THUNDER

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1.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 2

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2.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 3

File Index

3.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 4

Class Documentation

4.1 _complex_float_t Struct Reference

Public Attributes

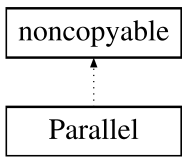
- double **dat** [2]

The documentation for this struct was generated from the following file:

- include/Precision.h

4.2 Parallel Class Reference

Inheritance diagram for Parallel:



Public Member Functions

- Parallel ()
- ~Parallel ()
- void setMPIEnv ()
- void setMPIEnv (const int commSize, const int commRank, const MPI_Comm &hemi, const MPI_Comm &slav)
- bool isMaster () const
- bool isA () const
- bool isB () const
- int commSize () const
- void setCommSize (const int commSize)
- int commRank () const
- void setCommRank (const int commRank)
- MPI_Comm hemi () const
- void setHemi (const MPI_Comm &hemi)
- MPI_Comm **slav** () const
- void **setSlav** (const MPI_Comm &slav)

Protected Attributes

- int _commSize
- int _commRank
- MPI_Comm _hemi
- MPI_Comm **_slav**

4.2.1 Constructor & Destructor Documentation

4.2.1.1 Parallel::Parallel ( )

default constructor

4.2.1.2 Parallel::∼Parallel ( )

default deconstructor

4.2.2 Member Function Documentation

4.2.2.1 int Parallel::commRank ( ) const

This function returns the rank ID of the current process in MPI_COMM_WORLD.

4.2.2.2 int Parallel::commSize ( ) const

This function returns the number of processes in MPI_COMM_WORLD.

4.2.2.3 MPI_Comm Parallel::hemi ( ) const

This function returns the hemisphere of the current process.

4.2.2.4 bool Parallel::isA ( ) const

This function returns whether the current process is in hemisphere A or not.

4.2.2.5 bool Parallel::isB ( ) const

This function returns whether the current process is in hemisphere B or not.

4.2.2.6 bool Parallel::isMaster ( ) const

This function returns whether the current process is the master process or not.

4.2.2.7 void Parallel::setCommRank (const int *commRank*)

This function sets the rank ID of the current process in MPI_COMM_WORLD.

Parameters

commRank	the rank ID of the current process in MPI_COMM_WORLD

4.2.2.8 void Parallel::setCommSize (const int *commSize*)

This function sets the number of processes in MPI_COMM_WORLD.

Parameters

commSize	the number of processes in MPI_COMM_WORLD

4.2.2.9 void Parallel::setHemi (const MPI_Comm & *hemi*)

This function sets the hemisphere of the current process.

Parameters

hemi	the hemisphere of the current process

4.2.2.10 void Parallel::setMPIEnv ( )

This function detects the number of processes in MPI_COMM_WORLD and the rank ID of the current process in MPI_COMM_WORLD. Moreover, it will assign all process in MPI_COMM_WORLD into three parts: master, hemisphere A and hemisphere B.

4.2.2.11 void Parallel::setMPIEnv (const int *commSize,* const int *commRank,* const MPI_Comm & *hemi,* const MPI_Comm & *slav*)

This function inherits the MPI information by parameters.

Parameters

commSize	the numbber of process in MPI_COMM_WORLD
commRank	the rank ID of the current process in MPI_COMM_WORLD
hemi	the hemisphere of the current process

4.2.3 Member Data Documentation

4.2.3.1 int Parallel::_commRank [protected]

the rank ID of the current process in MPI_COMM_WORLD

4.2.3.2 int Parallel::_commSize [protected]

number of processes in MPI_COMM_WORLD

4.2.3.3 MPI_Comm Parallel::_hemi [protected]

communicator of hemisphere A(B)

The documentation for this class was generated from the following file:

- include/Parallel.h

Chapter 5

File Documentation

5.1 include/Complex.h File Reference

Complex.h defines complex number related operations like +,-,$*$,/,|a|, $|a|^2$ and so on.

```
#include <gsl/gsl_complex.h>
#include <gsl/gsl_complex_math.h>
#include <math.h>
#include "Config.h"
#include "Precision.h"
#include "Typedef.h"
```

