# **NIRFASTerFF**

Release 1.1.0

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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 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, fluorecence, and DCS

FEM solver calculates: CW fluence, FD fluence, TPSF, direct TR moments for standard and fluorecence mesh, and G1/g1 curve for DCS mesh

Analytical solution in semi-infinite medium for: CW/FD fluence, TPSF, and DCS G1/g1 curves

Jacobian matrices: CW for standard, fluorescence, and DCS mesh, and FD for standard and fluorescence mesh

# **TWO**

# **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

**THREE** 

# **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

# **FOUR**

# **API DOCUMENTATION**

# 4.1 nirfasterff

# Modules

nirfasterff.base	Core classes used in the pacakge
nirfasterff.forward	Funtions for forward data calculation
nirfasterff.inverse	Calculation of the Jacobian matrices and a basic
	Tikhonov regularization function
nirfasterff.io	Some functions for reading/writing certain data types.
nirfasterff.lib	Low-level functions implemented in C/C++, on both
	GPU and CPU
nirfasterff.math	Some low-level functions used by the forward solvers.
nirfasterff.meshing	Functions used for mesh generation and quality check
nirfasterff.utils	Utility functions and auxiliary classes frequently used in
	the package.
nirfasterff.visualize	Functions for basic data visualization

# 4.1.1 nirfasterff.base

Core classes used in the pacakge

# Modules

nirfasterff.base.data	Defining some data classes, which are the return types of the fem data calculation functions
nirfasterff.base.dcs_mesh	Define the DCS mesh class.
nirfasterff.base.fluor_mesh	Define the fluorescence mesh class
nirfasterff.base.optodes	Define the optode class, an instance of which can be either a source or a detector
nirfasterff.base.stnd_mesh	Define the standard mesh class

## nirfasterff.base.data

Defining some data classes, which are the return types of the fem data calculation functions

#### **Classes**

DCSdata()	Class holding DCS data.
FDdata()	Class holding FD/CW data.
FLdata()	Class holding FD/CW fluorescence data.
TPSFdata()	Class holding time-resolved TPSF data.
TRMomentsdata()	Class holding time-resolved moments data calculated us-
	ing Mellin transform.
flTPSFdata()	Class holding fluorescence time-resolved TPSF data.
flTRMomentsdata()	Class holding fluorescence TR moments data calculated
	using Mellin transform.
meshvol()	Small class holding the information needed for convert-
	ing between mesh and volumetric space.

## nirfasterff.base.data.DCSdata

## class nirfasterff.base.data.DCSdata

Bases: object

Class holding DCS data.

# phi

steady-state 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

This is the same as nirfasterff.base.FDdata.phi, when modulation frequency is zero

# **Type**

double NumPy array

#### link

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

#### **Type**

int32 NumPy array

# amplitude

Steady-state amplitude of each channel. Size (NChannel,)

This is the same as nirfasterff.base.FDdata.amplitude, when modulation frequency is zero

# **Type**

double NumPy vector

# tau\_DCS

time vector in seconds

# **Type**

double NumPy vector

# phi\_DCS

G1 in medium from each source at each time step . If mesh contains non-tempty field vol, this will be represented on the grid

shape[-1] equals length of tau\_DCS, and shape[-2] equals number of sources

#### Type

double NumPy array

## G1\_DCS

G1 curve as is calculated from the correlation diffusion equation. Size: (NChannel, NTime)

#### Type

double NumPy array

#### g1\_DCS

g1 curve, i.e. G1 normalized by amplitudes. Size: (NChannel, NTime)

#### Type

double NumPy array

#### vol

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

#### **Type**

nirfaseterff.base.meshvol

# \_\_init\_\_()

#### **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 fields phi and phi\_DCS

## **Parameters**

 ${\it mesh}~(nirfasterff.base.dcsmesh)$  — 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 fields phi and phi\_DCS

#### **Parameters**

 $\mathbf{mesh}$  (nirfasterff.base.dcsmesh) — mesh whose .vol attribute is used to do the conversion.

# Return type

None.

#### nirfasterff.base.data.FDdata

# class nirfasterff.base.data.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

# \_\_init\_\_()

#### **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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**

 $egin{aligned} \textbf{mesh} \ (nirfasterff.base.stndmesh) - \text{mesh whose .vol attribute is used to do the conversion.} \end{aligned}$ 

# **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** (*nirfasterff.base.stndmesh*) – mesh whose .vol attribute is used to do the conversion.

# Return type

None.

## nirfasterff.base.data.FLdata

## class nirfasterff.base.data.FLdata

Bases: object

Class holding FD/CW fluorescence data.

### phix

intrinsic fluence from each source at excitation wavelength. 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

## phimm

intrinsic from each source at emission wavelength.

# **Type**

double Numpy array

## phifl

fluorescence emission fluence

## **Type**

double Numpy array

#### complexx

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

#### **Type**

double or complex double Numpy vector

# complexmm

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

#### **Type**

double or complex double Numpy vector

# complexfl

Complex amplitude of each channel, fluorescence emission. 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

# amplitudex

Absolute amplitude of each channel, intrinsic excitation. I.e. amplitudex=abs(complexx)

#### **Type**

double Numpy vector

# amplitudemm

Absolute amplitude of each channel, intrinsic emission. I.e. amplitudemm=abs(complexmm)

#### **Type**

double Numpy vector

## amplitudefl

Absolute amplitude of each channel, fluorescence emission. I.e. amplitudefl=abs(complexfl)

# **Type**

double Numpy vector

### phasex

phase data of each channel, intrinsic excitation. All zero in case of CW data

## **Type**

double Numpy vector

# phasemm

phase data of each channel, intrinsic emission. All zero in case of CW data

## **Type**

double Numpy vector

# phasefl

phase data of each channel, fluorescence emission. 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

## \_\_init\_\_()

# **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 fields phix, phimm, and phifl, if they are defined

#### **Parameters**

**mesh** (*nirfasterff.base.fluormesh*) – 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 fields phix, phimm, and phifl, if they are defined

#### **Parameters**

 ${\it mesh}\ (nirfaster ff.\ base.\ fluor mesh)$  — mesh whose .vol attribute is used to do the conversion.

#### **Return type**

None.

## nirfasterff.base.data.TPSFdata

# class nirfasterff.base.data.TPSFdata

Bases: object

Class holding time-resolved TPSF data.

### phi

TPSF from each source at each spatial location. If mesh contains non-tempty field vol, this will be represented on the grid

Shape: NNodes x num\_sources x time\_steps

OR: len(xgrid) x len(ygrid) x len(zgrid) x num\_sources x time\_steps

None by default, and only contains data if 'field' option is set to True when calculating forward data.

#### **Type**

double NumPy array or None

# time

time vector, in seconds

## **Type**

double NumPy vector

## tpsf

TPSF measured at each channel. Size: (NChannels, time\_steps)

### **Type**

double NumPy array

#### link

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

# Type

int32 NumPy array

#### vol

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

# **Type**

nirfaseterff.base.meshvol

## \_\_init\_\_()

# **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 or data.phi==None, 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, if it is defined

# **Parameters**

 ${\it mesh}\;(nirfaster ff. base.stndmesh) - {\it mesh}\;{\it whose}\;.vol\; attribute\; is\; used\; to\; do\; the\; conversion.$ 

## Return type

None.

# tomesh(mesh)

Convert data back to mesh space using information defined in mesh.vol. If data.vol is empty or data.phi==None, the function does nothing.

CAUTION: This OVERRIDES field phi, if it is defined

#### **Parameters**

 $\mathbf{mesh}$  (nirfasterff.base.fluormesh) – mesh whose .vol attribute is used to do the conversion.

# Return type

None.

## nirfasterff.base.data.TRMomentsdata

## class nirfasterff.base.data.TRMomentsdata

Bases: object

Class holding time-resolved moments data calculated using Mellin transform.

### phi

moments from each source at each spatial location. If mesh contains non-tempty field vol, this will be represented on the grid

Shape: NNodes x num\_sources x (max\_moment\_order + 1)

OR: len(xgrid) x len(ygrid) x len(zgrid) x num\_sources x (max\_moment\_order + 1)

None by default, and only contains data if 'field' option is set to True when calculating forward data.

### **Type**

double Numpy array or None

#### moments

moments for each channel. i-th column contains i-th moment as measured at each channel. Size: (NChannels, max\_moment\_order + 1)

# **Type**

double Numpy vector

#### link

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

#### Type

int32 NumPy array

# vol

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

#### Type

nirfaseterff.base.meshvol

```
__init__()
```

#### **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 or data.phi==None, 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, if it is defined

#### **Parameters**

**mesh** (*nirfasterff.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 or data.phi==None, the function does nothing.

CAUTION: This OVERRIDES field phi, if it is defined

#### **Parameters**

 $\mathbf{mesh}$  (nirfasterff.base.fluormesh) – mesh whose .vol attribute is used to do the conversion.

# **Return type**

None.

#### nirfasterff.base.data.fITPSFdata

#### class nirfasterff.base.data.flTPSFdata

Bases: object

Class holding fluorescence time-resolved TPSF data.

# phix

TPSF at exciation wavelength from each source at each spatial location. If mesh contains non-tempty field vol, this will be represented on the grid

Shape: NNodes x num\_sources x time\_steps

OR: len(xgrid) x len(ygrid) x len(zgrid) x num sources x time steps

None by default, and only contains data if 'field' option is set to True when calculating forward data.

# **Type**

double NumPy array

# phifl

similar to phix, but for fluorescence emission

#### **Type**

double NumPy array

#### time

time vector, in seconds

# **Type**

double NumPy vector

#### tpsfx

TPSF measured at each channel, excitation. Size: (NChannels, time\_steps)

#### Type

double NumPy array

## link

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

#### Type

int32 NumPy array

#### vol

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

#### Type

nirfaseterff.base.meshvol

# \_\_init\_\_()

# **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 or data.phix==None, the function does nothing.

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

CAUTION: This OVERRIDES the fields phix and phifl, if they are defined

# **Parameters**

 ${\it mesh}\ (nirfaster ff.\ base.\ fluor mesh)$  — 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 or data.phix==None, the function does nothing.

CAUTION: This OVERRIDES fields phix and phifl, if they are defined

#### **Parameters**

 $\mathbf{mesh}$  (nirfasterff.base.fluormesh) – mesh whose .vol attribute is used to do the conversion.

## Return type

None.

## nirfasterff.base.data.flTRMomentsdata

# class nirfasterff.base.data.flTRMomentsdata

Bases: object

Class holding fluorescence TR moments data calculated using Mellin transform.

# phix

moments at excitation wavelength from each source at each spatial location. If mesh contains non-tempty field vol, this will be represented on the grid

Shape: NNodes x num\_sources x (max\_moment\_order + 1)

OR: len(xgrid) x len(ygrid) x len(zgrid) x num\_sources x (max\_moment\_order + 1)

None by default, and only contains data if 'field' option is set to True when calculating forward data.

# **Type**

double NumPy array

# phifl

similar to phix, but for fluorescence emission

#### **Type**

double NumPy array

# momentsx

moments for each channel, exciation. i-th column contains i-th moment. Size: (NChannels, max moment order + 1)

#### **Type**

double NumPy array

## momentsfl

moments for each channel, fluorescence emission. i-th column contains i-th moment. Size: (NChannels,  $max\_moment\_order + 1$ )

## **Type**

double NumPy array

#### link

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

# Type

int32 NumPy array

#### vol

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

## **Type**

nirfaseterff.base.meshvol

```
__init__()
```

# **Methods**

init()	
isvol()	Checks if data is in volumetric space.
togrid(mesh)	Convert data to volumetric space as is defined in mesh.vol.
tomesh(mesh)	Convert data back to mesh space using information defined in mesh.vol.

# 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 or data.phix==None, the function does nothing.

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

CAUTION: This OVERRIDES the fields phix and phifl, if they are defined

# **Parameters**

 $\mathbf{mesh}$  (nirfasterff.base.fluormesh) — 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 or data.phix==None, the function does nothing.

CAUTION: This OVERRIDES fields phix and phifl, if they are defined

#### **Parameters**

 ${\it mesh}\ (nirfaster ff. \ base. \ fluor mesh)$  — mesh whose .vol attribute is used to do the conversion.

# Return type

None.

## nirfasterff.base.data.meshvol

```
class nirfasterff.base.data.meshvol
     Bases: object
     Small class holding the information needed for converting between mesh and volumetric space. Values calculated
     by nirfasterff.base.*mesh.gen_intmat
     Note that the volumetric space, defined by xgrid, ygrid, and zgrid (empty for 2D mesh), must be uniform
           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))
               Type
                   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
```

```
__init__()
```

# **Methods**

```
__init__()
```

# nirfasterff.base.dcs\_mesh

Define the DCS mesh class. Assuming all motions are Brownian.

## **Classes**

dcsmesh()

Main class for standard mesh.

## nirfasterff.base.dcs mesh.dcsmesh

```
class nirfasterff.base.dcs_mesh.dcsmesh
```

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,)

# **Type**

double NumPy array

# type

type of the mesh. It is always 'dcs'.

