Ecosystem

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1.1 Class Hierarchy

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2.1 Class List

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

Chapter 3

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3.1 File List

Here is a list of all files with brief descriptions:

Chapter 4

Class Documentation

4.1 ARNOLDI_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int k
- int iter
- double beta
- double hp1
- bool Output = true
- std::vector< Matrix< double > > Vk
- Matrix< double > Hkp1
- Matrix< double > yk
- Matrix< double > e1
- Matrix< double > w
- Matrix< double > v
- Matrix< double > sum

4.1.1 Member Data Documentation

4.1.1.1 double ARNOLDI_DATA::beta

4.1.1.2 Matrix<double> ARNOLDI_DATA::e1

4.1.1.3 Matrix<double> ARNOLDI_DATA::Hkp1

4.1.1.4 double ARNOLDI_DATA::hp1

4.1.1.5 int ARNOLDI_DATA::iter

4.1.1.6 int ARNOLDI_DATA::k

4.1.1.7 bool ARNOLDI_DATA::Output = true

4.1.1.8 Matrix<double> ARNOLDI_DATA::sum

4.1.1.9 Matrix<double> ARNOLDI_DATA::v

4.1.1.10 std::vector< Matrix<double> > ARNOLDI_DATA::Vk

4.1.1.11 Matrix<double> ARNOLDI_DATA::w

4.1.1.12 Matrix<double> ARNOLDI_DATA::yk

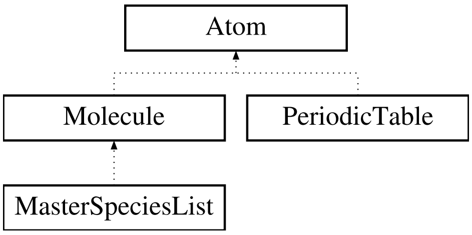
The documentation for this struct was generated from the following file:

- lark.h

4.2 Atom Class Reference

```
#include <eel.h>
```

Inheritance diagram for Atom:



Public Member Functions

- Atom ()
- ∼Atom ()
- Atom (std::string Name)
- Atom (int number)
- void Register (std::string Symbol)
- void Register (int number)
- void editAtomicWeight (double AW)
- void editOxidationState (int state)
- void editProtons (int proton)
- void editNeutrons (int neutron)
- void editElectrons (int electron)
- void editValence (int val)
- void removeProton ()
- void removeNeutron ()
- void removeElectron ()
- double AtomicWeight ()
- int OxidationState ()
- int Protons ()
- int Neutrons ()
- int Electrons ()
- int BondingElectrons ()
- std::string AtomName ()
- std::string AtomSymbol ()
- std::string AtomCategory ()
- std::string AtomState ()
- int AtomicNumber ()
- void DisplayInfo ()

Protected Attributes

- double atomic_weight
- int oxidation_state
- int protons
- int neutrons
- int electrons
- int valence_e

Private Attributes

- std::string Name
- std::string Symbol
- std::string Category
- std::string NaturalState
- int atomic_number

4.2.1 Constructor & Destructor Documentation

4.2.1.1 Atom::Atom ( )

4.2.1.2 Atom::∼Atom ( )

4.2.1.3 Atom::Atom (std::string *Name*)

4.2.1.4 Atom::Atom (int *number*)

4.2.2 Member Function Documentation

4.2.2.1 std::string Atom::AtomCategory ( )

4.2.2.2 int Atom::AtomicNumber ( )

4.2.2.3 double Atom::AtomicWeight ( )

4.2.2.4 std::string Atom::AtomName ( )

4.2.2.5 std::string Atom::AtomState ( )

4.2.2.6 std::string Atom::AtomSymbol ( )

4.2.2.7 int Atom::BondingElectrons ( )

4.2.2.8 void Atom::DisplayInfo ( )

4.2.2.9 void Atom::editAtomicWeight (double *AW*)

4.2.2.10 void Atom::editElectrons (int *electron*)

4.2.2.11 void Atom::editNeutrons (int *neutron*)

