Alliance

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# **Chapter 1**

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# 1.1 File List

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2 File Index

# **Chapter 2**

# **File Documentation**

# 2.1 array.c File Reference

array manipulation module

```
#include "array.h"
#include "utils_fftw.h"
#include "space_config.h"
```

## **Macros**

- #define CHI\_EM 3
- #define CHI\_EL 1
- #define FFT\_OFFSET 2

## **Functions**

```
    size_t get_flat_c (size_t is, size_t il, size_t im, size_t ix, size_t iy, size_t iz)
        returns flat index of the element of complex 6D array
    size_t getIndChiBufEM_c (size_t ix, size_t iy, size_t iz, size_t is, size_t ifield)
        returns flat index of an element of electromagnetic gyrokinetic potential in FOURIER SPACE
    size_t getIndChiBufEM_r (size_t ix, size_t iy, size_t iz, size_t is, size_t ifield)
        returns flat index of an element of electromagnetic gyrokinetic potential in POSITION SPACE
    size_t getIndChiBufEL_c (size_t ix, size_t iy, size_t iz, size_t is)
        returns returns flat index of an element of electrostatic gyrokinetic potential in FOURIER SPACE
    size_t getIndChiBufEL_r (size_t ix, size_t iy, size_t iz, size_t is)
        returns returns flat index of an element of electrostatic gyrokinetic potential in REAL SPACE
```

• size\_t get\_flat\_r (size\_t is, size\_t il, size\_t im, size\_t ix, size\_t iy, size\_t iz)

returns flat index of the element of real 6D array

• size\_t get\_flatIndexComplex3D (size\_t ix, size\_t iy, size\_t iz)

returns flat array of complex 3D array

- size\_t getIndChi (size\_t ix, size\_t iy, size\_t iz, size\_t is)
- void multiply\_ar\_c (COMPLEX \*ar1, COMPLEX \*ar2, COMPLEX \*ret)
- void multiply\_ar\_r (const double \*ar1, const double \*ar2, double \*ret)

## **Variables**

- struct array\_size array\_local\_size
- struct array\_size array\_global\_size
- · struct offset size array offset
- struct offset\_size array\_offset3D

# 2.1.1 Detailed Description

array manipulation module

contains functions which are supposed to make array manipulation simpler

# 2.1.2 Function Documentation

# 2.1.2.1 get\_flat\_c()

returns flat index of the element of complex 6D array

## **Parameters**

is	species type	
il	Laguerre moment	
im	Hermite moment	
ix	kx index	
iy	ky index	
iz	kz index	

returns flattened index of a complex array from its 6D index. Flattened index then can be passed to distribution function 6D array to get a required element at position (is,il,im,ix,iy,iz).

# 2.1.2.2 get\_flat\_r()

```
size_t iy,
size_t iz )
```

returns flat index of the element of real 6D array

### **Parameters**

is	species type	
il	Laguerre moment	
im	Hermite moment	
ix	ix x index	
iy	y y index	
iz	z index	

returns flattened index of a real array from its 6D index. Flattened index then can be passed to distribution function 6D array to get a required element at position (is,il,im,ix,iy,iz).

## 2.1.2.3 get\_flatIndexComplex3D()

returns flat array of complex 3D array

## **Parameters**

ix	kx index
iy	ky index
iz	kz index

returns flattened index of a complex array from its 3D position index. Flattened index then can be passed to one of the fields (  $\phi(\mathbf{k}), A_{||}(\mathbf{k}), B_{||}(\mathbf{k})$ ) 6D array to get a required element at position (ix,iy,iz).

## 2.1.2.4 getIndChi()

getIndChi(size\_t ix,size\_t iy, size\_t iz, size\_t is)

# 2.1.2.5 getIndChiBufEL\_c()

```
size_t iy,
size_t iz,
size_t is)
```

returns returns flat index of an element of electrostatic gyrokinetic potential in FOURIER SPACE

### **Parameters**

ix	kx index
iy	ky index
iz	kz index
is	particle species index

returns flattened index of a gyrokinetic potential  $\chi^{\phi}(\mathbf{k})$  from its 4D index in FOURIER SPACE. flattened index is then can be used to access required value of the gyrokinetic potential at position (ix,iy,iz,is).

## 2.1.2.6 getIndChiBufEL\_r()

returns returns flat index of an element of electrostatic gyrokinetic potential in REAL SPACE

#### **Parameters**

ix	x index
iy	y index
iz	z index
is	particle species index

returns flattened index of a gyrokinetic potential  $\chi^{\phi}(\mathbf{r})$  from its 4D index in REAL SPACE. flattened index is then can be used to access required value of the gyrokinetic potential at position (ix,iy,iz,is).

# 2.1.2.7 getIndChiBufEM\_c()

returns flat index of an element of electromagnetic gyrokinetic potential in FOURIER SPACE

## **Parameters**

ix	kx index
iy	ky index
iz	kz index
is	particle species index
ifield	field type

returns flattened index of a gyrokinetic potential  $\chi^{\phi,A,B}$  from its 4D index in FOURIER SPACE. flattened index is then can be used to access required value of the gyrokinetic potential at position (ix,iy,iz,is). Type of gyrokinetic potential is specified by ifield parameter. Use 0 is to access  $\chi^{\phi}(\mathbf{k})$ , 1 to access  $\chi^{A}(\mathbf{k})$  and 2 to access  $\chi^{B}(\mathbf{k})$ .

## 2.1.2.8 getIndChiBufEM\_r()

returns flat index of an element of electromagnetic gyrokinetic potential in POSITION SPACE

#### **Parameters**

ix	x index
iy	y index
iz	z index
is	particle species index
ifield	field type

returns flattened index of a gyrokinetic potential  $\chi^{\phi,A,B}(\mathbf{k})$  from its 4D index in POSITION SPACE. flattened index is then can be used to access required value of the gyrokinetic potential at position (ix,iy,iz,is). Type of gyrokinetic potential is specified by ifield parameter. Use 0 is to access  $\chi^{\phi}(\mathbf{r})$ , 1 to access  $\chi^{A}(\mathbf{r})$  and 2 to access  $\chi^{B}(\mathbf{r})$ .