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,)
         Type
             (double NumPy array
wv_DCS
     wavelength used (nm)
         Type
             double
alpha
     fraction of photon scattering events that occur from moving particles in the medium (a.u.). Size (NNodes,
     NFlow)
         Type
             double NumPy array
Db
     effective diffusion coefficient in Brownian motion (mm^2/s). Size (NNodes, NFlow)
         Type
              double NumPy array
aDb
     Defined as np.sum(a*Db,axis=1). This lumped parameter (mm^2/s) is what is actually used in data gen-
     reation. Size (NNodes,)
         Type
             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,)
          Type
              double NumPy array
source
     information about the sources
          Type
              nirfasterff.base.optode
meas
     information about the the detectors
          Type
              nirfasterff.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<sup>3</sup> or mm<sup>2</sup>) of each element. Size (NElements,)
          Type
              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
              nirfasterff.base.meshvol
__init__()
```

# **Methods**

init()	
()	
change_prop(idx, prop)	Change optical properties (mua, musp, ri, alpha and Db) at nodes specified in idx, and automatically change fields kappa, c, and ksi as well
<pre>femdata(tvec[, solver, opt])</pre>	Calculates steady-state fluences and G1/g1 curves for each source using a FEM solver, and then the boudary measurables for each channel
<pre>from_copy(mesh)</pre>	Deep copy all fields from another mesh.
<pre>from_file(file)</pre>	Read from classic NIRFAST mesh (ASCII) format, not checking the correctness of the loaded integration functions.
<pre>from_mat(matfile[, varname])</pre>	Read from Matlab .mat file that contains a NIR-FASTer mesh struct.
<pre>from_solid(ele, nodes[, prop, src, det, link])</pre>	Construct a NIRFASTer mesh from a 3D solid mesh generated by a mesher.
<pre>from_volume(vol[, param, prop, src, det, link])</pre>	Construct mesh from a segmented 3D volume using the built-in CGAL mesher.
<pre>gen_intmat(xgrid, ygrid[, zgrid])</pre>	Calculate the information needed to convert data between mesh and volumetric space, specified by x, y, z (if 3D) grids.
isvol()	Check if convertion matrices between mesh and vol- umetric spaces are calculated
<pre>jacobian(tvec[, normalize, solver, opt])</pre>	Calculates the Jacobian matrix
<pre>save_nirfast(filename)</pre>	Save mesh in the classic NIRFASTer ASCII format, which is directly compatible with the Matlab version
set_prop(prop)	Set optical properties of the whole mesh, using information provided in prop.
touch_optodes()	Moves all optodes (if non fixed) and recalculate the integration functions (i.e. barycentric coordinates).

# change\_prop(idx, prop)

Change optical properties (mua, musp, ri, alpha and Db) at nodes specified in idx, and automatically change fields kappa, c, and ksi as well

#### **Parameters**

- $idx(list\ or\ NumPy\ array\ or\ -1)$  zero-based indices of nodes to change. If idx == -1, function changes all the nodes
- **prop** (*list or NumPy array of length 6*) new optical properties to be assigned to the specified nodes. [region mua(mm-1) musp(mm-1) ri alpha Db].

# Return type

None.

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

Calculates steady-state fluences and G1/g1 curves for each source using a FEM solver, and then the boudary measurables for each channel

Assumes Brownian motion, that is,  $\langle \Delta r^2 \rangle = 6 * \alpha Db * \tau$ 

If mesh.vol is set, fluence and G1 data will be represented in volumetric space

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

#### **Parameters**

- **tvec** (*double NumPy array*) time vector (i.e. :math:`au`) for the G1 curve, in seconds. It is usually a good idea to use log scale
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Returns

• data (*nirfasterff.base.DCSdata*) – contains fluence, G1 curve, and g1 curve calculated at each spatial location, and also the boundary data.

See DCSdata() for details.

• **info** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver when calculating the fluence field.

See ConvergenceInfo() for details

## from\_copy(mesh)

Deep copy all fields from another mesh.

#### **Parameters**

**mesh** (nirfasterff.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 = nirfasterff.base.dcsmesh()
>>> 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 NIRFASTer 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 (NN-odes.3).
- **prop** (*double NumPy array*, *optional*) If not *None*, calls *dcsmesh.set\_prop(*) and sets the optical properties in the mesh. The default is None.

See set\_prop() for details.

• **src** (*nirfasterff.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** (*nirfasterff.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.

**from\_volume**(vol, param=utils.MeshingParams(), prop=None, src=None, det=None, 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 (nirfasterff.utils.MeshingParams, optional) parameters used in the CGAL mesher. If not specified, uses the default parameters defined in nirfasterff.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 dcsmesh.set\_prop() and sets the optical properties in the mesh. The default is None.

See set\_prop() for details.

• **src** (*nirfasterff.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** (*nirfasterff.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 nirfasterff.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

jacobian(tvec, normalize=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates the Jacobian matrix

Returns the Jacobian, direct field data, and the adjoint data

One Jacobian is calcualted at each time point in tvec, and the derivative is taken with regard to aDb

### **Parameters**

- tvec (double NumPy vector) time vector used.
- **normalize** (*bool*, *optional*) if True, Jacobbians are normalized to the measured boundary amplitude. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Returns

- J (double NumPy array) The Jacobian matrix. Size (NChannel, NVoxel, NTime)
- **data1** (*nirfasterff.base.FLdata*) The calculated direct field. The same as directly calling mesh.femdata(tvec)
- data2 (nirfasterff.base.FLdata) The calculated adjoint field. The same as calling mesh.femdata(tvec) AFTER swapping the locations of sources and detectors

#### See also:

```
jacobian_DCS()
```

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

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.

# nirfasterff.base.fluor mesh

Define the fluorescence mesh class

#### **Classes**

fluormesh()

Main class for fluorescence mesh.

# nirfasterff.base.fluor\_mesh.fluormesh

```
class nirfasterff.base.fluor_mesh.fluormesh
     Bases: object
     Main class for fluorescence 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,)
               Type
                   double NumPy array
     type
           type of the mesh. It is always 'fluor'.
               Type
                   str
     muax
           intrisic absorption coefficient (mm^-1) at excitation wavelength at each node. Size (NNodes,)
               Type
                   double NumPy array
     muam
           intrisic absorption coefficient (mm^-1) at emission wavelength at each node. Size (NNodes,)
               Type
                   double NumPy array
     muaf
           intrisic absorption coefficient (mm^-1) of the fluorophores at each node. Size (NNodes,)
               Type
                   double NumPy array
```

```
kappax
     intrisic diffusion coefficient (mm) at excitation wavelength at each node. Size (NNodes,). Defined as
     1/(3*(muax + musx))
         Type
             double NumPy array
kappam
     intrisic diffusion coefficient (mm) at emission wavelength at each node. Size (NNodes,). Defined as
     1/(3*(muam + musm))
         Type
             double NumPy array
ri
     refractive index at each node. Size (NNodes,)
         Type
             double NumPy array
musx
     intrisic reduced scattering coefficient (mm^-1) at excitation wavelength at each node. Size (NNodes,)
         Type
             double NumPy array
musm
     intrisic reduced scattering coefficient (mm^-1) at emission wavelength at each node. Size (NNodes,)
         Type
             double NumPy array
eta
     quantum efficiency (a.u.) of the fluorophores. Size (NNodes,)
         Type
             double NumPy array
tau
     time coefficient (second) of the fluorophores. Size (NNodes,)
         Type
             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,)
         Type
             double NumPy array
```

```
source
     information about the sources
          Type
              nirfasterff.base.optode
meas
     information about the the detectors
          Type
              nirfasterff.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<sup>3</sup> or mm<sup>2</sup>) of each element. Size (NElements,)
          Type
              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
              nirfasterff.base.meshvol
__init__()
```

# **Methods**

init()	
change_prop(idx, prop)	Change optical properties (muax, musxp, ri, muam, musmp, muaf, eta, and tau) at nodes specified in idx, and automatically change fields kappax, kappam, c, and ksi as well
femdata(freq[, solver, opt, xflag, mmflag,])	Calculates fluences for each source using a FEM solver, and then the boudary measurables for each channel
<pre>femdata_moments([max_moments, savefield,])</pre>	Calculates TR moments at each location in the mesh for each source directly using Mellin transform, and then the boudary measurables for each channel
<pre>femdata_tpsf(tmax, dt[, savefield,])</pre>	Calculates TPSF at each location in the mesh for each source using a FEM solver, and then the boudary measurables for each channel
<pre>from_copy(mesh)</pre>	Deep copy all fields from another mesh.
<pre>from_file(file)</pre>	Read from classic NIRFAST mesh (ASCII) format, not checking the correctness of the loaded integration functions.
<pre>from_mat(matfile[, varname])</pre>	Read from Matlab .mat file that contains a NIR-FASTer mesh struct.
<pre>from_solid(ele, nodes[, prop, src, det, link])</pre>	Construct a NIRFASTer mesh from a 3D solid mesh generated by a mesher.
<pre>from_volume(vol[, param, prop, src, det, link])</pre>	Construct mesh from a segmented 3D volume using the built-in CGAL mesher.
<pre>gen_intmat(xgrid, ygrid[, zgrid])</pre>	Calculate the information needed to convert data between mesh and volumetric space, specified by x, y, z (if 3D) grids.
isvol()	Check if convertion matrices between mesh and vol- umetric spaces are calculated
<pre>jacobian([freq, normalize, solver, opt])</pre>	Calculates the Jacobian matrix
save_nirfast(filename)	Save mesh in the classic NIRFASTer ASCII format, which is directly compatible with the Matlab version
set_prop(prop)	Set optical properties of the whole mesh, using information provided in prop.
touch_optodes()	Moves all optodes (if non fixed) and recalculate the integration functions (i.e. barycentric coordinates).

# change\_prop(idx, prop)

Change optical properties (muax, musxp, ri, muam, musmp, muaf, eta, and tau) at nodes specified in idx, and automatically change fields kappax, kappam, c, and ksi as well

# **Parameters**

- idx (list 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 8*) new optical properties to be assigned to the specified nodes. [muax(mm-1) musxp(mm-1) ri muam(mm-1) musmp(mm-1) muaf(mm-1) eta tau(sec)].

# **Return type**

None.

**femdata**(*freq*, *solver*=*utils*.*get*\_*solver*(), *opt*=*utils*.*SolverOptions*(), *xflag*=*True*, *mmflag*=*True*, *flflag*=*True*)

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\_fl\_CW() and femdata\_fl\_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** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

- **xflag** (bool, optional) if intrinsic excitation field is calculated. The default is True.
- mmflag (bool, optional) if intrinsic emission field is calculated. The default is True.
- **flflag** (bool, optional) if fluorescence field is calculated. If set True, xflag must also be True. The default is True.

#### Returns

• data (nirfasterff.base.FLdata) – fluence and boundary measurables given the mesh and optodes.

See *FLdata()* for details.

• **infox** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver, for intrinsic excitation.

See ConvergenceInfo() for details

• **infom** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver, for intrinsic emission.

See ConvergenceInfo() for details

• **infofl** (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, for fluorescence emission.

See ConvergenceInfo() for details

**femdata\_moments**(max\_moments=3, savefield=False, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates TR moments at each location in the mesh for each source directly using Mellin transform, and then the boudary measurables for each channel

This is done for both excitation and fluorescence emission

If mesh.vol is set and savefield is set to True, internal moments data will be represented in volumetric space

See femdata\_fl\_TR\_moments() for details

# **Parameters**

• max\_moments (int32, optional) – max order of moments to calculate. That is, 0th, 1st, 2nd, ..., max moments-th will be calculated. The default is 3.

• **savefield** (*bool*, *optional*) – If True, the internal moments are also returned. If False, only boundary moments are returned and data.phix and data.phifl will be empty.

The default is False.

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

See SolverOptions() for details

### **Returns**

• **data** (*nirfasterff.base.flTRMomentsdata*) – internal and boundary moments given the mesh and optodes, both excitation and fluorescence emission.

See flTRMomentsdata() for details.

• **infox** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver, excitation.

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

• **infom** (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, fluorescence emission.

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

**femdata\_tpsf**(tmax, dt, savefield=False, beautify=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates TPSF at each location in the mesh for each source using a FEM solver, and then the boudary measurables for each channel

This is done for both excitation and fluorescence emission

If mesh.vol is set and savefield is set to True, internal TPSF data will be represented in volumetric space

See femdata\_fl\_TR() for details

# **Parameters**

- **tmax** (*double*) maximum time simulated, in seconds.
- **dt** (*double*) size of each time step, in seconds.
- **savefield** (*bool*, *optional*) If True, the internal TPSFs are also returned. If False, only boundary TPSFs are returned and data.phix and data.phifl will be empty.

The default is False.

- **beautify** (*bool*, *optional*) If true, zeros the initial unstable parts of the boundary TPSFs. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- opt (nirfasterff.utils.SolverOptions, optional) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

### Returns

• **data** (*nirfasterff.base.ftTPSFdata*) – internal and boundary TPSFs given the mesh and optodes, both excitation and fluorescence emission.

```
See flTPSFdata() for details.
```

• **infox** (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, excitation.

Only the convergence info of the last time step is returned.

```
See ConvergenceInfo() for details
```

• **infom** (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, fluorescence emission.

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

# from\_copy(mesh)

Deep copy all fields from another mesh.

#### **Parameters**

**mesh** (nirfasterff.base.fluormesh) – 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 = nirfasterff.base.fluormesh()
>>> 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 NIRFASTer 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 (NN-odes,3).
- **prop** (double NumPy array, optional) If not None, calls fluormesh.set\_prop() and sets the optical properties in the mesh. The default is None.

See set\_prop() for details.

• **src** (*nirfasterff.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** (*nirfasterff.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.

**from\_volume**(vol, param=utils.MeshingParams(), prop=None, src=None, det=None, link=None)

Construct mesh from a segmented 3D volume using the built-in CGAL mesher. Calls fluormesh.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 (nirfasterff.utils.MeshingParams, optional) parameters used in the CGAL mesher. If not specified, uses the default parameters defined in nirfasterff.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 fluormesh.set\_prop() and sets the optical properties in the mesh. The default is None.

See *set\_prop()* for details.

• **src** (*nirfasterff.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** (*nirfasterff.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 nirfasterff.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

**jacobian**(freq=0, normalize=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates the Jacobian matrix

Returns the Jacobian, direct field data, and the adjoint data

Structure of the Jacobian is detailed in jacobian\_fl\_CW() and jacobian\_fl\_FD()

# **Parameters**

- **freq** (*double*) modulation frequency in Hz.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements at excitation wavelength ('Born ratio').

The default is True.

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

See SolverOptions() for details

#### Raises

**ValueError** – if modulation frequency is negative.

### Returns

- **J** (double NumPy array) The Jacobian matrix. Size (NChannel, NVoxel\*2) or (NChannel, NVoxel)
- **data1** (*nirfasterff.base.FLdata*) The calculated direct field. The same as directly calling mesh.femdata(freq)
- data2 (nirfasterff.base.FLdata) The calculated adjoint field. The same as calling mesh.femdata(freq) AFTER swapping the locations of sources and detectors

# 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 muax(mm-1) musxp(mm-1) ri muam(mm-1) musmp(mm-1) muaf(mm-1)

→eta tau]
[region muax(mm-1) musxp(mm-1) ri muam(mm-1) musmp(mm-1) muaf(mm-1)

→eta tau]
[...]
```

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.

# nirfasterff.base.optodes

Define the optode class, an instance of which can be either a source or a detector

#### **Classes**

```
optode([coord]) Class for NIRFASTer optodes, which can be either a group of sources or a group of detectors.
```

# nirfasterff.base.optodes.optode

```
class nirfasterff.base.optodes.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
     __init__(coord=[])
```

## **Methods**

init([coord])	
<pre>move_detectors(mesh)</pre>	Moves detector to the appropriate locations in the mesh.
move_sources(mesh)	Moves sources to the appropriate locations in the mesh.
touch_detectors(mesh)	Recalculate/fill in all other fields based on 'fixed' and 'coord'.
touch_sources(mesh)	Recalculate/fill in all other fields based on 'fixed' and 'coord'.