4.2.2.12 void Atom::editOxidationState (int *state*)

4.2.2.13 void Atom::editProtons (int *proton*)

4.2.2.14 void Atom::editValence (int *val*)

4.2.2.15 int Atom::Electrons ( )

4.2.2.16 int Atom::Neutrons ( )

4.2.2.17 int Atom::OxidationState ( )

4.2.2.18 int Atom::Protons ( )

4.2.2.19 void Atom::Register (std::string *Symbol*)

4.2.2.20 void Atom::Register (int *number*)

4.2.2.21 void Atom::removeElectron ( )

4.2.2.22 void Atom::removeNeutron ( )

4.2.2.23 void Atom::removeProton ( )

4.2.3 Member Data Documentation

4.2.3.1 int Atom::atomic_number `[private]`

4.2.3.2 double Atom::atomic_weight `[protected]`

4.2.3.3 std::string Atom::Category `[private]`

4.2.3.4 int Atom::electrons `[protected]`

4.2.3.5 std::string Atom::Name `[private]`

4.2.3.6 std::string Atom::NaturalState `[private]`

4.2.3.7 int Atom::neutrons `[protected]`

4.2.3.8 int Atom::oxidation_state `[protected]`

4.2.3.9 int Atom::protons `[protected]`

4.2.3.10 std::string Atom::Symbol `[private]`

4.2.3.11 int Atom::valence_e `[protected]`

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

- eel.h
- eel.cpp

4.3 BACKTRACK_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- double alpha = 1e-4
- double rho = 0.1
- double lambdaMin =DBL_EPSILON
- double normFkp1
- bool constRho = false
- Matrix< double > Fk
- Matrix< double > xk

4.3.1 Member Data Documentation

4.3.1.1 double BACKTRACK_DATA::alpha = 1e-4

4.3.1.2 bool BACKTRACK_DATA::constRho = false

4.3.1.3 Matrix<double> BACKTRACK_DATA::Fk

4.3.1.4 double BACKTRACK_DATA::lambdaMin =DBL_EPSILON

4.3.1.5 double BACKTRACK_DATA::normFkp1

4.3.1.6 double BACKTRACK_DATA::rho = 0.1

4.3.1.7 Matrix<double> BACKTRACK_DATA::xk

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

- lark.h

4.4 BiCGSTAB_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int maxit = 0
- int iter = 0
- bool breakdown
- double alpha
- double beta
- double rho
- double rho_old
- double omega
- double omega_old
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x

- Matrix< double > bestx
- Matrix< double > r
- Matrix< double > r0
- Matrix< double > v
- Matrix< double > p
- Matrix< double > y
- Matrix< double > s
- Matrix< double > z
- Matrix< double > t