# 2.1.2.9 multiply\_ar\_c()

multiply\_ar\_c(COMPLEX \*ar1, COMPLEX \*ar2, COMPLEX \*ret)

## 2.1.2.10 multiply\_ar\_r()

multiply\_ar\_r(const double \*ar1, const double \*ar2, double \*ret)

# 2.2 diagnostics.c File Reference

### diagnostics module

```
#include "diagnostics.h"
#include "parameters_io.h"
```

## **Macros**

- #define TO\_ROOT 0
- #define BUFFER\_SIZE 1

### **Functions**

- void diag\_computeSpectra (const COMPLEX \*g, const COMPLEX \*h, int timestep) general function to compute k or m spectra
- · void diag\_initSpec ()

initialize spectra computation

void diag\_computeFreeEnergy (COMPLEX \*g, COMPLEX \*h)

compute free energy

- void diag\_computeKSpectrum (const COMPLEX \*g, const COMPLEX \*h, double \*spec)
- void diag\_computeMSpectrum (const COMPLEX \*g, const COMPLEX \*h, double \*spec)

computes free energy spectra in m space

void diag\_getShells ()

computes shells from parameters

• double diag\_computeFreeEnergyFields (COMPLEX \*g, COMPLEX \*fields)

to be done later

• void diag\_compute (COMPLEX \*g, COMPLEX \*h, int timestep)

computes all diagnostics

#### **Variables**

```
double * diag_kSpec = 0
```

used to store free energy k spectra

• double \* diag\_mSpec = 0

used to store free energy m spectra

• double \* diag\_shells = 0

used to store positions of k shells required to compute k spectra

double diag\_freeEnergy

free energy

# 2.2.1 Detailed Description

diagnostics module

different diagnostic tools are gathered in this module

## 2.2.2 Function Documentation

## 2.2.2.1 diag\_compute()

computes all diagnostics

## **Parameters**

g	modified distribution function
h	distribution function
iter	current time step

# 2.2.2.2 diag\_computeFreeEnergy()

# compute free energy

#### **Parameters**

g	modified gyrokinetic distribution function
h	gyrokintic distribution function

computes free energy as  $W=2.\Re(\sum_{k_x,k_y,k_z>0,m,l,s}g*\bar{h})$ , taking into account reality condition.

# 2.2.2.3 diag\_computeFreeEnergyFields()

to be done later

### **Parameters**

g	
fields	computes free energy from the fields and distribution function.

# 2.2.2.4 diag\_computeKSpectrum()

### **Parameters**

g modified gyrokinetic distribution fund	
h	gyrokinetic distribution function
spec	spectra array

computes free energy  $k_{\perp}$  spectra  $W(k_i^{shell})=\frac{1}{N}\sum_{k_{i-1}^{shell}<|\mathbf{k}_{\perp}|< k_i^{shell}}\sum_{k_z,l,m,s}g\bar{h}$  where N is a number of wave vectors between shells  $k_{i-1}^{shell}$  and  $k_i^{shell}$ 

### 2.2.2.5 diag\_computeMSpectrum()

computes free energy spectra in m space

#### **Parameters**

g	modified gyrokinetic distribution function
h	gyrokinetic distribution function
spec	spectra array

computes free energy m spectra as  $W(m) = \sum_{k_x, k_y, k_z, l, s} g \bar{h}$ 

## 2.2.2.6 diag\_computeSpectra()

general function to compute k or m spectra

## Parameters

g	gyrokinetic distribution function
h	distribution function
timestep	current time step

function computes spectra at timestep as given in parameter file.  $k_{\perp}$  spectra is computed using diag\_computeKSpectrum, and m spectra is computed using diag\_computeMSpectrum

### 2.2.2.7 diag\_getShells()

```
diag_getShells ( )
```

computes shells from parameters

computes positions of k\_shells in between last\_shell and first\_shell as provided by user in parameter file. Position of  $i^{th}$  shell is computed as  $k_i^{shell} = (last\_shell - first\_shell)/(k\_shells) \cdot i$ 

## 2.2.2.8 diag\_initSpec()

```
void diag_initSpec ( )
```

initialize spectra computation

Prepares free energy spectra computation. For spectra in k: allocates diag\_kSpec array used to store k spectra. Allocates diag\_shells array and fills it with shell positions  $k^{shells}$ , used for binning of wave vectors when computing  $k_{\perp}$  spectra. For spectra in m: allocates diag\_mSpec array used to store m spectra. Called in init\_start function

# 2.3 distrib.c File Reference

```
gyrokinetic distribution function module
```

```
#include "distrib.h"
```

### **Functions**

- void distrib\_getH (COMPLEX \*h, const COMPLEX \*g)
   computes h from g
- $\bullet \ \ \text{void} \ \ \frac{\text{distrib\_getG}}{\text{getG}} \ \ (\text{COMPLEX} \ *g, \ \text{const} \ \ \text{COMPLEX} \ *h) \\$

computes g from h

• void distrib\_getXGrad (const COMPLEX \*in, COMPLEX \*out)

Computes gradient in kx direction.

void distrib\_getYGrad (const COMPLEX \*in, COMPLEX \*out)

Computes gradient in ky direction.

• void distrib\_getZGrad (const COMPLEX \*in, COMPLEX \*out)

Computes gradient in kz direction.

- void distrib\_enforceReality (COMPLEX \*f)
  - enforces reality condition on distribution function array
- void distrib\_setZeroNHalf (COMPLEX \*f)

sets all Nk/2 modes to zero

## 2.3.1 Detailed Description

gyrokinetic distribution function module

everything required to perform different manipulations to distribution functions

## 2.3.2 Function Documentation

# 2.3.2.1 distrib\_enforceReality()

```
void distrib_enforceReality ( {\tt COMPLEX} * f )
```

enforces reality condition on distribution function array

2.3 distrib.c File Reference

#### **Parameters**

f complex array for which reality condition will be forced.