Functions

- Complex **COMPLEX_POLAR** (const RFLOAT phi)
- Complex **ts_complex_polar** (const RFLOAT r, const RFLOAT phi)
- Complex **CONJUGATE** (const Complex &a)
- RFLOAT **ABS** (const Complex &a)
- RFLOAT **ABS2** (const Complex &a)
- Complex **COMPLEX** (RFLOAT a, RFLOAT b)
- RFLOAT **REAL** (const Complex &a)
- RFLOAT **IMAG** (const Complex &a)
- RFLOAT **gsl_real** (const Complex &a)
- RFLOAT **gsl_imag** (const Complex &a)
- RFLOAT **gsl_real_imag_sum** (const Complex &a)
- Complex **operator-** (const Complex &a)
- Complex **operator+** (const Complex &a, const Complex &b)
- Complex **operator-** (const Complex &a, const Complex &b)
- Complex **operator*** (const Complex &a, const Complex &b)
- Complex **operator/** (const Complex &a, const Complex &b)
- void **operator+=** (Complex &a, const Complex b)
- void **operator-=** (Complex &a, const Complex b)
- void **operator*=** (Complex &a, const Complex b)
- void **operator/=** (Complex &a, const Complex b)
- Complex **operator*** (const Complex a, const RFLOAT x)
- Complex **operator*** (const RFLOAT x, const Complex a)
- void **operator*=** (Complex &a, const RFLOAT x)
- Complex **operator/** (const Complex a, const RFLOAT x)
- void **operator/=** (Complex &a, const RFLOAT x)

5.1.1 Detailed Description

Complex.h defines complex number related operations like +,-,$*$,/,|a|, $|a|^2$ and so on.

5.2 include/Geometry/Euler.h File Reference

Euler.h contains several functions, for operations of quaternions, converting between Euler angles, rotation matrices and unit quaternions and sampling rotation matrices from even distribution.

```
#include <cmath>
#include <gsl/gsl_math.h>
#include "Macro.h"
#include "Typedef.h"
#include "Precision.h"
#include "Random.h"
#include "Functions.h"
```

Functions

- void quaternion_mul (dvec4 &dst, const dvec4 &a, const dvec4 &b)

  Calculate the product of two quaternions $\mathbf{q_1}$ *and* $\mathbf{q_2}$*.*
- dvec4 quaternion_conj (const dvec4 &quat)

  Calculate the conjugate quaternion of a quaternion.
- void angle (double &phi, double &theta, const dvec3 &src)

  Calculate ϕ *and* θ *given a certain direction* $\mathbf{v}$*.*
- void angle (double &phi, double &theta, double &psi, const dmat33 &src)

  Calculate ϕ*,* θ *and* ψ *of the rotation represented by the rotation matrix* $\mathbf{R}$*.*
- void angle (double &phi, double &theta, double &psi, const dvec4 &src)

  Calculate ϕ*,* θ *and* ψ *of the rotation represented by the unit quaternion* $\mathbf{q}$*.*
- void quaternion (dvec4 &dst, const double phi, const double theta, const double psi)

  Calculate the unit quaternion $\mathbf{q}$ *for representing the rotation, given 3 Euler angles* ϕ*,* θ *and* ψ*.*
- void quaternion (dvec4 &dst, const double phi, const dvec3 &axis)

  Calculate the unit quaternion $\mathbf{q}$ *for representing the rotation, given the rotation axis* $\mathbf{r}$ *and the rotation angle around this axis* ϕ*.*
- void quaternion (dvec4 &dst, const dmat33 &src)

  Calculate the unit quaternion $\mathbf{q}$ *for representing the rotation, given the rotation matrix* $\mathbf{R}$*.*
- void rotate2D (dmat22 &dst, const dvec2 &vec)