4.4.1 Member Data Documentation

4.4.1.1 double BiCGSTAB_DATA::alpha

4.4.1.2 double BiCGSTAB_DATA::bestres

4.4.1.3 Matrix<double> BiCGSTAB_DATA::bestx

4.4.1.4 double BiCGSTAB_DATA::beta

4.4.1.5 bool BiCGSTAB_DATA::breakdown

4.4.1.6 int BiCGSTAB_DATA::iter = 0

4.4.1.7 int BiCGSTAB_DATA::maxit = 0

4.4.1.8 double BiCGSTAB_DATA::omega

4.4.1.9 double BiCGSTAB_DATA::omega_old

4.4.1.10 bool BiCGSTAB_DATA::Output = true

4.4.1.11 Matrix<double> BiCGSTAB_DATA::p

4.4.1.12 Matrix<double> BiCGSTAB_DATA::r

4.4.1.13 Matrix<double> BiCGSTAB_DATA::r0

4.4.1.14 double BiCGSTAB_DATA::relres

4.4.1.15 double BiCGSTAB_DATA::relres_base

4.4.1.16 double BiCGSTAB_DATA::res

4.4.1.17 double BiCGSTAB_DATA::rho

4.4.1.18 double BiCGSTAB_DATA::rho_old

4.4.1.19 Matrix<double> BiCGSTAB_DATA::s

4.4.1.20 Matrix<double> BiCGSTAB_DATA::t

4.4.1.21 double BiCGSTAB_DATA::tol_abs = 1e-6

4.4.1.22 double BiCGSTAB_DATA::tol_rel = 1e-6

4.4.1.23 Matrix<double> BiCGSTAB_DATA::v

4.4.1.24 Matrix<double> BiCGSTAB_DATA::x

4.4.1.25 Matrix<double> BiCGSTAB_DATA::y

4.4.1.26 Matrix<double> BiCGSTAB_DATA::z

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

- lark.h

4.5 CGS_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int maxit = 0
- int iter = 0
- bool breakdown
- double alpha
- double beta
- double rho
- double sigma
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x
- Matrix< double > bestx
- Matrix< double > r
- Matrix< double > r0
- Matrix< double > u
- Matrix< double > w
- Matrix< double > v
- Matrix< double > p
- Matrix< double > c
- Matrix< double > z

4.5.1 Member Data Documentation

4.5.1.1 double CGS_DATA::alpha

4.5.1.2 double CGS_DATA::bestres

4.5.1.3 Matrix<double> CGS_DATA::bestx

4.5.1.4 double CGS_DATA::beta

4.5.1.5 bool CGS_DATA::breakdown

4.5.1.6 Matrix<double> CGS_DATA::c

4.5.1.7 int CGS_DATA::iter = 0

4.5.1.8 int CGS_DATA::maxit = 0

4.5.1.9 bool CGS_DATA::Output = true

4.5.1.10 Matrix<double> CGS_DATA::p

4.5.1.11 Matrix<double> CGS_DATA::r

4.5.1.12 Matrix<double> CGS_DATA::r0

4.5.1.13 double CGS_DATA::relres

4.5.1.14 double CGS_DATA::relres_base

4.5.1.15 double CGS_DATA::res

4.5.1.16 double CGS_DATA::rho

4.5.1.17 double CGS_DATA::sigma

4.5.1.18 double CGS_DATA::tol_abs = 1e-6

4.5.1.19 double CGS_DATA::tol_rel = 1e-6

4.5.1.20 Matrix<double> CGS_DATA::u

4.5.1.21 Matrix<double> CGS_DATA::v

4.5.1.22 Matrix<double> CGS_DATA::w

4.5.1.23 Matrix<double> CGS_DATA::x

4.5.1.24 Matrix<double> CGS_DATA::z

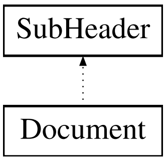
The documentation for this struct was generated from the following file:

- lark.h

4.6 Document Class Reference

```
#include <yaml_wrapper.h>
```

Inheritance diagram for Document:



Public Member Functions

- Document ()
- ∼Document ()
- Document (const Document &doc)
- Document (std::string name)
- Document (const KeyValueMap &map)
- Document (std::string name, const KeyValueMap &map)
- Document (std::string key, const Header &head)
- Document & operator= (const Document &doc)
- ValueTypePair & operator[ ] (const std::string key)
- ValueTypePair operator[ ] (const std::string key) const
- Header & operator() (const std::string key)
- Header operator() (const std::string key) const
- std::map< std::string, Header > & getHeadMap ()
- KeyValueMap & getDataMap ()
- Header & getHeader (std::string key)
- std::map< std::string, Header >
  ::const_iterator end () const
- std::map< std::string, Header >
  ::iterator end ()
- std::map< std::string, Header >
  ::const_iterator begin () const
- std::map< std::string, Header >
  ::iterator begin ()
- void clear ()
- void resetKeys ()
- void changeKey (std::string oldKey, std::string newKey)
- void revalidateAllKeys ()
- void addPair (std::string key, std::string val)
- void addPair (std::string key, std::string val, int t)
- void setName (std::string name)
- void setAlias (std::string alias)
- void setNameAliasPair (std::string n, std::string a, int s)
- void setState (int state)
- void DisplayContents ()
- void addHeadKey (std::string key)
- void copyAnchor2Alias (std::string alias, Header &ref)
- int size ()
- std::string getName ()
- std::string getAlias ()
- int getState ()
- bool isAlias ()
- bool isAnchor ()
- Header & getAnchoredHeader (std::string alias)
- Header & getHeadFromSubAlias (std::string alias)

