# **WBFMM**

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# **Chapter 1**

# **WBFMM: A Wide Band Fast Multipole Method library**

WBFMM is a library and collection of associated tools for the efficient solution of the Helmholtz equation and in particular the summation of fields generated by large numbers of acoustic sources.

- 1.1 Getting started
- 1.2 What WBFMM does

## 1.3 References

The following papers and links have been used in some way in developing WBFMM:

- Nail A. Gumerov and Ramani Duraiswami, Recursions for the Computation of Multipole Translation and Rotation Coefficients for the 3-D Helmholtz Equation, SIAM J. Sci. Comput., 25(4), 1344-1381, http://dx.
  doi.org/10.1137/S1064827501399705
- 2. Gumerov, Duraiswami, and Borovikov, Data Structures, Optimal Choice of Parameters, and Complexity Results for Generalized Multilevel Fast Multipole Methods in d Dimensions, 2003, http://users.

  umiacs.umd.edu/~gumerov/PDFs/cs-tr-4458.pdf
- 3. Nail A. Gumerov and Ramani Duraiswami, A broadband fast multipole accelerated boundary element method for the three dimensional Helmholtz equation, J. Acoust. Soc. Am., 125(1), http://dx.doi.org/10. ← 1121/1.3021297
- 4. Nail A. Gumerov and Ramani Duraiswami, Comparison of the efficiency of translation operators used in the fast multipole method for the 3D Laplace equation, 2005, http://www.umiacs.umd.←edu/~ramani/pubs/comparisontranslationmethods\_041205.pdf

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# **Chapter 5**

# **Module Documentation**

# 5.1 Boxes and octrees

Operations on octree boxes and trees.

#### **Data Structures**

- struct wbfmm\_box\_t
- struct wbfmm\_tree\_t
- struct wbfmm\_target\_list\_t
- struct wbfmm\_shift\_operators\_t

#### **Enumerations**

enum wbfmm\_problem\_t { WBFMM\_PROBLEM\_LAPLACE = 1, WBFMM\_PROBLEM\_HELMHOLTZ = 2 }

# **Functions**

• gint wbfmm tree add points (wbfmm tree t \*t, gpointer pts, guint npts, gsize pstr)

Add points to an octree.

• wbfmm\_tree\_t \* wbfmm\_tree\_new (gdouble \*x, gdouble D, guint maxpoints)

Allocate a new octree.

• gint wbfmm\_tree\_leaf\_expansions (wbfmm\_tree\_t \*t, gdouble k, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gboolean zero\_expansions, gdouble \*work)

Generate leaf expansions for a tree.

• gint wbfmm\_tree\_box\_field (wbfmm\_tree\_t \*t, guint level, guint b, gdouble k, gdouble \*x, gdouble \*f, gdouble \*work)

Evaluate singular expansion about a box centre.

• gint wbfmm\_tree\_box\_local\_field (wbfmm\_tree\_t \*t, guint level, guint b, gdouble k, gdouble \*x, gdouble \*f, gdouble \*src, gint sstr, gboolean eval\_neighbours, gdouble \*work)

Evaluate local field from regular expansion in box.

• guint64 wbfmm\_point\_index\_3d (gdouble \*x, gdouble \*c, gdouble D)

Find Morton index for point in a cubic domain.

• gint wbfmm\_tree\_coefficient\_init (wbfmm\_tree\_t \*t, guint I, guint nr, guint ns)

Initialize expansion coefficient data in an octree.

gint wbfmm\_tree\_refine (wbfmm\_tree\_t \*t)

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level.

gint wbfmm\_tree\_laplace\_box\_local\_field (wbfmm\_tree\_t \*t, guint level, guint b, gdouble \*x, gdouble \*f, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*d, gint dstr, gboolean eval\_neighbours, gdouble \*work)

Evaluate local Laplace field from regular expansion in box.

• gint wbfmm\_tree\_laplace\_leaf\_expansions (wbfmm\_tree\_t \*t, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gboolean zero\_expansions, gdouble \*work)

Generate leaf expansions for a tree in the Laplace problem.

gint wbfmm\_tree\_add\_points\_f (wbfmm\_tree\_t \*t, gpointer pts, guint npts, gsize pstr)

Add points to an octree.

wbfmm\_tree\_t \* wbfmm\_tree\_new\_f (gfloat \*x, gfloat D, guint maxpoints)

Allocate a new octree.

• gint wbfmm\_tree\_leaf\_expansions\_f (wbfmm\_tree\_t \*t, gfloat k, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gboolean zero\_expansions, gfloat \*work)

Generate leaf expansions for a tree.

• gint wbfmm\_tree\_box\_field\_f (wbfmm\_tree\_t \*t, guint level, guint b, gfloat k, gfloat \*x, gfloat \*f, gfloat \*work)

Evaluate singular expansion about a box centre.

gint wbfmm\_tree\_box\_local\_field\_f (wbfmm\_tree\_t \*t, guint level, guint b, gfloat k, gfloat \*x, gfloat \*f, gfloat \*src, gint sstr, gboolean eval neighbours, gfloat \*work)

Evaluate local field from regular expansion in box.

• guint64 wbfmm\_point\_index\_3d\_f (gfloat \*x, gfloat \*c, gfloat D)

Find Morton index for point in a cubic domain.

• gint wbfmm\_tree\_coefficient\_init\_f (wbfmm\_tree\_t \*t, guint I, guint nr, guint ns)

Initialize expansion coefficient data in an octree.

gint wbfmm\_tree\_refine\_f (wbfmm\_tree\_t \*t)

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level.

• gint wbfmm\_tree\_laplace\_box\_local\_field\_f (wbfmm\_tree\_t \*t, guint level, guint b, gfloat \*x, gfloat \*f, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*d, gint dstr, gboolean eval\_neighbours, gfloat \*work)

Evaluate local Laplace field from regular expansion in box.

• gint wbfmm\_tree\_laplace\_leaf\_expansions\_f (wbfmm\_tree\_t \*t, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gboolean zero\_expansions, gfloat \*work)

Generate leaf expansions for a tree in the Laplace problem.

• gint wbfmm tree add level (wbfmm tree t \*t)

# 5.1.1 Detailed Description

Operations on octree boxes and trees.

## 5.1.2 Enumeration Type Documentation

5.1.2.1 enum wbfmm\_problem\_t

Selection of physical problem to be handled by a **wbfmm\_tree\_t** (p. 74)

Enumerator

WBFMM\_PROBLEM\_LAPLACE Laplace equation
WBFMM\_PROBLEM\_HELMHOLTZ Helmholtz equation

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# **5.1.3 Function Documentation**

5.1.3.1 guint64 wbfmm\_point\_index\_3d ( gdouble \* x, gdouble \* c, gdouble D )

Find Morton index for point in a cubic domain.

#### **Parameters**

	X	point in space (three components, densely packed);
ĺ	С	location of bottom left corner of domain;
Ì	D	width of domain.

### Returns

0 on success

5.1.3.2 guint64 wbfmm\_point\_index\_3d\_f ( gfloat \* x, gfloat \* c, gfloat D )

Find Morton index for point in a cubic domain.

#### **Parameters**

X	point in space (three components, densely packed);
С	location of bottom left corner of domain;
D	width of domain.

#### Returns

0 on success

5.1.3.3 gint wbfmm\_tree\_add\_level ( wbfmm\_tree\_t \*t )

Add a new level to an existing octree. The function assigns memory for, and initializes, a new layer of boxes of type **wbfmm\_box\_t** (p. 71)

#### **Parameters**

t	an existing wbfmm_tree_t (p. 74)

#### Returns

0 on success.

References wbfmm\_tree\_t::boxes, and wbfmm\_tree\_t::depth.

5.1.3.4 gint wbfmm\_tree\_add\_points ( wbfmm\_tree\_t \* t, gpointer pts, guint npts, gsize pstr )

Add points to an octree.

Add a set of source points to an octree. The points are assumed to be in an array of real values with components in a packed triple, indexed using a stride of pstr bytes (this allows for quite general handling of different source formats).

#### **Parameters**

	t	an existing wbfmm_tree_t (p. 74);
	pts	an array containing point coordinates;
ĺ	npts	the number of points in <i>pts</i> ;
Ì	pstr	stride between points in bytes.

### Returns

0 on success.

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5.1.3.5 gint wbfmm\_tree\_add\_points\_f ( wbfmm\_tree\_t \* t, gpointer pts, guint npts, gsize pstr )

Add points to an octree.

Add a set of source points to an octree. The points are assumed to be in an array of real values with components in a packed triple, indexed using a stride of pstr bytes (this allows for quite general handling of different source formats).

#### **Parameters**

t	an existing wbfmm_tree_t (p. 74);
pts	an array containing point coordinates;
npts	the number of points in <i>pts</i> ;
pstr	stride between points in bytes.

### Returns

0 on success.

5.1.3.6 gint wbfmm\_tree\_box\_field ( wbfmm\_tree\_t \* t, guint level, guint b, gdouble k, gdouble \* x, gdouble \* f, gdouble \* work )

Evaluate singular expansion about a box centre.

#### **Parameters**

t	octree for problem;
level	level in t;
b	index of box at level <i>level</i> of <i>t</i> ;
k	wavenumber;
X	field evaluation point;
f	on output field at x (not zeroed before evaluation);
work	workspace

# Returns

0 on success

5.1.3.7 gint wbfmm\_tree\_box\_field\_f ( wbfmm\_tree\_t \* t, guint level, guint b, gfloat \* x, gfloat \* x, gfloat \* work )

Evaluate singular expansion about a box centre.

#### **Parameters**

t	octree for problem;
level	level in t;
b	index of box at level <i>level</i> of <i>t</i> ;
k	wavenumber;
X	field evaluation point;
f	on output field at x (not zeroed before evaluation);
work	workspace

### Returns

0 on success

5.1.3.8 gint wbfmm\_tree\_box\_local\_field ( wbfmm\_tree\_t \* t, guint level, guint b, gdouble \* x, gdouble \* x, gdouble \* t, gdouble

Evaluate local field from regular expansion in box.

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#### **Parameters**

t	octree for domain;
level	level of t;
b	box index at level level of t;
k	wavenumber;
X	location of evaluation point;
f	on output, field value (not zeroed before evaluation);
src	source strengths;
sstr	stride of data in <i>src</i> ;
eval_neighbours	if TRUE compute contributions from sources in box b and neighbours;
work	workspace.

# Returns

0 on success

5.1.3.9 gint wbfmm\_tree\_box\_local\_field\_f ( wbfmm\_tree\_t \* t, guint level, guint b, gfloat k, gfloat \* x, gfloat \*

Evaluate local field from regular expansion in box.

# **Parameters**

t	octree for domain;
level	level of t;
b	box index at level level of t;
k	wavenumber;
X	location of evaluation point;
f	on output, field value (not zeroed before evaluation);
src	source strengths;
sstr	stride of data in <i>src</i> ;
eval_neighbours	if TRUE compute contributions from sources in box b and neighbours;
work	workspace.

# Returns

0 on success

5.1.3.10 gint wbfmm\_tree\_coefficient\_init ( wbfmm\_tree\_t \* t, guint l, guint nr, guint ns )

Initialize expansion coefficient data in an octree.

# **Parameters**

t	octree for problem;
1	level to initialize data for;
nr	order of regular expansions at level <i>I</i> ;
ns	order of singular expansions at level <i>I</i> .

# Returns

0 on success

5.1.3.11 gint wbfmm\_tree\_coefficient\_init\_f ( wbfmm\_tree\_t \* t, guint I, guint I, guint I guin

Initialize expansion coefficient data in an octree.

#### **Parameters**

t	octree for problem;
1	level to initialize data for;
nr	order of regular expansions at level <i>l</i> ;
ns	order of singular expansions at level I.

### Returns

0 on success

5.1.3.12 gint wbfmm\_tree\_laplace\_box\_local\_field ( wbfmm\_tree\_t \* t, guint level, guint b, gdouble \* x, gdouble \* f, gdouble \* src, gint sstr, gdouble \* normals, gint nstr, gdouble \* d, gint dstr, gboolean eval\_neighbours, gdouble \* work )

Evaluate local Laplace field from regular expansion in box.

### **Parameters**

t	octree for domain;
level	level of t;
b	box index at level <i>level</i> of <i>t</i> ;
X	location of evaluation point;
f	on output, field value (not zeroed before evaluation);
src	source strengths;
sstr	stride of data in <i>src</i> ;
normals	normals for dipole sources;
nstr	stride in normals;
d	dipole source strengths, or dipole vectors;
dstr	stride in d;
eval_neighbours	if TRUE compute contributions from sources in box b and neighbours;
work	workspace.

#### Returns

0 on success

5.1.3.13 gint wbfmm\_tree\_laplace\_box\_local\_field\_f ( wbfmm\_tree\_t \* t, guint level, guint b, gfloat \* x, gfloat \* src, gint sstr, gfloat \* normals, gint nstr, gfloat \* d, gint dstr, gboolean  $eval\_neighbours$ , gfloat \* mormals

Evaluate local Laplace field from regular expansion in box.

t	octree for domain;
level	level of t;
b	box index at level <i>level</i> of <i>t</i> ;
X	location of evaluation point;
f	on output, field value (not zeroed before evaluation);
src	source strengths;
sstr	stride of data in <i>src</i> ;

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normals	normals for dipole sources;
nstr	stride in <i>normals</i> ;
d	dipole source strengths, or dipole vectors;
dstr	stride in d;
eval_neighbours	if TRUE compute contributions from sources in box b and neighbours;
work	workspace.

#### Returns

0 on success

5.1.3.14 gint wbfmm\_tree\_laplace\_leaf\_expansions ( wbfmm\_tree\_t \* t, gdouble \* src, gint sstr, gdouble \* normals, gint nstr, gdouble \* dipoles, gint dstr, gboolean zero\_expansions, gdouble \* work )

Generate leaf expansions for a tree in the Laplace problem.

Generate leaf expansions for a tree for the Laplace problem given some combination of monopole and dipole sources. Source positions are those in the point list attached to the tree using **wbfmm\_tree\_add\_points** (p. 12)(...) and indexing in the array must correspond to that in the point list. Input arrays may be NULL: if *src* is not NULL, it is interpreted as a list of complex monopole strengths; if *normals* is not NULL, *dipoles* may not be NULL and they are interpreted respectively as a vector ('normal') at each source position and a scalar complex amplitude (this corresponds to surface normal and a normal velocity amplitude in a boundary element method calculation); if *normals* is NULL and *dipoles* is not NULL, *dipoles* is interpreted as a three-element complex vector specifying the dipole strength. The strides *sstr*, *nstr*, and *dstr* are the number of scalar elements between successive entries in the arrays, with the elements of each entry densely packed. For example, a list of normals might read:

$$[n_{x1} \quad n_{y1} \quad n_{z1} \quad a_1 \quad b_1 \quad n_{x2} \ldots]$$

where  $(n_{x1}, n_{y1}, n_{z1})$  is the first normal vector and  $a_1$  and  $b_1$  are arbitrary entries in the array. In this case, the stride *nstr* would be 5, the number of elements between successive values of  $n_{xi}$ .

#### **Parameters**

t	octree for problem;
src	monopole source strengths;
sstr	stride of data in <i>src</i> ;
normals	dipole normals;
nstr	stride of data in <i>normals</i> ;
dipoles	dipole source strengths (if normals is not NULL), or moment vectors (if normals is NULL);
dstr	stride of data in <i>dipoles</i> ;
zero_expansions	if TRUE, set expansion coefficients to zero before adding source terms;
work	workspace.

# Returns

0 on success

5.1.3.15 gint wbfmm\_tree\_laplace\_leaf\_expansions\_f ( wbfmm\_tree\_t \* t, gfloat \* src, gint sstr, gfloat \* normals, gint nstr, gfloat \* dipoles, gint dstr, gboolean zero\_expansions, gfloat \* work )

Generate leaf expansions for a tree in the Laplace problem.

Generate leaf expansions for a tree for the Laplace problem given some combination of monopole and dipole sources. Source positions are those in the point list attached to the tree using **wbfmm\_tree\_add\_points\_**  $\leftarrow$  **f** (p. 13)(...) and indexing in the array must correspond to that in the point list. Input arrays may be NULL: if *src* is not NULL, it is interpreted as a list of complex monopole strengths; if *normals* is not NULL, *dipoles* may not be NULL and they are interpreted respectively as a vector ('normal') at each source position and a scalar complex

amplitude (this corresponds to surface normal and a normal velocity amplitude in a boundary element method calculation); if *normals* is NULL and *dipoles* is not NULL, *dipoles* is interpreted as a three-element complex vector specifying the dipole strength. The strides *sstr*, *nstr*, and *dstr* are the number of scalar elements between successive entries in the arrays, with the elements of each entry densely packed. For example, a list of normals might read:

$$[n_{x1} \quad n_{y1} \quad n_{z1} \quad a_1 \quad b_1 \quad n_{x2} \ldots]$$

where  $(n_{x1}, n_{y1}, n_{z1})$  is the first normal vector and  $a_1$  and  $b_1$  are arbitrary entries in the array. In this case, the stride *nstr* would be 5, the number of elements between successive values of  $n_{xi}$ .

#### **Parameters**

t	octree for problem;
src	monopole source strengths;
sstr	stride of data in <i>src</i> ;
normals	dipole normals;
nstr	stride of data in <i>normals</i> ;
dipoles	dipole source strengths (if normals is not NULL), or moment vectors (if normals is NULL);
dstr	stride of data in <i>dipoles</i> ;
zero_expansions	if TRUE, set expansion coefficients to zero before adding source terms;
work	workspace.