Enforces reality condition f(k) = conj(f(-k)) in plane kz = 0. For a given kx, it first checks where modes -kx are located using the  $mpi_w$ -where  $mpi_w$ -where

```
where_neg = mpi_whereIsX[kxNeg * 2];
```

If -kx is stored on a different processor, MPI\_VECTOR with a 4D data slice f(kx,kz = 0) is sent to this processor, to the buffer array:

```
mpi_sendVector(&f[ind6D], buffer, where_pos, where_neg);
```

if the data stored on the same processor, no vector is being sent. Reality condition is fulfilled in a loop over all other coordinates:

```
f[ind6D_neg] = conj(buffer[ind6D_pos]);
```

# 2.3.2.2 distrib\_getG()

```
distrib_getG (  \label{eq:complex} {\tt COMPLEX} \, * \, g, \\ {\tt const} \, {\tt COMPLEX} \, * \, h \, )
```

computes g from h

#### **Parameters**

g	complex array to store g
h	complex array with h

computes modified gyrokinetic distribution function g from gyrokinetic distribution function h. Please note that before calling this function gyrokinetic potentials must be computed

## 2.3.2.3 distrib\_getH()

computes h from g

## **Parameters**

h	complex array to store h
g	complex array with g

computes gyrokinetic distribution function h from modified gyrokinetic distribution function g. Please note that before calling this function gyrokinetic potentials must be computed

### 2.3.2.4 distrib getXGrad()

```
void distrib_getXGrad (
```

```
const COMPLEX * in,
COMPLEX * out )
```

Computes gradient in kx direction.

### **Parameters**

in	complex array. Distribution function of which gradient will be taken
out	complex array, where gradient is stored

Computes gradient in kx direction as following: grad(f) = i \* kx \* f

# 2.3.2.5 distrib\_getYGrad()

Computes gradient in ky direction.

### **Parameters**

in	complex array. Distribution function of which gradient will be taken
out	complex array, where gradient is stored

Computes gradient in ky direction as following: grad(f) = i \* ky \* f

# 2.3.2.6 distrib\_getZGrad()

Computes gradient in kz direction.

### **Parameters**

in	complex array. Distribution function of which gradient will be taken
out	complex array, where gradient is stored

Computes gradient in kz direction as following: grad(f) = i \* kz \* f

# 2.3.2.7 distrib\_setZeroNHalf()

```
void distrib_setZeroNHalf ( {\tt COMPLEX} \ * \ f \ )
```

sets all Nk/2 modes to zero

#### **Parameters**

f complex array

sets Nkx/2, Nky/2 and Nz/2 modes of distribution function to zero. Due to reality condition, for kz yhe last mode should be set to zero.

# 2.4 equation.c File Reference

### equation module

```
#include "equation.h"
#include "array.h"
#include "fields.h"
#include "distrib.h"
```

### **Macros**

- #define CHI EM 3
- #define CHI EL 1
- #define CHI\_PHI 0
- #define CHI A 1
- #define CHI\_B 2

## **Functions**

void equation\_getLinearTerm (const COMPLEX \*in, const COMPLEX \*plus\_boundary, const COMPLEX \*minus\_boundary, COMPLEX \*out)

computes linear term

• void equation\_getNonlinearElectromagnetic (double \*in, double \*chiAr, double \*out, double sign)

returns nonlinear electromagnetic term

void equation\_getNonlinearElectrostatic (double \*in, double \*chiAr, double \*out, double sign)

returns nonlinear electrostatic term

• void equation\_getNonlinearProduct (double \*in, double \*chiAr, double \*out, double sign)

chooses between computing electrostatic or electromagnetic term

 $\bullet \ \ void\ equation\_getNonlinearTerm\ (const\ COMPLEX\ *h,\ COMPLEX\ *out)$ 

computes nonlinear term

void equation\_getRHS (const COMPLEX \*in\_g, COMPLEX \*in\_h, COMPLEX \*out)

# 2.4.1 Detailed Description

equation module

module required to compute RHS of the equation.

# 2.4.2 Function Documentation

# 2.4.2.1 equation\_getLinearTerm()

### computes linear term

#### **Parameters**

in	complex array
out	complex array
plus_boundary	complex array
minus_boundary	complex array

computes linear term  ${\tt out}$  from distribution function  ${\tt in}$  .

# 2.4.2.2 equation\_getNonlinearElectromagnetic()

returns nonlinear electromagnetic term

### **Parameters**

in	input double array
chiAr	input double array
out	output double array
sign	should be 1 or -1

performs multiplication between input 6D complex array in and gyrokinetic potential array chiAr, in such way that the structure of the product is the same as nonlinear term of drift-kinetic equations. Used by equation\_getNonlinearProduct. sign is used to determine the sign of the resulting product. See equation\_getNonlinearTerm for explanation.

# 2.4.2.3 equation\_getNonlinearElectrostatic()

```
double * chiAr,
double * out,
double sign )
```

returns nonlinear electrostatic term

### **Parameters**

in	input double array
chiAr	input double array
out	output double array
sign	should be 1 or -1

 $see\ equation\_getNonlinear Electromagnetic\ for\ explanation$ 

## 2.4.2.4 equation\_getNonlinearProduct()

chooses between computing electrostatic or electromagnetic term

## Parameters

in	input double array
chiAr	input double array
out	output double array
sign	should be 1 or -1

 $\label{thm:thm:depending} \begin{subarray}{l} depending on flag \verb| systemType| provided by user in parameter file, chooses between equation_getNonlinearElectrostatic and equation_getNonlinearElectromagnetic \\ \end{subarray}$ 

## 2.4.2.5 equation\_getNonlinearTerm()

computes nonlinear term

#### **Parameters**

h	input complex array
out	output complex array

function returns nonlinear term. First it takes y gradient of distribution function h, and x gradient of gyrokinetic

```
potentials chi, and transforms them to real space:
```

```
distrib_getYGrad(h, fftw_hBuf); fields_getGradX(fftw_chiBuf); fftw_c2r(); fftw_c2r_chi(); after that, it computes \frac{\partial h}{\partial y} \frac{\partial x}{\partial x} part of the poisson brackets: equation_getNonlinearProduct((double *)fftw_hBuf, (double *)fftw_chiBuf, buffer, 1.); with the result stored in buffer after that, it computes x gradient of h and y gradient of gyrokinetic potential chi, and transforms results to real space: distrib_getXGrad(h, fftw_hBuf); fields_getGradY(fftw_chiBuf); fftw_c2r(); fftw_c2r_chi();
```

and computes second part of the poisson brackets  $-\frac{\partial h}{\partial x}\frac{\partial \chi}{\partial y}$  and adds the result to buffer. buffer is then transformed back to Fourier space, and dealiasing is performed.