Private Attributes

- std::map< std::string, Header > Head_Map

Additional Inherited Members

4.6.1 Constructor & Destructor Documentation

4.6.1.1 Document::Document ( )

4.6.1.2 Document::∼Document ( )

4.6.1.3 Document::Document (const Document & *doc*)

4.6.1.4 Document::Document (std::string *name*)

4.6.1.5 Document::Document (const KeyValueMap & *map*)

4.6.1.6 Document::Document (std::string *name,* const KeyValueMap & *map*)

4.6.1.7 Document::Document (std::string *key,* const Header & *head*)

4.6.2 Member Function Documentation

4.6.2.1 void Document::addHeadKey (std::string *key*)

4.6.2.2 void Document::addPair (std::string *key,* std::string *val*)

4.6.2.3 void Document::addPair (std::string *key,* std::string *val,* int *t*)

4.6.2.4 std::map< std::string, Header >::const_iterator Document::begin ( ) const

4.6.2.5 std::map< std::string, Header >::iterator Document::begin ( )

4.6.2.6 void Document::changeKey (std::string *oldKey,* std::string *newKey*)

4.6.2.7 void Document::clear ( )

4.6.2.8 void Document::copyAnchor2Alias (std::string *alias,* Header & *ref*)

4.6.2.9 void Document::DisplayContents ( )

4.6.2.10 std::map< std::string, Header >::const_iterator Document::end ( ) const

4.6.2.11 std::map< std::string, Header >::iterator Document::end ( )

4.6.2.12 std::string Document::getAlias ( )

4.6.2.13 Header & Document::getAnchoredHeader (std::string *alias*)

4.6.2.14 KeyValueMap & Document::getDataMap ( )

4.6.2.15 Header & Document::getHeader (std::string *key*)

4.6.2.16 Header & Document::getHeadFromSubAlias (std::string *alias*)

4.6.2.17 std::map< std::string, Header > & Document::getHeadMap ( )

4.6.2.18 std::string Document::getName ( )

4.6.2.19 int Document::getState ( )

4.6.2.20 bool Document::isAlias ( )

4.6.2.21 bool Document::isAnchor ( )

4.6.2.22 Header & Document::operator() (const std::string *key*)

4.6.2.23 Header Document::operator() (const std::string *key*) const

4.6.2.24 Document & Document::operator= (const Document & *doc*)

4.6.2.25 ValueTypePair & Document::operator[ ] (const std::string *key*)

4.6.2.26 ValueTypePair Document::operator[ ] (const std::string *key*) const

4.6.2.27 void Document::resetKeys ( )

4.6.2.28 void Document::revalidateAllKeys ( )

4.6.2.29 void Document::setAlias (std::string *alias*)

4.6.2.30 void Document::setName (std::string *name*)

4.6.2.31 void Document::setNameAliasPair (std::string *n,* std::string *a,* int *s*)

4.6.2.32 void Document::setState (int *state*)

4.6.2.33 int Document::size ( )

4.6.3 Member Data Documentation

4.6.3.1 std::map<std::string, Header> Document::Head_Map [private]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.7 DOGFISH_DATA Struct Reference

`#include <dogfish.h>`

Public Attributes

- unsigned long int total_steps = 0
- double time_old = 0.0
- double time = 0.0
- bool Print2File = true
- bool Print2Console = true
- bool DirichletBC = false
- bool NonLinear = false
- double t_counter = 0.0
- double t_print