#### Returns

0 on success

5.1.3.16 gint wbfmm\_tree\_leaf\_expansions ( wbfmm\_tree\_t \* t, gdouble \* src, gint sstr, gdouble \* normals, gint nstr, gdouble \* dipoles, gint dstr, gboolean zero\_expansions, gdouble \* work )

Generate leaf expansions for a tree.

Generate leaf expansions for a tree given some combination of monopole and dipole sources. Source positions are those in the point list attached to the tree using **wbfmm\_tree\_add\_points** (p. 12)(...) and indexing in the array must correspond to that in the point list. Input arrays may be NULL: if *src* is not NULL, it is interpreted as a list of complex monopole strengths; if *normals* is not NULL, *dipoles* may not be NULL and they are interpreted respectively as a vector ('normal') at each source position and a scalar complex amplitude (this corresponds to surface normal and a normal velocity amplitude in a boundary element method calculation); if *normals* is NULL and *dipoles* is not NULL, *dipoles* is interpreted as a three-element complex vector specifying the dipole strength. The strides *sstr*, *nstr*, and *dstr* are the number of scalar elements between successive entries in the arrays, with the elements of each entry densely packed. For example, a list of normals might read:

$$[n_{x1} \quad n_{y1} \quad n_{z1} \quad a_1 \quad b_1 \quad n_{x2} \ldots]$$

where  $(n_{x1}, n_{y1}, n_{z1})$  is the first normal vector and  $a_1$  and  $b_1$  are arbitrary entries in the array. In this case, the stride *nstr* would be 5, the number of elements between successive values of  $n_{xi}$ .

t	octree for problem;
k	wavenumber;
src	monopole source strengths;
sstr	stride of data in <i>src</i> ;
normals	dipole normals;
nstr	stride of data in <i>normals</i> ;
dipoles	dipole source strengths (if normals is not NULL), or moment vectors (if normals is NULL);

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	dstr	stride of data in <i>dipoles</i> ;
ze	ero_expansions	if TRUE, set expansion coefficients to zero before adding source terms;
	work	workspace.

#### **Returns**

0 on success

5.1.3.17 gint wbfmm\_tree\_leaf\_expansions\_f ( wbfmm\_tree\_t \* t, gfloat \*, gfloat \* src, gint sstr, gfloat \* normals, gint nstr, gfloat \* dipoles, gint dstr, gboolean zero\_expansions, gfloat \* work )

Generate leaf expansions for a tree.

Generate leaf expansions for a tree given some combination of monopole and dipole sources. Source positions are those in the point list attached to the tree using **wbfmm\_tree\_add\_points\_f** (p. 13)(...) and indexing in the array must correspond to that in the point list. Input arrays may be NULL: if *src* is not NULL, it is interpreted as a list of complex monopole strengths; if *normals* is not NULL, *dipoles* may not be NULL and they are interpreted respectively as a vector ('normal') at each source position and a scalar complex amplitude (this corresponds to surface normal and a normal velocity amplitude in a boundary element method calculation); if *normals* is NULL and *dipoles* is not NULL, *dipoles* is interpreted as a three-element complex vector specifying the dipole strength. The strides *sstr*, *nstr*, and *dstr* are the number of scalar elements between successive entries in the arrays, with the elements of each entry densely packed. For example, a list of normals might read:

$$[n_{x1} \quad n_{y1} \quad n_{z1} \quad a_1 \quad b_1 \quad n_{x2} \ldots]$$

where  $(n_{x1}, n_{y1}, n_{z1})$  is the first normal vector and  $a_1$  and  $b_1$  are arbitrary entries in the array. In this case, the stride *nstr* would be 5, the number of elements between successive values of  $n_{xi}$ .

#### **Parameters**

t	octree for problem;
k	wavenumber;
src	monopole source strengths;
sstr	stride of data in <i>src</i> ;
normals	dipole normals;
nstr	stride of data in <i>normals</i> ;
dipoles	dipole source strengths (if normals is not NULL), or moment vectors (if normals is NULL);
dstr	stride of data in <i>dipoles</i> ;
zero_expansions	if TRUE, set expansion coefficients to zero before adding source terms;
work	workspace.

### Returns

0 on success

5.1.3.18 wbfmm tree t\* wbfmm\_tree\_new ( gdouble \* x, gdouble D, guint maxpoints )

Allocate a new octree.

X	location of origin of tree;
D	width of domain;

maxpoints	maximum number of source points in tree.
-----------	--

# Returns

pointer to newly allocated tree.

5.1.3.19 wbfmm\_tree\_t\* wbfmm\_tree\_new\_f ( gfloat \* x, gfloat D, guint maxpoints )

Allocate a new octree.

#### **Parameters**

X	location of origin of tree;
D	width of domain;
maxpoints	maximum number of source points in tree.

### Returns

pointer to newly allocated tree.

5.1.3.20 gint wbfmm\_tree\_refine ( wbfmm\_tree\_t \* t )

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level.

# **Parameters**

t	an existing wbfmm_tree_t (p. 74).

# Returns

0 on success.

5.1.3.21 gint wbfmm\_tree\_refine\_f ( wbfmm\_tree\_t \* t )

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level

# **Parameters**

t	an existing wbfmm_tree_t (p. 74).

### Returns

0 on success.

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# 5.2 Shift operations

Shift operations (combined rotation and translation) for upward and downward passes, and same-level interactions.

#### **Functions**

• gint wbfmm\_child\_parent\_shift (gdouble \*Cp, gint Np, gdouble \*Cc, gint Nc, gdouble \*H03, gdouble \*H47, gint Lh, gdouble \*trans, gint Ls, gdouble \*work)

Upward shift of singular expansion from eight children to common parent.

• gint **wbfmm\_child\_parent\_shift\_bw** (gdouble \*Cp, gint Np, gdouble \*Cc, gint Nc, gdouble \*H03, gint Lh, gdouble \*transf, gdouble \*transb, gint Ls, gdouble \*work)

Upward shift of singular expansion from eight children to common parent, using backward translations.

gint wbfmm\_parent\_child\_shift (gdouble \*Cc, gint Nc, gdouble \*Cp, gint Np, gdouble \*H03, gdouble \*H47, gint Lh, gdouble \*trans, gint Ls, gdouble \*work)

Downward shift of parent expansion to child box centres.

- gint **wbfmm\_shift\_angles\_list4** (gint i, gint j, gint k, gdouble \*th, gdouble \*ph, gdouble \*ch, gdouble \*rs)

  Extract the rotation angles for boxes on interaction list 4.
- gint wbfmm\_shift\_angle\_table\_init (void)

Initialize table of angles for shift operations.

• wbfmm shift operators t \* wbfmm shift operators new (quint L, gdouble \*work)

Allocate shift operators and initialize rotations.

 gint wbfmm\_shift\_operators\_coaxial\_SR\_init (wbfmm\_shift\_operators\_t \*w, gdouble D, guint level, guint L, gdouble k, gdouble \*work)

Initialize singular-to-regular translation operators.

• gint wbfmm\_shift\_operators\_coaxial\_SS\_init (wbfmm\_shift\_operators\_t \*w, gdouble D, guint level, guint L, gdouble k, gdouble \*work)

Initialize singular-to-singular (regular-to-regular) translation operators.

• gint wbfmm\_child\_parent\_shift\_f (gfloat \*Cp, gint Np, gfloat \*Cc, gint Nc, gfloat \*H03, gfloat \*H47, gint Lh, gfloat \*trans, gint Ls, gfloat \*work)

Upward shift of singular expansion from eight children to common parent.

• gint wbfmm\_child\_parent\_shift\_bw\_f (gfloat \*Cp, gint Np, gfloat \*Cc, gint Nc, gfloat \*H03, gint Lh, gfloat \*transf, gfloat \*transb, gint Ls, gfloat \*work)

Upward shift of singular expansion from eight children to common parent, using backward translations.

• gint wbfmm\_parent\_child\_shift\_f (gfloat \*Cc, gint Nc, gfloat \*Cp, gint Np, gfloat \*H03, gfloat \*H47, gint Lh, gfloat \*trans, gint Ls, gfloat \*work)

Downward shift of parent expansion to child box centres.

• gint wbfmm\_shift\_angles\_list4\_f (gint i, gint j, gint k, gfloat \*th, gfloat \*ph, gfloat \*ch, gfloat \*rs)

Extract the rotation angles for boxes on interaction list 4.

gint wbfmm\_shift\_angle\_table\_init\_f (void)

Initialize table of angles for shift operations.

• wbfmm\_shift\_operators\_t \* wbfmm\_shift\_operators\_new\_f (guint L, gfloat \*work)

Allocate shift operators and initialize rotations.

gint wbfmm\_shift\_operators\_coaxial\_SR\_init (wbfmm\_shift\_operators\_t \*w, gfloat D, guint level, guint L, gfloat k, gfloat \*work)

Initialize singular-to-regular translation operators.

• gint wbfmm\_shift\_operators\_coaxial\_SS\_init (wbfmm\_shift\_operators\_t \*w, gfloat D, guint level, guint L, gfloat k, gfloat \*work)

Initialize singular-to-singular (regular-to-regular) translation operators.

## 5.2.1 Detailed Description

Shift operations (combined rotation and translation) for upward and downward passes, and same-level interactions.

### 5.2.2 Function Documentation

5.2.2.1 gint wbfmm\_child\_parent\_shift ( gdouble \* Cp, gint Np, gdouble \* Cc, gint Nc, gdouble \* H03, gdouble \* H47, gint Lh, gdouble \* trans, gint Ls, gdouble \* work )

Upward shift of singular expansion from eight children to common parent.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index.

#### **Parameters**

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
trans	coaxial translation operator for distance between child and parent box centres;
Ls	order of trans;
work	workspace

#### Returns

0 on success

5.2.2.2 gint wbfmm\_child\_parent\_shift\_bw ( gdouble \* Cp, gint Np, gdouble \* Cc, gint Nc, gdouble \* H03, gint Lh, gdouble \* transf, gdouble \* transb, gint Ls, gdouble \* work )

Upward shift of singular expansion from eight children to common parent, using backward translations.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index. The method is the same as for **wbfmm\_child\_parent\_shift** (p. 22)(...), except that the child boxes with Morton indices 4-7 are rotated in the same sense as the diagonally opposite child boxes 0-3 and a reverse (negative distance) coaxial translation is used to combine them with the lower child box data with the same rotation. The reverse rotation is then applied to the summed data meaning that only four reverse rotations rather than eight are required to transfer the data to the parent box orientation.

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
Lh	maximum order of rotation coefficients;
transf	forward ( $+kr$ ) coaxial translation operator for distance between child and parent box centres;
transb	backward ( $-kr$ ) coaxial translation operator for distance between child and parent box cen-
	tres;
Ls	order of trans;

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	d
work	workspace

#### Returns

0 on success

5.2.2.3 gint wbfmm\_child\_parent\_shift\_bw\_f ( gfloat \* Cp, gint Np, gfloat \* Cc, gint Nc, gfloat \* H03, gint Lh, gfloat \* transf, gfloat \* transb, gint Ls, gfloat \* work )

Upward shift of singular expansion from eight children to common parent, using backward translations.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index. The method is the same as for **wbfmm\_child\_parent\_shift\_f** (p. 23)(...), except that the child boxes with Morton indices 4-7 are rotated in the same sense as the diagonally opposite child boxes 0-3 and a reverse (negative distance) coaxial translation is used to combine them with the lower child box data with the same rotation. The reverse rotation is then applied to the summed data meaning that only four reverse rotations rather than eight are required to transfer the data to the parent box orientation.

#### **Parameters**

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
Lh	maximum order of rotation coefficients;
transf	forward ( $+kr$ ) coaxial translation operator for distance between child and parent box centres;
transb	backward ( $-kr$ ) coaxial translation operator for distance between child and parent box cen-
	tres;
Ls	order of trans;
work	workspace

#### Returns

0 on success

5.2.2.4 gint wbfmm\_child\_parent\_shift\_f ( gfloat \* Cp, gint Np, gfloat \* Cc, gint Nc, gfloat \* H03, gfloat \* H47, gint Lh, gfloat \* trans, gint Ls, gfloat \* work )

Upward shift of singular expansion from eight children to common parent.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index.

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;
H03	rotation coefficients for 'lower' children (Morton index 0-3);

H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
trans	coaxial translation operator for distance between child and parent box centres;
Ls	order of trans;
work	workspace

#### Returns

0 on success

5.2.2.5 gint wbfmm\_parent\_child\_shift ( gdouble \* *Cc*, gint *Nc*, gdouble \* *Cp*, gint *Np*, gdouble \* *H03*, gdouble \* *H47*, gint *Lh*, gdouble \* *trans*, gint *Ls*, gdouble \* *work* )

Downward shift of parent expansion to child box centres.

Shift the (regular) expansion data from a parent box to each of its child boxes, assuming the same packing as in **wbfmm\_child\_parent\_shift** (p. 22)(...). Note that the rotation matrices for this function are switched relative to the rotations of the same name in **wbfmm\_child\_parent\_shift** (p. 22)(...), because the 'upper' children rotate 'down' to be shifted to the parent centre but the rotation is 'up' to shift from the parent to those children, and similarly for the 'lower' children.

#### **Parameters**

Cc	child expansion array;
Nc	order of child expansions;
Ср	parent expansion array;
Np	order of parent expansion;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
trans	coaxial translation operator for distance between child and parent box centres;
Ls	order of trans;
work	workspace

## Returns

0 on success

5.2.2.6 gint wbfmm\_parent\_child\_shift\_f ( gfloat \* Cc, gint Nc, gfloat \* Cp, gint Np, gfloat \* H03, gfloat \* H47, gint Lh, gfloat \* trans, gint Ls, gfloat \* work )

Downward shift of parent expansion to child box centres.

Shift the (regular) expansion data from a parent box to each of its child boxes, assuming the same packing as in **wbfmm\_child\_parent\_shift\_f** (p. 23)(...). Note that the rotation matrices for this function are switched relative to the rotations of the same name in **wbfmm\_child\_parent\_shift\_f** (p. 23)(...), because the 'upper' children rotate 'down' to be shifted to the parent centre but the rotation is 'up' to shift from the parent to those children, and similarly for the 'lower' children.

Сс	child expansion array;
Nc	order of child expansions;

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Ср	parent expansion array;
Np	order of parent expansion;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
trans	coaxial translation operator for distance between child and parent box centres;
Ls	order of trans;
work	workspace

#### Returns

0 on success

# 5.2.2.7 gint wbfmm\_shift\_angle\_table\_init ( void )

Initialize table of angles for shift operations.

This function must be called before any interaction calculations are performed, in particular before any call to **wbfmm\_shift\_operators\_new** (p. 27)(...), in order to initialize the look-up table of orientations between boxes in interaction lists.

### Returns

0 on success

# 5.2.2.8 gint wbfmm\_shift\_angle\_table\_init\_f ( void )

Initialize table of angles for shift operations.

This function must be called before any interaction calculations are performed, in particular before any call to **wbfmm\_shift\_operators\_new\_f** (p. 28)(...), in order to initialize the look-up table of orientations between boxes in interaction lists.

## Returns

0 on success

5.2.2.9 gint wbfmm\_shift\_angles\_list4 ( gint i, gint j, gint k, gdouble \* th, gdouble \*

Extract the rotation angles for boxes on interaction list 4.

Find the rotation angles  $(\theta, \phi \chi)$  between a box at integer coordinates (i, j, k), using a look-up table which should be initialized with **wbfmm\_shift\_angle\_table\_init** (p. 25)(...)

i	integer $x$ coordinate of box on interaction list;
j	integer $y$ coordinate of box on interaction list;
k	integer $z$ coordinate of box on interaction list;
th	heta for rotation between boxes;
ph	$\phi$ for rotation between boxes;
ch	$\chi$ for rotation between boxes;

rs	scaling factor for distance between box centres, distance is <i>rs</i> multiplied by box width.
10	Scaling factor for distance between box centres, distance is 13 multiplied by box width

### Returns

0 on success

5.2.2.10 gint wbfmm\_shift\_angles\_list4\_f ( gint i, gint j, gint k, gfloat \* th, gfloat \* ph, gfloat \* ch, gfloat \* rs)

Extract the rotation angles for boxes on interaction list 4.

Find the rotation angles  $(\theta, \phi \chi)$  between a box at integer coordinates (i, j, k), using a look-up table which should be initialized with **wbfmm\_shift\_angle\_table\_init\_f** (p. 25)(...)

#### **Parameters**

i	integer $x$ coordinate of box on interaction list;
j	integer $y$ coordinate of box on interaction list;
k	integer $z$ coordinate of box on interaction list;
th	heta for rotation between boxes;
ph	$\phi$ for rotation between boxes;
ch	$\chi$ for rotation between boxes;
rs	scaling factor for distance between box centres, distance is rs multiplied by box width.

### **Returns**

0 on success

5.2.2.11 gint wbfmm\_shift\_operators\_coaxial\_SR\_init ( wbfmm\_shift\_operators\_t \* w, gdouble D, guint C, gdouble C,

Initialize singular-to-regular translation operators.

## **Parameters**

W	a <b>wbfmm_shift_operators_t</b> (p. 71) allocated with wbfmm_shift_operators_new();
D	width of the problem domain;
level	level for which to generate translations;
L	order of translations;
k	wavenumber;
work	workspace

# Returns

0 on success

5.2.2.12 gint wbfmm\_shift\_operators\_coaxial\_SR\_init ( wbfmm\_shift\_operators\_t \* w, gfloat D, guint level, guint L, gfloat \* w gflo

Initialize singular-to-regular translation operators.