# 2.5 fields.c File Reference

field computation and manipulation module

```
#include "fields.h"
```

#### **Macros**

- #define CHI\_PHI 0
- #define CHI A 1
- #define CHI\_B 2

## **Functions**

```
· void fields_init ()
     intializes fields

    void fields_getA (const COMPLEX *g)

      compute A field

    void fields_getB (const COMPLEX *g0, const COMPLEX *g1)

      computes B potential

    void fields_getPhi (const COMPLEX *g0, const COMPLEX *g1)

      computes phi potential

    void fields getFields (COMPLEX *g00, COMPLEX *g10, COMPLEX *g01)

      wrapper to get all the fields simultaneously

    void fields_getChi ()

     computes gyrokinetic potentials chi
void fields_getChiPhi ()
     computes chiPhi gyrokinetic potential from phi potential

    void fields getChiB ()

     computes chiB gyrokinetic potential from B potential

    void fields getChiA ()
```

computes chiA gyrokinetic potential from A potential

2.5 fields.c File Reference 19

```
    void fields_sendG (COMPLEX *g)
```

sends moments of gyrokinetic distribution function which are required to compute fields

• void fields\_getFieldsFromH (COMPLEX \*h00, COMPLEX \*h10, COMPLEX \*h01)

wrapper to get all the fields simultaneously, computed from gyrokinetic distribution function

void fields\_getAFromH (const COMPLEX \*h)

compute A field

• void fields\_getBFromH (const COMPLEX \*h0, const COMPLEX \*h1)

computes B potential

void fields\_getPhiFromH (const COMPLEX \*h)

computes phi potential

void fields getGradX (COMPLEX \*out)

computes chi gradient in x direction

void fields\_getGradY (COMPLEX \*out)

computes chi gradient in y direction

### **Variables**

- · struct fields\_fields fields\_fields
- struct fields\_chi fields\_chi
- double \* A denom
- double \* qnvTsJ
- double \* I B
- double \* I\_phi
- double \* a\_pot
- double \* b\_pot
- double \* c\_pot
- double \* phiB\_denom
- int \* global\_nm\_index
- COMPLEX \* g00
- COMPLEX \* g10
- COMPLEX \* g01

## 2.5.1 Detailed Description

field computation and manipulation module

Rerquired to compute  $A_{||}(\mathbf{k}), B_{||}(\mathbf{k}), \phi(\mathbf{k})$  potentials, as well as gyrokinetic potentials  $\chi_s^A(\mathbf{k}), \chi_s^B(\mathbf{k}), \chi_s^\phi(\mathbf{k})$ 

## 2.5.2 Function Documentation

## 2.5.2.1 fields\_getA()

```
void fields_getA ( {\tt const~COMPLEX~*~g~)}
```

compute A field

#### **Parameters**

g

4D complex array (kx,ky,kz,s). Must be first Hermite and zeroth Laguerre moment of modified gyrokinetic distribution function g.

computes  $A_{||}(\mathbf{k})$  potential from  $g_{s0}^1$  (g parameter)

# 2.5.2.2 fields\_getAFromH()

```
void fields_getAFromH ( {\tt const~COMPLEX~*~h~)}
```

### compute A field

### **Parameters**

h 4D complex array (kx,ky,kz,s). Must be first Hermite and zeroth Laguerre moment of gyrokinetic distribution function h.

computes  $A_{||}(\mathbf{k})$  potential from  $h^1_{s0}$  (h parameter)

# 2.5.2.3 fields\_getB()

```
void fields_getB ( {\tt const~COMPLEX~*~g0,} {\tt const~COMPLEX~*~g1~)}
```

computes B potential

#### **Parameters**

g0	4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of modified gyrokinetic distribution
	function.
g1	4D complex array (kx,ky,kz,s). Zeroth Hermite and first Laguerre moment of the modified distribution
	function.

Computes  $B_{\perp}(\mathbf{k})$  from  $g_{s0}^0$  (g0 parameter) and  $g_{s0}^1$  (g1 parameter).

## 2.5.2.4 fields\_getBFromH()

## computes B potential

#### **Parameters**

h0	4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of gyrokinetic distribution function.
h1	4D complex array (kx,ky,kz,s). Zeroth Hermite and first Laguerre moment of distribution function.

2.5 fields.c File Reference 21

Computes  $B_{\perp}({\bf k})$  from  $h_{s0}^0$  (h0 parameter) and  $h_{s0}^1$  (h1 parameter).

# 2.5.2.5 fields\_getChi()

```
void fields_getChi ( )
```

computes gyrokinetic potentials chi

Wrapper for functions fields\_getChiPhi, fields\_getChiA, fields\_getChiB

# 2.5.2.6 fields\_getChiA()

```
void fields_getChiA ( )
```

computes chiA gyrokinetic potential from A potential

computes  $chi_s^A(\mathbf{k})$ 

# 2.5.2.7 fields\_getChiB()

```
void fields_getChiB ( )
```

computes chiB gyrokinetic potential from B potential

computes  $\chi_s^B(\mathbf{k})$ 

# 2.5.2.8 fields\_getChiPhi()

```
fields_getChiPhi ( )
```

computes chiPhi gyrokinetic potential from phi potential

computes  $chi_s^{\phi}(\mathbf{k})$ 

# 2.5.2.9 fields\_getFields()

wrapper to get all the fields simultaneously

## **Parameters**

g00	4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of modified gyrokinetic distribution function.
g10	4D complex array (kx,ky,kz,s). Must be first Hermite and zeroth Laguerre moment of modified gyrokinetic distribution function g.
Generate	4D complex array (kx,ky,kz,s). Zeroth Hermite and first Laguerre moment of the modified distribution function.

Wrapper for functions fields\_getPhi, fields\_getB, fields\_getA.