- int NumComp
- double end_time
- double total_sorption_old
- double total_sorption
- double fiber_length
- double fiber_diameter
- FILE ∗ OutputFile
- double(∗ eval_R)(int i, int l, const void ∗data)
- double(∗ eval_DI)(int i, int l, const void ∗data)
- double(∗ eval_kf)(int i, const void ∗data)
- double(∗ eval_qs)(int i, const void ∗data)
- const void ∗ user_data
- std::vector< FINCH_DATA > finch_dat
- std::vector< DOGFISH_PARAM > param_dat

4.7.1 Member Data Documentation

4.7.1.1 bool DOGFISH_DATA::DirichletBC = false

4.7.1.2 double DOGFISH_DATA::end_time

4.7.1.3 double(∗ DOGFISH_DATA::eval_DI)(int i, int l, const void ∗data)

4.7.1.4 double(∗ DOGFISH_DATA::eval_kf)(int i, const void ∗data)

4.7.1.5 double(∗ DOGFISH_DATA::eval_qs)(int i, const void ∗data)

4.7.1.6 double(∗ DOGFISH_DATA::eval_R)(int i, int l, const void ∗data)

4.7.1.7 double DOGFISH_DATA::fiber_diameter

4.7.1.8 double DOGFISH_DATA::fiber_length

4.7.1.9 std::vector<FINCH_DATA> DOGFISH_DATA::finch_dat

4.7.1.10 bool DOGFISH_DATA::NonLinear = false

4.7.1.11 int DOGFISH_DATA::NumComp

4.7.1.12 FILE∗ DOGFISH_DATA::OutputFile

4.7.1.13 std::vector<DOGFISH_PARAM> DOGFISH_DATA::param_dat

4.7.1.14 bool DOGFISH_DATA::Print2Console = true

4.7.1.15 bool DOGFISH_DATA::Print2File = true

4.7.1.16 double DOGFISH_DATA::t_counter = 0.0

4.7.1.17 double DOGFISH_DATA::t_print

4.7.1.18 double DOGFISH_DATA::time = 0.0

4.7.1.19 double DOGFISH_DATA::time_old = 0.0

4.7.1.20 double DOGFISH_DATA::total_sorption

4.7.1.21 double DOGFISH_DATA::total_sorption_old

4.7.1.22 unsigned long int DOGFISH_DATA::total_steps = 0

4.7.1.23 const void∗ DOGFISH_DATA::user_data

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

- dogfish.h

4.8 DOGFISH_PARAM Struct Reference

```
#include <dogfish.h>
```

Public Attributes

- double intraparticle_diffusion
- double film_transfer_coeff
- double surface_concentration
- double initial_sorption
- double sorbed_molefraction
- Molecule species

4.8.1 Member Data Documentation

4.8.1.1 double DOGFISH_PARAM::film_transfer_coeff

4.8.1.2 double DOGFISH_PARAM::initial_sorption

4.8.1.3 double DOGFISH_PARAM::intraparticle_diffusion

4.8.1.4 double DOGFISH_PARAM::sorbed_molefraction

4.8.1.5 Molecule DOGFISH_PARAM::species

4.8.1.6 double DOGFISH_PARAM::surface_concentration

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

- dogfish.h

4.9 EX01_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- Matrix< double > M
- Matrix< double > b

4.9.1 Member Data Documentation

4.9.1.1 Matrix<double> EX01_DATA::b

4.9.1.2 Matrix<double> EX01_DATA::M

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

- lark.h

4.10 EX02_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- Matrix< double > M
- Matrix< double > b

4.10.1 Member Data Documentation

4.10.1.1 Matrix<double> EX02_DATA::b

4.10.1.2 Matrix<double> EX02_DATA::M

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

- lark.h

4.11 EX04_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- Matrix< double > M
- Matrix< double > b

4.11.1 Member Data Documentation

4.11.1.1 Matrix<double> EX04_DATA::b

4.11.1.2 Matrix<double> EX04_DATA::M

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

- lark.h

4.12 EX09_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- double h
- double k
- int N
- Matrix< double > x
- Matrix< double > M
- Matrix< double > s
- Matrix< double > p