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W	a wbfmm_shift_operators_t (p. 71) allocated with wbfmm_shift_operators_new_f();
D	width of the problem domain;
level	level for which to generate translations;
L	order of translations;
k	wavenumber;
work	workspace

#### Returns

0 on success

5.2.2.13 gint wbfmm\_shift\_operators\_coaxial\_SS\_init ( wbfmm\_shift\_operators\_t \* w, gdouble D, guint C, gdouble C,

Initialize singular-to-singular (regular-to-regular) translation operators.

#### **Parameters**

W	a wbfmm_shift_operators_t (p. 71) allocated with wbfmm_shift_operators_new();
D	width of the problem domain;
level	level for which to generate translations;
L	order of translations;
k	wavenumber;
work	workspace

# Returns

0 on success

5.2.2.14 gint wbfmm\_shift\_operators\_coaxial\_SS\_init ( wbfmm\_shift\_operators\_t \* w, gfloat D, guint level, guint L, gfloat \* w gflo

Initialize singular-to-singular (regular-to-regular) translation operators.

# Parameters

W	a wbfmm_shift_operators_t (p. 71) allocated with wbfmm_shift_operators_new_f();
D	width of the problem domain;
level	level for which to generate translations;
L	order of translations;
k	wavenumber;
work	workspace

#### Returns

0 on success

5.2.2.15 wbfmm\_shift\_operators\_t\* wbfmm\_shift\_operators\_new ( guint L, gdouble \* work )

Allocate shift operators and initialize rotations.

Allocate a new **wbfmm\_shift\_operators\_t** (p. 71) of given maximum order and initialize the rotation coefficients needed for same-level interaction calculations and upward and downward passes.

## **Parameters**

L	maximum order of expansions;
work	workspace.

# Returns

0 on success

5.2.2.16 wbfmm\_shift\_operators\_t\* wbfmm\_shift\_operators\_new\_f ( guint L, gfloat \* work )

Allocate shift operators and initialize rotations.

Allocate a new **wbfmm\_shift\_operators\_t** (p. 71) of given maximum order and initialize the rotation coefficients needed for same-level interaction calculations and upward and downward passes.

# **Parameters**

L	maximum order of expansions;
work	workspace.

# Returns

# 5.3 Generation and evaluation of expansions

Generation of regular and singular expansions and evaluation of them at field points.

#### **Functions**

• gint **wbfmm\_expansion\_h\_cfft** (gdouble k, gint N, gdouble \*x0, gdouble \*xs, gdouble \*q, gdouble \*cfft, gint cstr, gdouble \*work)

Generation of singular expansion coefficients for point source.

• gint **wbfmm\_expansion\_dipole\_h\_cfft** (gdouble k, gint N, gdouble \*x0, gdouble \*xs, gdouble \*fx, gdouble \*fx, gdouble \*fx, gdouble \*fx, gdouble \*sty, gdouble \*fx, gdouble \*work)

Generation of singular expansion coefficients for point dipole source.

• gint **wbfmm\_expansion\_h\_evaluate** (gdouble k, gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate a singular expansion.

• gint **wbfmm\_expansion\_j\_evaluate** (gdouble k, gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate a regular expansion.

• gint wbfmm\_expansion\_h\_cfft\_f (gfloat k, gint N, gfloat \*x0, gfloat \*xs, gfloat \*q, gfloat \*cfft, gint cstr, gfloat \*work)

Generation of singular expansion coefficients for point source.

• gint **wbfmm\_expansion\_dipole\_h\_cfft\_f** (gfloat k, gint N, gfloat \*x0, gfloat \*xs, gfloat \*fx, gfloat \*fy, gfloat \*fx, gfloat \*stx, gfloat \*fx, gfloat \*stx, gfloat \*fx, gfloat \*stx, gflo

Generation of singular expansion coefficients for point dipole source.

• gint wbfmm\_expansion\_h\_evaluate\_f (gfloat k, gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gfloat \*xf, gfloat \*field, gfloat \*work)

Evaluate a singular expansion.

• gint wbfmm\_expansion\_j\_evaluate\_f (gfloat k, gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gfloat \*xf, gfloat \*field, gfloat \*work)

Evaluate a regular expansion.

# 5.3.1 Detailed Description

Generation of regular and singular expansions and evaluation of them at field points.

The functions described here handle spherical harmonic expansions of complex variables, solutions of the Helmholtz equations. Expansions of real variables are dealt with in a separate set of functions, for the Laplace equation (**Evaluation of the Laplace potential** (p. 58)). The expansion coefficients are packed in single- or double-precision arrays with the index of coefficient  $C_n^m$ ,  $-n \le m \le n$  given by i = n(n+1) + m. Coefficients are represented as real and imaginary parts, so that the coefficient is given by array entries  $C_{si+0} + jC_{si+1}$  where i is the index, s is a stride allowing interleaved packing of data, and  $C_n$  is an array entry.

# 5.3.2 Function Documentation

5.3.2.1 gint wbfmm\_expansion\_dipole\_h\_cfft ( gdouble k, gint N, gdouble \* x0, gdouble \* xs, gdouble \* tx, gdouble \* tx

Generation of singular expansion coefficients for point dipole source.

#### **Parameters**

k	wavenumber;
N	order of expansion;
х0	centre of expansion;
XS	source position;
fx	component of complex source strength;
fy	component of complex source strength;
fz	component of complex source strength;
cfft	incremented with expansion coefficients;
cstr	stride in cfft, in number of complex elements;
work	workspace

# Returns

0 on success

5.3.2.2 gint wbfmm\_expansion\_dipole\_h\_cfft\_f ( gfloat k, gint N, gfloat \*x0, gfloat \*xs, gf

Generation of singular expansion coefficients for point dipole source.

## **Parameters**

k	wavenumber;
N	order of expansion;
x0	centre of expansion;
XS	source position;
fx	component of complex source strength;
fy	component of complex source strength;
fz	component of complex source strength;
cfft	incremented with expansion coefficients;
cstr	stride in cfft, in number of complex elements;
work	workspace

#### Returns

0 on success

5.3.2.3 gint wbfmm\_expansion\_h\_cfft ( gdouble k, gint N, gdouble \* x0, gdouble \* xs, gdouble \* q, gdouble \*

Generation of singular expansion coefficients for point source.

k	wavenumber;
N	order of expansion;
x0	centre of expansion;
XS	source position;
q	complex source strength;
cfft	incremented with expansion coefficients;

cstr	stride in cfft, in number of complex elements;
work	workspace

## **Returns**

0 on success

5.3.2.4 gint wbfmm\_expansion\_h\_cfft\_f ( gfloat k, gint N, gfloat \* x0, gfloat \* xs, gfloat \* q, gfloat \* cfft, gint cstr, gfloat \* work )

Generation of singular expansion coefficients for point source.

## **Parameters**

k	wavenumber;
N	order of expansion;
х0	centre of expansion;
XS	source position;
q	complex source strength;
cfft	incremented with expansion coefficients;
cstr	stride in cfft, in number of complex elements;
work	workspace

#### Returns

0 on success

5.3.2.5 gint wbfmm\_expansion\_h\_evaluate ( gdouble \* x0, gdouble \* x0, gdouble \* cfft, gint cstr, gint N, gdouble \* xf, gdouble \*

Evaluate a singular expansion.

## **Parameters**

k	wavenumber;
x0	centre of expansion;
cfft	expansion coefficients;
cstr	stride in cfft, in number of complex elements;
N	order of expansion;
xf	field point;
field	incremented with computed field;
work	workspace

# Returns

0 on success

5.3.2.6 gint wbfmm\_expansion\_h\_evaluate\_f ( gfloat k, gfloat \*x0, g

Evaluate a singular expansion.

## **Parameters**

k	wavenumber;
x0	centre of expansion;
cfft	expansion coefficients;
cstr	stride in cfft, in number of complex elements;
N	order of expansion;
xf	field point;
field	incremented with computed field;
work	workspace

# Returns

0 on success

5.3.2.7 gint wbfmm\_expansion\_j\_evaluate ( gdouble \* x0, gdouble \* x0, gdouble \* cfft, gint cstr, gint N, gdouble \* xf, gdouble \*

Evaluate a regular expansion.

# **Parameters**

k	wavenumber;
x0	centre of expansion;
cfft	expansion coefficients;
cstr	stride in cfft, in number of complex elements;
N	order of expansion;
xf	field point;
field	incremented with computed field;
work	workspace

# Returns

0 on success

5.3.2.8 gint wbfmm\_expansion\_j\_evaluate\_f ( gfloat k, gfloat \*x0, gfloat \*xf, gint cstr, gint N, gfloat \*xf, gfloat

Evaluate a regular expansion.

# **Parameters**

k	wavenumber;
x0	centre of expansion;
cfft	expansion coefficients;
cstr	stride in cfft, in number of complex elements;
N	order of expansion;
xf	field point;
field	incremented with computed field;
work	workspace

# Returns

# 5.4 Upward and downward passes

Upward and downward pass operations in octrees.

#### **Functions**

gint wbfmm\_downward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform downward pass at one level of an octree.

- gint wbfmm\_upward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

  Perform upward pass at one level of an octree.
- gint wbfmm\_laplace\_downward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform downward pass at one level of an octree for the Laplace problem.

gint wbfmm\_laplace\_upward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform upward pass at one level of an octree for the Laplace problem.

• gint wbfmm\_downward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform downward pass at one level of an octree.

- gint wbfmm\_upward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

  Perform upward pass at one level of an octree.
- gint wbfmm\_laplace\_downward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform downward pass at one level of an octree for the Laplace problem.

• gint wbfmm\_laplace\_upward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform upward pass at one level of an octree for the Laplace problem.

# 5.4.1 Detailed Description

Upward and downward pass operations in octrees.

#### 5.4.2 Function Documentation

5.4.2.1 gint wbfmm\_downward\_pass ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gdouble \* work )

Perform downward pass at one level of an octree.

Perform one stage of a downward pass for tree levels greater than or equal to two. The actions performed are the evaluation of the list 4 contribution to the regular expansion and, for non-leaf boxes, a downward shift of the regular expansions to the child boxes at the next level.

t	an initialized octree which has had the upward pass performed;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform downward pass;

work	workspace
------	-----------

#### Returns

0 on success

5.4.2.2 gint wbfmm\_downward\_pass\_f ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gfloat \* work )

Perform downward pass at one level of an octree.

Perform one stage of a downward pass for tree levels greater than or equal to two. The actions performed are the evaluation of the list 4 contribution to the regular expansion and, for non-leaf boxes, a downward shift of the regular expansions to the child boxes at the next level.

#### **Parameters**

t	an initialized octree which has had the upward pass performed;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform downward pass;
work	workspace

#### Returns

0 on success

5.4.2.3 gint wbfmm\_laplace\_downward\_pass ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gdouble \* work )

Perform downward pass at one level of an octree for the Laplace problem.

Perform one stage of a downward pass for tree levels greater than or equal to two. The actions performed are the evaluation of the list 4 contribution to the regular expansion and, for non-leaf boxes, a downward shift of the regular expansions to the child boxes at the next level.

#### **Parameters**

t	an initialized octree which has had the upward pass performed;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform downward pass;
work	workspace

#### Returns

0 on success

5.4.2.4 gint wbfmm\_laplace\_downward\_pass\_f ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gfloat \* work )

Perform downward pass at one level of an octree for the Laplace problem.

Perform one stage of a downward pass for tree levels greater than or equal to two. The actions performed are the evaluation of the list 4 contribution to the regular expansion and, for non-leaf boxes, a downward shift of the regular expansions to the child boxes at the next level.

#### **Parameters**

t	an initialized octree which has had the upward pass performed;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform downward pass;
work	workspace

#### Returns

0 on success

5.4.2.5 gint wbfmm\_laplace\_upward\_pass ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gdouble \* work )

Perform upward pass at one level of an octree for the Laplace problem.

Perform one stage of the upward pass in an octree. The action performed is the upward shift of the singular expansions from boxes at level *level* to their parents.

#### **Parameters**

t	an initialized octree;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform upward pass;
work	workspace

#### Returns

0 on success

5.4.2.6 gint wbfmm\_laplace\_upward\_pass\_f ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gfloat \* work )

Perform upward pass at one level of an octree for the Laplace problem.

Perform one stage of the upward pass in an octree. The action performed is the upward shift of the singular expansions from boxes at level *level* to their parents.

# **Parameters**

t	an initialized octree;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform upward pass;
work	workspace

#### Returns

0 on success

5.4.2.7 gint wbfmm\_upward\_pass ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gdouble \* work )

Perform upward pass at one level of an octree.

Perform one stage of the upward pass in an octree. The action performed is the upward shift of the singular expansions from boxes at level *level* to their parents.

## **Parameters**

t	an initialized octree;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform upward pass;
work	workspace

## Returns

0 on success

5.4.2.8 gint wbfmm\_upward\_pass\_f ( wbfmm\_tree\_t \* t, wbfmm\_shift\_operators\_t \* op, guint level, gfloat \* work )

Perform upward pass at one level of an octree.

Perform one stage of the upward pass in an octree. The action performed is the upward shift of the singular expansions from boxes at level *level* to their parents.

## **Parameters**

t	an initialized octree;
ор	shift operators allocated for <i>t</i> ;
level	level at which to perform upward pass;
work	workspace

# Returns

# 5.5 Rotation coefficients and operations

Computation and application of rotation operators.

#### **Functions**

• gint **wbfmm\_rotation\_angles** (gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*jx, gdouble \*jx, gdouble \*jx, gdouble \*jx, gdouble \*jx, gdouble \*ch)

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

• gint wbfmm\_coefficients\_H\_rotation (gdouble \*H, gint N, gdouble th, gdouble \*work)

Compute rotation coefficients for angle  $\theta$ .

• gint **wbfmm\_rotate\_H** (gdouble \*Co, gint cstro, gdouble \*Ci, gint cstri, gint N, gdouble \*H, gdouble ph, gdouble ch)

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients.

• gint **wbfmm\_laplace\_rotate\_H** (gdouble \*Co, gint cstro, gdouble \*Ci, gint cstri, gint N, gint nq, gdouble \*H, gdouble ph, gdouble ch)

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

• gint **wbfmm\_rotation\_angles\_f** (gfloat \*ix, gfloat \*iy, gfloat \*jx, gfloat \*jx, gfloat \*jy, gfloat \*jy, gfloat \*th, gfloat \*ph, gfloat \*ch)

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

• gint wbfmm\_coefficients\_H\_rotation\_f (gfloat \*H, gint N, gfloat th, gfloat \*work)

Compute rotation coefficients for angle  $\theta$ .

- gint wbfmm\_rotate\_H\_f (gfloat \*Co, gint cstro, gfloat \*Ci, gint cstri, gint N, gfloat \*H, gfloat ph, gfloat ch)
   Apply rotation (θ, φ χ) to multipole coefficients.
- gint wbfmm\_laplace\_rotate\_H\_f (gfloat \*Co, gint cstro, gfloat \*Ci, gint cstri, gint N, gint nq, gfloat \*H, gfloat ph, gfloat ch)

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

## 5.5.1 Detailed Description

Computation and application of rotation operators.

Recursive computation of rotation coefficients using the methods of Gumerov and Duraiswami,  $http://dx. \leftarrow doi.org/10.1137/S1064827501399705$ 

#### 5.5.2 Function Documentation

5.5.2.1 gint wbfmm\_coefficients\_H\_rotation ( gdouble \* H, gint N, gdouble th, gdouble \* work )

Compute rotation coefficients for angle  $\theta$ .

Generate the coefficients required to rotate one multipole expansion to a new orientation, using Gumerov and Duraiswami, Section 5, equation (5.48) and recursion (5.55). Coefficients H are real and densely packed on output.

#### **Parameters**

	Н	on output rotation coefficients;
Ī	N	maximum order of coefficients to compute;
Ī	th	rotation angle $\theta$ , from <b>wbfmm_rotation_angles</b> (p. 40)();
ſ	work	workspace

## Returns

5.5.2.2 gint wbfmm\_coefficients\_H\_rotation\_f ( gfloat \* H, gint N, gfloat th, gfloat \* work )

Compute rotation coefficients for angle  $\theta$ .

Generate the coefficients required to rotate one multipole expansion to a new orientation, using Gumerov and Duraiswami, Section 5, equation (5.48) and recursion (5.55). Coefficients *H* are real and densely packed on output.

#### **Parameters**

Н	on output rotation coefficients;
N	maximum order of coefficients to compute;
th	rotation angle $\theta$ , from <b>wbfmm_rotation_angles_f</b> (p. 40)();
work	workspace

#### Returns

0 on success

5.5.2.3 gint wbfmm\_laplace\_rotate\_H ( gdouble \* Co, gint cstro, gdouble \* Ci, gint cstri, gint N, gint nq, gdouble \* H, gdouble ph, gdouble ch )

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

Given the rotation coefficients H for angle  $\theta$  from **wbfmm\_coefficients\_H\_rotation** (p. 37)(...), rotate input coefficients to new system of axes, using H and angles  $\phi$  and  $\chi$ . Input and output are strided arrays of dense complex data with spacing between adjacent complex values given as cstri and cstro elements respectively. Thus, Co for example is packed as:

$$[\Re(C_{00}) \quad \Im(C_{00}) \dots (2 \times \mathsf{cstro}) \dots \Re(C_{0,-1}) \quad \Im(C_{0,-1})]$$

This stride system allows for packing data more conveniently for upward and downward passes in the FMM proper.