## 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. Can be a 'stndmesh', 'fluormesh', or 'dcsmesh', 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  $1/\mu'_s$  for stnd and dcs mesh, and  $1/\mu'_{sx}$  for fluor mesh

Integration functions are also calculated after moving.

### **Parameters**

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

# Return type

None.

# nirfasterff.base.stnd\_mesh

Define the standard mesh class

## **Classes**

stndmesh()

Main class for standard mesh.

# nirfasterff.base.stnd mesh.stndmesh

# class nirfasterff.base.stnd\_mesh.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,)
          Type
              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,)
          Type
              (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,)
          Type
              double NumPy array
source
     information about the sources
          Type
              nirfasterff.base.optode
meas
     information about the the detectors
```

```
Type
              nirfasterff.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
С
     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<sup>3</sup> or mm<sup>2</sup>) of each element. Size (NElements,)
          Type
              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
              nirfasterff.base.meshvol
__init__()
```

# **Methods**

init()	
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
<pre>femdata(freq[, solver, opt])</pre>	Calculates fluences for each source using a FEM solver, and then the boudary measurables for each channel
<pre>femdata_moments([max_moments, savefield,])</pre>	Calculates TR moments at each location in the mesh for each source directly using Mellin transform, and then the boudary measurables for each channel
<pre>femdata_tpsf(tmax, dt[, savefield,])</pre>	Calculates TPSF at each location in the mesh for each source using a FEM solver, and then the boudary measurables for each channel
<pre>from_copy(mesh)</pre>	Deep copy all fields from another mesh.
<pre>from_file(file)</pre>	Read from classic NIRFAST mesh (ASCII) format, not checking the correctness of the loaded integration functions.
<pre>from_mat(matfile[, varname])</pre>	Read from Matlab .mat file that contains a NIR-FASTer mesh struct.
<pre>from_solid(ele, nodes[, prop, src, det, link])</pre>	Construct a NIRFASTer mesh from a 3D solid mesh generated by a mesher.
<pre>from_volume(vol[, param, prop, src, det, link])</pre>	Construct mesh from a segmented 3D volume using the built-in CGAL mesher.
<pre>gen_intmat(xgrid, ygrid[, zgrid])</pre>	Calculate the information needed to convert data between mesh and volumetric space, specified by x, y, z (if 3D) grids.
isvol()	Check if convertion matrices between mesh and vol- umetric spaces are calculated
<pre>jacobian([freq, normalize, mus, solver, opt])</pre>	Calculates the Jacobian matrix
save_nirfast(filename)	Save mesh in the classic NIRFASTer ASCII format, which is directly compatible with the Matlab version
set_prop(prop)	Set optical properties of the whole mesh, using information provided in prop.
touch_optodes()	Moves all optodes (if non fixed) and recalculate the integration functions (i.e. barycentric coordinates).

# 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 (list 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** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

#### Returns

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

See FDdata() for details.

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

See ConvergenceInfo() for details

**femdata\_moments**(max\_moments=3, savefield=False, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates TR moments at each location in the mesh for each source directly using Mellin transform, and then the boudary measurables for each channel

If mesh.vol is set and savefield is set to True, internal moments data will be represented in volumetric space

See femdata\_stnd\_TR\_moments() for details

### **Parameters**

- max\_moments (int32, optional) max order of moments to calculate. That is, 0th, 1st, 2nd, ..., max\_moments-th will be calculated. The default is 3.
- **savefield** (*bool*, *optional*) If True, the internal moments are also returned. If False, only boundary moments are returned and data.phi will be empty.

The default is False.

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

See SolverOptions() for details

### Returns

• **data** (*nirfasterff.base.TRMomentsdata*) – internal and boundary moments given the mesh and optodes.

See TRMomentsdata() for details.

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

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

**femdata\_tpsf**(tmax, dt, savefield=False, beautify=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates TPSF at each location in the mesh for each source using a FEM solver, and then the boudary measurables for each channel

If mesh.vol is set and savefield is set to True, internal TPSF data will be represented in volumetric space

See femdata\_stnd\_TR() for details

### **Parameters**

- tmax (double) maximum time simulated, in seconds.
- **dt** (*double*) size of each time step, in seconds.
- **savefield** (*bool*, *optional*) If True, the internal TPSFs are also returned. If False, only boundary TPSFs are returned and data.phi will be empty.

The default is False.

- **beautify** (*bool*, *optional*) If true, zeros the initial unstable parts of the boundary TPSFs. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

# Returns

data (nirfasterff.base.TPSFdata) – internal and boundary TPSFs given the mesh and optodes.

See TPSFdata() for details.

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

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

# from\_copy(mesh)

Deep copy all fields from another mesh.

## Parameters

**mesh** (nirfasterff.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 = nirfasterff.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 NIRFASTer 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 (NN-odes,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**(*nirfasterff.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** (*nirfasterff.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.

**from\_volume**(vol, param=utils.MeshingParams(), prop=None, src=None, det=None, 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 (nirfasterff.utils.MeshingParams, optional) parameters used in the CGAL mesher. If not specified, uses the default parameters defined in nirfasterff.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** (*nirfasterff.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** (*nirfasterff.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 nirfasterff.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

jacobian(freq=0, normalize=True, mus=False, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates the Jacobian matrix

Returns the Jacobian, direct field data, and the adjoint data

Structure of the Jacobian is detailed in jacobian\_stnd\_CW() and jacobian\_stnd\_FD()

#### **Parameters**

- **freq** (*double*) modulation frequency, in Hz.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements, i.e. use Rytov approximation.

The default is True.

- **mus** (*bool*, *optional*) whether derivates wrt mus (left half of the 'full' Jacobian) is calculated. Only has effect when freq=0. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

## Raises

**ValueError** – if freq is negative.

### Returns

- **J** (double or complex double NumPy array) The Jacobian matrix. Size (NChannel\*2, NVoxel\*2) if freq>0, (NChannel, NVoxel\*2) if freq=0 and mus=True, (NChannel, NVoxel) if freq=0 and mus=False
- **data1** (*nirfasterff.base.FDdata*) The calculated direct field. The same as directly calling mesh.femdata(freq)
- data2 (nirfasterff.base.FDdata) The calculated adjoint field. The same as calling mesh.femdata(freq) AFTER swapping the locations of sources and detectors

### save\_nirfast(filename)

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

### Parameter:

**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.

# 4.1.2 nirfasterff.forward

Funtions for forward data calculation

## **Modules**

nirfasterff.forward.analytical	Analytical solutions to the diffusion equation in semi-infinite media
nirfasterff.forward.femdata	The FEM solvers.

# nirfasterff.forward.analytical

Analytical solutions to the diffusion equation in semi-infinite media

# **Functions**

<pre>semi_infinite_CW(mua, musp, n, rho[, z,])</pre>	Calculates the continuous-wave fluence in space using the analytical solution to the diffusion equation in semi- infinite media.
<pre>semi_infinite_DCS(mua, musp, n, rho, aDb,)</pre>	Calculates DCS G1 curve using the analytical solution to the correlation diffusion equation in semi-infinite media
semi_infinite_FD(mua, musp, n, freq, rho[,])	Calculates the frequency-domain fluence in space using the analytical solution to the diffusion equation in semi- infinite media.
<pre>semi_infinite_TR(mua, musp, n, rho, T, dt[,])</pre>	Calculates TPSF at a given location using the analytical solution to the diffusion equation in semi-infinite media

# nirfasterff.forward.analytical.semi\_infinite\_CW

nirfasterff.forward.analytical.semi\_infinite\_CW(mua, musp, n, rho, z=0, boundary='exact', n air=1.0)

Calculates the continuous-wave fluence in space using the analytical solution to the diffusion equation in semi-infinite media.

Internaly calls the FD version with freq set to zero

#### **Parameters**

- **mua** (*double*) absorption coefficient of the medium, in mm^-1.
- **musp** (*double*) reduced scattering coefficient of the medium, in mm^-1.
- **n** (double) refractive index of the medium.
- **rho** (*double NumPy vector or scalar*) distance to the light source, projected to the x-y (i.e. boundary plane of the semi-infinite space) plane, in mm.

Can be a vector, in which case fluences calculated at multiple locations will be returned

• **z** (*double NumPy vector or scalar*, *optional*) – depth of the location(s) of interest. 0 for boundary measurement.

If a vector, it must have the same length as rho

The default is 0.

• **boundary** (*str*, *optional*) – type of the boundary condition, which can be 'robin', 'approx', or 'exact'. The default is 'exact'.

See boundary\_attenuation() for details.

• **n\_air** (*double*, *optional*) – refratcive index outside of the semi-infinite space, which is typically assumed to be air. The default is 1.0.

## Returns

calculated fluence, where each element corresponds to a location, as specified by rho and z. Size (NLocation,)

# Return type

double NumPy vector

## References

Durduran et al, 2010, Rep. Prog. Phys. doi:10.1088/0034-4885/73/7/076701

# nirfasterff.forward.analytical.semi infinite DCS

```
nirfasterff.forward.analytical.semi_infinite_DCS(mua, musp, n, rho, aDb, wvlength, tvec, z=0, boundary='exact', n_air=1.0, normalize=0)
```

Calculates DCS G1 curve using the analytical solution to the correlation diffusion equation in semi-infinite media Function assumes Brownian motion, that is,  $\langle \Delta r^2 \rangle = 6\alpha Db\tau$ 

### **Parameters**

- mua (double) absorption coefficient of the medium, in mm^-1.
- **musp** (*double*) reduced scattering coefficient of the medium, in mm^-1.

- **n** (double) refractive index of the medium.
- **rho** (*scalar*) distance to the light source, projected to the x-y (i.e. boundary plane of the semi-infinite space) plane, in mm.
- aDb (double) The lumped flow parameter  $\alpha Db$  in Brownian motion.
- wvlength (double or int) wavelength used, in nm.
- **tvec** (*double Numpy vector*) time vector used to calculate the G1 curve. It is usually a good idea to use log space.
- **z** (double, optional) depth of the location of interest. 0 for boundary measurement. The default is 0.
- **boundary** (*str*, *optional*) type of the boundary condition, which can be 'robin', 'approx', or 'exact'. The default is 'exact'.

See boundary\_attenuation() for details.

- **n\_air** (*double*, *optional*) refratcive index outside of the semi-infinite space, which is typically assumed to be air. The default is 1.0.
- **normalize** (*bool*, *optional*) if true, returns the normalized g1 curve, instead of G1. The default is 0.

### Returns

G1 or g1 curve calculated at the given location and time points.

## Return type

double NumPy vector

### References

Durduran et al, 2010, Rep. Prog. Phys. doi:10.1088/0034-4885/73/7/076701

# nirfasterff.forward.analytical.semi infinite FD

```
nirfasterff.forward.analytical.semi_infinite_FD(mua, musp, n, freq, rho, z=0, boundary='exact', n_air=1.0)
```

Calculates the frequency-domain fluence in space using the analytical solution to the diffusion equation in semi-infinite media.

### **Parameters**

- **mua** (*double*) absorption coefficient of the medium, in mm^-1.
- **musp** (*double*) reduced scattering coefficient of the medium, in mm^-1.
- **n** (double) refractive index of the medium.
- **freq** (double NumPy vector or scalar) modulation frequency, in Hz.
- **rho** (*double NumPy vector or scalar*) distance to the light source, projected to the x-y (i.e. boundary plane of the semi-infinite space) plane, in mm.

Can be a vector, in which case fluences calculated at multiple locations will be returned

• **z** (*double NumPy vector or scalar, optional*) – depth of the location(s) of interest. 0 for boundary measurement.

If a vector, it must have the same length as rho

The default is 0.

• **boundary** (*str*, *optional*) – type of the boundary condition, which can be 'robin', 'approx', or 'exact'. The default is 'exact'.

See boundary\_attenuation() for details.

• **n\_air** (*double*, *optional*) – refratcive index outside of the semi-infinite space, which is typically assumed to be air. The default is 1.0.

#### Returns

calculated complex fluence, where each row (or element in vector) corresponds to a location, as specified by rho and z,

and each column corresponds to a modulation frequency. Size (NLocation,), or (NLocation, NFreq)

## **Return type**

complex double NumPy array

## References

Durduran et al, 2010, Rep. Prog. Phys. doi:10.1088/0034-4885/73/7/076701

# nirfasterff.forward.analytical.semi\_infinite\_TR