### 2.5.2.10 fields getFieldsFromH()

wrapper to get all the fields simultaneously, computed from gyrokinetic distribution function

#### **Parameters**

h00	4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of gyrokinetic distribution function.
h10	4D complex array (kx,ky,kz,s). Must be first Hermite and zeroth Laguerre moment of gyrokinetic distribution
	function h.
h01	4D complex array (kx,ky,kz,s). Zeroth Hermite and first Laguerre moment of the distribution function.

Wrapper for functions fields\_getPhiFromH, #fields\_get\_BFromH, fields\_getAFromH.

### 2.5.2.11 fields getGradX()

computes chi gradient in x direction

### **Parameters**

```
out output complex array of size (kx,ky,kz,s,Nfields).
```

computes gradient in x direction for chi potentials. Nfields<\tt> can be 1 or 3, and chosen automatically at start of the simulation depending on the simulation type (electrostatic or electromagnetic)

## 2.5.2.12 fields\_getGradY()

computes chi gradient in y direction

## **Parameters**

```
out output complex array of size (kx,ky,kz,s,Nfields).
```

computes gradient in y direction for chi potentials. Nfields < tt> can be 1 or 3, and chosen automatically at start of the simulation depending on the simulation type

2.5 fields.c File Reference 23

```
(electrostatic or electromagnetic)
```

### 2.5.2.13 fields getPhi()

computes phi potential

#### **Parameters**

g0	4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of modified gyrokinetic distribution
	function.
g1	4D complex array (kx,ky,kz,s). Zeroth Hermite and first Laguerre moment of the modified distribution
	function.

Computes  $\phi(\mathbf{k})$  from  $g_{s0}^0$  (g0 parameter) and  $g_{s0}^1$  (g1 parameter).

## 2.5.2.14 fields\_getPhiFromH()

```
void fields_getPhiFromH ( {\tt const~COMPLEX~*~h~)}
```

computes phi potential

## **Parameters**

h | 4D complex array (kx,ky,kz,s). Zeroth Hermite and Laguerre moment of gyrokinetic distribution function.

Computes  $\phi(\mathbf{k})$  from  $h_{s0}^0$  (h parameter)

## 2.5.2.15 fields\_init()

```
void fields_init ( )
```

intializes fields

pre-computes some comstants required to compute fields. Called in init\_start function

## 2.5.2.16 fields\_sendG()

```
fields_sendG ( {\tt COMPLEX} \ * \ g \ )
```

sends moments of gyrokinetic distribution function which are required to compute fields

#### **Parameters**

g complex array. Modified or non-modified gyrokinetic distribution function

```
sends g_{s0}^{1}(\mathbf{k})f, g_{s1}^{0}(\mathbf{k})f, g_{s0}^{0}(\mathbf{k})f
```

to all processes to compute potentials locally.

# 2.6 init.c File Reference

initialization module for alliance.

```
#include "init.h"
#include "distrib.h"
```

### **Macros**

• #define RANK\_IO 0

### **Functions**

```
• void init_start (char *filename)
```

initialization of ALLIANCE

void init\_printParameters ()

parameter output

• void init\_initEnums ()

enumerator initialization

void fill\_rand (COMPLEX \*ar1)

fills the inital conditions randomly

• void fill\_randM0 (COMPLEX \*ar1)

fill zeroth Hermite moment with random values

void fill\_randSingleKM (COMPLEX \*ar1)

fill single chosen wavevector and Hermite moment

void init\_conditions (COMPLEX \*data)

distribution function initialization

• double init\_energySpec (double k, double m, double amp, double disp)

returns energy spectrum

## **Variables**

- · enum adiabatic kinetic
- enum electromagnetic systemType
- · enum initial initialConditions

2.6 init.c File Reference 25

# 2.6.1 Detailed Description

initialization module for alliance.

all the inititalization routines are here.

# 2.6.2 Macro Definition Documentation

# 2.6.2.1 RANK\_IO

```
#define RANK_IO 0
```

defines rank of the processor used to output information to console

## 2.6.3 Function Documentation

# 2.6.3.1 fill\_rand()

fills the inital conditions randomly

#### **Parameters**

data

complex 6d array to fill initializes distribution with spectrum defined in init\_energySpec This function is supposed to be used in-module only and should not be used elsewhere outside init.c file.

# 2.6.3.2 fill\_randM0()

```
void fill_randM0 ( {\tt COMPLEX * data })
```

fill zeroth Hermite moment with random values

#### **Parameters**

data | complex 6D array to fill

fills 0-th Hermite moment of a distribution function ar1 with random values This function is supposed to be used in-module only and should not be used elsewhere outside init.c file.

## 2.6.3.3 fill\_randSingleKM()

fill single chosen wavevector and Hermite moment

#### **Parameters**

```
data complex 6D array
```

initializes single wavevector and Hermite moment of a distribution function with random variable. This function is only for in-module use and should not be used elsewhere outside init.c file.

## 2.6.3.4 init\_conditions()

```
void init_conditions ( {\tt COMPLEX} \ * \ {\tt data} \ )
```

distribution function initialization

## **Parameters**

data	complex 6D array
------	------------------

initializes distribution function with chosen method (see fill\_rand, fill\_randM0, fill\_randSingleKM)

## 2.6.3.5 init\_energySpec()

returns energy spectrum

## **Parameters**

k	a wavenumber at which spectrum is computed
m	Hermite moment at which amplitude is computed
amp	amplitude of the spectrum
disp	dispersion of the spectrum

computes spectrum of form  $A \cdot k^2 exp(-2k^2/\sigma^2)$ , where  $\sigma = disp$ , and A = amp This function is supposed to be

used in-module only and should not be used elsewhere outside init.c file.

### 2.6.3.6 init\_initEnums()

```
void init_initEnums ( )
```

enumerator initialization

initializes enumerators, which are then used to define if system is adiabatic or kinetic, electromagnetic or electrostatic, and type of initial conditions

## 2.6.3.7 init\_printParameters()

```
void init_printParameters ( )
```

parameter output

prints parameters of the simulation

## 2.6.3.8 init\_start()

initialization of ALLIANCE

**Parameters** 

lename specifies parameter filena	ne
-----------------------------------	----

initializes all the modules required for ALLIANCE to work.