#### **Parameters**

Со	on output contains rotated coefficients;
cstro	stride in Co, in number of complex elements;
Ci	input coefficients, to be rotated;
cstri	stride in Ci, in number of complex elements;
N	maximum order of coefficients;
nq	number of source terms;
Н	rotation coefficients for angle $\theta$ , from <b>wbfmm_coefficients_H_rotation</b> (p. 37)();
ph	angle $\phi$ for rotation;
ch	angle $\chi$ for rotation.

# Returns

0 on success

5.5.2.4 gint wbfmm\_laplace\_rotate\_H\_f ( gfloat \* Co, gint cstro, gfloat \* Ci, gint cstri, gint N, gint nq, gfloat \* H, gfloat ph, gfloat ch )

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

Given the rotation coefficients H for angle  $\theta$  from **wbfmm\_coefficients\_H\_rotation\_f** (p. 38)(...), rotate input coefficients to new system of axes, using H and angles  $\phi$  and  $\chi$ . Input and output are strided arrays of dense complex data with spacing between adjacent complex values given as cstri and cstro elements respectively. Thus, Co for example is packed as:

$$[\Re(C_{00}) \ \Im(C_{00}) \dots (2 \times \mathsf{cstro}) \dots \Re(C_{0,-1}) \ \Im(C_{0,-1})]$$

This stride system allows for packing data more conveniently for upward and downward passes in the FMM proper.

#### **Parameters**

Со	on output contains rotated coefficients;
cstro	stride in Co, in number of complex elements;
Ci	input coefficients, to be rotated;
cstri	stride in Ci, in number of complex elements;
N	maximum order of coefficients;
nq	number of source terms;
Н	rotation coefficients for angle $\theta$ , from <b>wbfmm_coefficients_H_rotation_f</b> (p. 38)();
ph	angle $\phi$ for rotation;
ch	angle $\chi$ for rotation.

#### Returns

0 on success

5.5.2.5 gint wbfmm\_rotate\_H ( gdouble \* Co, gint cstro, gdouble \* Ci, gint cstri, gint N, gdouble \* H, gdouble ph, gdouble ch )

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients.

Given the rotation coefficients H for angle  $\theta$  from **wbfmm\_coefficients\_H\_rotation** (p. 37)(...), rotate input coefficients to new system of axes, using H and angles  $\phi$  and  $\chi$ . Input and output are strided arrays of dense complex data with spacing between adjacent complex values given as cstri and cstro elements respectively. Thus, Co for example is packed as:

$$[\Re(C_{00}) \ \Im(C_{00}) \dots (2 \times \mathsf{cstro}) \dots \Re(C_{0,-1}) \ \Im(C_{0,-1})]$$

This stride system allows for packing data more conveniently for upward and downward passes in the FMM proper.

The function is available as a reference version wbfmm\_rotate\_H\_ref(...) and an optimized version wbfmm\_rotate ← \_H\_avx(...) which uses AVX optimizations if available. The compile time switch -DWBFMM\_USE\_AVX selects the AVX version.

#### **Parameters**

Ca	an output contains retated coefficients.
Со	on output contains rotated coefficients;
cstro	stride in <i>Co</i> , in number of complex elements;
Ci	input coefficients, to be rotated;
cstri	stride in Ci, in number of complex elements;
N	maximum order of coefficients;
Н	rotation coefficients for angle $\theta$ , from <b>wbfmm_coefficients_H_rotation</b> (p. 37)();
ph	angle $\phi$ for rotation;
ch	angle $\chi$ for rotation.

#### Returns

0 on success

5.5.2.6 gint wbfmm\_rotate\_H\_f ( gfloat \* Co, gint cstro, gfloat \* Ci, gint cstri, gint N, gfloat \* H, gfloat ph, gfloat ch )

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients.

Given the rotation coefficients H for angle  $\theta$  from **wbfmm\_coefficients\_H\_rotation\_f** (p. 38)(...), rotate input coefficients to new system of axes, using H and angles  $\phi$  and  $\chi$ . Input and output are strided arrays of dense complex data with spacing between adjacent complex values given as cstri and cstro elements respectively. Thus, Co for example is packed as:

$$[\Re(C_{00}) \quad \Im(C_{00}) \dots (2 \times \mathsf{cstro}) \dots \Re(C_{0,-1}) \quad \Im(C_{0,-1})]$$

This stride system allows for packing data more conveniently for upward and downward passes in the FMM proper.

The function is available as a reference version wbfmm\_rotate\_H\_ref\_f(...) and an optimized version wbfmm← \_rotate\_H\_avx\_f(...) which uses AVX optimizations if available. The compile time switch -DWBFMM\_USE\_AVX selects the AVX version.

#### **Parameters**

Со	on output contains rotated coefficients;
cstro	stride in Co, in number of complex elements;
Ci	input coefficients, to be rotated;
cstri	stride in Ci, in number of complex elements;
N	maximum order of coefficients;
Н	rotation coefficients for angle $\theta$ , from <b>wbfmm_coefficients_H_rotation_f</b> (p. 38)();
ph	angle $\phi$ for rotation;
ch	angle $\chi$ for rotation.

#### Returns

0 on success

5.5.2.7 gint wbfmm\_rotation\_angles ( gdouble \* ix, gdouble \* iy, gdouble \* ix, gdouble \*

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

Compute the angles for rotation between two systems of axes  $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$  and  $(\mathbf{j}_x, \mathbf{j}_y, \mathbf{j}_z)$ , as defined in Section 5 of Gumerov and Duraiswami. All vectors should be unit length and form a right-handed coordinate system (no check is performed).

# **Parameters**

ix	initial coordinate system $x$ axis;
iy	initial coordinate system $y$ axis;
iz	initial coordinate system $z$ axis;
jx	rotated coordinate system $x$ axis;
jу	rotated coordinate system $y$ axis;
jz	rotated coordinate system $z$ axis;
th	on exit, $\theta$ for rotation;
ph	on exit, $\phi$ for rotation;
ch	on exit, $\chi$ for rotation.

#### Returns

0 on success

5.5.2.8 gint wbfmm\_rotation\_angles\_f ( gfloat \* ix, gfloat \* iy, gfloat \* iz, gfloat \* jx, gfloa

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

Compute the angles for rotation between two systems of axes  $(\mathbf{i}_x, \mathbf{i}_y, \mathbf{i}_z)$  and  $(\mathbf{j}_x, \mathbf{j}_y, \mathbf{j}_z)$ , as defined in Section 5 of Gumerov and Duraiswami. All vectors should be unit length and form a right-handed coordinate system (no check is performed).

# **Parameters**

ix	initial coordinate system $x$ axis;
iy	initial coordinate system $y$ axis;
iz	initial coordinate system $z$ axis;
jx	rotated coordinate system $x$ axis;
jу	rotated coordinate system $y$ axis;
jz	rotated coordinate system $z$ axis;
th	on exit, $\theta$ for rotation;
ph	on exit, $\phi$ for rotation;
ch	on exit, $\chi$ for rotation.

# Returns

# 5.6 Translation operators

Translation of expansions.

## **Functions**

• gint wbfmm\_coefficients\_SR\_coaxial (gdouble \*cfftSR, gint L, gdouble kr, gdouble \*work)

Generate coefficients for coaxial singular-to-regular translation.

• gint wbfmm\_coaxial\_translate (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gdouble \*cfft, gint L, gboolean complex)

Perform coaxial translation of multipole expansion.

• gint wbfmm\_coefficients\_SR\_coaxial\_f (gfloat \*cfftSR, gint L, gfloat kr, gfloat \*work)

Generate coefficients for coaxial singular-to-regular translation.

gint wbfmm\_coaxial\_translate\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gfloat \*cfft, gint L, gboolean complex)

Perform coaxial translation of multipole expansion.

• gint wbfmm\_coefficients\_RR\_coaxial (gdouble \*cfftRR, gint L, gdouble kr, gdouble \*work)

Generate coefficients for coaxial regular-to-regular translation.

• gint wbfmm\_coefficients\_RR\_coaxial\_f (gfloat \*cfftRR, gint L, gfloat kr, gfloat \*work)

Generate coefficients for coaxial regular-to-regular translation.

# 5.6.1 Detailed Description

Translation of expansions.

## 5.6.2 Function Documentation

5.6.2.1 gint wbfmm\_coaxial\_translate ( gdouble \* Co, gint cstro, gint No, gdouble \* Ci, gint cstri, gint Ni, gdouble \* cfft, gint L, gboolean complex )

Perform coaxial translation of multipole expansion.

Compute the coaxial translation of a multipole expansion along its z axis, using coefficients from **wbfmm** $_{\leftarrow}$  **coefficients\_SR\_coaxial** (p. 44)(...) (complex) or **wbfmm\_coefficients\_RR\_coaxial** (p. 43)(...) (real). Input and output coefficients are strided data as described for **wbfmm\_rotate H** (p. 39)(...).

#### **Parameters**

Со	on output contains translated multipole expansion;
cstro	stride for output data in number of complex elements;
No	order of output expansion;
Ci	input multipole expansion;
cstri	stride for input data in number of complex elements;
Ni	order of input expansion;
cfft	translation coefficients;
L	maximum order of translation coefficients;
complex	if TRUE treat cfft as complex (e.g. for singular-to-regular translation); if FALSE treat as real
	(e.g. regular-to-regular or singular-to-singular).

# Returns

5.6.2.2 gint wbfmm\_coaxial\_translate\_f ( gfloat \* Co, gint cstro, gint No, gfloat \* Ci, gint cstri, gint Ni, gfloat \* cfft, gint L, gboolean complex )

Perform coaxial translation of multipole expansion.

Compute the coaxial translation of a multipole expansion along its z axis, using coefficients from **wbfmm** $_{\leftarrow}$  **coefficients\_SR\_coaxial\_f** (p. 44)(...) (complex) or **wbfmm\_coefficients\_RR\_coaxial\_f** (p. 43)(...) (real). Input and output coefficients are strided data as described for **wbfmm\_rotate\_H\_f** (p. 39)(...).

#### **Parameters**

Со	on output contains translated multipole expansion;
cstro	stride for output data in number of complex elements;
No	order of output expansion;
Ci	input multipole expansion;
cstri	stride for input data in number of complex elements;
Ni	order of input expansion;
cfft	translation coefficients;
L	maximum order of translation coefficients;
complex	if TRUE treat cfft as complex (e.g. for singular-to-regular translation); if FALSE treat as real
	(e.g. regular-to-regular or singular-to-singular).

## Returns

0 on success

5.6.2.3 gint wbfmm\_coefficients\_RR\_coaxial ( gdouble \* cfftRR, gint L, gdouble kr, gdouble \* work )

Generate coefficients for coaxial regular-to-regular translation.

Generate translation coefficients for a regular-to-regular coaxial shift along the z axis of the local coordinate system, by distance r for wavenumber k, using the methods of Section 4.8 of Gumerov and Duraiswami. The regular-to-regular translation coefficients are identical to the singular-to-singular coefficients and are real.

#### **Parameters**

cfftRR	on output contains (real) translation coefficients;
L	maximum order of multipole expansion to be translated;
kr	coaxial translation parameter (wavenumber times distance);
work	workspace

# Returns

0 on success

5.6.2.4 gint wbfmm\_coefficients\_RR\_coaxial\_f ( gfloat \* cfftRR, gint L, gfloat \* work )

Generate coefficients for coaxial regular-to-regular translation.

Generate translation coefficients for a regular-to-regular coaxial shift along the z axis of the local coordinate system, by distance r for wavenumber k, using the methods of Section 4.8 of Gumerov and Duraiswami. The regular-to-regular translation coefficients are identical to the singular-to-singular coefficients and are real.

cfftRR	on output contains (real) translation coefficients;
L	maximum order of multipole expansion to be translated;
kr	coaxial translation parameter (wavenumber times distance);
work	workspace

## Returns

0 on success

5.6.2.5 gint wbfmm\_coefficients\_SR\_coaxial ( gdouble \* cfftSR, gint L, gdouble \*kr, gdouble \* work )

Generate coefficients for coaxial singular-to-regular translation.

Generate translation coefficients for a singular-to-regular coaxial shift along the z axis of the local coordinate system, by distance r for wavenumber k, using the methods of Section 4.8 of Gumerov and Duraiswami. The output coefficients are complex.

## **Parameters**

	cfftSR	on output contains (complex) translation coefficients;
ĺ	L	maximum order of multipole expansion to be translated;
ſ	kr	coaxial translation parameter (wavenumber times distance);
ĺ	work	workspace

#### Returns

0 on success

5.6.2.6 gint wbfmm\_coefficients\_SR\_coaxial\_f ( gfloat \* cfftSR, gint L, gfloat \* w ork )

Generate coefficients for coaxial singular-to-regular translation.

Generate translation coefficients for a singular-to-regular coaxial shift along the z axis of the local coordinate system, by distance r for wavenumber k, using the methods of Section 4.8 of Gumerov and Duraiswami. The output coefficients are complex.

# **Parameters**

cfftSR	on output contains (complex) translation coefficients;
L	maximum order of multipole expansion to be translated;
kr	coaxial translation parameter (wavenumber times distance);
work	workspace

#### Returns

# 5.7 Utility and convenience functions

Various functions of use in debugging or underlying utilities.

#### **Functions**

- gint **wbfmm\_cartesian\_to\_spherical** (gdouble \*x0, gdouble \*x, gdouble \*r, gdouble \*th, gdouble \*ph) Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .
- gint wbfmm\_legendre\_recursion\_array (gdouble \*\*Pnm1, gdouble \*\*Pn, gint n, gdouble C, gdouble S)

  Perform recursion on normalized associated Legendre functions.
- gint wbfmm\_legendre\_init (gdouble C, gdouble S, gdouble \*P0, gdouble \*P10, gdouble \*P11)
   Initialize normalized associated Legendre functions.
- gint wbfmm\_bessel\_j\_recursion (gdouble \*jnm1, gdouble \*jn, gdouble x, gint n)

Perform recursion on spherical Bessel function  $j_n(x)$ .

• gint wbfmm\_bessel\_j\_init (gdouble x, gdouble \*j0, gdouble \*j1)

Initialize the spherical Bessel function recursion.

• gint wbfmm bessel h init (gdouble x, gdouble \*h0, gdouble \*h1)

Initialize spherical Hankel function recursion.

• gint wbfmm bessel h recursion (gdouble \*hnm1, gdouble \*hn, gdouble x, gint n)

Perform one step of spherical Hankel recursion.

• gint wbfmm\_total\_dipole\_field (gdouble k, gdouble \*xs, gint xstride, gdouble \*src, gint sstride, gint nsrc, gdouble \*xf, gdouble \*field)

Compute total field from dipole sources by direct evaluation.

• gint **wbfmm\_total\_field** (gdouble k, gdouble \*xs, gint xstride, gdouble \*src, gint sstride, gint nsrc, gdouble \*xf, gdouble \*field)

Compute total field by direct evaluation.

• gint wbfmm\_coordinate\_transform (gdouble \*x, gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*y)

Transform coordinates to rotated axes.

- gint **wbfmm\_shift\_coordinates** (gdouble \*x, gdouble \*y, gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*r)

  Find system of axes for coordinate shift.
- gint **wbfmm\_box\_location\_from\_index** (guint64 idx, guint32 level, gdouble \*x0, gdouble D, gdouble \*x, gdouble \*wb)

Find the coordinates of a box from its Morton index.

- gint wbfmm\_tree\_box\_centre (wbfmm\_tree\_t \*t, guint32 level, guint64 b, gdouble \*xb, gdouble \*wb)

  Find centre and width of box in an octree.
- gint **wbfmm\_points\_origin\_width** (gdouble \*x, gint str, gint n, gdouble \*xmin, gdouble \*D, gboolean init\_← limits)

Find limits of a cube containing a set of points.

- gint **wbfmm\_shift\_angles** (gdouble \*xi, gdouble \*xj, gdouble \*th, gdouble \*ph, gdouble \*ch, gdouble \*r)

  Compute angles and distance to shift expansion between two points.
- $\bullet \ \, \text{gint wbfmm\_tree\_write\_sources (wbfmm\_tree\_t *t, gdouble *q, gint stride, FILE *f)} \\$

Write a tree source list to file.

gint wbfmm\_cartesian\_to\_spherical\_f (gfloat \*x0, gfloat \*x, gfloat \*r, gfloat \*th, gfloat \*ph)

Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .

• gint wbfmm legendre recursion array f (gfloat \*\*Pnm1, gfloat \*\*Pn, gint n, gfloat C, gfloat S)

Perform recursion on normalized associated Legendre functions.

• gint wbfmm\_legendre\_init\_f (gfloat C, gfloat S, gfloat \*P0, gfloat \*P10, gfloat \*P11)

Initialize normalized associated Legendre functions.

• gint wbfmm bessel j recursion f (gfloat \*jnm1, gfloat \*jn, gfloat x, gint n)

Perform recursion on spherical Bessel function  $j_n(x)$ .

gint wbfmm\_bessel\_j\_init\_f (gfloat x, gfloat \*j0, gfloat \*j1)

Initialize the spherical Bessel function recursion.

• gint wbfmm\_bessel\_h\_init\_f (gfloat x, gfloat \*h0, gfloat \*h1)

Initialize spherical Hankel function recursion.

• gint wbfmm\_bessel\_h\_recursion\_f (gfloat \*hnm1, gfloat \*hn, gfloat x, gint n)

Perform one step of spherical Hankel recursion.

• gint **wbfmm\_total\_dipole\_field\_f** (gfloat k, gfloat \*xs, gint xstride, gfloat \*src, gint sstride, gint nsrc, gfloat \*xf, gfloat \*field)

Compute total field from dipole sources by direct evaluation.