4.12.1 Member Data Documentation

4.12.1.1 double EX09_DATA::h

4.12.1.2 double EX09_DATA::k

4.12.1.3 Matrix<double> EX09_DATA::M

4.12.1.4 int EX09_DATA::N

4.12.1.5 Matrix<double> EX09_DATA::p

4.12.1.6 Matrix<double> EX09_DATA::s

4.12.1.7 Matrix<double> EX09_DATA::x

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

- lark.h

4.13 EX15_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int N
- int m
- Matrix< double > b

4.13.1 Member Data Documentation

4.13.1.1 Matrix<double> EX15_DATA::b

4.13.1.2 int EX15_DATA::m

4.13.1.3 int EX15_DATA::N

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

- lark.h

4.14 FINCH_DATA Struct Reference

```
#include <finch.h>
```

Public Attributes

- int d = 0
- double dt = 0.0125
- double dt_old = 0.0125
- double T = 1.0
- double dz = 0.1
- double L = 1.0
- double s = 1.0
- double t = 0.0
- double t_old = 0.0
- double uT = 0.0
- double uT_old = 0.0
- double uAvg = 0.0
- double uAvg_old = 0.0
- double uIC = 0.0
- double vIC = 1.0
- double DIC = 1.0
- double kIC = 1.0
- double RIC = 1.0
- double uo = 1.0
- double vo = 1.0
- double Do = 1.0
- double ko = 1.0
- double Ro = 1.0
- double kfn = 1.0
- double kfnp1 = 1.0
- double lambda_I
- double lambda_E
- int LN = 10
- bool CN = true
- bool Update = false
- bool Dirichlet = false
- bool CheckMass = false
- bool ExplicitFlux = false
- bool Iterative = true
- bool SteadyState = false
- bool NormTrack = true
- double beta = 0.5
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- int max_iter = 20
- int total_iter = 0

- int nl_method = FINCH_Picard
- std::vector< double > CL_I
- std::vector< double > CL_E
- std::vector< double > CC_I
- std::vector< double > CC_E
- std::vector< double > CR_I
- std::vector< double > CR_E
- std::vector< double > fL_I
- std::vector< double > fL_E
- std::vector< double > fC_I
- std::vector< double > fC_E
- std::vector< double > fR_I
- std::vector< double > fR_E
- std::vector< double > OI
- std::vector< double > OE
- std::vector< double > NI
- std::vector< double > NE
- std::vector< double > MI
- std::vector< double > ME
- std::vector< double > uz_l_I
- std::vector< double > uz_lm1_I
- std::vector< double > uz_lp1_I
- std::vector< double > uz_l_E
- std::vector< double > uz_lm1_E
- std::vector< double > uz_lp1_E
- Matrix< double > unm1
- Matrix< double > un
- Matrix< double > unp1
- Matrix< double > u_star
- Matrix< double > ubest
- Matrix< double > vn
- Matrix< double > vnp1
- Matrix< double > Dn
- Matrix< double > Dnp1
- Matrix< double > kn
- Matrix< double > knp1
- Matrix< double > Sn
- Matrix< double > Snp1
- Matrix< double > Rn
- Matrix< double > Rnp1
- Matrix< double > Fn
- Matrix< double > Fnp1
- Matrix< double > gI
- Matrix< double > gE
- Matrix< double > res
- Matrix< double > pres
- int(∗ callroutine)(const void ∗user_data)
- int(∗ setic)(const void ∗user_data)
- int(∗ settime)(const void ∗user_data)
- int(∗ setpreprocess)(const void ∗user_data)
- int(∗ solve)(const void ∗user_data)
- int(∗ setparams)(const void ∗user_data)
- int(∗ discretize)(const void ∗user_data)
- int(∗ setbcs)(const void ∗user_data)
- int(∗ evalres)(const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)

- int(∗ evalprecon)(const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)
- int(∗ setpostprocess)(const void ∗user_data)
- int(∗ resettime)(const void ∗user_data)
- PICARD_DATA picard_dat
- PJFNK_DATA pjfnk_dat
- const void ∗ param_data

