop=None, src=None, det=None, link=None)

Construct a NIRFASTer mesh from a 3D solid mesh generated by a mesher. Similar to the solidmesh2nirfast function in Matlab version.

Can also set the optical properties and optodes if supplied

#### **Parameters**

• **ele**(*int/double NumPy array*) – element list in one-based indexing. If four columns, all nodes will be labeled as region 1

If five columns, the last column will be used for region labeling.

- **nodes** (*double NumPy array*) node locations in the mesh. Unit: mm. Size (NNodes,3).
- **prop** (double NumPy array, optional) If not None, calls stndmesh.set\_prop() and sets the optical properties in the mesh. The default is None.

See set\_prop() for details.

• **src** (nirfasteruff.base.optode, *optional*) – If not *None*, sets the sources and moves them to the appropriate locations. The default is None.

See touch\_sources() for details.

• **det** (nirfasteruff.base.optode, *optional*) – If not *None*, sets the detectors and moves them to the appropriate locations. The default is None.

See touch\_detectors() for details.

• link (int32 NumPy array, optional) — If not None, sets the channel information. Uses one-based indexing. The default is None.

Each row represents a channel, in the form of [src, det, active], where active is 0 or 1

If *link* contains only two columns, all channels are considered active.

# Return type

None.

 $\textbf{from\_volume}(\textit{vol}, \textit{param=utils.MeshingParams}(), \textit{prop=None}, \textit{src=None}, \textit{det=None}, \textit{link=None})$ 

Construct mesh from a segmented 3D volume using the built-in CGAL mesher. Calls stndmesh.from solid after meshing step.

#### **Parameters**

• **vol** (*uint8 NumPy array*) – 3D segmented volume to be meshed. 0 is considered as outside. Regions labeled using unique integers.

• param (nirfasteruff.utils.MeshingParams, optional) — parameters used in the CGAL mesher. If not specified, uses the default parameters defined in nirfasteruff.utils.MeshingParams().

Please modify fields xPixelSpacing, yPixelSpacing, and SliceThickness if your volume doesn't have [1,1,1] resolution

See MeshingParams() for details.

• **prop** (double NumPy array, optional) – If not None, calls stndmesh.set\_prop() and sets the optical properties in the mesh. The default is None.

See set\_prop() for details.

• **src** (nirfasteruff.base.optode, optional) – If not *None*, sets the sources and moves them to the appropriate locations. The default is None.

See touch\_sources() for details.

• **det** (nirfasteruff.base.optode, optional) – If not *None*, sets the detectors and moves them to the appropriate locations. The default is None.

See touch\_detectors() for details.

• link (int32 NumPy array, optional) — If not None, sets the channel information. Uses one-based indexing. The default is None.

Each row represents a channel, in the form of [src, det, active], where active is 0 or 1

If link contains only two columns, all channels are considered active.

### Return type

None.

# gen\_intmat(xgrid, ygrid, zgrid=[])

Calculate the information needed to convert data between mesh and volumetric space, specified by x, y, z (if 3D) grids.

All grids must be uniform. The results will from a nirfasteruff.base.meshvol object stored in field .vol

If field .vol already exists, it will be calculated again, and a warning will be thrown

#### **Parameters**

- **xgrid** (double NumPy array) x grid in mm.
- ygrid (double NumPy array) x grid in mm.
- **zgrid** (double NumPy array, optional) x grid in mm. Leave empty for 2D meshes. The default is [].

#### Raises

**ValueError** – if grids not uniform, or zgrid empty for 3D mesh

#### Return type

None.

#### isvol()

Check if convertion matrices between mesh and volumetric spaces are calculated

#### Returns

True if attribute .vol is calculate, False if not.

### Return type

bool

#### save\_nirfast(filename)

Save mesh in the classic NIRFASTer ASCII format, which is directly compatible with the Matlab version

# **Parameters**

**filename** (*str*) – name of the file to be saved as. Should have no extensions.

# Return type

None.

# set\_prop(prop)

Set optical properties of the whole mesh, using information provided in prop.