• gint wbfmm\_total\_field\_f (gfloat k, gfloat \*xs, gint xstride, gfloat \*src, gint sstride, gint nsrc, gfloat \*xf, gfloat \*field)

Compute total field by direct evaluation.

• gint wbfmm\_coordinate\_transform\_f (gfloat \*x, gfloat \*ix, gfloat \*iy, gfloat \*iz, gfloat \*y)

Transform coordinates to rotated axes.

• gint wbfmm\_shift\_coordinates\_f (gfloat \*x, gfloat \*y, gfloat \*ix, gfloat \*ix, gfloat \*iz, gfloat \*r)

Find system of axes for coordinate shift.

• gint wbfmm\_box\_location\_from\_index\_f (guint64 idx, guint32 level, gfloat \*x0, gfloat D, gfloat \*x, gfloat \*wb)

Find the coordinates of a box from its Morton index.

• gint wbfmm\_tree\_box\_centre\_f (wbfmm\_tree\_t \*t, guint32 level, guint64 b, gfloat \*xb, gfloat \*wb)

Find centre and width of box in an octree.

- gint wbfmm\_points\_origin\_width\_f (gfloat \*x, gint str, gint n, gfloat \*xmin, gfloat \*D, gboolean init\_limits)

  Find limits of a cube containing a set of points.
- gint wbfmm\_shift\_angles\_f (gfloat \*xi, gfloat \*xj, gfloat \*th, gfloat \*ph, gfloat \*ch, gfloat \*r)

Compute angles and distance to shift expansion between two points.

gint wbfmm\_tree\_write\_sources\_f (wbfmm\_tree\_t \*t, gfloat \*q, gint stride, FILE \*f)

Write a tree source list to file.

## 5.7.1 Detailed Description

Various functions of use in debugging or underlying utilities.

#### 5.7.2 Function Documentation

5.7.2.1 gint wbfmm\_bessel\_h\_init ( gdouble x, gdouble \*h0, gdouble \*h1 )

Initialize spherical Hankel function recursion.

## **Parameters**

X	argument of $h_n(x)$ ;
h0	on exit $h_0(x)$ ;
h1	on exit $h_1(x)$

## Returns

0 on success

5.7.2.2 gint wbfmm\_bessel\_h\_init\_f ( gfloat x, gfloat \* h0, gfloat \* h1 )

Initialize spherical Hankel function recursion.

#### **Parameters**

X	argument of $h_n(x)$ ;
h0	on exit $h_0(x)$ ;
h1	on exit $h_1(x)$

#### Returns

0 on success

5.7.2.3 gint wbfmm\_bessel\_h\_recursion ( gdouble \* hnm1, gdouble \* hn, gdouble x, gint n )

Perform one step of spherical Hankel recursion.

Perform one step of the spherical Hankel function recursion. On entry hnm1 and hnm contain  $h_{n-1}(x)$  and  $h_n(x)$  respectively. On exit they contain equivalent values but for n incremented by one. When x falls below a small order-dependent cutoff, where the recursion is unreliable,  $h_n(x)$  is computed directly using a power series.

#### **Parameters**

hnm1	$h_{n-1}(x);$
hn	$h_n(x)$ ;
X	argument of spherical Hankel function;
n	order of spherical Hankel function

## Returns

0 on success

5.7.2.4 gint wbfmm\_bessel\_h\_recursion\_f ( gfloat \* hnm1, gfloat \* hn, gfloat x, gint n)

Perform one step of spherical Hankel recursion.

Perform one step of the spherical Hankel function recursion. On entry hnm1 and hnm contain  $h_{n-1}(x)$  and  $h_n(x)$  respectively. On exit they contain equivalent values but for n incremented by one. When x falls below a small order-dependent cutoff, where the recursion is unreliable,  $h_n(x)$  is computed directly using a power series.

# **Parameters**

hnm1	$h_{n-1}(x);$
hn	$h_n(x)$ ;
X	argument of spherical Hankel function;
n	order of spherical Hankel function

#### Returns

0 on success

5.7.2.5 gint wbfmm\_bessel\_j\_init ( gdouble x, gdouble \*j0, gdouble \*j1 )

Initialize the spherical Bessel function recursion.

#### **Parameters**

X	argument of $j_n(x)$ ;
j0	on exit $j_0(x)$ ;
j1	on exit $j_1(x)$

#### Returns

0 on success

5.7.2.6 gint wbfmm\_bessel\_j\_init\_f ( gfloat x, gfloat \*j0, gfloat \*j1 )

Initialize the spherical Bessel function recursion.

#### **Parameters**

X	argument of $j_n(x)$ ;
j0	on exit $j_0(x)$ ;
j1	on exit $j_1(x)$

#### Returns

0 on success

5.7.2.7 gint wbfmm\_bessel\_j\_recursion ( gdouble \* jnm1, gdouble \* jn, gdouble x, gint n )

Perform recursion on spherical Bessel function  $j_n(x)$ .

Perform one step of the spherical Bessel function recursion. On entry jnm1 and jnm contain  $j_{n-1}(x)$  and  $j_n(x)$  respectively. On exit they contain equivalent values but for n incremented by one. When x falls below a small order-dependent cutoff, where the recursion is unreliable,  $j_n(x)$  is computed directly using a power series.

# Parameters

jnm1	$j_{n-1}(x)$ ;
jn	$j_n(x)$ ;
X	argument of spherical Bessel function;
n	order of spherical Bessel function

# Returns

0 on success

5.7.2.8 gint wbfmm\_bessel\_j\_recursion\_f ( gfloat \* jnm1, gfloat \* jn, gfloat x, gint n)

Perform recursion on spherical Bessel function  $j_n(x)$ .

Perform one step of the spherical Bessel function recursion. On entry jnm1 and jnm contain  $j_{n-1}(x)$  and  $j_n(x)$  respectively. On exit they contain equivalent values but for n incremented by one. When x falls below a small order-dependent cutoff, where the recursion is unreliable,  $j_n(x)$  is computed directly using a power series.

#### **Parameters**

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jnm1	$j_{n-1}(x);$
jn	$j_n(x)$ ;
X	argument of spherical Bessel function;
n	order of spherical Bessel function

## Returns

0 on success

5.7.2.9 gint wbfmm\_box\_location\_from\_index ( guint64 *idx*, guint32 *level*, gdouble \* x0, gdouble \* x, gdouble \* x, gdouble \* x, gdouble \* wb )

Find the coordinates of a box from its Morton index.

## **Parameters**

idx	Morton index of box;
level	level in octree of box;
x0	origin of top-level box;
D	width of top-level box;
X	coordinates of box idx at level level;
wb	width of box at level level

# Returns

0 on success

5.7.2.10 gint wbfmm\_box\_location\_from\_index\_f ( guint64 idx, guint32 level, gfloat \* x0, gfloat \* x, gfloat \* x, gfloat \* xb )

Find the coordinates of a box from its Morton index.

#### **Parameters**

idx	Morton index of box;
level	level in octree of box;
x0	origin of top-level box;
D	width of top-level box;
X	coordinates of box idx at level level;
wb	width of box at level level

# Returns

0 on success

5.7.2.11 gint wbfmm\_cartesian\_to\_spherical ( gdouble \*x0, gdouble \*x, gdouble \*x

Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .

х0	centre of coordinate system;

X	point whose coordinates are to be found;
r	r;
th	$\mid  heta;$
ph	$ \phi $

## Returns

0 on success

5.7.2.12 gint wbfmm\_cartesian\_to\_spherical\_f ( gfloat \*x0, gfloat \*x, gfloat

Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .

#### **Parameters**

х0	centre of coordinate system;
X	point whose coordinates are to be found;
r	r;
th	$\theta$ ;
ph	$\phi$

# Returns

0 on success

5.7.2.13 gint wbfmm\_coordinate\_transform ( gdouble \* x, gdouble \* ix, gdouble \* iy, gdouble \* iz, gdouble \* y )

Transform coordinates to rotated axes.

# Parameters

	point coordinates in original axes;
i	unit vector in new axes;
iy	unit vector in new axes;
iz	unit vector in new axes;
J	point coordinates in new axes

#### **Returns**

0 on success

5.7.2.14 gint wbfmm\_coordinate\_transform\_f ( gfloat \* x, gfloat \* ix, gfloat \* iy, gfloat \* iy, gfloat \* iv, gfloat

Transform coordinates to rotated axes.

X	point coordinates in original axes;
ix	unit vector in new axes;
	,
ly	unit vector in new axes;
iz	unit vector in new axes;

_		
		naint an audinates in nauceur
	V	point coordinates in new axes
	y I	point coordinates in new axes

## Returns

0 on success

5.7.2.15 gint wbfmm\_legendre\_init ( gdouble C, gdouble S, gdouble P0, gdouble P10, gdouble P11)

Initialize normalized associated Legendre functions.

## **Parameters**

С	$\cos \theta$ ;
S	$\sin \theta$ ;
	on output $P_1^0(\cos \theta)$ ;
P11	on output $P_1^1(\cos\theta)$ ;

## Returns

0 on success

5.7.2.16 gint wbfmm\_legendre\_init\_f ( gfloat C, gfloat S, gfloat P0, gfloat P10, gfloat P11)

Initialize normalized associated Legendre functions.

#### **Parameters**

С	$\cos \theta$ ;
S	$\sin \theta$ ;
	on output $P_0^0(\cos  heta)$ ;
	on output $P_1^0(\cos \theta)$ ;
P11	on output $P_1^1(\cos\theta)$ ;

# Returns

0 on success

5.7.2.17 gint wbfmm\_legendre\_recursion\_array ( gdouble \*\* Pnm1, gdouble \*\* Pn, gint n, gdouble C, gdouble S)

Perform recursion on normalized associated Legendre functions.

Perform recursion on normalized associated Legendre functions with input  $P_{n-1}^m(\cos\theta),\ 0\le m\le n-1$ , and  $P_n^m(\cos\theta),\ 0\le m\le n$ , generating equivalent outputs with n incremented by one. Note that the arrays of associated Legendre functions are switched internally to ensure that the ordering remains correct after the recursion step.

Pnm1	pointer to array of normalized associated Legendre functions for $n-1$ ;
Pn	pointer to array of normalized associated Legendre functions for $n$ ;
n	order of <i>Pn</i> ;

С	$\cos \theta$ ;
S	$\sin \theta$ ;

## Returns

0 on success

5.7.2.18 gint wbfmm\_legendre\_recursion\_array\_f ( gfloat \*\* Pnm1, gfloat \*\* Pn, gint n, gfloat C, gfloat S)

Perform recursion on normalized associated Legendre functions.

Perform recursion on normalized associated Legendre functions with input  $P_{n-1}^m(\cos\theta),\ 0\le m\le n-1$ , and  $P_n^m(\cos\theta),\ 0\le m\le n$ , generating equivalent outputs with n incremented by one. Note that the arrays of associated Legendre functions are switched internally to ensure that the ordering remains correct after the recursion step.

## **Parameters**

Pnm1	pointer to array of normalized associated Legendre functions for $n-1$ ;
Pn	pointer to array of normalized associated Legendre functions for $n$ ;
n	order of <i>Pn</i> ;
С	$\cos \theta$ ;
S	$\sin \theta$ ;

## Returns

0 on success

5.7.2.19 gint wbfmm\_points\_origin\_width ( gdouble \* x, gint str, gint n, gdouble \* xmin, gdouble \* D, gboolean init\_limits )

Find limits of a cube containing a set of points.

# **Parameters**

X	array of points coordinates;
str	stride of points in x;
n	number of points in <i>x</i> ;
xmin	origin of cube containing all points in x;
D	width of cube containing all points in x;
init_limits	if TRUE initialize limits overwriting any data in xmin

#### Returns

0 on success

5.7.2.20 gint wbfmm\_points\_origin\_width\_f ( gfloat \*x, gint str, gint n, gfloat \*xmin, gfloat \*D, gboolean  $init\_limits$  )

Find limits of a cube containing a set of points.

_		
	Χ	array of points coordinates;

str	stride of points in x;
n	number of points in x;
xmin	origin of cube containing all points in x;
D	width of cube containing all points in x;
init_limits	if TRUE initialize limits overwriting any data in xmin

## Returns

0 on success

5.7.2.21 gint wbfmm\_shift\_angles ( gdouble \*xi, gdouble \*xi, gdouble \*th, gdouble \*th,

Compute angles and distance to shift expansion between two points.

This is a combination of a call to **wbfmm\_shift\_coordinates** (p. 53)(...) and **wbfmm\_rotation\_angles** (p. 40)(...)

## **Parameters**

xi	origin of shift;
xj	destination of shift;
th	heta for shift;
ph	$\phi$ for shift;
ch	$\chi$ for shift;
r	distance between source and destination points

## Returns

0 on success

5.7.2.22 gint wbfmm\_shift\_angles\_f ( gfloat \* xi, gfloat \* xj, gfloat \* th, gfloat \* ph, gfloat \* ch, gfloat \* r)

Compute angles and distance to shift expansion between two points.

This is a combination of a call to  $wbfmm\_shift\_coordinates\_f$  (p. 54)(...) and  $wbfmm\_rotation\_angles\_ \leftarrow f$  (p. 40)(...)

# **Parameters**

xi	origin of shift;
xj	destination of shift;
th	heta for shift;
ph	$\phi$ for shift;
ch	$\chi$ for shift;
r	distance between source and destination points

## Returns

0 on success

5.7.2.23 gint wbfmm\_shift\_coordinates ( gdouble \* x, gdouble \* y, gdouble \* ix, gdouble

Find system of axes for coordinate shift.

#### **Parameters**

X	origin of shift;
У	point to shift to;
ix	on output unit vector of shift axes;
iy	on output unit vector of shift axes;
iz	on output unit vector of shift axes in direction of shift;
r	distance between two input points

#### Returns

0 on success

5.7.2.24 gint wbfmm\_shift\_coordinates\_f ( gfloat \* x, gfloat \* y, gfloat \* ix, gfloat \* iy, gfloat \* iv, gfloat \*

Find system of axes for coordinate shift.

#### **Parameters**

X	origin of shift;
у	point to shift to;
ix	on output unit vector of shift axes;
iy	on output unit vector of shift axes;
iz	on output unit vector of shift axes in direction of shift;
r	distance between two input points

#### Returns

0 on success

5.7.2.25 gint wbfmm\_total\_dipole\_field ( gdouble \* xs, gint xstride, gdouble \* src, gint sstride, gint nsrc, gdouble \* xf, gdouble \* field )

Compute total field from dipole sources by direct evaluation.

Evaluate the field at some point  $\mathbf{x}$  by direct evaluation of the sum over sources at  $\mathbf{x}_n \sum_{n=1}^{N} \mathbf{f}_n \cdot \nabla h_0(\mathbf{x} - \mathbf{x}_n) / 4\pi$ .

# Parameters

k	wavenumber;
XS	array of source positions;
xstride	stride in xs between source positions;
src	array of complex vector source strengths;
sstride	stride in <i>src</i> ;
nsrc	number of sources;
xf	point for field evaluation;
field	incremented with computed field

# Returns

0 on success

5.7.2.26 gint wbfmm\_total\_dipole\_field\_f ( gfloat \* xs, gint xstride, gfloat \* src, gint sstride, gint sstride, gfloat \* src, gint sstride, gint sstride, gfloat \* src, gint sstride, gint sstride, gint sstride, gfloat \* src, gint sstride, gfloat \* src, gint sstride, gint sstride, gint sstride, gfloat \* src, gint sstride, gint sstride

Compute total field from dipole sources by direct evaluation.

Evaluate the field at some point  $\mathbf{x}$  by direct evaluation of the sum over sources at  $\mathbf{x}_n \sum_{n=1}^N \mathbf{f}_n \cdot \nabla h_0(\mathbf{x} - \mathbf{x}_n) / 4\pi$ .

#### **Parameters**

k	wavenumber;
XS	array of source positions;
xstride	stride in xs between source positions;
src	array of complex vector source strengths;
sstride	stride in <i>src</i> ;
nsrc	number of sources;
xf	point for field evaluation;
field	incremented with computed field

# Returns

0 on success

5.7.2.27 gint wbfmm\_total\_field ( gdouble \* xs, gint xstride, gdouble \* src, gint sstride, gint nsrc, gdouble \* xf, gdouble \* field )

Compute total field by direct evaluation.

Evaluate the field at some point  $\mathbf{x}$  by direct evaluation of the sum over sources at  $\mathbf{x}_n \sum_{n=1}^N s_n h_0(\mathbf{x} - \mathbf{x}_n)/4\pi$ .

#### **Parameters**

k	wavenumber;
XS	array of source positions;
xstride	stride in xs between source positions;
src	array of complex scalar source strengths;
sstride	stride in <i>src</i> ;
nsrc	number of sources;
xf	point for field evaluation;
field	incremented with computed field

# Returns

0 on success

5.7.2.28 gint wbfmm\_total\_field\_f ( gfloat k, gfloat \* xs, gint xstride, gfloat \* src, gint sstride, gint nsrc, gfloat \* field )

Compute total field by direct evaluation.

Evaluate the field at some point  $\mathbf{x}$  by direct evaluation of the sum over sources at  $\mathbf{x}_n \sum_{n=1}^N s_n h_0(\mathbf{x} - \mathbf{x}_n)/4\pi$ .

k	wavenumber;
XS	array of source positions;
xstride	stride in xs between source positions;
src	array of complex scalar source strengths;
sstride	stride in <i>src</i> ;
nsrc	number of sources;
xf	point for field evaluation;

field	incremented with computed field
-------	---------------------------------

## Returns

0 on success

5.7.2.29 gint wbfmm\_tree\_box\_centre ( wbfmm\_tree\_t \* t, guint32 level, guint64 b, gdouble \* xb, gdouble \* wb )

Find centre and width of box in an octree.