# 2.7 parameters\_io.c File Reference

reads inpuit parameters from parameter file provided by user

```
#include "parameters_io.h"
#include "utils_fftw.h"
```

#### **Macros**

• #define VERBOSE 0

# **Functions**

```
• void init_global_size ()
```

initializes global size of the 6D array

• void read\_parameters (char \*filename)

reads parameters from user parameter file.

• void read\_parametersFromFile (char \*filename)

## **Variables**

• struct system\_param parameters

# 2.7.1 Detailed Description

reads inpuit parameters from parameter file provided by user

## 2.7.2 Function Documentation

## 2.7.2.1 init\_global\_size()

```
void init_global_size ( )
```

initializes global size of the 6D array

 $initializes \verb| array_local_size| | \textit{structure with global simulation size}.$ 

# 2.7.2.2 read\_parameters()

reads parameters from user parameter file.

Reads parameters from user parameter file. All the parameters are stored in the parameters structure

## 2.7.2.3 read\_parametersFromFile()

read\_parametersFromFile(char \*filename):

2.8 solver.c File Reference

# 2.8 solver.c File Reference

```
numerical solver
```

```
#include "solver.h"
```

### **Macros**

- #define **SOLVERTYPE** RK4
- #define IORANK 0

# **Functions**

```
    void solver_init ()
        initializes solver
    void solver_makeStep (COMPLEX **g, COMPLEX *h)
        iterate solver forward
```

# **Variables**

- enum solverType solverType
- struct solver solver
- struct rk4 rk4

# 2.8.1 Detailed Description

numerical solver

## 2.8.2 Function Documentation

# 2.8.2.1 solver\_init()

```
void solver_init ( )
initializes solver
initializes solver with the solverType.
```

# 2.8.2.2 solver\_makeStep()

```
void solver_makeStep ( \label{eq:complex} \mbox{COMPLEX ** } g \mbox{,} \mbox{COMPLEX ** } h \mbox{ )}
```

iterate solver forward

#### **Parameters**

g	address of the 6D complex array. Modified gyrokinetic distribution function	
h	6D complex array. Gyrokinetic distribution function	l

solves one simulation time step

# 2.9 space\_config.c File Reference

space configuration module

```
#include "space_config.h"
#include <complex.h>
```

## **Macros**

• #define MINUS\_I -1.j

# **Functions**

```
    void space_init ()
        initializes wave space. Called in init_start() function.
    void space_generateWaveSpace ()
```

void space\_generatevvaveopace (

generates wave space.

• void space\_generateMSpace () generates Hermite space.

• void free\_wavespace ()

deallocates all the arrays.

# **Variables**

```
• double space_Lx = 100
```

- double space\_Ly = 100
- double **space\_Lz** = 100
- double \* space\_kx
- double \* space\_ky
- double \* space\_kz
- double \* space\_kPerp
- double \* space\_kPerp2
- double \* space\_kSq
- double \* space\_sqrtM
- size t \* space\_globalMIndex
- COMPLEX \* space\_iKx
- COMPLEX \* space\_iKy
- COMPLEX \* space\_iKz

# 2.9.1 Detailed Description

space configuration module

creates k and m spaces

#### 2.9.2 Function Documentation

#### 2.9.2.1 free\_wavespace()

```
free_wavespace ( )
```

deallocates all the arrays.

to be added...

#### 2.9.2.2 space\_generateMSpace()

```
space_generateMSpace ( )
```

generates Hermite space.

to be added

#### 2.9.2.3 space generateWaveSpace()

```
void space_generateWaveSpace ( )
```

generates wave space.

generates wave number arrays space\_kx, space\_ky, space\_kz of lengths nkx,nky,nkz for a numerical box of size [lx, ly, lz] in kx,ky,kz directions as following:

```
[0, pi / lx, 2 pi / lx, ..., (n / 2 + 1) pi / lx, - (n / 2) pi / lx, ..., - pi / lx] generates arrays space_iKx, space_iKy, space_iKz, of lengths nkx,nky,nkz. These arrays are later used to compute gradients by fields_getGradX, fields_getGradY, distrib_getXGrad, distrib_getYGrad, distrib_getZGrad.
```

# 2.10 utils\_fftw.c File Reference

```
FFT module.
```

```
#include "utils_fftw.h"
```

#### **Macros**

- #define FFTW\_RANK 3
- · #define CHI EL 1
- #define CHI EM 3
- #define VERBOSE 0

#### **Functions**

```
• void fftw_init (MPI_Comm communicator)
     initializes fftw transform.
• void fftw r2c ()
     real to complex fft transform.
void fftw_c2r ()
     complex to real fft transform.
• void fftw r2c chi ()
     real to complex transform of chi potentials
• void fftw_c2r_chi ()
     complex to real transform of chi potentials
• void fftw r2c field ()
     real to complex transform of field potentials
void fftw_c2r_field ()
     complex to real transform of field potentials
• void fftw kill ()
     kills fftw

    void fftw_copy_buffer_r (double *to, double *from)

     copy 6D real array

    void fftw_copy_buffer_c (COMPLEX *to, COMPLEX *from)

     copy 6D complex array

    void fftw_copyChiBuf_r (double *ar1, double *ar2)

     copy 5D real array

    void fftw_copyChiBuf_c (COMPLEX *ar1, COMPLEX *ar2)

     copy 5D complex array.

    void fftw copyFieldBuf r (double *to, double *from)

     copy 3D real data array.

    void fftw_copyFieldBuf_c (COMPLEX *to, COMPLEX *from)

     copy 3D complex data array.
• double cosinus (double f, int ix)

    void fftw_test_fill (double *ar, double f)

    void fftw_normalise_data (COMPLEX *data)

    void fftw_normalise_data_r (double *data)

      normalise data.
• void fftw_normalise_chi_r (double *data)
     notmalase chi data
• void fftw_normalise_field_r (double *data)
     normalise real 3D data

    void dealiasing23 (COMPLEX *data_c)

     2/3 rule dealiasing
```