  Calculate the rotation matrix (2D) $\mathbf{R}$*, which rotates the unit vector* $\mathbf{v_0} = \{1,0\}$ *to the given unit vector* $\mathbf{v}$*.*
- void rotate2D (dmat22 &dst, const double phi)

  Calculate the rotation matrix (2D) $\mathbf{R}$*, given the rotation angle* ϕ*.*
- void direction (dvec3 &dst, const double phi, const double theta)

  Caclulate the unit direction vector $\mathbf{v}$*, given the rotation angle* ϕ *and* θ*.*
- void rotate3D (dmat33 &dst, const double phi, const double theta, const double psi)

  Caclulate the rotation matrix $\mathbf{R}$*, given the rotation angle* ϕ*,* θ *and* ψ*.*
- void rotate3D (dmat33 &dst, const dvec4 &src)

  Calculate the rotation matrix $\mathbf{R}$*, given the unit quaternion* $\mathbf{q}$ *which represents this rotation.*
- void rotate3DX (dmat33 &dst, const double phi)

  Calculate the rotation matrix $\mathbf{R}$ *which represents the rotation along X-axis with rotation angle* ϕ*.*
- void rotate3DY (dmat33 &dst, const double phi)

  Calculate the rotation matrix $\mathbf{R}$ *which represents the rotation along Y-axis with rotation angle* ϕ*.*
- void rotate3DZ (dmat33 &dst, const double phi)

Calculate the rotation matrix $\mathbf{R}$ *which represents the rotation along Z-axis with rotation angle* ϕ*.*

- void alignZ (dmat33 &dst, const dvec3 &vec)

  Calculate the rotation matrix $\mathbf{R}$ *which aligns a direction vector* $\mathbf{v}$ *to Z-axis.*
- void rotate3D (dmat33 &dst, const double phi, const dvec3 &axis)

  Calculate the rotation matrix $\mathbf{R}$ *which represents the rotation along the axis* $\mathbf{v}$ *with rotation angle* ϕ*.*
- void reflect3D (dmat33 &dst, const dvec3 &plane)

  Calculate the transformation matrix $\mathbf{M}$ *of reflection against a certian plane, which is represented by its normal vector* $\mathbf{n}$*.*
- void swingTwist (dvec4 &swing, dvec4 &twist, const dvec4 &src, const dvec3 &vec)

  Calculate the two quaternions $\mathbf{q_s}$ *and* $\mathbf{q_t}$*, which represent swing and twist along axis* $\mathbf{v}$ *respectively, representing the rotation represented by quaternion* $\mathbf{q}$*.*
- void randRotate2D (dmat22 &rot)

  Sample a 2D rotation matrix $\mathbf{R}$ *from even distribution.*
- void randRotate3D (dmat33 &rot)

  Sample a 3D rotation matrix $\mathbf{R}$ *from even distribution.*

5.2.1 Detailed Description

Euler.h contains several functions, for operations of quaternions, converting between Euler angles, rotation matrices and unit quaternions and sampling rotation matrices from even distribution. Quaternions are a number system that extends the complex numbers. Unit quaternions provide a convenient mathematical notation for representing rotations of objects in 3D. Compared to Euler angles, they are simpler to compose and aovid the problem of glimbal lock. Compared to rotation matrices, they are more compact and more efficient. Moroever, unlike Euler angles, unit quaternions do not rely on the choosing and order of the rotation axes.

To be noticed, Euler angles in this file follow the standard of ZXZ Euler system. In other words, Euler angle set $\{\phi, \theta, \psi\}$ stands for rotating along Z axis with ϕ, followed by rotating along X axis with θ, and followed by rotating along Z axis with ψ.

5.2.2 Function Documentation

5.2.2.1 void alignZ (dmat33 & *dst,* const dvec3 & *vec*)

Calculate the rotation matrix $\mathbf{R}$ which aligns a direction vector $\mathbf{v}$ to Z-axis.