## **Parameters**

t	an octree;
level	level inside <i>t</i> ;
b	Morton index of box at level <i>level</i> ;
xb	centre of box with index b at level level;
wb	width of box at level <i>level</i> ;

#### Returns

0 on success

5.7.2.30 gint wbfmm\_tree\_box\_centre\_f ( wbfmm\_tree\_t \* t, guint32 level, guint64 b, gfloat \* xb, gfloat \* xb, gfloat \* xb )

Find centre and width of box in an octree.

#### **Parameters**

t	an octree;
level	level inside t;
b	Morton index of box at level <i>level</i> ;
xb	centre of box with index b at level level;
wb	width of box at level <i>level</i> ;

## Returns

0 on success

5.7.2.31 gint wbfmm\_tree\_write\_sources ( wbfmm\_tree\_t \* t, gdouble \* q, gint stride, FILE \* f )

Write a tree source list to file.

Write to file a list of source positions attached to an octree, in order of Morton index by which they are attached to leaf boxes. If source strengths are supplied (*q* not NULL) these are also written to file.

# **Parameters**

t	an octree with a list of sources attached;
q	source strengths (if NULL, source strengths are not written);
stride	source strength stride in q;
f	output file to write to

# Returns

5.7.2.32 gint wbfmm\_tree\_write\_sources\_f ( wbfmm\_tree\_t \* t, gfloat \* q, gint stride, FILE \* f )

Write a tree source list to file.

Write to file a list of source positions attached to an octree, in order of Morton index by which they are attached to leaf boxes. If source strengths are supplied (q not NULL) these are also written to file.

#### Parameters

t	an octree with a list of sources attached;
q	source strengths (if NULL, source strengths are not written);
stride	source strength stride in q;
f	output file to write to

## Returns

# 5.8 Evaluation of the Laplace potential

Variants on standard functions to allow WBFMM to be used for the Laplace equation.

#### **Functions**

• gint **wbfmm\_laplace\_expansion\_cfft** (gint N, gdouble \*x0, gdouble \*xs, gdouble \*q, gint nq, gdouble \*cfft, gint cstr, gdouble \*work)

Generation of singular expansion coefficients for point source in Laplace problem.

• gint wbfmm\_expansion\_laplace\_evaluate (gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gint nq, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate a singular expansion for Laplace problem.

• gint wbfmm\_laplace\_coaxial\_translate\_SS (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Singular to singular translation for Laplace expansion.

• gint wbfmm\_laplace\_child\_parent\_shift (gdouble \*Cp, gint Np, gdouble \*Cc, gint Nc, gint nq, gdouble \*H03, gdouble \*H47, gint Lh, gdouble wb, gdouble \*work)

Upward shift of singular expansion from eight children to common parent in Laplace problem.

• gint wbfmm\_laplace\_parent\_child\_shift (gdouble \*Cc, gint Nc, gdouble \*Cp, gint Np, gint nq, gdouble \*H03, gdouble \*H47, gint Lh, gdouble wb, gdouble \*work)

Downward shift of regular expansion from parent to eight children in Laplace problem.

- gint wbfmm\_laplace\_field\_coefficients (gdouble \*x, gint N, gboolean grad, gdouble \*cfft, gdouble \*work)

  Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using wbfmm\_laplace\_expansion\_apply (p. 65)(...)
- gint wbfmm laplace expansion apply (gdouble \*C, gint cstr, gint nq, gdouble \*ec, gint N, gdouble \*f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

- gint wbfmm\_laplace\_local\_coefficients (gdouble \*x, gint N, gboolean grad, gdouble \*cfft, gdouble \*work)
  - Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply** (p. 65)(...)
- gint wbfmm\_box\_fields\_laplace (wbfmm\_tree\_t \*t, gint level, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate the Laplace field generated by all boxes on a given level of an octree.

• gint wbfmm\_laplace\_coaxial\_translate\_init (gint N)

Initialize lookup tables of Laplace translation coefficients.

• gint wbfmm\_laplace\_coaxial\_translate\_SR (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Singular to regular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_RR (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Regular to regular translation for Laplace expansion.

- gint wbfmm\_laplace\_field (gdouble \*xs, gint xstride, gdouble \*src, gint sstride, gint nq, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gint nsrc, gdouble \*xf, gdouble \*field)
- gint **wbfmm\_laplace\_expansion\_local\_evaluate** (gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gint nq, gdouble \*xf, gdouble \*field, gdouble \*work)
- gint wbfmm\_laplace\_expansion\_cfft\_f (gint N, gfloat \*x0, gfloat \*xs, gfloat \*q, gint nq, gfloat \*cfft, gint cstr, gfloat \*work)

Generation of singular expansion coefficients for point source in Laplace problem.

• gint wbfmm\_expansion\_laplace\_evaluate\_f (gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gint nq, gfloat \*xf, gfloat \*field, gfloat \*work)

Evaluate a singular expansion for Laplace problem.

• gint wbfmm\_laplace\_coaxial\_translate\_SS\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Singular to singular translation for Laplace expansion.

• gint wbfmm\_laplace\_child\_parent\_shift\_f (gfloat \*Cp, gint Np, gfloat \*Cc, gint Nc, gint nq, gfloat \*H03, gfloat \*H47, gint Lh, gfloat wb, gfloat \*work)

Upward shift of singular expansion from eight children to common parent in Laplace problem.

• gint wbfmm\_laplace\_parent\_child\_shift\_f (gfloat \*Cc, gint Nc, gfloat \*Cp, gint Np, gint nq, gfloat \*H03, gfloat \*H47, gint Lh, gfloat wb, gfloat \*work)

Downward shift of regular expansion from parent to eight children in Laplace problem.

• gint wbfmm laplace field coefficients f (gfloat \*x, gint N, gboolean grad, gfloat \*cfft, gfloat \*work)

Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

gint wbfmm\_laplace\_expansion\_apply\_f (gfloat \*C, gint cstr, gint nq, gfloat \*ec, gint N, gfloat \*f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

• gint wbfmm\_laplace\_local\_coefficients\_f (gfloat \*x, gint N, gboolean grad, gfloat \*cfft, gfloat \*work)

Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

• gint wbfmm\_box\_fields\_laplace\_f (wbfmm\_tree\_t \*t, gint level, gfloat \*xf, gfloat \*field, gfloat \*work)

Evaluate the Laplace field generated by all boxes on a given level of an octree.

gint wbfmm laplace coaxial translate init f (gint N)

Initialize lookup tables of Laplace translation coefficients.

• gint wbfmm\_laplace\_coaxial\_translate\_SR\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Singular to regular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_RR\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Regular to regular translation for Laplace expansion.

- gint **wbfmm\_laplace\_field\_f** (gfloat \*xs, gint xstride, gfloat \*src, gint sstride, gint nq, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gint nsrc, gfloat \*xf, gfloat \*field)
- gint wbfmm\_laplace\_expansion\_local\_evaluate\_f (gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gint nq, gfloat \*xf, gfloat \*field, gfloat \*work)

# 5.8.1 Detailed Description

Variants on standard functions to allow WBFMM to be used for the Laplace equation.

# 5.8.2 Function Documentation

5.8.2.1 gint wbfmm box fields laplace ( wbfmm tree t \* t, gint level, gdouble \* xf, gdouble \* field, gdouble \* work )

Evaluate the Laplace field generated by all boxes on a given level of an octree.

t	octree;
level	level at which to use expansions;
xf	field evaluation point;
field	on output contains the sum of singular expansions from each box on level level evaluated at
	xf,

work	workspace.
------	------------

## Returns

0 on success

5.8.2.2 gint wbfmm\_box\_fields\_laplace\_f ( wbfmm\_tree\_t \* t, gint level, gfloat \* xf, gfloat \* field, gfloat \* work )

Evaluate the Laplace field generated by all boxes on a given level of an octree.

# **Parameters**

t	octree;
level	level at which to use expansions;
xf	field evaluation point;
field	on output contains the sum of singular expansions from each box on level level evaluated at
	xf;
work	workspace.

## Returns

0 on success

5.8.2.3 gint wbfmm\_expansion\_laplace\_evaluate ( gdouble \* x0, gdouble \* cft, gint cst, gint N, gint nq, gdouble \* xt, gdouble \* tield, gdouble \* work )

Evaluate a singular expansion for Laplace problem.

# **Parameters**

x0	origin of expansion;
cfft	on output, incremented with coefficients of expansion;
cstr	stride in cfft (must be at least equal to nq);
N	order of expansion;
nq	number of components in $q$ ;
xf	field point;
field	computed potential for each of the <i>nq</i> components;
work	workspace.

# Returns

0 on success

5.8.2.4 gint wbfmm\_expansion\_laplace\_evaluate\_f ( gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gint nq, gfloat \*xf, gfloat  $*title{field}$ , gfloat  $*title{work}$ )

Evaluate a singular expansion for Laplace problem.

х0	origin of expansion;

cfft	on output, incremented with coefficients of expansion;
cstr	stride in cfft (must be at least equal to nq);
N	order of expansion;
nq	number of components in <i>q</i> ;
xf	field point;
field	computed potential for each of the <i>nq</i> components;
work	workspace.

#### Returns

0 on success

5.8.2.5 gint wbfmm\_laplace\_child\_parent\_shift ( gdouble \* Cp, gint Np, gdouble \* Cc, gint Nc, gint nq, gdouble \* H03, gdouble \* H47, gint Lh, gdouble \* b, gdouble \* work )

Upward shift of singular expansion from eight children to common parent in Laplace problem.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index.

#### **Parameters**

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;
nq	number of elements in source;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
wb	child box width;
work	workspace

# Returns

0 on success

5.8.2.6 gint wbfmm\_laplace\_child\_parent\_shift\_f ( gfloat \* Cp, gint Np, gfloat \* Cc, gint Nc, gint nq, gfloat \* H03, gfloat \* H47, gint Lh, gfloat wb, gfloat \* work )

Upward shift of singular expansion from eight children to common parent in Laplace problem.

Shift the expansion of eight child boxes to their parent and sum into the parent expansion. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index.

Ср	parent expansion array;
Np	order of parent expansion;
Сс	child expansion array;
Nc	order of child expansions;

nq	number of elements in source;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
wb	child box width;
work	workspace

#### Returns

0 on success

5.8.2.7 gint wbfmm\_laplace\_coaxial\_translate\_init ( gint N )

Initialize lookup tables of Laplace translation coefficients.

Initialize lookup tables of Laplace translation coefficients for use in coaxial translation of Laplace expansions. This function must be called before any coaxial translation is performed in a Laplace problem.

#### **Parameters**

-		
	Ν	maximum order of expansion to be translated.

#### Returns

0 on success

5.8.2.8 gint wbfmm\_laplace\_coaxial\_translate\_init\_f ( gint N )

Initialize lookup tables of Laplace translation coefficients.

Initialize lookup tables of Laplace translation coefficients for use in coaxial translation of Laplace expansions. This function must be called before any coaxial translation is performed in a Laplace problem.

# Parameters

N	maximum order of expansion to be translated.
	<u>'</u>

## Returns

0 on success

5.8.2.9 gint wbfmm\_laplace\_coaxial\_translate\_RR ( gdouble \* Co, gint cstro, gint No, gdouble \* Ci, gint cstri, gint Ni, gint nq, gdouble t)

Regular to regular translation for Laplace expansion.

Translate a regular expansion for the Laplace problem along the z axis to a regular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to  ${\bf wbfmm\_laplace\_coaxial\_translate\_init}$  (p. 62)(...)

Со	on output, expansion about new centre;
----	--

cstro	stride in <i>Co</i> ;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in <i>Ci</i> ;
Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

## Returns

0 on success

5.8.2.10 gint wbfmm\_laplace\_coaxial\_translate\_RR\_f ( gfloat \* Co, gint cstro, gint No, gfloat \* Ci, gint cstri, gint Ni, gint nq, gfloat t)

Regular to regular translation for Laplace expansion.

Translate a regular expansion for the Laplace problem along the z axis to a regular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to **wbfmm\_laplace\_coaxial\_translate\_init\_f** (p. 62)(...)

#### **Parameters**

Со	on output, expansion about new centre;
cstro	stride in <i>Co</i> ;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in <i>Ci</i> ;
Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

## Returns

0 on success

5.8.2.11 gint wbfmm\_laplace\_coaxial\_translate\_SR ( gdouble \* Co, gint cstro, gint No, gdouble \* Ci, gint cstri, gint Ni, gint nq, gdouble t )

Singular to regular translation for Laplace expansion.

Translate a singular expansion for the Laplace problem along the z axis to a regular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to  ${\bf wbfmm\_laplace\_coaxial\_translate\_init}$  (p. 62)(...)

#### **Parameters**

Со	on output, expansion about new centre;
cstro	stride in Co;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in Ci;

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Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

## Returns

0 on success

5.8.2.12 gint wbfmm\_laplace\_coaxial\_translate\_SR\_f ( gfloat \* Co, gint cstro, gint No, gfloat \* Ci, gint cstri, gint Ni, gint nq, gfloat t)

Singular to regular translation for Laplace expansion.

Translate a singular expansion for the Laplace problem along the z axis to a regular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to  $\mathbf{wbfmm\_laplace\_coaxial\_translate\_init\_f}$  (p. 62)(...)

#### **Parameters**

Со	on output, expansion about new centre;
cstro	stride in <i>Co</i> ;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in <i>Ci</i> ;
Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

#### Returns

0 on success

5.8.2.13 gint wbfmm\_laplace\_coaxial\_translate\_SS ( gdouble \* Co, gint cstro, gint No, gdouble \* Ci, gint cstri, gint Ni, gint nq, gdouble t )

Singular to singular translation for Laplace expansion.

Translate a singular expansion for the Laplace problem along the z axis to a singular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to **wbfmm\_laplace\_coaxial\_translate\_init** (p. 62)(...)

## **Parameters**

Со	on output, expansion about new centre;
cstro	stride in Co;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in <i>Ci</i> ;
Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

## Returns

0 on success

5.8.2.14 gint wbfmm\_laplace\_coaxial\_translate\_SS\_f ( gfloat \* Co, gint cstro, gint No, gfloat \* Ci, gint cstri, gint Ni, gint nq, gfloat t )

Singular to singular translation for Laplace expansion.

Translate a singular expansion for the Laplace problem along the z axis to a singular expansion about a new centre. Before any Laplace translation function is called, the translation coefficients must be initialized with a call to  $wbfmm_laplace_coaxial_translate_init_f$  (p. 62)(...)

#### **Parameters**

Со	on output, expansion about new centre;
cstro	stride in Co;
No	order of expansion in <i>Co</i> ;
Ci	input expansion coefficients;
cstri	stride in Ci;
Ni	order of expansion in <i>Ci</i> ;
nq	number of source terms in expansion;
t	distance to translate expansion.

#### Returns

0 on success

5.8.2.15 gint wbfmm\_laplace\_expansion\_apply ( gdouble \* C, gint cstr, gint nq, gdouble \* ec, gint N, gdouble \* f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

## **Parameters**

С	coefficients of expansion;
cstr	stride in C;
nq	number of source terms in C;
ec	evaluation coefficients;
N	order of expansion;
f	on exit contains evaluated field.

# Returns

0 on success

5.8.2.16 gint wbfmm\_laplace\_expansion\_apply\_f ( gfloat \* C, gint cstr, gint nq, gfloat \* ec, gint N, gfloat \* f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

## **Parameters**

С	coefficients of expansion;
cstr	stride in C;

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nq	number of source terms in C;
ec	evaluation coefficients;
N	order of expansion;
f	on exit contains evaluated field.

## Returns

0 on success

5.8.2.17 gint wbfmm\_laplace\_expansion\_cfft ( gint N, gdouble \* x0, gdouble \* xs, gdouble \* q, gint nq, gdouble \* cfft, gint cstr, gdouble \* work )

Generation of singular expansion coefficients for point source in Laplace problem.

#### **Parameters**

N	order of expansion;
х0	origin of expansion;
XS	source position;
q	source strength(s);
nq	number of components in $q$ ;
cfft	on output, incremented with coefficients of expansion;
cstr	stride in cfft (must be at least equal to nq);
work	workspace.

## Returns

0 on success

5.8.2.18 gint wbfmm\_laplace\_expansion\_cfft\_f ( gint N, gfloat \* x0, gfloat \* xs, gfloat \* q, gint nq, gfloat \* cfft, gint cstr, gfloat \* work )

Generation of singular expansion coefficients for point source in Laplace problem.

# Parameters

N	order of expansion;
х0	origin of expansion;
XS	source position;
q	source strength(s);
nq	number of components in <i>q</i> ;
cfft	on output, incremented with coefficients of expansion;
cstr	stride in cfft (must be at least equal to nq);
work	workspace.

# Returns

0 on success

5.8.2.19 gint wbfmm\_laplace\_expansion\_local\_evaluate ( gdouble \* x0, gdouble \* cfft, gint cstr, gint N, gint nq, gdouble \* xf, gdouble \* field, gdouble \* work )

**Parameters** 

5.8.2.20 gint wbfmm\_laplace\_expansion\_local\_evaluate\_f ( gfloat \* x0, gfloat \* cfft, gint cstr, gint N, gint nq, gfloat \* xf, gfloat \* field, gfloat \* work )

#### **Parameters**

1	
1	
1	

5.8.2.21 gint wbfmm\_laplace\_field ( gdouble \* xs, gint xstride, gdouble \* src, gint sstride, gint nq, gdouble \* normals, gint nstr, gdouble \* dipoles, gint dstr, gint nsrc, gdouble \* xf, gdouble \* field )

#### **Parameters**

5.8.2.22 gint wbfmm\_laplace\_field\_coefficients ( gdouble \* x, gint N, gboolean grad, gdouble \* cfft, gdouble \* work )

Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply** (p. 65)(...)