#### **Variables**

- ptrdiff\_t size\_c [3]
- ptrdiff\_t size\_r [3]
- · ptrdiff\_t howmany
- ptrdiff\_t howmany\_chi
- · ptrdiff t local size
- ptrdiff\_t local\_n0
- ptrdiff\_t local\_0\_start
- ptrdiff\_t local\_size\_chi
- ptrdiff\_t local\_n0\_chi
- ptrdiff\_t local\_0\_start\_chi
- ptrdiff\_t local\_size\_field
- ptrdiff\_t local\_n0\_field
- ptrdiff\_t local\_0\_start\_field
- fftw plan plan c2r
- fftw\_plan plan\_r2c
- fftw\_plan plan\_c2r\_chi
- fftw\_plan plan\_r2c\_chi
- fftw\_plan plan\_c2r\_field
- fftw\_plan plan\_r2c\_field
- COMPLEX \* fftw\_hBuf
- $COMPLEX * fftw\_chiBuf$
- COMPLEX \* fftw\_field
- double fftw\_norm
- void(\* fftw\_dealiasing )(COMPLEX \*) = NULL
- int \* global\_nkx\_index

# 2.10.1 Detailed Description

FFT module.

contains FFT related routines

# 2.10.2 Function Documentation

#### 2.10.2.1 cosinus()

```
double cosinus ( \label{eq:double f, int } \mbox{double } f, \mbox{int } ix \mbox{)}
```

### cosinus(double f,int ix)

#### 2.10.2.2 dealiasing23()

```
void dealiasing23 ( {\tt COMPLEX * data\_c })
```

2/3 rule dealiasing

#### **Parameters**

data↩	complex 6D data array
_c	

#### 2.10.2.3 fftw\_c2r()

```
fftw_c2r ( )
```

complex to real fft transform.

Performs complex to real in-place fft transform on array fftw\_hBuf. Used to transform 6D arrays (x,y,z,m,l,s).

# 2.10.2.4 fftw\_c2r\_chi()

```
void fftw_c2r_chi ( )
```

complex to real transform of chi potentials

Performs complex to real in-place fft transform on array fftw\_chiBuf. Used to transform 5D arrays (kx,ky,kz,s,field).

### 2.10.2.5 fftw\_c2r\_field()

```
void fftw_c2r_field ( )
```

complex to real transform of field potentials

Performs complex to real in-place fft transform on array fftw\_field. Used to transform 3D arrays (kx,ky,kz).

# 2.10.2.6 fftw\_copy\_buffer\_c()

copy 6D complex array

### **Parameters**

to	where to copy array	
from	array which will be copied	

copies complex data from array to array to

# 2.10.2.7 fftw\_copy\_buffer\_r()

copy 6D real array

#### **Parameters**

to	where to copy array
from	array which will be copied

copies real data from array to array to

# 2.10.2.8 fftw\_copyChiBuf\_c()

copy 5D complex array.

#### **Parameters**

ar1	destination
ar2	source

copies complex  $\chi$  array from ar1 to ar2.

# 2.10.2.9 fftw\_copyChiBuf\_r()

copy 5D real array

# **Parameters**

ar1	destination
ar2	source

copies real  $\chi$  array from ar1 to ar2.

# 2.10.2.10 fftw\_copyFieldBuf\_c()

```
fftw_copyFieldBuf_c (
```

```
COMPLEX * to,
COMPLEX * from )
```

copy 3D complex data array.

#### **Parameters**

to	
from	copies 3D complex data array from to

# 2.10.2.11 fftw\_copyFieldBuf\_r()

copy 3D real data array.

#### **Parameters**

to	
from	copies 3D data array from to

# 2.10.2.12 fftw\_kill()

```
void fftw_kill ( )
```

kills fftw

to be added

# 2.10.2.13 fftw\_normalise\_chi\_r()

notmalase chi data

### **Parameters**

data	5D real data array

normalises data by #fftw\_norm.

### 2.10.2.14 fftw\_normalise\_data()

fftw\_normalise\_data(double \*data)

# 2.10.2.15 fftw\_normalise\_data\_r()

normalise data.

#### **Parameters**

```
data 6D data array
```

normalises data by #fftw\_norm.

# 2.10.2.16 fftw\_normalise\_field\_r()

normalise real 3D data

#### **Parameters**

data	3D real array
------	---------------

normalises data by #fftw\_norm.

# 2.10.2.17 fftw\_r2c()

```
fftw_r2c ( )
```

real to complex fft transform.

Performs real to complex in-place fft transform of on array  $fftw_hBuf$ . Used to transform 6D arrays (kx,ky,kz,m,l,s).

# 2.10.2.18 fftw\_r2c\_chi()

```
void fftw_r2c_chi ( )
```

real to complex transform of chi potentials

 $Performs \ real \ to \ complex \ in-place \ fft \ transform \ on \ array \ \texttt{fftw\_chiBuf.} \ Used \ to \ transform \ 5D \ arrays \ (x,y,z,s,field).$ 

#### 2.10.2.19 fftw\_r2c\_field()

```
void fftw_r2c_field ( )
```

real to complex transform of field potentials

Performs real to complex in-place fft transform on array fftw\_field. Used to transform 3D arrays (x,y,z).

# 2.10.2.20 fftw\_test\_fill()

fftw test fill(double \*ar,double f)

# 2.11 utils\_hdf.c File Reference

#### hdf module

```
#include "utils_hdf.h"
#include <unistd.h>
#include <sys/stat.h>
```

#### **Macros**

- #define BASE DIR "."
- #define WORK\_DIR "."
- #define CHCK\_DIR "checkpoint"
- #define CHCK\_NAME "chk"
- #define PATH\_SEPARATOR "/"
- #define VERBOSE 1
- #define FILENAME ID LEN 128
- #define CHECKPOINT\_ROOT 0
- #define PATH\_LEN 128

#### **Functions**

- void complex\_t\_init ()
- void hdf\_init ()
- void hdf\_createSaveDirs ()
- void hdf\_create\_file\_c (char \*filename, COMPLEX \*data)
- void hdf\_create\_file\_r (char \*filename, double \*data)
- void hdf\_initChi ()
- void hdf\_createChiFile\_r (char \*filename, double \*data)
- void hdf\_createChiFile\_c (char \*filename, COMPLEX \*data)
- void hdf\_initField ()
- void hdf\_saveFieldA (char \*filename)
- void hdf\_saveField\_r (double \*f, char \*filename)