Parameters

out	*dst*	$\mathbf{R}$
in	*vec*	$\mathbf{v}$

5.2.2.2 void angle (double & *phi,* double & *theta,* const dvec3 & *src*)

Calculate ϕ and θ given a certain direction $\mathbf{v}$.

$\mathbf{v}$ must be a unit vector. Output value ϕ ranges $[0, 2\pi)$, and θ ranges $[0, \pi]$.

Parameters

out	*phi*	ϕ
out	*theta*	θ
in	*src*	$\mathbf{v}$

5.2.2.3 void angle (double & *phi,* double & *theta,* double & *psi,* const dmat33 & *src*)

Calculate ϕ, θ and ψ of the rotation represented by the rotation matrix $\mathbf{R}$.

$\mathbf{R}$ must be an orthogonal matirx and determinant of which equals to 1. In other words, $RR^T = I$ and $\det A = 1$. Output value ϕ ranges $[0, 2\pi)$, θ ranges $[0, \pi]$, and ψ ranges $[0, 2\pi)$.

Parameters

out	*phi*	ϕ
out	*theta*	θ
out	*psi*	ψ
in	*src*	$\mathbf{R}$

5.2.2.4 void angle (double & *phi,* double & *theta,* double & *psi,* const dvec4 & *src*)

Calculate ϕ, θ and ψ of the rotation represented by the unit quaternion $\mathbf{q}$.

Parameters

out	*phi*	ϕ
out	*theta*	θ
out	*psi*	ψ
in	*src*	$\mathbf{q}$

5.2.2.5 void direction (dvec3 & *dst,* const double *phi,* const double *theta*)

Caclulate the unit direction vector $\mathbf{v}$, given the rotation angle ϕ and θ.

Parameters

out	*dst*	$\mathbf{v}$
in	*phi*	ϕ
in	*theta*	θ

5.2.2.6 void quaternion (dvec4 & *dst,* const double *phi,* const double *theta,* const double *psi*)

Calculate the unit quaternion $\mathbf{q}$ for representing the rotation, given 3 Euler angles ϕ, θ and ψ.

Parameters

out	*dst*	$\mathbf{q}$
in	*phi*	ϕ
in	*theta*	θ
in	*psi*	ψ

5.2.2.7 void quaternion (dvec4 & *dst,* const double *phi,* const dvec3 & *axis*)

Calculate the unit quaternion $\mathbf{q}$ for representing the rotation, given the rotation axis $\mathbf{r}$ and the rotation angle around this axis ϕ.

This rotation axis $\mathbf{r}$ must be a unit vector, while the rotation angle ϕ ranges $(-\infty, +\infty)$.

Parameters

out	*dst*	$\mathbf{q}$
in	*phi*	ϕ
in	*axis*	$\mathbf{r}$

5.2.2.8 void quaternion (dvec4 & *dst*, const dmat33 & *src*)

Calculate the unit quaternion $\mathbf{q}$ for representing the rotation, given the rotation matrix $\mathbf{R}$.

Parameters

out	*dst*	$\mathbf{q}$
in	*src*	$\mathbf{R}$

5.2.2.9 dvec4 quaternion_conj (const dvec4 & *quat*)

Calculate the conjugate quaternion of a quaternion.

Returns

the conjugate quaternion

Parameters

in	*quat*	a quaternion

5.2.2.10 void quaternion_mul (dvec4 & *dst*, const dvec4 & *a*, const dvec4 & *b*)

Calculate the product of two quaternions $\mathbf{q_1}$ and $\mathbf{q_2}$.