#### **Parameters**

X	location of evaluation point relative to centre of expansion;
N	order of expansion;
grad	if TRUE generate coefficients for gradient of field;
cfft	on exit contains evaluation coefficients;
work	workspace.

#### Returns

0 on success

5.8.2.23 gint wbfmm\_laplace\_field\_coefficients\_f ( gfloat \*x, gint N, gboolean grad, gfloat \*x gf

Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

#### **Parameters**

X	location of evaluation point relative to centre of expansion;
N	order of expansion;
grad	if TRUE generate coefficients for gradient of field;
cfft	on exit contains evaluation coefficients;
work	workspace.

## Returns

0 on success

5.8.2.24 gint wbfmm\_laplace\_field\_f ( gfloat \* xs, gint xstride, gfloat \* src, gint sstride, gint nq, gfloat \* normals, gint nstr, gfloat \* dipoles, gint dstr, gint nsrc, gfloat \* xf, gfloat \* field )

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#### **Parameters**

5.8.2.25 gint wbfmm\_laplace\_local\_coefficients ( gdouble \* x, gint N, gboolean grad, gdouble \* cfft, gdouble \* work )

Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm laplace expansion apply** (p. 65)(...)

## **Parameters**

X	location of evaluation point relative to centre of expansion;
N	order of expansion;
grad	if TRUE generate coefficients for gradient of field;
cfft	on exit contains evaluation coefficients;
work	workspace.

## Returns

0 on success

5.8.2.26 gint wbfmm\_laplace\_local\_coefficients\_f ( gfloat \*x, gint N, gboolean grad, gfloat \*cfft, gfloat \*work )

Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

#### **Parameters**

X	location of evaluation point relative to centre of expansion;
N	order of expansion;
grad	if TRUE generate coefficients for gradient of field;
cfft	on exit contains evaluation coefficients;
work	workspace.

#### Returns

0 on success

5.8.2.27 gint wbfmm\_laplace\_parent\_child\_shift ( gdouble \* Cc, gint Nc, gdouble \* Cp, gint Np, gint nq, gdouble \* H03, gdouble \* H47, gint Lh, gdouble \* b, gdouble \* work )

Downward shift of regular expansion from parent to eight children in Laplace problem.

Shift the expansion of a parent box to its eight child boxes. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index. Note that rotation coefficients *H03* and *H47* are the same as for the upward pass but switched (because the rotations are performed in the opposite direction).

#### **Parameters**

Сс	child expansion array;
Nc	order of child expansions;

Ср	parent expansion array;
Np	order of parent expansion;
nq	number of elements in source;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
wb	parent box width;
work	workspace

## Returns

0 on success

5.8.2.28 gint wbfmm\_laplace\_parent\_child\_shift\_f ( gfloat \* Cc, gint Nc, gfloat \* Cp, gint Np, gint nq, gfloat \* H03, gfloat \* H47, gint Lh, gfloat wb, gfloat \* work )

Downward shift of regular expansion from parent to eight children in Laplace problem.

Shift the expansion of a parent box to its eight child boxes. This function assumes data are packed with a stride of eight elements so that all expansion coefficients of a given order are contiguous in memory, ordered by Morton index. Note that rotation coefficients *H03* and *H47* are the same as for the upward pass but switched (because the rotations are performed in the opposite direction).

#### **Parameters**

Сс	child expansion array;
Nc	order of child expansions;
Ср	parent expansion array;
Np	order of parent expansion;
nq	number of elements in source;
H03	rotation coefficients for 'lower' children (Morton index 0-3);
H47	rotation coefficients for 'upper' children (Morton index 4-7);
Lh	maximum order of rotation coefficients;
wb	parent box width;
work	workspace

# Returns

0 on success

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# 5.9 Indexing and lookup operations

Indexing functions for accessing tree data structures.

#### **Functions**

- guint64 wbfmm\_box\_index (guint32 i, guint32 j, guint32 k)
- gint wbfmm\_box\_location (guint64 idx, guint32 \*i, guint32 \*j, guint32 \*k)

# 5.9.1 Detailed Description

Indexing functions for accessing tree data structures.

Functions for indexing and lookup in tree data structures, including finding neighbours and interaction lists, based on the methods of Gumerov, Duraiswami, and Borovikov, Data Structures, Optimal Choice of Parameters, and Complexity Results for Generalized Multilevel Fast Multipole Methods in d Dimensions, 2003

http://users.umiacs.umd.edu/~gumerov/PDFs/cs-tr-4458.pdf

Code for Morton indexing operations is taken from: https://www.forceflow.be/2013/10/07/morton-encodingdeco

# 5.9.2 Function Documentation

5.9.2.1 guint64 wbfmm\_box\_index ( guint32 i, guint32 j, guint32 k )

Generate a Morton index for a box with corner at integer coordinates (i,j,k).

#### **Parameters**

i	x index of bottom left hand corner;
j	y index of bottom left hand corner;
k	z index of bottom left hand corner.

### Returns

Morton index for (i, j, k).

5.9.2.2 gint wbfmm\_box\_location ( guint64 idx, guint32 \* i, guint32 \* j, guint32 \* k )

Compute indices for bottom left hand corner of box defined by its Morton index, as generated by **wbfmm\_box\_index** (p. 70)

## **Parameters**

idx	index of box corner;
i	on output, x index of bottom left hand corner of box;
j	on output, y index of bottom left hand corner of box;
k	on output, z index of bottom left hand corner of box.

#### Returns

0 on success.

# **Chapter 6**

# **Data Structure Documentation**

# 6.1 wbfmm\_box\_t Struct Reference

# **Data Fields**

- guint32 i
- guint32 **n**
- gpointer mps
- gpointer mpr

# 6.1.1 Detailed Description

Data type for octree boxes

# 6.1.2 Field Documentation

6.1.2.1 guint32 wbfmm\_box\_t::i

index of first source point in box

6.1.2.2 gpointer wbfmm\_box\_t::mpr

pointer to regular multipole expansion data

6.1.2.3 gpointer wbfmm\_box\_t::mps

pointer to singular multipole expansion data

6.1.2.4 guint32 wbfmm\_box\_t::n

number of points in box

# 6.2 wbfmm\_shift\_operators\_t Struct Reference

## **Data Fields**

- gsize size
- guint nlevels
- guint L [WBFMM\_TREE\_MAX\_DEPTH+1]
- guint nerot
- gpointer **SR** [WBFMM\_TREE\_MAX\_DEPTH+1]
- gpointer SS [WBFMM\_TREE\_MAX\_DEPTH+1]
- gpointer rotations

# 6.2.1 Detailed Description

Data type holding operators for upward and downward passes and interaction calculations at each level

## 6.2.2 Field Documentation

```
6.2.2.1 guint wbfmm_shift_operators_t::L[WBFMM_TREE_MAX_DEPTH+1]
```

< number of levels in tree

```
6.2.2.2 guint wbfmm_shift_operators_t::nerot
```

< maximum order of expansion per level

6.2.2.3 guint wbfmm\_shift\_operators\_t::nlevels

< maximum order of expansions

6.2.2.4 gpointer wbfmm\_shift\_operators\_t::rotations

< singular-to-singular (regular-to-regular) coaxial translations

6.2.2.5 gsize wbfmm\_shift\_operators\_t::size

size of data type, i.e. float or double

6.2.2.6 gpointer wbfmm\_shift\_operators\_t::SR[WBFMM\_TREE\_MAX\_DEPTH+1]

< number of elements in rotation operators

6.2.2.7 gpointer wbfmm\_shift\_operators\_t::SS[WBFMM\_TREE\_MAX\_DEPTH+1]

< singular-to-regular coaxial translations

# 6.3 wbfmm\_target\_list\_t Struct Reference

## **Data Fields**

 $\bullet \ \ wbfmm\_tree\_t*t$ 

- · guint maxpoints
- guint **npoints**
- guint \* **ip**
- guint nc
- guint32 \* boxes
- gchar \* points
- gsize size
- gsize pstr
- gint \* ibox
- gint \* isrc
- gint \* ics
- · gpointer cfft
- gpointer csrc
- · gboolean grad

# 6.3.1 Detailed Description

Data type for target point lists

## 6.3.2 Field Documentation

6.3.2.1 guint32\* wbfmm\_target\_list\_t::boxes

box indices of points

6.3.2.2 gpointer wbfmm\_target\_list\_t::cfft

coefficients of regular expansions in boxes

6.3.2.3 gpointer wbfmm\_target\_list\_t::csrc

coefficients of near-field (direct) interactions, point-by-point

6.3.2.4 gboolean wbfmm\_target\_list\_t::grad

gradient computations included

6.3.2.5 gint\* wbfmm\_target\_list\_t::ibox

start and end of source index lists for each box

 $\textbf{6.3.2.6} \quad \textbf{gint} * \textbf{wbfmm\_target\_list\_t::ics}$ 

start of near-field coefficients for each target

6.3.2.7 guint \* wbfmm\_target\_list\_t::ip

indices of points, sorted by Morton index

```
6.3.2.8 gint * wbfmm_target_list_t::isrc
source index lists for each box
6.3.2.9 guint wbfmm_target_list_t::maxpoints
maximum number of points in target list
6.3.2.10 guint wbfmm_target_list_t::nc
number of coefficients (size of blocks of coefficients)
6.3.2.11 guint wbfmm_target_list_t::npoints
number of points in target list
6.3.2.12 gchar* wbfmm_target_list_t::points
point coordinates
6.3.2.13 gsize wbfmm_target_list_t::pstr
stride in point data
6.3.2.14 gsize wbfmm_target_list_t::size
size of floating point type in data (float, double, etc)
6.3.2.15 wbfmm tree t* wbfmm_target_list_t::t
```

# 6.4 wbfmm\_tree\_t Struct Reference

# **Data Fields**

- wbfmm\_box\_t \* boxes [WBFMM\_TREE\_MAX\_DEPTH+1]
- guint maxpoints

tree containing source data

- guint **npoints**
- guint \* **ip**
- guint **nq**
- guint depth
- guint order\_s [WBFMM\_TREE\_MAX\_DEPTH+1]
- guint order\_r [WBFMM\_TREE\_MAX\_DEPTH+1]
- gchar x [24]
- gchar \* points
- gpointer \* **mps** [WBFMM\_TREE\_MAX\_DEPTH+1]
- gpointer \* mpr [WBFMM\_TREE\_MAX\_DEPTH+1]
- gsize size
- gsize pstr
- gdouble **D**

# 6.4.1 Detailed Description

Data type for octrees

## 6.4.2 Field Documentation

 $6.4.2.1 \quad wbfmm\_box\_t* wbfmm\_tree\_t::boxes[WBFMM\_TREE\_MAX\_DEPTH+1]$ 

arrays of boxes at each level

Referenced by wbfmm\_tree\_add\_level().

6.4.2.2 gdouble wbfmm\_tree\_t::D

width of domain cube

6.4.2.3 guint wbfmm\_tree\_t::depth

depth of tree

Referenced by wbfmm\_tree\_add\_level().

6.4.2.4 guint \* wbfmm\_tree\_t::ip

indices of points, sorted by Morton index

6.4.2.5 guint wbfmm\_tree\_t::maxpoints

maximum number of points in tree

 $6.4.2.6 \quad gpointer*wbfmm\_tree\_t::mpr[WBFMM\_TREE\_MAX\_DEPTH+1]$ 

regular expansion data at each level

 $6.4.2.7 \quad gpointer*\ wbfmm\_tree\_t::mps[WBFMM\_TREE\_MAX\_DEPTH+1]$ 

singular expansion data at each level

6.4.2.8 guint wbfmm\_tree\_t::npoints

number of points in tree

6.4.2.9 guint wbfmm\_tree\_t::nq

number of source components

6.4.2.10 guint wbfmm\_tree\_t::order\_r[WBFMM\_TREE\_MAX\_DEPTH+1]

order of regular expansions at each level

6.4.2.11 guint wbfmm\_tree\_t::order\_s[WBFMM\_TREE\_MAX\_DEPTH+1]

order of singular expansions at each level

 $\textbf{6.4.2.12} \quad \textbf{gchar} * \textbf{wbfmm\_tree\_t::points}$ 

point coordinates

6.4.2.13 gsize wbfmm\_tree\_t::pstr

stride in point data

6.4.2.14 gsize wbfmm\_tree\_t::size

size of floating point type in data (float, double, etc)

6.4.2.15 gchar wbfmm\_tree\_t::x[24]

origin of tree domain cube

# **Chapter 7**

# **File Documentation**

# 7.1 tree.c File Reference

# **Functions**

• gint wbfmm\_tree\_add\_level (wbfmm\_tree\_t \*t)

# 7.1.1 Detailed Description

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Date

Mon Jun 24 14:51:21 2019

# 7.2 wbfmm.h File Reference

Header for Wide Band FMM library.

# **Data Structures**

- struct wbfmm\_box\_t
- struct wbfmm tree t
- struct wbfmm\_target\_list\_t
- struct wbfmm\_shift\_operators\_t

# **Enumerations**

enum wbfmm\_problem\_t { WBFMM\_PROBLEM\_LAPLACE = 1, WBFMM\_PROBLEM\_HELMHOLTZ = 2 }

# **Functions**

• gint **wbfmm\_cartesian\_to\_spherical** (gdouble \*x0, gdouble \*x, gdouble \*r, gdouble \*th, gdouble \*ph) Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .

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• gint **wbfmm\_shift\_coordinates** (gdouble \*x, gdouble \*y, gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*r)

Find system of axes for coordinate shift.

• gint wbfmm\_legendre\_recursion\_array (gdouble \*\*Pnm1, gdouble \*\*Pn, gint n, gdouble C, gdouble S)

Perform recursion on normalized associated Legendre functions.

• gint **wbfmm\_bessel\_j\_recursion** (gdouble \*jnm1, gdouble \*jn, gdouble x, gint n)

Perform recursion on spherical Bessel function  $j_n(x)$ .

• gint wbfmm\_bessel\_h\_recursion (gdouble \*hnm1, gdouble \*hn, gdouble x, gint n)

Perform one step of spherical Hankel recursion.

• gint wbfmm\_bessel\_j\_init (gdouble x, gdouble \*j0, gdouble \*j1)

Initialize the spherical Bessel function recursion.

• gint wbfmm bessel\_h init (gdouble x, gdouble \*h0, gdouble \*h1)

Initialize spherical Hankel function recursion.

• gint wbfmm\_legendre\_init (gdouble C, gdouble S, gdouble \*P0, gdouble \*P10, gdouble \*P11)

Initialize normalized associated Legendre functions.

gint wbfmm\_expansion\_h\_cfft (gdouble k, gint N, gdouble \*x0, gdouble \*xs, gdouble \*q, gdouble \*cfft, gint cstr, gdouble \*work)

Generation of singular expansion coefficients for point source.

• gint **wbfmm\_expansion\_dipole\_h\_cfft** (gdouble k, gint N, gdouble \*x0, gdouble \*xs, gdouble \*fx, gdouble \*fx, gdouble \*fx, gdouble \*fx, gdouble \*sty, gdouble \*fx, gdouble \*work)

Generation of singular expansion coefficients for point dipole source.

• gint **wbfmm\_expansion\_h\_evaluate** (gdouble k, gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate a singular expansion.

• gint **wbfmm\_expansion\_j\_evaluate** (gdouble k, gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gdouble \*xf, gdouble \*field, gdouble \*work)

Evaluate a regular expansion.

• gint **wbfmm\_total\_dipole\_field** (gdouble k, gdouble \*xs, gint xstride, gdouble \*src, gint sstride, gint nsrc, gdouble \*xf, gdouble \*field)

Compute total field from dipole sources by direct evaluation.

gint wbfmm\_coordinate\_transform (gdouble \*x, gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*y)

Transform coordinates to rotated axes.

• gint wbfmm\_coefficients\_RR\_coaxial (gdouble \*cfftRR, gint L, gdouble kr, gdouble \*work)

Generate coefficients for coaxial regular-to-regular translation.

• gint wbfmm\_coefficients\_SR\_coaxial (gdouble \*cfftSR, gint L, gdouble kr, gdouble \*work)

Generate coefficients for coaxial singular-to-regular translation.

• gint **wbfmm\_rotation\_angles** (gdouble \*ix, gdouble \*iy, gdouble \*iz, gdouble \*jx, gdouble \*jy, gdouble \*jy,

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

gint wbfmm\_coefficients\_H\_rotation (gdouble \*H, gint N, gdouble th, gdouble \*work)

Compute rotation coefficients for angle  $\theta$ .

• gint **wbfmm\_laplace\_expansion\_cfft** (gint N, gdouble \*x0, gdouble \*xs, gdouble \*q, gint nq, gdouble \*cfft, gint cstr, gdouble \*work)

Generation of singular expansion coefficients for point source in Laplace problem.