```
nirfasterff.forward.analytical.semi_infinite_TR(mua, musp, n, rho, T, dt, z=0, boundary='EBC-Robin')
```

Calculates TPSF at a given location using the analytical solution to the diffusion equation in semi-infinite media

### **Parameters**

- mua (double) absorption coefficient of the medium, in mm^-1.
- **musp** (*double*) reduced scattering coefficient of the medium, in mm^-1.
- **n** (double) refractive index of the medium.
- **rho** (*scalar*) distance to the light source, projected to the x-y (i.e. boundary plane of the semi-infinite space) plane, in mm.
- **T**(double NumPy vector or scalar) if a scalar, it is the total amount of time and time vector will be generated also based on dt (see below).

if a vector, it is directly used as the time vector, and the argument dt will be ignored. Unit: seconds

- **dt** (*double*) step size of the time vector (in seconds). If the argument T is a vector, it will be ignored.
- **z** (double, optional) depth of the location of interest. 0 for boundary measurement. The default is 0.

Note that when z=0, the function returns reflectance, instead of fluence. Please refer to the References for detail.

• **boundary** (*str*, *optional*) – type of the boundary condition, which can be (case insensitive),

'PCB-exact' - partial current boundary condition, with exact internal reflectance

'PCB-approx' - partial current boundary condition, with Groenhuis internal reflectance approximation

'PCB-Robin' - partial current boundary condition, with internal reflectance derived from Fresnel's law

'EBC-exact' - extrapolated boundary condition, with exact internal reflectance

'EBC-approx' - extrapolated boundary condition, with Groenhuis internal reflectance approximation

'EBC-Robin' - extrapolated boundary condition, with internal reflectance derived from Fresnel's law

'ZBC' - zero boundary condition

The default is 'EBC-Robin'.

See boundary\_attenuation() for the differences between 'exact', 'approx' and 'robin'

## Raises

**ValueError** – if boundary condition is not of a recognized kind.

#### Returns

**phi** – Coumn 0: the time vector; Column 1: calculated TPSF at the given location. Size (NTime, 2)

## **Return type**

double Numpy array

## References

Hielscher et al., 1995, Phys. Med. Biol. doi:10.1088/0031-9155/40/11/013

Kienle and Patterson, 1997, JOSA A. doi:10.1364/JOSAA.14.000246

### nirfasterff.forward.femdata

The FEM solvers. It is usually recommended to use the high-level wrappers in the mesh classes by calling the mesh.femdata\* functions.

## **Functions**

<pre>femdata_DCS(mesh, tvec[, solver, opt])</pre>	Forward modeling calculating steady-state fluences and G1/g1 curves by solving the correlation diffusion equation.
<pre>femdata_fl_CW(mesh[, solver, opt, xflag,])</pre>	Forward modeling for CW in fluorescence meshes.
<pre>femdata_fl_FD(mesh, freq[, solver, opt,])</pre>	Forward modeling for FD in fluorescence meshes.
<pre>femdata_fl_TR(mesh, tmax, dt[, savefield,])</pre>	Forward modeling calculating TPSF on a fluorescence mesh.
<pre>femdata_fl_TR_moments(mesh[, max_moments,])</pre>	Forward modeling calculating TR moments using Mellin transform on a fluorescence mesh.
<pre>femdata_stnd_CW(mesh[, solver, opt])</pre>	Forward modeling for CW.
<pre>femdata_stnd_FD(mesh, freq[, solver, opt])</pre>	Forward modeling for FD.
<pre>femdata_stnd_TR(mesh, tmax, dt[, savefield,])</pre>	Forward modeling calculating TPSF on a standard mesh.
<pre>femdata_stnd_TR_moments(mesh[, max_moments,])</pre>	Forward modeling calculating TR moments using Mellin transform on a standard mesh.

# nirfasterff.forward.femdata.femdata DCS

nirfasterff.forward.femdata\_DCS(mesh, tvec, solver=utils.get\_solver(), opt=utils.SolverOptions())

Forward modeling calculating steady-state fluences and G1/g1 curves by solving the correlation diffusion equation. Please consider using mesh.femdata(tvec) instead.

The fluences as well as its boundary amplitudes are exactly the same as what the CW solver would give when tau=0.

g1 curve is simple G1 curve normalized by the boundary amplitudes.

The function calculates the MASS matrices, the source vectors, and calls the G1 solver, which internally utilizes the CW solver.

When calculating the flow-related term, the function assumes Brownian motion and uses only mesh.aDb (that is, mesh.a and mesh.Db are ignored).

This is to say, we assume  $\langle \Delta r^2 \rangle = 6\alpha Db\tau$ 

# **Parameters**

- **mesh** (nirfasterff.base.dcsmesh) the mesh used to calcuate the forward data.
- **tvec** (*double NumPy array*) time vector (i.e. :math:` au`) for the G1 curve, in seconds. It is usually a good idea to use log scale
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 dcs mesh.

# Returns

• **data** (*nirfasterff.base.DCSdata*) – contains fluence, G1 curve, and g1 curve calculated at each spatial location, and also the boundary data.

If mesh.vol is set, internal G1 curves will be returned in volumetric space

See DCSdata() for details.

• **info** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver when calculating the fluence field.

See *ConvergenceInfo()* for details

#### See also:

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

#### References

Durduran et al, 2010, Rep. Prog. Phys. doi:10.1088/0034-4885/73/7/076701

# nirfasterff.forward.femdata\_femdata\_fl\_CW

 $\label{eq:cward} \begin{tabular}{ll} \textbf{nirfasterff.forward.femdata\_fl\_CW} (mesh, solver=utils.get\_solver(), opt=utils.SolverOptions(), \\ xflag=True, mmflag=True, flflag=True) \end{tabular}$ 

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

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

The optional flags can be used to determine which fields are calculated. By default all true.

Note that when flflag is set to True, xflag must also be True.

# **Parameters**

- **mesh** (nirfasterff.base.fluormesh) 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** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

- **xflag** (bool, optional) if intrinsic excitation field is calculated. The default is True.
- mmflag (bool, optional) if intrinsic emission field is calculated. The default is True.
- **flflag** (*bool*, *optional*) if fluorescence field is calculated. If set True, xflag must also be True. The default is True.

# Raises

- **TypeError** If mesh is not a fluor mesh.
- **ValueError** If flflag is set True but xflag is not.

### Returns

data (nirfasterff.base.FLdata) – fluence and boundary measurables given the mesh and optodes.

If mesh.vol is defined, the returned fluences will be in volumetric space See *FLdata()* for details.

• infox (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, for intrinsic excitation.

See ConvergenceInfo() for details

infom (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, for intrinsic emission.

See ConvergenceInfo() for details

• **infofl** (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, for fluorescence emission.

See ConvergenceInfo() for details

#### See also:

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

# nirfasterff.forward.femdata\_fl\_FD

```
\label{eq:continuous_solver} \begin{split} \textit{nirfasterff.forward.femdata_fl_FD}(\textit{mesh}, \textit{freq}, \textit{solver} = \textit{utils.get\_solver}(), \\ \textit{opt} = \textit{utils.SolverOptions}(), \textit{xflag} = \textit{True}, \textit{mmflag} = \textit{True}, \\ \textit{flflag} = \textit{True}) \end{split}
```

Forward modeling for FD in fluorescence meshes. Please consider using mesh.femdata(frequency) instead.

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

The optional flags can be used to determine which fields are calculated. By default all true.

Note that when flflag is set to True, xflag must also be True.

## **Parameters**

- **mesh** (nirfasterff.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** (nirfasterff.utils.SolverOptions, *optional*) Solver options. Uses default parameters if not specified, and they should suffice in most cases.

See SolverOptions() for details

- **xflag** (bool, optional) if intrinsic excitation field is calculated. The default is True.
- mmflag (bool, optional) if intrinsic emission field is calculated. The default is True.
- **flflag** (*bool*, *optional*) if fluorescence field is calculated. If set True, xflag must also be True. The default is True.

### Raises

- **TypeError** If mesh is not a fluor mesh.
- **ValueError** If flflag is set True but xflag is not.

# Returns

data (nirfasterff.base.FLdata) – fluence and boundary measurables given the mesh and optodes.

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

See FLdata() for details.

• infox (nirfasterff.utils. ConvergenceInfo) – convergence information of the solver, for intrinsic excitation.

See ConvergenceInfo() for details

• **infom** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver, for intrinsic emission.

See ConvergenceInfo() for details

• infofl (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, for fluorescence emission.

See ConvergenceInfo() for details

### See also:

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

## nirfasterff.forward.femdata.femdata fl TR

```
nirfasterff.forward.femdata_fl_TR(mesh, tmax, dt, savefield=False, beautify=True, solver=utils.get_solver(), opt=utils.SolverOptions())
```

Forward modeling calculating TPSF on a fluorescence mesh. Please consider using mesh.femdata\_tpsf(tmax, dt) instead.

The function calculates the MASS matrices, the source vectors, and calls two separate TPSF solvers (both preconditioned conjugated gradient):

First time calculates the TPSF for the excitation field, the result of which is consequently convolved with the decay.

The second solver is called with the convolved excitation field as its input to calculate the TPSF for fluorescence emission.

# **Parameters**

- **mesh** (nirfasterff.base.fluormesh) the mesh used to calcuate the forward data.
- tmax (double) maximum time simulated, in seconds.
- **dt** (*double*) size of each time step, in seconds.
- **savefield** (*bool*, *optional*) If True, the internal TPSFs are also returned. If False, only boundary TPSFs are returned and data.phix and data.phifl will be empty.

The default is False.

- **beautify** (*bool*, *optional*) If true, zeros the initial unstable parts of the boundary TPSFs. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 fluor mesh.

#### Returns

• **data** (*nirfasterff.base.flTPSFdata*) – internal and boundary TPSFs given the mesh and optodes, both excitation and fluorescence emission.

If *mesh.vol* is set and *savefield* is set to *True*, internal TPSF data will be represented in volumetric space

See flTPSFdata() for details.

• infox (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, excitation.

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

infom (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, fluorescence emission.

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

### See also:

```
gen_mass_matrix(), get_field_TR(), and get_field_TRFL()
```

## nirfasterff.forward.femdata.femdata fl TR moments

Forward modeling calculating TR moments using Mellin transform on a fluorescence mesh. Please consider using mesh.femdata\_moments() instead.

The function calculates the MASS matrix, the source vectors, and calls the two Mellin moments solver (both preconditioned conjugated gradient):

First time calculates the moments for the excitation field, the result of which is consequently used as the input of the second solver.

which calculates the moments of fluorescence emission based on the excitation moments

Calculates 0th, 1st, 2nd, ..., max\_moments-th moments directly without calculating TPSF first, and this is done for both excitation and fluorescence emission.

This is more efficient, if the time series are not of concern.

# **Parameters**

- **mesh** (nirfasterff.base.fluormesh) the mesh used to calculate the forward data.
- max\_moments (int32, optional) max order of moments to calculate. That is, 0th, 1st, 2nd, ... max moments-th will be calculated. The default is 3.
- **savefield** (*bool*, *optional*) If True, the internal moments are also returned. If False, only boundary moments are returned and data.phix and data.phifl will be empty.

The default is False.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 fluor mesh.
- **ValueError** if max\_moments is negative.

#### Returns

• **data** (*nirfasterff.base.flTRMomentsdata*) – internal and boundary moments given the mesh and optodes, both excitation and fluorescence emission.

If *mesh.vol* is set and *savefield* is set to *True*, internal moments will be represented in volumetric space

See flTRMomentsdata() for details.

• infox (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, excitation.

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

infom (nirfasterff.utils.ConvergenceInfo) – convergence information of the solver, fluorescence emission.

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

## See also:

```
gen_mass_matrix(), get_field_TRmoments(), and get_field_TRFLmoments()
```

# nirfasterff.forward.femdata.femdata\_stnd\_CW

nirfasterff.forward.femdata\_stnd\_CW(mesh, 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** (*nirfasterff.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** (nirfasterff.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 (nirfasterff.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** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver.

See *ConvergenceInfo()* for details

### See also:

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

# nirfasterff.forward.femdata\_femdata\_stnd\_FD

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 (nirfasterff.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** (nirfasterff.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 (nirfasterff.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** (*nirfasterff.utils.ConvergenceInfo*) – convergence information of the solver.

See ConvergenceInfo() for details

# See also:

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

# nirfasterff.forward.femdata\_femdata\_stnd\_TR

nirfasterff.forward.femdata.femdata\_stnd\_TR(mesh, tmax, dt, savefield=False, beautify=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Forward modeling calculating TPSF on a standard mesh. Please consider using mesh.femdata\_tpsf(tmax, dt) instead.

The function calculates the MASS matrices, the source vectors, and calls the standard TPSF solver (preconditioned conjugated gradient).

#### **Parameters**

- mesh (nirfasterff.base.stndmesh) the mesh used to calcuate the forward data.
- tmax (double) maximum time simulated, in seconds.
- **dt** (*double*) size of each time step, in seconds.
- **savefield** (*bool*, *optional*) If True, the internal TPSFs are also returned. If False, only boundary TPSFs are returned and data.phi will be empty.

The default is False.

- **beautify** (*bool*, *optional*) If true, zeros the initial unstable parts of the boundary TPSFs. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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.
- ValueError If tmax is smaller than dt

## Returns

data (nirfasterff.base.TPSFdata) – internal and boundary TPSFs given the mesh and optodes.

If mesh.vol is defined and *savefield==True*, the returned internal TPSFs will be in volumetric space

See TPSFdata() for details.

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

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

## See also:

```
gen_mass_matrix(), gen_sources(), and get_field_TR()
```

# nirfasterff.forward.femdata.femdata stnd TR moments

Forward modeling calculating TR moments using Mellin transform on a standard mesh. Please consider using mesh.femdata\_moments() instead.

The function calculates the MASS matrices, the source vectors, and calls the Mellin moments solver (preconditioned conjugated gradient).

Calculates 0th, 1st, 2nd, .., max\_moments-th moments directly without calculating TPSF first.

This is more efficient, if the actual TPSFs are not of concern.

### **Parameters**

- mesh (nirfasterff.base.stndmesh) the mesh used to calcuate the forward data.
- max\_moments (int32, optional) max order of moments to calculate. That is, 0th, 1st, 2nd, ..., max\_moments-th will be calculated. The default is 3.
- **savefield** (*bool*, *optional*) If True, the internal moments are also returned. If False, only boundary moments are returned and data.phi will be empty.

The default is False.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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.
- **ValueError** If max\_moments is negative.

## Returns

• data (nirfasterff.base.TRMomentsdata) – internal and boundary moments given the mesh and optodes.

If mesh.vol is defined and *savefield==True*, the returned internal moments will be in volumetric space

See TRMomentsdata() for details.

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

Only the convergence info of highest order moments is returned.

See ConvergenceInfo() for details

# See also:

gen\_mass\_matrix(), gen\_sources(), and get\_field\_TRmoments()

## References

Arridge and Schweiger, Applied Optics, 1995. doi:10.1364/AO.34.002683

# 4.1.3 nirfasterff.inverse

Calculation of the Jacobian matrices and a basic Tikhonov regularization function

### **Functions**

<pre>jacobian_DCS(mesh, tvec[, normalize,])</pre>	Calculates the Jacobian matrix for a DCS mesh using the adjoint method
<pre>jacobian_fl_CW(mesh[, normalize, solver, opt])</pre>	Calculates the continuous-wave fluorescence Jacobian matrix using the adjoint method
<pre>jacobian_fl_FD(mesh, freq[, normalize,])</pre>	Calculates the frequency-domain fluorescence Jacobian matrix using the adjoint method
<pre>jacobian_stnd_CW(mesh[, normalize, mus,])</pre>	Calculates the continuous-wave Jacobian matrix using the adjoint method
<pre>jacobian_stnd_FD(mesh, freq[, normalize,])</pre>	Calculates the frequency-domain Jacobian matrix using the adjoint method
tikhonov(A, reg, y)	Solves Tikhonov regularization (ie ridge regression)

# nirfasterff.inverse.jacobian DCS

Calculates the Jacobian matrix for a DCS mesh using the adjoint method

One Jacobian is calcualted at each time point in tvec, and the derivative is taken with regard to aDb

## **Parameters**

- mesh (nirfasterff.base.dcsmesh) mesh on which the Jacobian is calculated.
- tvec (double NumPy vector) time vector used.
- **normalize** (*bool*, *optional*) if True, Jacobbians are normalized to the measured boundary amplitude. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 DCS mesh, or mesh.vol is not defined.

## Returns

- **J** (*double NumPy array*) The Jacobian matrix. Size (NChannel, NVoxel, NTime)
- **data1** (*nirfasterff.base.FLdata*) The calculated direct field. The same as directly calling mesh.femdata(tvec)

• data2 (nirfasterff.base.FLdata) – The calculated adjoint field. The same as calling mesh.femdata(tvec) AFTER swapping the locations of sources and detectors

# nirfasterff.inverse.jacobian\_fl\_CW

Calculates the continuous-wave fluorescence Jacobian matrix using the adjoint method