Assuming that $\mathbf{q_1} = (w_1, x_1, y_1, z_1)$ and $\mathbf{q_2} = (w_2, x_2, y_2, z_2)$, the product can be calculated as

$$\begin{pmatrix} w_1 \\ x_1 \\ y_1 \\ z_1 \end{pmatrix} \times \begin{pmatrix} w_2 \\ x_2 \\ y_2 \\ z_2 \end{pmatrix} = \begin{pmatrix} w_1w_2 - x_1x_2 - y_1y_2 - z_1z_2 \\ w_1x_2 + x_1w_2 + y_1z_2 - z_1y_2 \\ w_1y_2 - x_1z_2 + y_1w_2 + z_1x_2 \\ w_1z_2 + x_1y_2 - y_1x_2 + z_1w_2 \end{pmatrix}$$

Parameters

out	*dst*	product, a quaternion
in	*a*	left multiplier, $\mathbf{q_1}$
in	*b*	right multiplier, $\mathbf{q_2}$

5.2.2.11 void randRotate2D (dmat22 & *rot*)

Sample a 2D rotation matrix $\mathbf{R}$ from even distribution.

Parameters

out	*rot*	$\mathbf{R}$

5.2.2.12 void randRotate3D (dmat33 & *rot*)

Sample a 3D rotation matrix $\mathbf{R}$ from even distribution.

Parameters

out	*rot*	$\mathbf{R}$

5.2.2.13 void reflect3D (dmat33 & *dst*, const dvec3 & *plane*)

Calculate the transformation matrix $\mathbf{M}$ of reflection against a certian plane, which is represented by its normal vector $\mathbf{n}$.

Parameters

out	*dst*	$\mathbf{M}$
in	*plane*	$\mathbf{n}$

5.2.2.14 void rotate2D (dmat22 & *dst*, const dvec2 & *vec*)

Calculate the rotation matrix (2D) $\mathbf{R}$, which rotates the unit vector $\mathbf{v_0} = \{1, 0\}$ to the given unit vector $\mathbf{v}$.

Parameters

out	*dst*	$\mathbf{R}$
in	*vec*	$\mathbf{v}$

5.2.2.15 void rotate2D (dmat22 & *dst*, const double *phi*)

Calculate the rotation matrix (2D) $\mathbf{R}$, given the rotation angle ϕ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ

5.2.2.16 void rotate3D (dmat33 & *dst*, const double *phi*, const double *theta*, const double *psi*)

Caclulate the rotation matrix $\mathbf{R}$, given the rotation angle ϕ, θ and ψ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ
in	*theta*	θ
in	*psi*	ψ

5.2.2.17 void rotate3D (dmat33 & *dst*, const dvec4 & *src*)

Calculate the rotation matrix $\mathbf{R}$, given the unit quaternion $\mathbf{q}$ which represents this rotation.

Parameters

out	*dst*	$\mathbf{R}$
in	*src*	$\mathbf{q}$

5.2.2.18 void rotate3D (dmat33 & *dst,* const double *phi,* const dvec3 & *axis*)

Calculate the rotation matrix $\mathbf{R}$ which represents the rotation along the axis $\mathbf{v}$ with rotation angle ϕ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ
in	*axis*	$\mathbf{v}$

5.2.2.19 void rotate3DX (dmat33 & *dst*, const double *phi*)

Calculate the rotation matrix $\mathbf{R}$ which represents the rotation along X-axis with rotation angle ϕ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ

5.2.2.20 void rotate3DY (dmat33 & *dst*, const double *phi*)

Calculate the rotation matrix $\mathbf{R}$ which represents the rotation along Y-axis with rotation angle ϕ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ

5.2.2.21 void rotate3DZ (dmat33 & *dst*, const double *phi*)

Calculate the rotation matrix $\mathbf{R}$ which represents the rotation along Z-axis with rotation angle ϕ.

Parameters

out	*dst*	$\mathbf{R}$
in	*phi*	ϕ

5.2.2.22 void swingTwist (dvec4 & *swing*, dvec4 & *twist*, const dvec4 & *src*, const dvec3 & *vec*)

Calculate the two quaternions $\mathbf{q_s}$ and $\mathbf{q_t}$, which represent swing and twist along axis $\mathbf{v}$ respectively, representing the rotation represented by quaternion $\mathbf{q}$.

Parameters

out	*swing*	$\mathbf{q_s}$
out	*twist*	$\mathbf{q_t}$
in	*src*	$\mathbf{q}$
in	*vec*	$\mathbf{v}$

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