#### **Parameters**

**prop** (double NumPy array) – optical property info, similar to the MCX format:

```
[region mua(mm-1) musp(mm-1) ri]
[region mua(mm-1) musp(mm-1) ri]
[...]
```

where 'region' is the region label, and they should match exactly with unique(mesh.region). The order doesn't matter.

# Return type

None.

#### touch\_optodes()

Moves all optodes (if non fixed) and recalculate the integration functions (i.e. barycentric coordinates).

See touch\_sources() and touch\_detectors() for details

#### Return type

None.

### nirfasteruff.nirfasteruff.forward

#### class nirfasteruff.nirfasteruff.forward

Bases: object

Dummy class holding the forward modeling functions. Dummy class used so the function hierarchy can be compatible with the full version

```
__init__()
```

#### **Methods**

```
__init__()

femdata_stnd_CW([solver, opt]) Forward modeling for CW.

femdata_stnd_FD(freq[, solver, opt]) Forward modeling for FD.
```

# femdata\_stnd\_CW(solver=utils.get\_solver(), opt=utils.SolverOptions())

Forward modeling for CW. Please consider using mesh.femdata(0) instead.

The function calculates the FEM MASS matrix, the source vectors, and calls the CW solver (preconditioned conjugated gradient).

#### **Parameters**

- mesh (nirfasteruff.base.stndmesh) the mesh used to calcuate the forward data.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified

• **opt** (nirfasteruff.utils.SolverOptions, *optional*) – Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Raises

**TypeError** – If mesh is not a stnd mesh.

#### Returns

• **data** (*nirfasteruff.base.FDdata*) – fluence and boundary measurables given the mesh and optodes.

If mesh.vol is defined, the returned fluence will be in volumetric space

See FDdata() for details.

• **info** (*nirfasteruff.utils.ConvergenceInfo*) – convergence information of the solver.

See ConvergenceInfo() for details

#### See also:

```
get_field_CW(), gen_mass_matrix(), and gen_sources()
```

**femdata\_stnd\_FD**(freq, solver=utils.get\_solver(), opt=utils.SolverOptions())

Forward modeling for FD. Please consider using mesh.femdata(freq) instead. freq in Hz

The function calculates the MASS matrix, the source vectors, and calls the FD solver (preconditioned BiCGStab).

#### **Parameters**

- mesh (nirfasteruff.base.stndmesh) the mesh used to calcuate the forward data.
- **freq** (*double*) modulation frequency in Hz.

When it is 0, function continues with the BiCGstab solver, but generates a warning that the CW solver should be used for better performance

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasteruff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Raises

**TypeError** – If mesh is not a stnd mesh.

# Returns

• **data** (*nirfasteruff.base.FDdata*) – fluence and boundary measurables given the mesh and optodes.

If mesh.vol is defined, the returned fluence will be in volumetric space

See FDdata() for details.

• **info** (*nirfasteruff.utils.ConvergenceInfo*) – convergence information of the solver.

See ConvergenceInfo() for details

#### See also:

```
get_field_FD(), gen_mass_matrix(), and gen_sources()
```

# nirfasteruff.nirfasteruff.io

#### class nirfasteruff.nirfasteruff.io

Bases: object

Dummy class holding some I/O functions Dummy class used so the function hierarchy can be compatible with the full version

```
__init__()
```

#### **Methods**

init()	
readMEDIT()	Read a mesh generated by the CGAL mesher, which is saved in MEDIT format
saveinr(fname[, xPixelSpacing,])	Save a volume in the INRIA format.

# readMEDIT()

Read a mesh generated by the CGAL mesher, which is saved in MEDIT format

Directly translated from the Matlab version

#### **Parameters**

**fname** (str) – name of the file to be loaded.

#### **Returns**

- elements (NumPy array) list of elements in the mesh. Zero-based
- nodes (NumPy array) node locations of the mesh, in mm.
- **faces** (*NumPy array*) list of faces in the mesh. In case of 2D, it's the same as elements. Zero-based
- nnpe (int) size of dimension 1 of elements, i.e. 4 for 3D mesh and 3 for 2D mesh.

saveinr(fname, xPixelSpacing=1., yPixelSpacing=1., SliceThickness=1.)