```
J_{ij} = dA_i / d_gamma_j
```

where A is fluorescence amplitude if normalization is False, fluorescence amplitude divided by excitation amplitude ('Born ratio') if True

gamma\_j = mesh.eta[j]\*mesh.muaf[j]

### **Parameters**

- mesh (nirfasterff.base.fluormesh) mesh on which the Jacobian is calculated.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements at excitation wavelength ('Born ratio').

The default is True.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 fluor mesh, or mesh.vol is not defined.

### Returns

- J (double NumPy array) The Jacobian matrix. Size (NChannel, NVoxel)
- **data1** (*nirfasterff.base.FLdata*) The calculated direct field. The same as directly calling mesh.femdata(0)
- data2 (nirfasterff.base.FLdata) The calculated adjoint field. The same as calling mesh.femdata(0) AFTER swapping the locations of sources and detectors

# References

Milstein et al., JOSA A, 2004. doi:10.1364/JOSAA.21.001035

# nirfasterff.inverse.jacobian\_fl\_FD

Calculates the frequency-domain fluorescence Jacobian matrix using the adjoint method

The Jacobian is structured as, suppose we have M channels and N voxels:

```
[d_real{A_1}/d_gamma_1, d_real{A_1}/d_gamma_2, ..., d_real{A_1}/d_gamma_{N}, d_real $$A_1$/dtau_1, d_real{A_1}/dtau_2, ..., d_real{A_1}/dtau_{N}$$] [d_imag{A_1}/d_gamma_1, d_imag{A_1}/d_gamma_2, ..., d_imag{A_1}/d_gamma_{N}, d_imag $$A_1$/dtau_1, d_imag{A_1}/dtau_2, ..., d_imag{A_1}/dtau_{N}$$] [d_real{A_2}/d_gamma_1, d_real{A_2}/d_gamma_2, ..., d_real{A_2}/d_gamma_{N}, d_real $$A_2$/dtau_1, d_real{A_2}/dtau_2, ..., d_real{A_2}/dtau_{N}$$] [d_imag{A_2}/d_gamma_1, d_imag{A_2}/d_gamma_2, ..., d_imag{A_2}/d_gamma_{N}, d_imag $$A_2$/dtau_1, d_imag{A_2}/dtau_2, ..., d_imag{A_2}/dtau_{N}$$] ... [d_real{A_M}/d_gamma_1, d_real{A_M}/d_gamma_2, ..., d_real{A_M}/d_gamma_{N}, d_real $$$A_M}/dtau_1, d_real{A_M}/dtau_2, ..., d_real{A_M}/dtau_{N}$$] [d_imag{A_M}/d_gamma_1, d_imag{A_M}/d_gamma_2, ..., d_imag{A_M}/d_gamma_{N}, d_imag $$$A_M}/dtau_1, d_imag{A_M}/dtau_2, ..., d_imag{A_M}/dtau_{N}$$]
```

where A is fluorescence amplitude if normalization is False, fluorescence amplitude divided by excitation amplitude ('Born ratio') if True gamma\_j = mesh.eta[j]\*mesh.muaf[j]

### **Parameters**

- mesh (nirfasterff.base.fluormesh) mesh on which the Jacobian is calculated.
- **freq** (*double*) modulation frequency in Hz.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements at excitation wavelength ('Born ratio').

The default is True.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 fluor mesh, or mesh.vol is not defined.

## Returns

- **J** (double NumPy array) The Jacobian matrix. Size (NChannel\*2, NVoxel\*2)
- data1 (nirfasterff.base.FLdata) The calculated direct field. The same as directly calling mesh.femdata(freq)
- data2 (nirfasterff.base.FLdata) The calculated adjoint field. The same as calling mesh.femdata(freq) AFTER swapping the locations of sources and detectors

### References

Milstein et al., JOSA A, 2004. doi:10.1364/JOSAA.21.001035

## nirfasterff.inverse.jacobian stnd CW

nirfasterff.inverse.jacobian\_stnd\_CW(mesh, normalize=True, mus=False, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates the continuous-wave Jacobian matrix using the adjoint method

Calculates spatial distributions of sensitivity of field registerd on the mesh boundary to changes of optical properties per voxel.

When mus is set to True, the Jacobian is structured as, suppose we have M channels and N voxels:

where A and Phi denote the measured amplitude and the phase if *normalize=False*, and the log of them if *normalize=True* 

When mus is set to False, the returned Jacobian is only the right half of the above. That is, only derivatives wrt

Note that the calculation is only done in the volumetric space

### **Parameters**

- mesh (nirfasterff.base.stndmesh) mesh on which the Jacobian is calculated.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements, i.e. use Rytov approximation.

The default is True.

- **mus** (bool, optional) whether derivates wrt mus (left half of the 'full' Jacobian) is calculated. The default is False.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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, or mesh.vol is not defined.

#### Returns

- **J** (*double NumPy array*) The Jacobian matrix. Size (NChannel, NVoxel\*2) if mus=True, (NChannel, NVoxel) if mus=False
- data1 (nirfasterff.base.FDdata) The calculated direct field. The same as directly calling mesh.femdata(0)

• data2 (nirfasterff.base.FDdata) – The calculated adjoint field. The same as calling mesh.femdata(0) AFTER swapping the locations of sources and detectors

## nirfasterff.inverse.jacobian\_stnd\_FD

nirfasterff.inverse.jacobian\_stnd\_FD(mesh, freq, normalize=True, mus=True, solver=utils.get\_solver(), opt=utils.SolverOptions())

Calculates the frequency-domain Jacobian matrix using the adjoint method

Calculates spatial distributions of sensitivity of field registerd on the mesh boundary to changes of optical properties per voxel.

When freq=0, see <code>jacobian\_stnd\_CW()</code> for the structure of the Jacobian

When freq>0, the Jacobian is structured as, suppose we have M channels and N voxels:

where A and Phi denote the measured amplitude and the phase if *normalize=False*, and the log of them if *normalize=True* 

Note that the calculation is only done in the volumetric space

#### **Parameters**

- mesh (nirfasterff.base.stndmesh) mesh on which the Jacobian is calculated.
- **freq** (*double*) modulation frequency, in Hz.
- **normalize** (*bool*, *optional*) whether normalize the Jacobian to the amplitudes of boundary measurements, i.e. use Rytov approximation.

The default is True.

- **mus** (*bool*, *optional*) whether derivates wrt mus (left half of the 'full' Jacobian) is calculated. Only has effect when freq=0. The default is True.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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, or mesh.vol is not defined.

### Returns

- **J** (double or complex double NumPy array) The Jacobian matrix. Size (NChannel\*2, NVoxel\*2) if freq>0, (NChannel, NVoxel\*2) if freq=0 and mus=True, (NChannel, NVoxel) if freq=0 and mus=False
- **data1** (*nirfasterff.base.FDdata*) The calculated direct field. The same as directly calling mesh.femdata(freq)
- data2 (nirfasterff.base.FDdata) The calculated adjoint field. The same as calling mesh.femdata(freq) AFTER swapping the locations of sources and detectors

## References

Arridge, Applied Optics, 1995. doi:10.1364/AO.34.007395

#### nirfasterff.inverse.tikhonov

```
nirfasterff.inverse.tikhonov(A, reg, y)
```

Solves Tikhonov regularization (ie ridge regression)

That is, given a linear system y = Ax, it solves  $\arg\min_x ||Ax - y||_2^2 + ||\Gamma x||_2^2$ 

where A is the forward matrix, y is the recording, and  $\Gamma$  is the regularization matrix

### **Parameters**

- A (double NumPy array) forward matrix, e.g. the Jacobian in DOT.
- reg (double NumPy array or scalar) if a scalar, the same regularization is applied to all elements of x, i.e.  $\Gamma = reg * I$ .

if a vector, the regularization matrix is assumed to be diagonal, with the diagonal elements specified in reg, i.e.  $\Gamma = diag(reg)$ .

if a matrix, it must be symmetric. In this case,  $\Gamma = reg$ .

• y (double NumPy vector) – measurement vector, e.g. dOD at each channel in DOT.

### Raises

**ValueError** – if reg is of incompatible size or not symmetric (if matrix).

### Returns

**result** – Tikhonov regularized solution to the linear system.

### **Return type**

double NumPy vector

## 4.1.4 nirfasterff.io

Some functions for reading/writing certain data types.

As of now, they are only used by the CGAL mesher, and there should be no need for the user to directly call them.

# **Functions**

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

## nirfasterff.io.readMEDIT

## nirfasterff.io.readMEDIT(fname)

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.

## nirfasterff.io.saveinr

nirfasterff.io.saveinr(vol, 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.

# 4.1.5 nirfasterff.lib

Low-level functions implemented in C/C++, on both GPU and CPU

You should NOT directly call these functions. Please use the wrapper functions provided instead

### **Modules**

```
nirfasterff.lib.nirfasterff_cpu
nirfasterff.lib.nirfasterff_cuda
```

# nirfasterff.lib.nirfasterff\_cpu

## **Functions**

```
IntGradGrid(*args, **kwargs)
                                                     Overloaded function.
IntGrid(*args, **kwargs)
                                                     Overloaded function.
ele_area(arg0, arg1)
gen_mass_matrix(arg0, arg1, arg2, arg3, ...)
                                                     Overloaded function.
gen_source_fl(*args, **kwargs)
get_field_CW(*args, **kwargs)
                                                     Overloaded function.
get_field_FD(*args, **kwargs)
                                                     Overloaded function.
get_field_TR(*args, **kwargs)
                                                     Overloaded function.
get_field_TRFL(arg0, arg1, arg2, arg3, arg4, ...)
get_field_TRFL_moments(arg0, arg1, arg2, ...)
get_field_TR_moments(*args, **kwargs)
                                                     Overloaded function.
gradientIntfunc(arg0, arg1, arg2)
gradientIntfunc2(arg0, arg1, arg2)
isCUDA()
mesh_support(arg0, arg1, arg2)
pointLocation(arg0, arg1, arg2)
```

# nirfasterff.lib.nirfasterff\_cpu.IntGradGrid

nirfasterff.lib.nirfasterff\_cpu.IntGradGrid(\*args, \*\*kwargs)

Overloaded function.

- 1. IntGradGrid(arg0: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c contiguous], numpy.ndarray[numpy.complex128[m, flags.writeable, flags.c\_contiguous], arg1: n], arg2: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c contiguous], arg3: numpy.ndarray[numpy.complex128[m, flags.writeable, flags.c\_contiguous], n], arg4: numpy.ndarray[numpy.complex128[m, flags.writeable, flags.c contiguous], numpy.ndarray[numpy.complex128[m, flags.writeable, flags.c contiguous], arg5: n], arg6: numpy.ndarray[numpy.int32[m. nl. flags.writeable. flags.c contiguous], arg7: int) numpy.ndarray[numpy.complex128[m, n]]
- 2. IntGradGrid(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], numpy.ndarray[numpy.float64[m, flags.writeable, flags.c\_contiguous], arg1: n], arg2: numpy.ndarray[numpy.float64[m, flags.writeable, flags.c\_contiguous], n], arg3: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c contiguous], numpy.ndarray[numpy.float64[m, flags.writeable, flags.c\_contiguous], arg4: n], arg5: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c contiguous], arg6: numpy.ndarray[numpy.int32[m, n], flags.writeable, flags.c\_contiguous], arg7: int) numpy.ndarray[numpy.float64[m, n]]

## nirfasterff.lib.nirfasterff cpu.IntGrid

nirfasterff.lib.nirfasterff\_cpu.IntGrid(\*args, \*\*kwargs)

Overloaded function.

- 1. IntGrid(arg0: numpy.ndarray[numpy.complex128[m, flags.writeable, nl. flags.c contiguous], numpy.ndarray[numpy.complex128[m, flags.writeable, arg1: flags.c\_contiguous], n], numpy.ndarray[numpy.int32[m. arg2: n], flags.writeable, flags.c contiguous]) numpy.ndarray[numpy.complex128[m, n]]
- 2. IntGrid(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c contiguous], arg2: numpy.ndarray[numpy.int32[m, flags.writeable, flags.c\_contiguous]) n], numpy.ndarray[numpy.float64[m, n]]

## nirfasterff.lib.nirfasterff cpu.ele area

nirfasterff.lib.nirfasterff\_cpu.ele\_area(arg0:  $numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c_contiguous], <math>arg1$ :  $numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c_contiguous]) <math>\rightarrow$  numpy.ndarray[numpy.float64[m, 1]]

# nirfasterff.lib.nirfasterff\_cpu.gen\_mass\_matrix

```
nirfasterff.lib.nirfasterff_cpu.gen_mass_matrix(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg4: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg5: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg5: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg7: float) <math>\rightarrow tuple[numpy.ndarray[numpy.int32[m, 1]], numpy.ndarray[numpy.int32[m, 1]], numpy.ndarray[numpy.complex128[m, 1]]]
```

## nirfasterff.lib.nirfasterff cpu.gen source fl

nirfasterff.lib.nirfasterff\_cpu.gen\_source\_fl(\*args, \*\*kwargs)

Overloaded function.

- 2. gen\_source\_fl(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c\_contiguous]) -> numpy.ndarray[numpy.complex128[m, n]]

### nirfasterff.lib.nirfasterff cpu.get field CW

nirfasterff.lib.nirfasterff\_cpu.get\_field\_CW(\*args, \*\*kwargs)

Overloaded function.

- 2. get\_field\_CW(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff\_lib.nirfasterff\_cpu.ConvergenceInfoCPU]]

# nirfasterff.lib.nirfasterff\_cpu.get\_field\_FD

nirfasterff.lib.nirfasterff\_cpu.get\_field\_FD(\*args, \*\*kwargs)

Overloaded function.

- 1. get\_field\_FD(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.complex128[m, 1], flags.writeable], arg3: scipy.sparse.csc\_matrix[numpy.complex128], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 100000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.complex128[m, n]], list[nirfasterff.lib.nirfasterff\_cpu.ConvergenceInfoCPU]]
- 2. get\_field\_FD(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.complex128[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c\_contiguous], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.complex128[m, n]], list[nirfasterff\_lib.nirfasterff\_cpu.ConvergenceInfoCPU]]

# nirfasterff.lib.nirfasterff cpu.get field TR

nirfasterff.lib.nirfasterff\_cpu.get\_field\_TR(\*args, \*\*kwargs)

Overloaded function.

- 1. get field TR(arg0: numpy.ndarray[numpy.int32[m, flags.writeable], 1], numpy.ndarray[numpy.int32[m, flags.writeable], arg2: 1], numpy.ndarray[numpy.float64[m, numpy.ndarray[numpy.float64[m, flags.writeable], arg3: 1], flags.writeable], scipy.sparse.csc matrix[numpy.float64], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 100000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff cpu.ConvergenceInfoCPU]]
- 2. get field TR(arg0: numpy.ndarray[numpy.int32[m, flags.writeable], 1], arg1: numpy.ndarray[numpy.int32[m, flags.writeable], numpy.ndarray[numpy.float64[m, 1], arg2: flags.writeable], flags.writeable], arg3: numpy.ndarray[numpy.float64[m, 11. arg4: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff\_cpu.ConvergenceInfoCPU]]

## nirfasterff.lib.nirfasterff cpu.get field TRFL

nirfasterff.lib.nirfasterff\_cpu.get\_field\_TRFL(arg0: numpy.ndarray[numpy.int32[m, 1],

flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg4: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg5: int, max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0,  $nthread: int = 8) \rightarrow$  tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff\_cpu.ConvergenceInfoCPU]]

# nirfasterff.lib.nirfasterff\_cpu.get\_field\_TRFL\_moments