- gint wbfmm\_laplace\_field (gdouble \*xs, gint xstride, gdouble \*src, gint sstride, gint nq, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gint nsrc, gdouble \*xf, gdouble \*field)
- gint **wbfmm\_laplace\_expansion\_local\_evaluate** (gdouble \*x0, gdouble \*cfft, gint cstr, gint N, gint nq, gdouble \*xf, gdouble \*field, gdouble \*work)
- gint wbfmm\_laplace\_expansion\_local\_evaluate\_f (gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gint nq, gfloat \*xf, gfloat \*field, gfloat \*work)
- gint wbfmm\_laplace\_coaxial\_translate\_init (gint N)

Initialize lookup tables of Laplace translation coefficients.

gint wbfmm\_laplace\_coaxial\_translate\_init\_f (gint N)

Initialize lookup tables of Laplace translation coefficients.

gint wbfmm\_laplace\_expansion\_cfft\_f (gint N, gfloat \*x0, gfloat \*xs, gfloat \*q, gint nq, gfloat \*cfft, gint cstr, gfloat \*work)

Generation of singular expansion coefficients for point source in Laplace problem.

- gint wbfmm\_laplace\_field\_f (gfloat \*xs, gint xstride, gfloat \*src, gint sstride, gint nq, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gint nsrc, gfloat \*xf, gfloat \*field)
- gint wbfmm\_laplace\_coaxial\_translate\_SS (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Singular to singular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_SS\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Singular to singular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_RR (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Regular to regular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_RR\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Regular to regular translation for Laplace expansion.

• gint wbfmm\_laplace\_coaxial\_translate\_SR (gdouble \*Co, gint cstro, gint No, gdouble \*Ci, gint cstri, gint Ni, gint nq, gdouble t)

Singular to regular translation for Laplace expansion.

gint wbfmm\_laplace\_coaxial\_translate\_SR\_f (gfloat \*Co, gint cstro, gint No, gfloat \*Ci, gint cstri, gint Ni, gint nq, gfloat t)

Singular to regular translation for Laplace expansion.

• gint wbfmm\_laplace\_rotate\_H (gdouble \*Co, gint cstro, gdouble \*Ci, gint cstri, gint N, gint nq, gdouble \*H, gdouble ph, gdouble ch)

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

• gint wbfmm\_laplace\_rotate\_H\_f (gfloat \*Co, gint cstro, gfloat \*Ci, gint cstri, gint N, gint nq, gfloat \*H, gfloat ph, gfloat ch)

Apply rotation  $(\theta, \phi \chi)$  to multipole coefficients for the Laplace problem.

• gint wbfmm\_laplace\_child\_parent\_shift (gdouble \*Cp, gint Np, gdouble \*Cc, gint Nc, gint nq, gdouble \*H03, gdouble \*H47, gint Lh, gdouble t, gdouble \*work)

Upward shift of singular expansion from eight children to common parent in Laplace problem.

• gint wbfmm\_laplace\_child\_parent\_shift\_f (gfloat \*Cp, gint Np, gfloat \*Cc, gint Nc, gint nq, gfloat \*H03, gfloat \*H47, gint Lh, gfloat t, gfloat \*work)

Upward shift of singular expansion from eight children to common parent in Laplace problem.

• gint wbfmm\_laplace\_parent\_child\_shift (gdouble \*Cc, gint Nc, gdouble \*Cp, gint Np, gint nq, gdouble \*H03, gdouble \*H47, gint Lh, gdouble t, gdouble \*work)

Downward shift of regular expansion from parent to eight children in Laplace problem.

• gint wbfmm\_laplace\_parent\_child\_shift\_f (gfloat \*Cc, gint Nc, gfloat \*Cp, gint Np, gint nq, gfloat \*H03, gfloat \*H47, gint Lh, gfloat t, gfloat \*work)

Downward shift of regular expansion from parent to eight children in Laplace problem.

• gint wbfmm\_tree\_laplace\_leaf\_expansions (wbfmm\_tree\_t \*t, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gboolean zero expansions, gdouble \*work)

Generate leaf expansions for a tree in the Laplace problem.

• gint wbfmm\_tree\_laplace\_leaf\_expansions\_f (wbfmm\_tree\_t \*t, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gboolean zero expansions, gfloat \*work)

Generate leaf expansions for a tree in the Laplace problem.

• gint wbfmm\_laplace\_downward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform downward pass at one level of an octree for the Laplace problem.

gint wbfmm\_laplace\_downward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

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Perform downward pass at one level of an octree for the Laplace problem.

gint wbfmm\_laplace\_upward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform upward pass at one level of an octree for the Laplace problem.

gint wbfmm\_laplace\_upward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform upward pass at one level of an octree for the Laplace problem.

• gint wbfmm\_tree\_laplace\_box\_local\_field (wbfmm\_tree\_t \*t, guint level, guint b, gdouble \*x, gdouble \*f, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*d, gint dstr, gboolean eval\_neighbours, gdouble \*work)

Evaluate local Laplace field from regular expansion in box.

• gint wbfmm\_tree\_laplace\_box\_local\_field\_f (wbfmm\_tree\_t \*t, guint level, guint b, gfloat \*x, gfloat \*f, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*d, gint dstr, gboolean eval\_neighbours, gfloat \*work)

Evaluate local Laplace field from regular expansion in box.

• gint wbfmm\_laplace\_local\_coefficients (gdouble \*x, gint N, gboolean grad, gdouble \*cfft, gdouble \*work)

Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using wbfmm\_laplace\_expansion\_apply (p. 65)(...)

• gint wbfmm laplace local coefficients f (gfloat \*x, gint N, gboolean grad, gfloat \*cfft, gfloat \*work)

Generate coefficients for evaluation of local field from (regular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

• gint wbfmm\_laplace\_field\_coefficients (gdouble \*x, gint N, gboolean grad, gdouble \*cfft, gdouble \*work)

Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply** (p. 65)(...)

• gint wbfmm\_laplace\_field\_coefficients\_f (gfloat \*x, gint N, gboolean grad, gfloat \*cfft, gfloat \*work)

Generate coefficients for evaluation of field from (singular) expansion coefficients in the Laplace problem. The coefficients from this function can be applied to an expansion using **wbfmm\_laplace\_expansion\_apply\_f** (p. 65)(...)

• gint wbfmm\_laplace\_expansion\_apply (gdouble \*C, gint cstr, gint nq, gdouble \*ec, gint N, gdouble \*f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

• gint wbfmm\_laplace\_expansion\_apply\_f (gfloat \*C, gint cstr, gint nq, gfloat \*ec, gint N, gfloat \*f)

Apply evaluation coefficients to coefficients of an expansion to evaluate the Laplace potential. Evaluation coefficients can be evaluated using wbfmm\_laplace\_field\_coefficients) or wbfmm\_laplace\_local\_coefficients) for the field (singular) or local (regular) expansions respectively.

• gint **wbfmm\_child\_parent\_shift** (gdouble \*Cp, gint Np, gdouble \*Cc, gint Nc, gdouble \*H03, gdouble \*H47, gint Lh, gdouble \*shift, gint Ls, gdouble \*work)

Upward shift of singular expansion from eight children to common parent.

• gint **wbfmm\_parent\_child\_shift** (gdouble \*Cc, gint Nc, gdouble \*Cp, gint Np, gdouble \*H03, gdouble \*H47, gint Lh, gdouble \*shift, gint Ls, gdouble \*work)

Downward shift of parent expansion to child box centres.

• gint wbfmm\_shift\_angles\_list4 (gint i, gint j, gint k, gdouble \*th, gdouble \*ph, gdouble \*ch, gdouble \*rs)

Extract the rotation angles for boxes on interaction list 4.

• gint wbfmm shift angle table init (void)

Initialize table of angles for shift operations.

• wbfmm\_shift\_operators\_t \* wbfmm\_shift\_operators\_new (guint L, gdouble \*work)

Allocate shift operators and initialize rotations.

• gint wbfmm\_shift\_operators\_coaxial\_SR\_init (wbfmm\_shift\_operators\_t \*w, gdouble D, guint level, guint L, gdouble k, gdouble \*work)

Initialize singular-to-regular translation operators.

• gint wbfmm\_shift\_operators\_coaxial\_SS\_init (wbfmm\_shift\_operators\_t \*w, gdouble D, guint level, guint L, gdouble k, gdouble \*work)

Initialize singular-to-singular (regular-to-regular) translation operators.

• gint wbfmm\_upward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform upward pass at one level of an octree.

 gint wbfmm\_downward\_pass (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gdouble \*work)

Perform downward pass at one level of an octree.

• gint wbfmm\_tree\_box\_field (wbfmm\_tree\_t \*t, guint level, guint b, gdouble k, gdouble \*x, gdouble \*f, gdouble \*work)

Evaluate singular expansion about a box centre.

• gint wbfmm\_tree\_refine (wbfmm\_tree\_t \*t)

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level.

- gint wbfmm\_tree add level (wbfmm\_tree\_t \*tree)
- gint wbfmm tree add points (wbfmm tree t \*t, gpointer pts, guint npts, gsize stride)

Add points to an octree.

• guint64 **wbfmm\_point\_index\_3d** (gdouble \*x, gdouble \*c, gdouble D)

Find Morton index for point in a cubic domain.

wbfmm\_tree\_t \* wbfmm\_tree\_new (gdouble \*x, gdouble D, guint maxpoints)

Allocate a new octree.

• gint wbfmm\_tree\_coefficient\_init (wbfmm\_tree\_t \*t, guint I, guint nr, guint ns)

Initialize expansion coefficient data in an octree.

• gint wbfmm\_tree\_leaf\_expansions (wbfmm\_tree\_t \*t, gdouble k, gdouble \*src, gint sstr, gdouble \*normals, gint nstr, gdouble \*dipoles, gint dstr, gboolean zero\_expansions, gdouble \*work)

Generate leaf expansions for a tree.

• gint **wbfmm\_box\_location\_from\_index** (guint64 i, guint32 level, gdouble \*x0, gdouble D, gdouble \*x, gdouble \*wb)

Find the coordinates of a box from its Morton index.

• gint **wbfmm\_shift\_angles** (gdouble \*xi, gdouble \*xj, gdouble \*th, gdouble \*ph, gdouble \*ch, gdouble \*r)

Compute angles and distance to shift expansion between two points.

• gint wbfmm\_tree\_write\_sources (wbfmm\_tree\_t \*t, gdouble \*q, gint stride, FILE \*f)

Write a tree source list to file.

• gint wbfmm\_cartesian\_to\_spherical\_f (gfloat \*x0, gfloat \*x, gfloat \*r, gfloat \*th, gfloat \*ph)

Convert Cartesian to spherical coordinates  $(r, \theta, \phi)$ .

gint wbfmm\_shift\_coordinates\_f (gfloat \*x, gfloat \*y, gfloat \*ix, gfloat \*iy, gfloat \*iz, gfloat \*r)

Find system of axes for coordinate shift.

• gint wbfmm legendre recursion array f (gfloat \*\*Pnm1, gfloat \*\*Pn, gint n, gfloat C, gfloat S)

Perform recursion on normalized associated Legendre functions.

gint wbfmm\_bessel\_j\_recursion\_f (gfloat \*jnm1, gfloat \*jn, gfloat x, gint n)

Perform recursion on spherical Bessel function  $j_n(x)$ .

• gint wbfmm bessel h recursion f (gfloat \*hnm1, gfloat \*hn, gfloat x, gint n)

Perform one step of spherical Hankel recursion.

gint wbfmm\_bessel\_j\_init\_f (gfloat x, gfloat \*j0, gfloat \*j1)

Initialize the spherical Bessel function recursion.

gint wbfmm\_bessel\_h\_init\_f (gfloat x, gfloat \*h0, gfloat \*h1)

Initialize spherical Hankel function recursion.

• gint  $wbfmm_legendre_init_f$  (gfloat C, gfloat S, gfloat \*P0, gfloat \*P10, gfloat \*P11)

Initialize normalized associated Legendre functions.

gint wbfmm\_expansion\_h\_cfft\_f (gfloat k, gint N, gfloat \*x0, gfloat \*xs, gfloat \*q, gfloat \*cfft, gint cstr, gfloat \*work)

Generation of singular expansion coefficients for point source.

• gint **wbfmm\_expansion\_dipole\_h\_cfft\_f** (gfloat k, gint N, gfloat \*x0, gfloat \*xs, gfloat \*fx, gfloat \*fy, gfloat \*fx, gfloat \*stx, gfloat \*fx, gfloa

Generation of singular expansion coefficients for point dipole source.

• gint wbfmm\_expansion\_h\_evaluate\_f (gfloat k, gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gfloat \*xf, gfloat \*field, gfloat \*work)

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Evaluate a singular expansion.

• gint wbfmm\_expansion\_j\_evaluate\_f (gfloat k, gfloat \*x0, gfloat \*cfft, gint cstr, gint N, gfloat \*xf, gfloat \*field, gfloat \*work)

Evaluate a regular expansion.

• gint **wbfmm\_total\_dipole\_field\_f** (gfloat k, gfloat \*xs, gint xstride, gfloat \*src, gint sstride, gint nsrc, gfloat \*xf, gfloat \*field)

Compute total field from dipole sources by direct evaluation.

• gint wbfmm\_coordinate\_transform\_f (gfloat \*x, gfloat \*ix, gfloat \*iy, gfloat \*iz, gfloat \*y)

Transform coordinates to rotated axes.

gint wbfmm coefficients RR coaxial f (gfloat \*cfftRR, gint L, gfloat kr, gfloat \*work)

Generate coefficients for coaxial regular-to-regular translation.

gint wbfmm\_coefficients\_SR\_coaxial\_f (gfloat \*cfftSR, gint L, gfloat kr, gfloat \*work)

Generate coefficients for coaxial singular-to-regular translation.

• gint **wbfmm\_rotation\_angles\_f** (gfloat \*ix, gfloat \*ix, gfloat \*ix, gfloat \*jx, gfloat \*jx, gfloat \*jx, gfloat \*jx, gfloat \*th, gfloat \*ph, gfloat \*ch)

Compute the rotation angles  $(\theta, \phi, \chi)$  between axes.

• gint wbfmm\_coefficients\_H\_rotation\_f (gfloat \*H, gint N, gfloat th, gfloat \*work)

Compute rotation coefficients for angle  $\theta$ .

• guint64 wbfmm\_point\_index\_3d\_f (gfloat \*x, gfloat \*c, gfloat D)

Find Morton index for point in a cubic domain.

• wbfmm\_tree\_t \* wbfmm\_tree\_new\_f (gfloat \*x, gfloat D, guint maxpoints)

Allocate a new octree.

• gint wbfmm tree coefficient init f (wbfmm tree t \*t, guint I, guint nr, guint ns)

Initialize expansion coefficient data in an octree.

• gint wbfmm\_tree\_leaf\_expansions\_f (wbfmm\_tree\_t \*t, gfloat k, gfloat \*src, gint sstr, gfloat \*normals, gint nstr, gfloat \*dipoles, gint dstr, gboolean zero\_expansions, gfloat \*work)

Generate leaf expansions for a tree.

gint wbfmm\_tree\_refine\_f (wbfmm\_tree\_t \*t)

Refine an existing octree by adding a level and redistributing points attached to the tree to the boxes at the new level.

• gint wbfmm\_tree\_add\_points\_f (wbfmm\_tree\_t \*t, gpointer pts, guint npts, gsize stride)

Add points to an octree.

- gint wbfmm\_box\_location\_from\_index\_f (guint64 i, guint32 level, gfloat \*x0, gfloat D, gfloat \*x, gfloat \*wb)

  Find the coordinates of a box from its Morton index.
- gint **wbfmm\_child\_parent\_shift\_f** (gfloat \*Cp, gint Np, gfloat \*Cc, gint Nc, gfloat \*H03, gfloat \*H47, gint Lh, gfloat \*shift, gint Ls, gfloat \*work)

Upward shift of singular expansion from eight children to common parent.

• gint wbfmm\_parent\_child\_shift\_f (gfloat \*Cc, gint Nc, gfloat \*Cp, gint Np, gfloat \*H03, gfloat \*H47, gint Lh, gfloat \*shift, gint Ls, gfloat \*work)

Downward shift of parent expansion to child box centres.

gint wbfmm\_shift\_angles\_list4\_f (gint i, gint j, gint k, gfloat \*th, gfloat \*ph, gfloat \*ch, gfloat \*rs)

Extract the rotation angles for boxes on interaction list 4.

• gint wbfmm\_shift\_angles\_f (gfloat \*xi, gfloat \*xj, gfloat \*th, gfloat \*ph, gfloat \*ch, gfloat \*r)

Compute angles and distance to shift expansion between two points.

gint wbfmm\_tree\_write\_sources\_f (wbfmm\_tree\_t \*t, gfloat \*q, gint stride, FILE \*f)

Write a tree source list to file.

• gint wbfmm shift angle table init f (void)

Initialize table of angles for shift operations.

wbfmm\_shift\_operators\_t \* wbfmm\_shift\_operators\_new\_f (guint L, gfloat \*work)

Allocate shift operators and initialize rotations.

• gint wbfmm\_upward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform upward pass at one level of an octree.

gint wbfmm\_downward\_pass\_f (wbfmm\_tree\_t \*t, wbfmm\_shift\_operators\_t \*op, guint level, gfloat \*work)

Perform downward pass at one level of an octree.

• gint wbfmm\_tree\_box\_field\_f (wbfmm\_tree\_t \*t, guint level, guint b, gfloat k, gfloat \*x, gfloat \*f, gfloat \*work)

Evaluate singular expansion about a box centre.

- guint64 wbfmm\_box\_index (guint32 i, guint32 j, guint32 k)
- gint wbfmm\_box\_location (guint64 idx, guint32 \*i, guint32 \*j, guint32 \*k)

# 7.2.1 Detailed Description

Header for Wide Band FMM library.

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