Save a volume in the INRIA format. This is for the CGAL mesher.

Directly translated from the Matlab version

#### **Parameters**

- **vol** (*NumPy array*) the volume to be saved.
- **fname** (*str*) file name to be saved as.
- **xPixelSpacing** (*double*, *optional*) volume resolution in x direction. The default is 1..
- **yPixelSpacing** (*double*, *optional*) volume resolution in y direction. The default is 1..
- **SliceThickness** (*double*, *optional*) volume resolution in z direction. The default is 1..

### Return type

None.

#### nirfasteruff.nirfasteruff.math

#### class nirfasteruff.nirfasteruff.math

Bases: object

Dummy class holding some low-level functions. Be careful using them: they interact closely with the C++ functions and wrong arguments used can cause unexpected crashes. Dummy class used so the function hierarchy can be compatible with the full version

\_\_init\_\_()

#### **Methods**

init()	
<pre>gen_mass_matrix(omega[, solver, GPU])</pre>	Calculate the MASS matrix, and return the coordinates in CSR format.
gen_sources()	Calculate the source vectors (point source only) for the sources in mesh.source field
<pre>get_boundary_data(phi)</pre>	Calculates boundary data given the field data in mesh
<pre>get_field_CW(csrJ, csrV, qvec[, opt, solver])</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.
<pre>get_field_FD(csrJ, csrV, qvec[, opt, solver])</pre>	Call the Preconditioned BiConjugate Stablized solver with FSAI preconditioner.

### gen\_mass\_matrix(omega, solver=utils.get\_solver(), GPU=-1)

Calculate the MASS matrix, and return the coordinates in CSR format.

The current Matlab version outputs COO format, so the results are NOT directly compatible

If calculation fails on GPU (if chosen), it will generate a warning and automatically switch to CPU

#### **Parameters**

- mesh (nirfasteruff.base.stndmesh) the mesh used to calculate the MASS matrix.
- **omega** (*double*) modulation frequency, in radian.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **GPU** (*int*, *optional*) GPU selection. -1 for automatic, 0, 1, ... for manual selection on multi-GPU systems. The default is -1.

# Raises

- RuntimeError if both CUDA and CPU versions fail.
- **TypeError** if 'solver' is not 'CPU' or 'GPU'.

#### **Returns**

- **csrI** (*int32 NumPy vector, zero-based*) I indices of the MASS matrix, in CSR format. Size (NNodes,)
- **csrJ** (*int32 NumPy vector, zero-based*) J indices of the MASS matrix, in CSR format. Size (nnz(MASS),)

• **csrV** (*float64 or complex128 NumPy vector*) – values of the MASS matrix, in CSR format. Size (nnz(MASS),)

# gen\_sources()

Calculate the source vectors (point source only) for the sources in mesh.source field

#### **Parameters**

**mesh** (NIRFASTer mesh type) – mesh used to calculate the source vectors. Source information is also defined here.

#### Returns

**qvec** – source vectors, where each column corresponds to one source. Size (NNodes, Nsources).

# Return type

complex double NumPy array

#### get\_boundary\_data(phi)

Calculates boundary data given the field data in mesh

The field data can be any of the supported type: fluence, TPSF, or moments

#### **Parameters**

- **mesh** (*nirfasteruff mesh type*) the mesh whose boundary and detectors are used for the calculation.
- **phi** (double or complex double NumPy array) field data as calculated by one of the 'get\_field\_\*' solvers. Size (NNodes, NSources)

#### Returns

**data** – measured boundary data at each channel. Size (NChannels,).

# **Return type**

double or complex double NumPy array

get\_field\_CW(csrJ, csrV, qvec, opt=utils.SolverOptions(), solver=utils.get\_solver())

Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner. For CW data only.

The current Matlab version uses COO format input, so they are NOT directly compatible

If calculation fails on GPU (if chosen), it will generate a warning and automatically switch to CPU.