```
nirfasterff.lib.nirfasterff_cpu.get_field_TRFL_moments(arg0: numpy.ndarray[numpy.int32[m, 1],
                                                                 flags.writeable], arg1:
                                                                 numpy.ndarray[numpy.int32[m, 1],
                                                                 flags.writeable], arg2:
                                                                 numpy.ndarray[numpy.float64[m, 1],
                                                                flags.writeable], arg3:
                                                                 numpy.ndarray[numpy.float64[m, 1],
                                                                 flags.writeable], arg4:
                                                                 numpy.ndarray[numpy.float64[m, 1],
                                                                 flags.writeable], arg5:
                                                                 numpy.ndarray[numpy.float64[m, n],
                                                                 flags.writeable, flags.c contiguous], arg6:
                                                                 numpy.ndarray[numpy.float64[m, 1],
                                                                flags.writeable], arg7:
                                                                 numpy.ndarray[numpy.float64[m, 1],
                                                                 flags.writeable], arg8: int, max_iter: int =
                                                                 1000, AbsoluteTolerance: float = 1e-12,
                                                                 RelativeTolerance: float = 1e-12, divergence:
                                                                 tuple[numpy.ndarray[numpy.float64[m, n]],
                                                                 list[nirfasterff.lib.nirfasterff_cpu.ConvergenceInfoCPU]]
```

## nirfasterff.lib.nirfasterff cpu.get field TR moments

nirfasterff.lib.nirfasterff\_cpu.get\_field\_TR\_moments(\*args, \*\*kwargs)
 Overloaded function.

- 1. get field TR moments(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, flags.writeable], numpy.ndarray[numpy.float64[m, arg2: numpy.ndarray[numpy.float64[m, flags.writeable], arg3: 1], flags.writeable], arg4: scipy.sparse.csc matrix[numpy.float64], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff cpu.ConvergenceInfoCPU]]
- 2. get field TR moments(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.float64[m, flags.writeable], numpy.ndarray[numpy.float64[m, flags.writeable], 1], arg4: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg5: int, max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 100000000.0, nthread: int = 8) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff\_cpu.ConvergenceInfoCPU]]

# nirfasterff.lib.nirfasterff\_cpu.gradientIntfunc

```
\label{lib:nirfasterff_cpu.gradientIntfunc} nirfasterff\_cpu.gradientIntfunc(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous]) <math>\rightarrow tuple[numpy.ndarray[numpy.int32[m, 1]], numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous])
```

# nirfasterff.lib.nirfasterff\_cpu.gradientIntfunc2

# nirfasterff.lib.nirfasterff\_cpu.isCUDA

```
nirfasterff.lib.nirfasterff\_cpu.isCUDA() \rightarrow bool
```

# nirfasterff.lib.nirfasterff\_cpu.mesh\_support

```
nirfasterff.lib.nirfasterff_cpu.mesh_support(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c_contiguous], <math>arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c_contiguous], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable]) <math>\rightarrow numpy.ndarray[numpy.float64[m, 1]]
```

### nirfasterff.lib.nirfasterff cpu.pointLocation

```
\label{libnirfasterff_cpu.pointLocation} \begin{tabular}{l} nirfasterff\_cpu.pointLocation(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous]) $\rightarrow$ tuple[numpy.ndarray[numpy.int32[m, 1]], numpy.ndarray[numpy.float64[m, n]]] \end{tabular}
```

## **Classes**

 ${\it ConvergenceInfoCPU}$ 

# nirfasterff.lib.nirfasterff\_cpu.ConvergenceInfoCPU

```
class nirfasterff.lib.nirfasterff_cpu.ConvergenceInfoCPU
    Bases: pybind11_object
    __init__(self: nirfasterff.lib.nirfasterff_cpu.ConvergenceInfoCPU) → None
```

## **Methods**

```
__init__(self)
```

## **Attributes**

```
isConverged
isConvergedToAbsoluteTolerance
iteration
residual
```

# nirfasterff.lib.nirfasterff\_cuda

# **Functions**

```
gen_mass_matrix(arg0, arg1, arg2, arg3, ...)gen_source_fl(*args, **kwargs)Overloaded function.get_field_CW(*args, **kwargs)Overloaded function.get_field_FD(*args, **kwargs)Overloaded function.get_field_TR(*args, **kwargs)Overloaded function.get_field_TRFL(arg0, arg1, arg2, arg3, arg4, ...)overloaded function.get_field_TRFL_moments(arg0, arg1, arg2, ...)overloaded function.
```

# nirfasterff.lib.nirfasterff\_cuda.gen\_mass\_matrix

```
nirfasterff.lib.nirfasterff_cuda.gen_mass_matrix(arg0: numpy.ndarray[numpy.float64[m, n],
                                                             flags.writeable, flags.c contiguous], arg1:
                                                             numpy.ndarray[numpy.float64[m, n],
                                                             flags.writeable, flags.c_contiguous], arg2:
                                                             numpy.ndarray[numpy.float64[m, 1],
                                                             flags.writeable], arg3:
                                                             numpy.ndarray[numpy.float64[m, 1],
                                                             flags.writeable], arg4:
                                                             numpy.ndarray[numpy.float64[m, 1],
                                                             flags.writeable], arg5:
                                                             numpy.ndarray[numpy.float64[m, 1],
                                                             flags.writeable], arg6:
                                                             numpy.ndarray[numpy.float64[m, 1],
                                                             flags.writeable], arg7: float, GPU: int = -1) \rightarrow
                                                             tuple[numpy.ndarray[numpy.int32[m, 1]],
                                                             numpy.ndarray[numpy.int32[m, 1]],
                                                             numpy.ndarray[numpy.complex128[m, 1]]]
```

# nirfasterff.lib.nirfasterff\_cuda.gen\_source\_fl

 $\label{lib.nirfasterff_cuda.gen_source_fl(*args, **kwargs)} \\ \text{nirfasterff\_cuda.gen\_source\_fl(*} \\ \text{args, **kwargs)} \\$ 

Overloaded function.

- 1. gen\_source\_fl(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], GPU: int = -1) -> numpy.ndarray[numpy.float64[m, n]]
- 2. gen\_source\_fl(arg0: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg1: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg2: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c\_contiguous], GPU: int = -1) -> numpy.ndarray[numpy.complex128[m, n]]

## nirfasterff.lib.nirfasterff\_cuda.get\_field\_CW

nirfasterff.lib.nirfasterff\_cuda.get\_field\_CW(\*args, \*\*kwargs)

Overloaded function.

- 1. get\_field\_CW(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg3: scipy.sparse.csc\_matrix[numpy.float64], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff\_lib.nirfasterff\_cuda.ConvergenceInfoGPU]]
- 2. get\_field\_CW(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 100000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff cuda.ConvergenceInfoGPU]]

## nirfasterff.lib.nirfasterff cuda.get field FD

nirfasterff.lib.nirfasterff\_cuda.get\_field\_FD(\*args, \*\*kwargs)

Overloaded function.

- 1. get\_field\_FD(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.complex128[m, 1], flags.writeable], arg3: scipy.sparse.csc\_matrix[numpy.complex128], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.complex128[m, n]], list[nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU]]
- 2. get\_field\_FD(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg2: numpy.ndarray[numpy.complex128[m, 1], flags.writeable], arg3: numpy.ndarray[numpy.complex128[m, n], flags.writeable, flags.c\_contiguous], max\_iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.complex128[m, n]], list[nirfasterff\_lib.nirfasterff\_cuda.ConvergenceInfoGPU]]

# nirfasterff.lib.nirfasterff cuda.get field TR

nirfasterff.lib.nirfasterff\_cuda.get\_field\_TR(\*args, \*\*kwargs)

Overloaded function.

- 1. get\_field\_TR(arg0: numpy.ndarray[numpy.int32[m, flags.writeable], 1], numpy.ndarray[numpy.int32[m, flags.writeable], arg2: 1], numpy.ndarray[numpy.float64[m, numpy.ndarray[numpy.float64[m, flags.writeable], arg3: 1], flags.writeable], scipy.sparse.csc matrix[numpy.float64], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff cuda.ConvergenceInfoGPU]]
- 2. get field TR(arg0: numpy.ndarray[numpy.int32[m, flags.writeable], 1], numpy.ndarray[numpy.int32[m, flags.writeable], numpy.ndarray[numpy.float64[m, 1], arg2: flags.writeable], arg3: numpy.ndarray[numpy.float64[m, 1], flags.writeable], arg4: numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c\_contiguous], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, diverfloat = 100000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU]]

## nirfasterff.lib.nirfasterff cuda.get field TRFL

# nirfasterff.lib.nirfasterff\_cuda.get\_field\_TRFL\_moments

```
nirfasterff.lib.nirfasterff_cuda.get_field_TRFL_moments(arg0: numpy.ndarray[numpy.int32[m, 1],
                                                                      flags.writeable], arg1:
                                                                      numpy.ndarray[numpy.int32[m, 1],
                                                                      flags.writeable], arg2:
                                                                      numpy.ndarray[numpy.float64[m, 1],
                                                                      flags.writeable], arg3:
                                                                      numpy.ndarray[numpy.float64[m, 1],
                                                                      flags.writeable], arg4:
                                                                      numpy.ndarray[numpy.float64[m, 1],
                                                                      flags.writeable], arg5:
                                                                      numpy.ndarray[numpy.float64[m, n],
                                                                      flags.writeable, flags.c contiguous], arg6:
                                                                      numpy.ndarray[numpy.float64[m, 1],
                                                                      flags.writeable], arg7:
                                                                      numpy.ndarray[numpy.float64[m, 1],
                                                                      flags.writeable], arg8: int, max_iter: int =
                                                                      1000, AbsoluteTolerance: float = 1e-12,
                                                                      RelativeTolerance: float = 1e-12,
                                                                      divergence: float = 100000000.0, GPU: int
                                                                      =-1) \rightarrow
                                                                      tuple[numpy.ndarray[numpy.float64[m, n]],
                                                                      list[nirfasterff.lib.nirfasterff_cuda.ConvergenceInfoGPU]]
```

### nirfasterff.lib.nirfasterff cuda.get field TR moments

nirfasterff.lib.nirfasterff\_cuda.get\_field\_TR\_moments(\*args, \*\*kwargs)

Overloaded function.

1. get field TR moments(arg0: numpy.ndarray[numpy.int32[m, flags.writeable], 1], arg1: numpy.ndarray[numpy.int32[m, flags.writeable], arg2: numpy.ndarray[numpy.float64[m, numpy.ndarray[numpy.float64[m, flags.writeable], flags.writeable], arg3: 11. arg4: scipy.sparse.csc matrix[numpy.float64], arg5: int, max iter: int = 1000, AbsoluteTolerance: float = 1e-12, RelativeTolerance: float = 1e-12, divergence: float = 1000000000.0, GPU: int = -1) ->

tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff cuda.ConvergenceInfoGPU]]

2. get\_field\_TR\_moments(arg0: numpy.ndarray[numpy.int32[m, 1], flags.writeable], arg1: numpy.ndarray[numpy.int32[m, flags.writeable], numpy.ndarray[numpy.float64[m, arg2: flags.writeable], numpy.ndarray[numpy.float64[m, flags.writeable], arg3: 1], numpy.ndarray[numpy.float64[m, n], flags.writeable, flags.c contiguous], arg5: int, max iter: float = 1e-12, RelativeTolerance: int = 1000, AbsoluteTolerance: float = 1e-12, divergence: float = 100000000.0, GPU: int = -1) -> tuple[numpy.ndarray[numpy.float64[m, n]], list[nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU]]

## **Classes**

 ${\it ConvergenceInfoGPU}$ 

# nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU

class nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU

Bases: pybind11\_object

**\_\_init\_\_**(self: nirfasterff.lib.nirfasterff\_cuda.ConvergenceInfoGPU)  $\rightarrow$  None

## **Methods**

\_\_init\_\_(self)

# **Attributes**

isConverged

 $\verb|isConvergedToAbsoluteTolerance| \\$ 

iteration

residual

# 4.1.6 nirfasterff.math

Some low-level functions used by the forward solvers.

It is usually unnecessary to use them directly and caution must be excercised, as many of them interact closely with the C++ libraries and can cause crashes if used incorrectly

## **Functions**

<pre>gen_mass_matrix(mesh, omega[, solver, GPU])</pre>	Calculate the MASS matrix, and return the coordinates in CSR format.
gen_sources(mesh)	Calculate the source vectors (point source only) for the sources in mesh.source field
<pre>gen_sources_fl(mesh, phix[, frequency,])</pre>	Calculates FEM sources vector for re-emission.
<pre>get_boundary_data(mesh, phi)</pre>	Calculates boundary data given the field data in mesh
<pre>get_field_CW(csrI, csrJ, csrV, qvec[, opt,])</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.
<pre>get_field_FD(csrI, csrJ, csrV, qvec[, opt,])</pre>	Call the Preconditioned BiConjugate Stablized solver with FSAI preconditioner.
<pre>get_field_TR(csrI, csrJ, csrV, qvec, dt,)</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.
<pre>get_field_TRFL(csrI, csrJ, csrV, qvec_m, dt,)</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.
<pre>get_field_TRFLmoments(csrI, csrJ, csrV,)</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.
<pre>get_field_TRmoments(csrI, csrJ, csrV, qvec,)</pre>	Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner.

## nirfasterff.math.gen mass matrix

nirfasterff.math.gen\_mass\_matrix(mesh, 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 (nirfasterff.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),)

### nirfasterff.math.gen sources

### nirfasterff.math.gen\_sources(mesh)

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

# nirfasterff.math.gen\_sources\_fl

nirfasterff.math.gen\_sources\_fl (mesh, phix, frequency=0., solver=utils.get\_solver(), GPU=-1) Calculates FEM sources vector for re-emission.

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

### **Parameters**

- **mesh** (*nirfasterff.base.fluormesh*) mesh used to calcualte the source vectors. Source information is also defined here.
- **phix** (*double NumPy array*) excitation fluence calculated at each node for each source. Size (NNodes, NSources)
- **frequency** (*double*, *optional*) modulation frequency, in Hz. The default is 0..
- **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

qvec – calculated fluence emission source vectors. Size (NNodes, NSources)

## Return type

double or complex double NumPy array

# nirfasterff.math.get\_boundary\_data

nirfasterff.math.get\_boundary\_data(mesh, 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 (nirfasterff 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

# nirfasterff.math.get\_field\_CW

nirfasterff.math.get\_field\_CW(csrI, csrI, 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** (nirfasterff.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)
- $\bullet \ \ info\ (\textit{nirfasterff.utils.ConvergenceInfo}) convergence\ information\ of\ the\ solver.$

See ConvergenceInfo() for details

### See also:

gen\_mass\_matrix()

## nirfasterff.math.get field FD

nirfasterff.math.get\_field\_FD(csrI, 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** (nirfasterff.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** (*nirfasterff.utils.ConvergenceInfo*) convergence information of the solver.

See *ConvergenceInfo()* for details

### See also:

gen\_mass\_matrix()

# nirfasterff.math.get\_field\_TR

Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner. Calculates TPSF data

NOT interchangeable with the current MATLAB version

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

On both GPU and CPU, the algorithm solves the sources one by one

#### **Parameters**

- csrI (int32 NumPy vector, zero-based) I indices of the MASS matrices, in CSR format.
- csrJ (int32 NumPy vector, zero-based) J indices of the MASS matrices, in CSR format.
- csrV (complex double NumPy vector) values of the MASS matrices, in CSR format.

This is calculated using gen\_mass\_matrix with omega=1. The real part coincides with K+C, and the imaginary part coincides with -M.

See references for details

• **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.

- **dt** (*double*) time step size, in seconds.
- max\_step (int32) total number of time steps.
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 csrV is not complex, or if quec is not real, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

### Returns

• **phi** (*double NumPy array*) – Calculated TPSF at each source. Size (NNodes, Nsources\*max\_step), structured as,