4.14.1 Member Data Documentation

4.14.1.1 double FINCH_DATA::beta = 0.5

4.14.1.2 int(∗ FINCH_DATA::callroutine)(const void ∗user_data)

4.14.1.3 std::vector<double> FINCH_DATA::CC_E

4.14.1.4 std::vector<double> FINCH_DATA::CC_I

4.14.1.5 bool FINCH_DATA::CheckMass = false

4.14.1.6 std::vector<double> FINCH_DATA::CL_E

4.14.1.7 std::vector<double> FINCH_DATA::CL_I

4.14.1.8 bool FINCH_DATA::CN = true

4.14.1.9 std::vector<double> FINCH_DATA::CR_E

4.14.1.10 std::vector<double> FINCH_DATA::CR_I

4.14.1.11 int FINCH_DATA::d = 0

4.14.1.12 double FINCH_DATA::DIC = 1.0

4.14.1.13 bool FINCH_DATA::Dirichlet = false

4.14.1.14 int(∗ FINCH_DATA::discretize)(const void ∗user_data)

4.14.1.15 Matrix<double> FINCH_DATA::Dn

4.14.1.16 Matrix<double> FINCH_DATA::Dnp1

4.14.1.17 double FINCH_DATA::Do = 1.0

4.14.1.18 double FINCH_DATA::dt = 0.0125

4.14.1.19 double FINCH_DATA::dt_old = 0.0125

4.14.1.20 double FINCH_DATA::dz = 0.1

4.14.1.21 int(∗ FINCH_DATA::evalprecon)(const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)

4.14.1.22 int(∗ FINCH_DATA::evalres)(const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)

4.14.1.23 bool FINCH_DATA::ExplicitFlux = false

4.14.1.24 std::vector<double> FINCH_DATA::fC_E

4.14.1.25 std::vector<double> FINCH_DATA::fC_I

4.14.1.26 std::vector<double> FINCH_DATA::fL_E

4.14.1.27 std::vector<double> FINCH_DATA::fL_I

4.14.1.28 Matrix<double> FINCH_DATA::Fn

4.14.1.29 Matrix<double> FINCH_DATA::Fnp1

4.14.1.30 std::vector<double> FINCH_DATA::fR_E

4.14.1.31 std::vector<double> FINCH_DATA::fR_I

4.14.1.32 Matrix<double> FINCH_DATA::gE

4.14.1.33 Matrix<double> FINCH_DATA::gI

4.14.1.34 bool FINCH_DATA::Iterative = true

4.14.1.35 double FINCH_DATA::kfn = 1.0

4.14.1.36 double FINCH_DATA::kfnp1 = 1.0

4.14.1.37 double FINCH_DATA::kIC = 1.0

4.14.1.38 Matrix<double> FINCH_DATA::kn

4.14.1.39 Matrix<double> FINCH_DATA::knp1

4.14.1.40 double FINCH_DATA::ko = 1.0

4.14.1.41 double FINCH_DATA::L = 1.0

4.14.1.42 double FINCH_DATA::lambda_E

4.14.1.43 double FINCH_DATA::lambda_I

4.14.1.44 int FINCH_DATA::LN = 10

4.14.1.45 int FINCH_DATA::max_iter = 20

4.14.1.46 std::vector<double> FINCH_DATA::ME

4.14.1.47 std::vector<double> FINCH_DATA::MI

4.14.1.48 std::vector<double> FINCH_DATA::NE

4.14.1.49 std::vector<double> FINCH_DATA::NI

4.14.1.50 int FINCH_DATA::nl_method = FINCH_Picard

4.14.1.51 bool FINCH_DATA::NormTrack = true

4.14.1.52 std::vector<double> FINCH_DATA::OE

4.14.1.53 std::vector<double> FINCH_DATA::OI

4.14.1.54 const void* FINCH_DATA::param_data

4.14.1.55 PICARD_DATA FINCH_DATA::picard_dat

4.14.1.56 PJFNK_DATA FINCH_DATA::pjfnk_dat

4.14.1.57 Matrix<double> FINCH_DATA::pres

4.14.1.58 Matrix<double> FINCH_DATA::res

4.14.1.59 int(* FINCH_DATA::resettime)(const void *user_data)