On GPU, the algorithm first tries to solve for all sources simultaneously, but this can fail due to insufficient GPU memory.

If this is the case, it will generate a warning and solve the sources one by one. The latter is not as fast, but requires much less memory.

On CPU, the algorithm only solves the sources one by one.

#### **Parameters**

- csrI (int32 NumPy vector, zero-based) I indices of the MASS matrix, in CSR format.
- csrJ (int32 NumPy vector, zero-based) J indices of the MASS matrix, in CSR format.
- csrV (double NumPy vector) values of the MASS matrix, in CSR format.
- **qvec** (double NumPy array, or Scipy CSC sparse matrix) The source vectors. i-th column corresponds to source i. Size (NNode, NSource)

See gen\_sources() for details.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasteruff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Raises

- TypeError if MASS matrix and source vectors are not both real, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

#### Returns

- phi (double NumPy array) Calculated fluence at each source. Size (NNodes, Nsources)
- **info** (*nirfasteruff.utils.ConvergenceInfo*) convergence information of the solver. See ConvergenceInfo() for details

#### See also:

gen\_mass\_matrix()

get\_field\_FD(csrJ, csrV, qvec, opt=utils.SolverOptions(), solver=utils.get\_solver())

Call the Preconditioned BiConjugate Stablized solver with FSAI preconditioner.

This is designed for FD data, but can also work for CW is an all-zero imaginary part is added to the MASS matrix and source vectors.

The current Matlab version uses COO format input, so they are NOT directly compatible

If calculation fails on GPU (if chosen), it will generate a warning and automatically switch to CPU.

On GPU, the algorithm first tries to solve for all sources simultaneously, but this can fail due to insufficient GPU memory.

If this is the case, it will generate a warning and solve the sources one by one. The latter is not as fast, but requires much less memory.

On CPU, the algorithm only solves the sources one by one.

# **Parameters**

- csrI (int32 NumPy vector, zero-based) I indices of the MASS matrix, in CSR format.
- csrJ (int32 NumPy vector, zero-based) J indices of the MASS matrix, in CSR format.
- csrV (complex double NumPy vector) values of the MASS matrix, in CSR format.
- **qvec** (complex double NumPy array, or Scipy CSC sparse matrix) The source vectors. i-th column corresponds to source i. Size (NNode, NSource)

See gen\_sources() for details.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasteruff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Raises

- **TypeError** if MASS matrix and source vectors are not both complex, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

#### **Returns**

- **phi** (*complex double NumPy array*) Calculated fluence at each source. Size (NNodes, Nsources)
- **info** (*nirfasteruff.utils.ConvergenceInfo*) convergence information of the solver. See ConvergenceInfo() for details

#### See also:

```
gen_mass_matrix()
```

# nirfasteruff.nirfasteruff.meshing

# class nirfasteruff.nirfasteruff.meshing

```
Bases: object
__init__()
```

# **Methods**

RunCGALMeshGenerator([opt])	Generate a tetrahedral mesh from a volume using CGAL 6.0.1 mesher, where different regions are labeled used a distinct integer.
init()	

# RunCGALMeshGenerator(opt=utils.MeshingParams())

Generate a tetrahedral mesh from a volume using CGAL 6.0.1 mesher, where different regions are labeled used a distinct integer.

Internallly, the function makes a system call to the mesher binary, which can also be used standalone through the command line.

Also runs a pruning steps after the mesh generation, where nodes not referred to in the element list are removed.

#### **Parameters**

- mask (uint8 NumPy array) 3D volumetric data defining the space to mesh. Regions defined by different integers. 0 is background.
- **opt** (nirfasteruff.utils.MeshingParams, *optional*) meshing parameters used. Default values will be used if not specified.

See nirfasteruff.utils.MeshingParams() for details

#### Returns

• **ele** (*int NumPy array*) – element list calculated by the mesher, one-based. Last column indicates the region each element belongs to

• **nodes** (*double NumPy array*) – element list calculated by the mesher, in mm.