```
[src0_step0, src1_step0,...,src0_step1, src1_step1,...]
```

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

Only the convergence info of the last time step is returned.

See *ConvergenceInfo()* for details

### See also:

gen\_mass\_matrix()

### References

Arridges et al., Med. Phys., 1993. doi:10.1118/1.597069

# nirfasterff.math.get\_field\_TRFL

Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner. Calculates the TPSFs of fluorescence emission given the TPSFs of excitation

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

On both GPU and CPU, the algorithm solves the sources one by one

### **Parameters**

- **csrI** (*int32 NumPy vector*, *zero-based*)—I indices of the MASS matrices at emission wavelength, in CSR format.
- csrJ (int32 NumPy vector, zero-based) J indices of the MASS matrices at emission wavelength, in CSR format.
- **csrV**(complex double NumPy vector) values of the MASS matrices at emission wavelength, in CSR format.

This is calculated using gen\_mass\_matrix with omega=1.

• **qvec\_m** (*double NumPy array*) – TPSF of the excitation convolved with decay, and multiplied by the FEM matrix. Size (NNodes, NSources\*NTime), structured as,

```
[src0_step0, src1_step0,...,src0_step1, src1_step1,...]
```

- **dt** (*double*) time step size, in seconds.
- max\_step (int32) total number of time steps. It should match exactly with the number of steps in the excitation data
- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 csrV is not complex, or if phix is not real, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

#### Returns

• **phi** (*double NumPy array*) – Calculated TPSF at each source of fluorescence emission. Size (NNodes, Nsources\*max\_step), structured as,

```
[src0_step0, src1_step0,...,src0_step1, src1_step1,...]
```

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

Only the convergence info of the last time step is returned.

See ConvergenceInfo() for details

#### See also:

```
gen_mass_matrix(), get_field_TR()
```

# nirfasterff.math.get\_field\_TRFLmoments

nirfasterff.math.get\_field\_TRFLmoments(csrI, csrJ, csrV, csrV2, mx, gamma, tau, max\_moment, opt=utils.SolverOptions(), solver=utils.get\_solver())

Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner. Directly calculates moments of re-emission using Mellin transform, given the moments of excitation

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

On both GPU and CPU, the algorithm solves the sources one by one

## **Parameters**

- **csrI** (*int32 NumPy vector*, *zero-based*)—I indices of the MASS matrices at emission wavelength, in CSR format.
- **csrJ** (*int32 NumPy vector*, *zero-based*) J indices of the MASS matrices at emission wavelength, in CSR format.
- **csrV**(*complex double NumPy vector*) values of the MASS matrices at emission wavelength, in CSR format.

This is calculated using gen\_mass\_matrix with omega=1.

- $\hbox{\bf \bullet csrV2} \ (\textit{double NumPy vector}) values \ of the FEM \ integration \ matrix, in \ CSR \ format. \\$ 
  - This is calculated using gen\_mass\_matrix with omega=0, mua=1, kappa=0, and no boundary nodes.
- mx (double NumPy array) moments of the excitation. Size (NNodes, Nsources\*(max\_moment+1)), structured as,

```
[src0_m0, src1_m0,...,src0_m1, src1_m1,...]
```

- gamma (double NumPy array) defined as mesh.eta\*mesh.muaf.
- tau (double NumPy array) decay factor, as defined in mesh.tau.
- max\_moment (int32) max order of moments to calculate. That is, 0th, 1st, 2nd, .., max moments-th will be calculated.

This should match exact with the max\_moment of the excitation

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 csrV is not complex, or if mx is not real, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

#### Returns

• **phi** (*double NumPy array*) – Calculated Mellin transform of fluorecence emission at each source. Size (NNodes, Nsources\*(max\_moment+1)), structured as,

```
[src0_m0, src1_m0,...,src0_m1, src1_m1,...]
```

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

Only the convergence info of the highest order moments is returned.

See ConvergenceInfo() for details

#### See also:

gen\_mass\_matrix(), get\_field\_TRmoments()

## nirfasterff.math.get field TRmoments

Call the Preconditioned Conjugate Gradient solver with FSAI preconditioner. Directly calculates moments of TR data using Mellin transform

NOT interchangeable with the current MATLAB version

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

On both GPU and CPU, the algorithm solves the sources one by one

## **Parameters**

- csrI (int32 NumPy vector, zero-based) I indices of the MASS matrices, in CSR format.
- csrJ (int32 NumPy vector, zero-based) J indices of the MASS matrices, in CSR format.
- csrV (complex double NumPy vector) values of the MASS matrices, in CSR format.

This is calculated using gen\_mass\_matrix with omega=1. The real part coincides with K+C, and the imaginary part coincides with -B.

See references for details

- **qvec** (double NumPy array, or Scipy CSC sparse matrix) The source vectors. i-th column corresponds to source i. Size (NNode, NSource)
- max\_moment (int32) max order of moments to calculate. That is, 0th, 1st, 2nd, .., max\_moments-th will be calculated.

- **solver** (*str*, *optional*) Choose between 'CPU' or 'GPU' solver (case insensitive). Automatically determined (GPU prioritized) if not specified
- **opt** (nirfasterff.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 csrV is not complex, or if quec is not real, or if solver is not 'CPU' or 'GPU'.
- RuntimeError if both GPU and CPU solvers fail.

### Returns

• **phi** (*double NumPy array*) – Calculated Mellin transform at each source. Size (NNodes, Nsources\*(max\_moment+1)), structured as,

```
[src0_m0, src1_m0,...,src0_m1, src1_m1,...]
```

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

Only the convergence info of the highest order moments is returned.

See ConvergenceInfo() for details

## See also:

gen\_mass\_matrix()

## References

Arridge and Schweiger, Applied Optics, 1995. doi:10.1364/AO.34.002683

# 4.1.7 nirfasterff.meshing

Functions used for mesh generation and quality check

### **Modules**

nirfasterff.meshing.auxiliary	Auxiliary functions used for mesh quality check.
nirfasterff.meshing.meshutils	Functions used for mesh generation and mesh quality check

# nirfasterff.meshing.auxiliary

Auxiliary functions used for mesh quality check.

They are unlikely to become useful to an ordinary user, but still documented for completeness

Use with caution: no error checking mechanisms implemented

# **Functions**

check_facearea(nodes, ele)	Calculates the areas of each face, and check if they are close to zero
<pre>check_tetrahedron_faces(ele)</pre>	Check for faces shared by more than two tetrahedrons
checkedges(ele)	Check for orphan edges and edges shared by more than two triangles
<pre>quality_triangle_radius(nodes, ele)</pre>	Radius ratio: 2*inradius / circumradius
simpqual(nodes, ele)	For each tetrahedron, calculates the didehedral angles and returns the smallest sine of them
$vector\_vector\_angle(u, v)$	Calculates vector-vector angles, in radian

# nirfasterff.meshing.auxiliary.check\_facearea

nirfasterff.meshing.auxiliary.check\_facearea(nodes, ele)

Calculates the areas of each face, and check if they are close to zero

Close to zero defined as 1e6 of the max span of the mesh

#### **Parameters**

- **nodes** (double NumPy array) node locations of the mesh.
- **ele** (*int32 NumPy array*) element list of the mesh, zero-based.

### Returns

- area (double NumPy vector) areas of each face. Size (NElements,)
- **zeroflag** (*bool NumPy vector*) flags of whether the area is close to zero, for each face. Size (NElements,)

# nirfasterff.meshing.auxiliary.check\_tetrahedron\_faces

nirfasterff.meshing.auxiliary.check\_tetrahedron\_faces(ele)

Check for faces shared by more than two tetrahedrons

## **Parameters**

ele (int32 NumPy array) — element list of the mesh, zero-based.

## Returns

flag - 0 if no faulty faces found, and 2 if faces shared by more than two tetrahedrons are found.

## Return type

int

# nirfasterff.meshing.auxiliary.checkedges

```
nirfasterff.meshing.auxiliary.checkedges(ele)
```

Check for orphan edges and edges shared by more than two triangles

#### **Parameters**

ele (int32 NumPy array) – element list of the mesh, zero-based.

#### Returns

 $\mathbf{flag} - 0$  if no errors found; 1 if edges shared by more than two triangles found; 2 if dangling edges found; 3 if both errors found.

## Return type

int

# nirfasterff.meshing.auxiliary.quality\_triangle\_radius

```
nirfasterff.meshing.auxiliary.quality_triangle_radius(nodes, ele)
```

Radius ratio: 2\*inradius / circumradius

Value between 0 and 1. Equals 1 only when a triangle is equilateral

#### **Parameters**

- nodes (double NumPy array) node locations of the mesh.
- **ele** (*int32 NumPy array*) element list of the mesh, zero-based.

#### Returns

radius ratios for each triangle. Size (NElements,)

## **Return type**

double NumPy vector

## References

https://en.wikibooks.org/wiki/Trigonometry/Circles and Triangles/The Incircle

## nirfasterff.meshing.auxiliary.simpqual