- void hdf\_saveFieldB (char \*filename)
- void hdf saveFieldPhi (char \*filename)
- void hdf\_saveEnergy (int timestep)
- void hdf\_saveData (COMPLEX \*h, int timestep)
- void hdf\_createParamFile ()
- · void hdf createFiles ()
- void hdf saveKSpec (int timestep)
- void hdf\_saveMSpec (int timestep)
- void hdf initCheckpoints ()
- void hdf createCheckpoint (COMPLEX \*h, int timestep)
- void hdf\_dumpCheckpoint (COMPLEX \*h, int timestep, char \*filename)
- void hdf\_saveDistrib (COMPLEX \*h, int timestep)
- void hdf createFieldFile ()
- void hdf saveFields (int timestep)
- void hdf readData (char \*filename, COMPLEX \*h)

#### **Variables**

- int hdf rank = 6
- int hdf rankFields = 3
- int hdf rankChi = 5
- int hdf freeEnergyCalls = 0
- char \*\* hdf\_checkpointNames
- char hdf\_newCheckpointName [FILENAME\_ID\_LEN]
- char SIMULATION\_PATH [PATH\_LEN]
- char CHECKPOINT\_PATH [PATH\_LEN]
- char PARAMETER\_FILENAME [FILENAME\_ID\_LEN]
- char DISTRIBUTION\_FILENAME [FILENAME ID LEN]
- char FIELD\_FILENAME [FILENAME ID LEN]
- size t hdf checkpointCount = 0
- hid\_t complex\_id
- hsize t dataspace dims r [6]
- hsize t dataspace dims c [6]
- hsize\_t dataspace\_dimsFields [3]
- hsize t dataspace\_dimsFields\_r [3]
- hsize t dataspace dimsChi [5]
- hsize\_t dataspace\_dimsChi\_r [5]
- hsize\_t chunk\_dims\_r [6]
- hsize t chunk dims c [6]
- hsize\_t chunk\_dimsFields [3]
- hsize t chunk dimsFields r [3]
- hsize\_t chunk\_dimsChi [5]
- hsize\_t chunk\_dimsChi\_r [5]
- hsize t offset [6]
- hsize\_t offsetFields [3]
- hsize\_t offsetFields\_r [3]
- hsize\_t offsetChi [5]
- hsize\_t offsetChi\_r [5]
- hsize\_t count [6] = {1,1,1,1,1,1}
- hsize\_t **stride** [6] = {1,1,1,1,1,1}
- hsize\_t countFields [3] = {1,1,1}
- hsize\_t strideFields [3] = {1,1,1}
- hsize\_t countChi [5] = {1,1,1,1,1}
   hsize\_t ctrideChi [5] = {1,1,1,1,1}
- hsize\_t **strideChi** [5] = {1,1,1,1,1}
- · herr t status
- MPI\_Info info = MPI\_INFO\_NULL
- · complex\_t tmp

# 2.11.1 Detailed Description

hdf module

contains HDF related routines to save and read hdf files

#### 2.11.2 Function Documentation

# 2.11.2.1 hdf\_create\_file\_c()

hdf\_create\_file\_c

#### 2.11.2.2 hdf\_create\_file\_r()

hdf\_create\_file\_r

# 2.11.2.3 hdf\_createCheckpoint()

```
void hdf_createCheckpoint ( \label{eq:complex} {\tt COMPLEX} \, * \, h \text{,} \\ \\ {\tt int} \, \, timestep \, )
```

hdf\_createCheckpoint

# 2.11.2.4 hdf\_createChiFile\_c()

hdf\_createChiFile\_c

# 2.11.2.5 hdf\_createChiFile\_r()

hdf\_createChiFile\_r

### 2.11.2.6 hdf\_createFieldFile()

```
void hdf_createFieldFile ( )
```

FIELD FILE hdf\_createFieldFile

# 2.11.2.7 hdf\_createFiles()

```
void hdf_createFiles ( )
```

hdf\_createFiles

#### 2.11.2.8 hdf\_createParamFile()

```
void hdf_createParamFile ( )
```

PARAMETER FILE hdf\_createParamFile

# 2.11.2.9 hdf\_createSaveDirs()

```
void hdf_createSaveDirs ( )
```

hdf\_createSaveDirs

# 2.11.2.10 hdf\_dumpCheckpoint()

 $hdf\_dumpCheckpoint$ 

# 2.11.2.11 hdf\_init()

```
void hdf_init ( )
```

INITIALIZE HDF5 hdf\_init

# 2.11.2.12 hdf\_initCheckpoints()

```
void hdf_initCheckpoints ( )
```

CHECKPOINTS hdf\_initCheckpoints

# 2.11.2.13 hdf\_initChi()

```
void hdf_initChi ( )
hdf_initChi
```

### 2.11.2.14 hdf\_initField()

```
void hdf_initField ( )
```

hdf\_initField

# 2.11.2.15 hdf\_readData()

READ FILE hdf\_readData

# 2.11.2.16 hdf\_saveData()

```
void hdf_saveData ( \label{eq:complex} {\tt COMPLEX} \, * \, h, \\ \\ {\tt int} \, \, timestep \, )
```

hdf\_saveData

# 2.11.2.17 hdf\_saveEnergy()

hdf\_saveEnergy

#### 2.11.2.18 hdf\_saveField\_r()

hdf\_saveField\_r

# 2.11.2.19 hdf\_saveFieldA()

hdf\_saveFieldA

# 2.11.2.20 hdf\_saveFieldB()

 $hdf\_saveFieldB$ 

# 2.11.2.21 hdf\_saveFieldPhi()

hdf\_saveFieldPhi

# 2.11.2.22 hdf\_saveFields()

hdf\_saveFields

# 2.11.2.23 hdf\_saveKSpec()

hdf\_saveKSpec

# 2.11.2.24 hdf\_saveMSpec()

hdf\_saveMSpec

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