#### References

https://doc.cgal.org/latest/Mesh\_3/index.html#Chapter\_3D\_Mesh\_Generation

# nirfasteruff.nirfasteruff.utils

# class nirfasteruff.nirfasteruff.utils

Bases: object

Dummy class holding some helper functions and helper classes Dummy class used so the function hierarchy can be compatible with the full version

\_\_init\_\_()

#### **Methods**

init()	
<pre>check_element_orientation_2d(nodes)</pre>	Make sure the 2D triangular elements are oriented counter clock wise.
<pre>get_nthread()</pre>	Choose the number of OpenMP threads in CPU solvers
<pre>get_solver()</pre>	Get the default solver.
isCUDA()	Checks if system has a CUDA device with compute capability >=5.2
<pre>pointLineDistance(B, p)</pre>	Calculate the distance between a point and a line (defined by two points), and find the projection point
pointLocation(pointlist)	Similar to Matlab's pointLocation function, queries which elements in mesh the points belong to, and also calculate the barycentric coordinates.
pointTriangleDistance(P)	Calculate the distance between a point and a triangle (defined by three points), and find the projection point

# class ConvergenceInfo(info=None)

Bases: object

Convergence information of the FEM solvers. Only used internally as a return type of functions nir-fasteruff.math.get\_field $_*$ 

Constructed using the output of the internal C++ functions

# isConverged

if solver converged to relative tolerance, for each rhs **Type** 

bool array

# isConvergedToAbsoluteTolerance

if solver converged to absolute tolerance, for each rhs

Type

bool array

```
iteration
         iterations taken to converge, for each rhs
              Type
                int array
     residual
         final residual, for each rhs
              Type
                double array
class MeshingParams(xPixelSpacing=1., yPixelSpacing=1., SliceThickness=1., facet_angle=25.,
                         facet_size=3., facet_distance=2., cell_radius_edge=3., general_cell_size=3.,
                         subdomain=np.array([0., 0.]), lloyd_smooth=True, offset=None)
     Bases: object
     Parameters to be used by the CGAL mesher. Note: they should all be double
     xPixelSpacing
         voxel distance in x direction. Default: 1.0
             Type
                double
     yPixelSpacing
         voxel distance in y direction. Default: 1.0
              Type
                double
     SliceThickness
         voxel distance in z direction. Default: 1.0
              Type
                double
     facet_angle
         lower bound for the angle (in degrees) of surface facets. Default: 25.0
              Type
                double
     facet_size
         upper bound for the radii of surface Delaunay balls circumscribing the facets. Default: 3.0
              Type
                double
     facet_distance
         upper bound for the distance between the circumcenter of a surface facet and the center of its surface
         Delaunay ball. Default: 2.0
              Type
                double
     cell_radius_edge
         upper bound for the ratio between the circumradius of a mesh tetrahedron and its shortest edge. Default:
         3.0
              Type
                double
     general_cell_size
         upper bound on the circumradii of the mesh tetrahedra, when no region-specific parameters (see below)
```

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are provided. Default: 3.0

```
Type double
```

#### subdomain

Specify cell size for each region, in format:

```
[region_label1, cell_size1]
[region_label2, cell_size2]
...
```

If a region is not specified, value in "general\_cell\_size" will be used. Default: np.array([0., 0.])

#### Type

double Numpy array

# lloyd\_smooth

Switch for Lloyd smoother before local optimization. This can take up to 120s (hard limit set) but improves mesh quality. Default: True

Type

bool

# offset

offset value to be added to the nodes after meshing. Size (3,). Defualt: None

#### Type

double Numpy array

#### **Notes**

Refer to CGAL documentation for details of the meshing algorithm as well as its parameters

https://doc.cgal.org/latest/Mesh\_3/index.html#Chapter\_3D\_Mesh\_Generation

```
class SolverOptions(max_iter=1000, AbsoluteTolerance=1e-12, RelativeTolerance=1e-12, divergence=1e8, GPU=-1)
```

Bases: object

Parameters used by the FEM solvers, Equivalent to 'solver options' in the Matlab version