```
nirfasterff.meshing.auxiliary.simpqual(nodes, ele)
```

For each tetrahedron, calculates the didehedral angles and returns the smallest sine of them

## **Parameters**

- **nodes** (*double NumPy array*) node locations of the mesh.
- **ele** (*int32 NumPy array*) element list of the mesh, zero-based.

#### Returns

smallest sine of the dihedral angles for each element. Size (NElements,)

#### Return type

double NumPy vector

### References

https://en.wikipedia.org/wiki/Dihedral\_angle

# nirfasterff.meshing.auxiliary.vector\_vector\_angle

nirfasterff.meshing.auxiliary.vector\_vector\_angle(u, v)

Calculates vector-vector angles, in radian

Each row of u, v is a vector, and the angles are calculated pairwise row by row

### **Parameters**

- **u** (double NumPy array) first set of vectors.
- v (double NumPy array) second set of vectors.

#### Returns

pairwise vector-vector angles, in radian. Same number of rows as u and v

## **Return type**

double NumPy vector

# nirfasterff.meshing.meshutils

Functions used for mesh generation and mesh quality check

## **Functions**

<pre>CheckMesh2D(elements, nodes[, base, verbose])</pre>	Main function that calculates and checks the quality of a 2D mesh
<pre>CheckMesh3D(elements, nodes[, base, verbose])</pre>	Main function that calculates and checks the quality of a 3D mesh, which can be either a solid or surface mesh
RunCGALMeshGenerator(mask[, opt])	Generate a tetrahedral mesh from a volume using CGAL 6.0.1 mesher, where different regions are labeled used a distinct integer.
<pre>boundfaces(nodes, elements[, base, renumber])</pre>	Finds the boundary faces of a 3D tetrahedral mesh
<pre>checkmesh3d_solid(ele, nodes[, verbose])</pre>	Calculates and returns the quality metrics of the tetrahedrons in a 3D tetrahedral mesh
<pre>checkmesh3d_surface(ele, nodes[, verbose])</pre>	Calculates and returns the quality metrics of the triangles in a 3D surface mesh

# nirfasterff.meshing.meshutils.CheckMesh2D

nirfasterff.meshing.meshutils.CheckMesh2D(elements, nodes, base=1, verbose=False)

Main function that calculates and checks the quality of a 2D mesh

## **Parameters**

- elements (int32 NumPy array) element list of the mesh, zero-based.
- **nodes** (double NumPy array) node locations of the mesh, in mm.

- base (int, optional) one- or zero-based indexing of the element list. Can be 1, or 0. The default is 1.
- verbose (bool, optional) whether print the problematic elements to stdout, if any. The
  default is False.

### Raises

**TypeError** – if elements and nodes do not define a valid 2D mesh.

#### Returns

- flag (int) flags of mesh quality, set by bits: 'b2b1b0'.
   b1 set if faulty edges found; b2 set if triangles with small area found
- q\_radius\_ratio (double NumPy array) radius ratio of each triangle, defined as 2\*inradius / circumradius.
- **area** (*double NumPy array*) area of each triangle in mesh.

# nirfasterff.meshing.meshutils.CheckMesh3D

nirfasterff.meshing.meshutils.CheckMesh3D(elements, nodes, base=1, verbose=False)

Main function that calculates and checks the quality of a 3D mesh, which can be either a solid or surface mesh

If surface mesh, checkmesh3d\_surface() is called

If solid mesh, checkmesh3d\_solid() is first used, and checkmesh3d\_surface() is subsequently used to check its outer surface

#### **Parameters**

- **ele** (*int32 NumPy array*) element list of the mesh, zero-based.
- nodes (double NumPy array) node locations of the mesh, in mm.
- base (int, optional) one- or zero-based indexing of the element list. Can be 1, or 0. The default is 1.
- **verbose** (*bool*, *optional*) whether print the problematic elements to stdout, if any. The default is False.

### Raises

**TypeError** – if elements and nodes do not define a valid 3D mesh.

#### Returns

- vol (double NumPy vector) Volume (for solid mesh) or area (for surface mesh) of each element.
- **vol\_ratio** (*double NumPy vector*) volume ratio for each tetrahedron in a solid mesh. Returns scalar 0.0 in case of a surface mesh.
- **q\_area** (*double NumPy vector*) area ratio for each triangle in a surface mesh. Returns scalar 0.0 in case of a solid mesh.
- status\_solid (int) flags of solid mesh quality, set by bits: 'b3b2b1b0'.

b1 set if small volumes found; b2 set if small volume ratios found; b3 set if faces shared by more than two tetrahedrons found

• status\_surface (int) – flags of surface mesh quality, set by bits: 'b3b2b1b0'.

b1 set if edges shared by more than two triangles found; b2 set if dangling edges found; b3 triangles with small area found

#### See also:

nirfasterff.meshing.checkmesh3d\_solid(), nirfasterff.meshing.checkmesh3d\_surface()

## nirfasterff.meshing.meshutils.RunCGALMeshGenerator

nirfasterff.meshing.meshutils.RunCGALMeshGenerator(mask, 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** (nirfasterff.utils.MeshingParams, *optional*) meshing parameters used. Default values will be used if not specified.

See nirfasterff.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

# nirfasterff.meshing.meshutils.boundfaces

nirfasterff.meshing.meshutils.boundfaces(nodes, elements, base=0, renumber=True)

Finds the boundary faces of a 3D tetrahedral mesh

### **Parameters**

- nodes (double NumPy array) node locations of the mesh. Size (NNodes, 3)
- **elements** (*NumPy array*) element list of the mesh, can be either one-based or zero-based, which must be specified using the 'base' argument.
- base(int, optional) one- or zero-based indexing of the element list. Can be 1, or 0. The default is 0.
- **renumber** (*bool*, *optional*) whether renumber of the node indices in the extracted surface mesh. The default is True.

#### Returns

• **new\_faces** (*int32 NumPy array*) – list of boundary faces of the mesh. Base of indexing is consistent with input element list

If *renumber=True*, node indices are renumbered; if not, same node indices as in 'elements' are used

• **new\_points** (*double NumPy array*) – point locations of the boundary nodes.

If *renumber=True*, returns the subset of node loations that are on the surface; if not, it is the same as input *nodes* 

## nirfasterff.meshing.meshutils.checkmesh3d solid

nirfasterff.meshing.meshutils.checkmesh3d\_solid(ele, nodes, verbose=False)

Calculates and returns the quality metrics of the tetrahedrons in a 3D tetrahedral mesh

Please consider using nirfasterff.meshing.CheckMesh3D() instead.

### **Parameters**

- **ele** (*int32 NumPy array*) element list of the mesh, zero-based.
- **nodes** (*double NumPy array*) node locations of the mesh, in mm.
- verbose (bool, optional) whether print the problematic tetrahedrons to stdout, if any.
   The default is False.

#### Raises

**TypeError** – if mesh is not 3D tetrahedral, or if element list uses undefined nodes.

#### Returns

- **vol** (*double NumPy vector*) volume of each tetrahedron, mm<sup>3</sup>.
- **vol\_ratio** (*double NumPy vector*) volume ratio, defined as the smallest sine of dihedral angles of each tetrahedron.
- zeroflag (bool NumPy vector) flags of whether the volume of a tetrahedron is too small.
- faceflag (bool) whether there are faces shared by more than two tetrahedrons.

### nirfasterff.meshing.meshutils.checkmesh3d surface

nirfasterff.meshing.meshutils.checkmesh3d\_surface(ele, nodes, verbose=False)

Calculates and returns the quality metrics of the triangles in a 3D surface mesh

Please consider using nirfasterff.meshing.CheckMesh3D() instead.

### **Parameters**

- **ele** (int32 NumPy array) element list of the mesh, zero-based.
- **nodes** (*double NumPy array*) node locations of the mesh, in mm.
- verbose (bool, optional) whether print the problematic triangles to stdout, if any. The
  default is False.

#### Raises

**TypeError** – if mesh is not 3D tetrahedral, or if element list uses undefined nodes.

#### Returns

- **q\_radius\_ratio** (*double NumPy vector*) radius ratio of each triangle, defined as 2\**inradius* / *circumradius*.
- **q\_area\_ratio** (*double NumPy vector*) face area divided by 'ideal area' for each triangle, where ideal area is the area of an equilateral triangle whose edge length equals the longest edge in the face.
- **area** (*double NumPy vector*) area of each triangle, in mm<sup>2</sup>.
- **zeroflag** (*bool NumPy vector*) flags whether the area a triangle is close to zero.
- edgeflag (*int*) flag if any problematic edges. Flag set by bits 'b1b0': b1=1 if dangling edges found, b0=1 if there exist edges shared by more than two triangles

# 4.1.8 nirfasterff.utils

Utility functions and auxiliary classes frequently used in the package.

## **Functions**

boundary_attenuation(n_incidence[,])	Calculate the boundary attenuation factor between two media.
<pre>check_element_orientation_2d(ele, nodes)</pre>	Make sure the 2D triangular elements are oriented counter clock wise.
compress_coo(coo_idx, N)	Convert COO indices to compressed.
<pre>gen_intmat_impl(mesh, xgrid, ygrid, zgrid)</pre>	YOU SHOULD NOT USE THIS FUNCTION DIRECTLY.
<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(A, B, p)</pre>	Calculate the distance between a point and a line (defined by two points), and find the projection point
pointLocation(mesh, pointlist)	Similar to Matlab's pointLocation function, queries which elements in mesh the points belong to, and also calculate the barycentric coordinates.
<pre>pointTriangleDistance(TRI, P)</pre>	Calculate the distance between a point and a triangle (defined by three points), and find the projection point
uncompress_coo(compressed_idx)	Convert compressed indices to COO.

# nirfasterff.utils.boundary\_attenuation

 $\label{lem:nirfasterff.utils.boundary_attenuation} (\textit{n\_incidence}, \textit{n\_transmission} = 1.0, \textit{method} = 'robin')$ 

Calculate the boundary attenuation factor between two media.

If vectors are used as inputs, they must have the same size and calculation is done for each pair

If n\_incidence is a vector but n\_transmission is a scalar, code assumes n\_transmission to be the same for each value in n\_incidence

### **Parameters**

- n\_incidence (double Numpy vector or scalar) refractive index of the medium within the boundary, e.g. a tissue.
- n\_transmission (double Numpy vector or scalar, optional) refractive index of the medium outside of the boundary, e.g. air. The default is 1.0.
- **method** (str, optional) boundary type, which can be,

'robin' - internal reflectance derived from Fresnel's law

'approx' - Groenhuis internal reflectance approximation  $(1.440n^{-2}+0.710n^{-1}+0.668+0.00636n)$ 

'exact' - exact internal reflectance (integrals of polarised reflectances, etc.)

The default is 'robin'.

#### Raises

**ValueError** – if n\_incidence and n\_transmission are both vectors and have difference sizes, or if method is not of a recognized kind

#### Returns

A – calculated boundary attenuation factor.

# Return type

double Numpy vector or scalar

### References

Durduran et al, 2010, Rep. Prog. Phys. doi:10.1088/0034-4885/73/7/076701

## nirfasterff.utils.check element orientation 2d

## nirfasterff.utils.check\_element\_orientation\_2d(ele, 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

### nirfasterff.utils.compress coo

nirfasterff.utils.compress\_coo(coo idx, N)

Convert COO indices to compressed.

#### **Parameters**

- coo\_idx (int NumPy array) Input indices in COO format, zero-based.
- N (int) Number of rows in the sparse matrix.

#### Returns

Output indices in compressed format, zero-based. Size (N+1,)

## Return type

int NumPy array

## nirfasterff.utils.gen intmat impl

nirfasterff.utils.gen\_intmat\_impl(mesh, xgrid, ygrid, zgrid)

YOU SHOULD NOT USE THIS FUNCTION DIRECTLY. USE MESH.GEN\_INTMAT INSTEAD.

Heart of the gen\_intmat function, which calculates the necessary information for converting between mesh and grid space

#### **Parameters**

- **mesh** (nirfasterff.base.stndmesh or nirfasterff.base.fluormesh) The original mesh with with FEM data is calculated.
- **xgrid** (*float64 NumPy 1-D array*) x grid in mm. Must be regular.
- ygrid (float64 NumPy 1-D array) y grid in mm. Must be regular.
- **zgrid** (float64 NumPy 1-D array, or [] if 2D mesh) z grid in mm. Must be regular.

### Returns

- **gridinmesh** (*int32 NumPy array*) Col 0: indices of grid points that are in the mesh; Col 1: indeces of the elements the grid point is in. Flattened in 'F' order, one-based.
- meshingrid (int32 NumPy array) Indices of mesh nodes that are in the grid. One-based.
- int\_mat\_mesh2grid (CSC sparse matrix, float64) Sparse matrix converting data from mesh space to grid space. Size (NGrid, NNodes).
- int\_mat\_mesh2grid (CSC sparse matrix, float64) Sparse matrix converting data from grid space to mesh space. Size (NNodes, NGrid).

## nirfasterff.utils.get\_nthread

## nirfasterff.utils.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

# nirfasterff.utils.get\_solver

```
nirfasterff.utils.get_solver()
```

Get the default solver.

### Returns

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

## **Return type**

str

#### nirfasterff.utils.isCUDA

# nirfasterff.utils.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

# nirfasterff.utils.pointLineDistance

```
nirfasterff.utils.pointLineDistance(A, 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.

## nirfasterff.utils.pointLocation

# nirfasterff.utils.pointLocation(mesh, 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 any of the NIRFASTer mesh types (stnd, fluor, dcs). 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<sub>i</sub>).
- 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

## nirfasterff.utils.pointTriangleDistance

## nirfasterff.utils.pointTriangleDistance(TRI, 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

# nirfasterff.utils.uncompress\_coo

```
nirfasterff.utils.uncompress_coo(compressed_idx)
```

Convert compressed indices to COO.

#### **Parameters**

compressed\_idx (int NumPy array) - Input indices in compressed format, zero-based.

#### Returns

**coo\_idx** – Output indices in COO format, zero-based.

# Return type

int NumPy array

## **Classes**

ConvergenceInfo([info])	Convergence information of the FEM solvers.
<pre>MeshingParams([xPixelSpacing,])</pre>	Parameters to be used by the CGAL mesher.
<pre>SolverOptions([max_iter, AbsoluteTolerance,])</pre>	Parameters used by the FEM solvers, Equivalent to
	'solver_options' in the Matlab version

# nirfasterff.utils.ConvergenceInfo

# class nirfasterff.utils.ConvergenceInfo(info=None)

Bases: object

Convergence information of the FEM solvers. Only used internally as a return type of functions nirfasterff.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

# $\verb|isConvergedToAbsoluteTolerance| \\$

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

\_\_init\_\_(info=None)

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## **Methods**

```
__init__([info])
```

# nirfasterff.utils.MeshingParams

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) 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
```

```
__init__(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)
```

#### **Methods**

```
__init__([xPixelSpacing, yPixelSpacing, ...])
```

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# nirfasterff.utils.SolverOptions

```
class nirfasterff.utils.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
     __init__(max iter=1000, AbsoluteTolerance=1e-12, RelativeTolerance=1e-12, divergence=1e8, GPU=-1)
     Methods
       __init__([max iter, AbsoluteTolerance, ...])
```

# 4.1.9 nirfasterff.visualize

Functions for basic data visualization

# **Functions**

<pre>plot3dmesh(mesh[, data, selector, alpha])</pre>	Fast preview of data within a 3D FEM mesh in the nir-fasterff format.
<pre>plotimage(mesh[, data])</pre>	Fast preview of data within a 2D FEM mesh in the nir-fasterff format.

# nirfasterff.visualize.plot3dmesh

nirfasterff.visualize.plot3dmesh(mesh, data=None, selector=None, alpha=0.8)

Fast preview of data within a 3D FEM mesh in the nirfasterff format.

Plots an image of the values on the mesh at the intersection specified by "selector".

For 2D mesh, use plotimage() instead

#### **Parameters**

- **mesh** (*nirfasterff* mesh type) a 3D nirfasterff mesh to plot the data on.
- data (double NumPy vector, optional) data to be plotted, with size (NNode,). If not specified, treated as all zero.
- **selector** (str, optional) Specifies the intersection at which the data will be plotted, e.g. 'x>50', or '(x>50) | (y<100)', or 'x + y + z < 200'.

Note that "=" is not supported. When "|" or "&" are used, make sure that all conditions are put in parantheses separately

If not specified, function plots the outermost shell of the mesh.

• alpha (float, optional) - transparency, between 0-1. Default is 0.8

#### Raises

**TypeError** – if mesh not 2D.

## Returns

- matplotlib.figure.Figure the figure to be displayed
- *mpl\_toolkits.mplot3d.axes3d.Axes3D* Current axes of the plot. Can be subsequently used for further plotting.

### **Notes**

This function is adapted from the 'plotmesh' function in the iso2mesh toolbox

https://iso2mesh.sourceforge.net/cgi-bin/index.cgi

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# nirfasterff.visualize.plotimage

nirfasterff.visualize.plotimage(mesh, data=None)

Fast preview of data within a 2D FEM mesh in the nirfasterff format.

Plots an image of the values on the mesh. For 3D mesh, use plot3dmesh() instead

## **Parameters**

- mesh (nirfasterff mesh type) a 2D nirfasterff mesh to plot the data on.
- data (double NumPy vector, optional) data to be plotted, with size (NNode,). If not specified, treated as all zero.

#### Raises

**TypeError** – if mesh not 2D.

## **Returns**

- matplotlib.figure.Figure the figure to be displayed
- *mpl\_toolkits.mplot3d.axes3d.Axes3D* Current axes of the plot. Can be subsequently used for further plotting.

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