#### max\_iter

```
maximum number of iterations allowed. Default: 1000
```

Type int

#### AbsoluteTolerance

Absolute tolerance for convergence. Default: 1e-12

**Type** 

double

# RelativeTolerance

Relative (to the initial residual norm) tolerance for convergence. Default: 1e-12

Type

double

#### divergence

Stop the solver when residual norm greater than this value. Default: 1e8

Type

double

```
GPU
         GPU selection. -1 for automatic, 0, 1, ... for manual selection on multi-GPU systems. Default: -1
             Type
               int
check_element_orientation_2d(nodes)
     Make sure the 2D triangular elements are oriented counter clock wise.
     This is a direct translation from the Matlab version.
         Parameters
              • ele (NumPy array) – Elements in a 2D mesh. One-based. Size: (NNodes, 3).
              • nodes (NumPy array) – Node locations in a 2D mesh. Size: (NNodes, 2).
         Raises
             TypeError – If ele does not have three rows, i.e. not a 2D triangular mesh.
         Returns
             ele - Re-oriented element list.
         Return type
             NumPy array
get_nthread()
     Choose the number of OpenMP threads in CPU solvers
```

On CPUs with no hyperthreading, all physical cores are used Otherwise use min(physical\_core, 8), i.e. no more than 8

This is heuristically determined to avoid performance loss due to memory bottlenecking

Advanced user can directly modify this function to choose the appropriate number of threads

#### **Returns**

nthread - number of OpenMP threads to use in CPU solvers.

#### **Return type**

int

# get\_solver()

Get the default solver.

#### Returns

If isCUDA is true, returns 'GPU', otherwise 'CPU'.

# Return type

str

# isCUDA()

Checks if system has a CUDA device with compute capability >=5.2

On a Mac machine, it automatically returns False without checking

#### Returns

True if a CUDA device with compute capability >=5.2 exists, False if not.

#### Return type

bool

#### pointLineDistance(B, p)

Calculate the distance between a point and a line (defined by two points), and find the projection point

This is a direct translation from the Matlab version

#### **Parameters**

- A (NumPy array) first point on the line. Size (2,) or (3,)
- **B** (NumPy array) second point on the line. Size (2,) or (3,)
- **p** (NumPy array) point of query. Size (2,) or (3,)

#### Returns

- **dist** (*double*) point-line distance.
- **point** (*NumPy array*) projection point on the line.

#### pointLocation(pointlist)

Similar to Matlab's pointLocation function, queries which elements in mesh the points belong to, and also calculate the barycentric coordinates.

This is a wrapper of the C++ function pointLocation, which implements an AABB tree based on Darren Engwirda's findtria package

#### **Parameters**

- mesh (NIRFASTer mesh) Can be 2D or 3D.
- **pointlist** (*NumPy array*) A list of points to query. Shape (N, dim), where N is number of points.

#### **Returns**

- **ind** (*double NumPy array*) i-th queried point is in element *ind[i]* of mesh (zero-based). If not in mesh, *ind[i]=-1*. Size: (N,).
- **int\_func** (*double NumPy array*) i-th row is the barycentric coordinates of i-th queried point. If not in mesh, corresponding row is all zero. Size: (N, dim+1).

#### References

https://github.com/dengwirda/find-tria

# pointTriangleDistance(P)

Calculate the distance between a point and a triangle (defined by three points), and find the projection point

#### Parameters

- TRI (Numpy array) The three points (per row) defining the triangle. Size: (3,3)
- **P** (*Numpy array*) point of query. Size (3,).

#### Returns

- **dist** (*double*) point-triangle distance.
- **PP0** (*NumPy array*) projection point on the triangular face.

# **Notes**

This is modified from Joshua Shaffer's code, available at: https://gist.github.com/joshuashaffer/99d58e4ccbd37ca5d96e

which is based on Gwendolyn Fischer's Matlab code: https://uk.mathworks.com/matlabcentral/fileexchange/22857-distance-between-a-point-and-a-triangle-in-3d

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