4.14.1.60 double FINCH_DATA::RIC = 1.0

4.14.1.61 Matrix<double> FINCH_DATA::Rn

4.14.1.62 Matrix<double> FINCH_DATA::Rnp1

4.14.1.63 double FINCH_DATA::Ro = 1.0

4.14.1.64 double FINCH_DATA::s = 1.0

4.14.1.65 int(* FINCH_DATA::setbcs)(const void *user_data)

4.14.1.66 int(* FINCH_DATA::setic)(const void *user_data)

4.14.1.67 int(* FINCH_DATA::setparams)(const void *user_data)

4.14.1.68 int(* FINCH_DATA::setpostprocess)(const void *user_data)

4.14.1.69 int(* FINCH_DATA::setpreprocess)(const void *user_data)

4.14.1.70 int(* FINCH_DATA::settime)(const void *user_data)

4.14.1.71 Matrix<double> FINCH_DATA::Sn

4.14.1.72 Matrix<double> FINCH_DATA::Snp1

4.14.1.73 int(* FINCH_DATA::solve)(const void *user_data)

4.14.1.74 bool FINCH_DATA::SteadyState = false

4.14.1.75 double FINCH_DATA::T = 1.0

4.14.1.76 double FINCH_DATA::t = 0.0

4.14.1.77 double FINCH_DATA::t_old = 0.0

4.14.1.78 double FINCH_DATA::tol_abs = 1e-6

4.14.1.79 double FINCH_DATA::tol_rel = 1e-6

4.14.1.80 int FINCH_DATA::total_iter = 0

4.14.1.81 Matrix<double> FINCH_DATA::u_star

4.14.1.82 double FINCH_DATA::uAvg = 0.0

4.14.1.83 double FINCH_DATA::uAvg_old = 0.0

4.14.1.84 Matrix<double> FINCH_DATA::ubest

4.14.1.85 double FINCH_DATA::uIC = 0.0

4.14.1.86 Matrix<double> FINCH_DATA::un

4.14.1.87 Matrix<double> FINCH_DATA::unm1

4.14.1.88 Matrix<double> FINCH_DATA::unp1

4.14.1.89 double FINCH_DATA::uo = 1.0

4.14.1.90 bool FINCH_DATA::Update = false

4.14.1.91 double FINCH_DATA::uT = 0.0

4.14.1.92 double FINCH_DATA::uT_old = 0.0

4.14.1.93 std::vector<double> FINCH_DATA::uz_l_E

4.14.1.94 std::vector<double> FINCH_DATA::uz_l_I

4.14.1.95 std::vector<double> FINCH_DATA::uz_lm1_E

4.14.1.96 std::vector<double> FINCH_DATA::uz_lm1_I

4.14.1.97 std::vector<double> FINCH_DATA::uz_lp1_E

4.14.1.98 std::vector<double> FINCH_DATA::uz_lp1_I

4.14.1.99 double FINCH_DATA::vIC = 1.0

4.14.1.100 Matrix<double> FINCH_DATA::vn

4.14.1.101 Matrix<double> FINCH_DATA::vnp1

4.14.1.102 double FINCH_DATA::vo = 1.0

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

- finch.h

4.15 GCR_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int restart = -1
- int maxit = 0
- int iter_outer = 0
- int iter_inner = 0
- int total_iter = 0
- bool breakdown = false
- double alpha
- double beta
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x
- Matrix< double > bestx
- Matrix< double > r
- Matrix< double > c_temp
- Matrix< double > u_temp
- std::vector< Matrix< double > > u
- std::vector< Matrix< double > > c
- OPTRANS_DATA transpose_dat

4.15.1 Member Data Documentation

4.15.1.1 double GCR_DATA::alpha

4.15.1.2 double GCR_DATA::bestres

4.15.1.3 Matrix<double> GCR_DATA::bestx

4.15.1.4 double GCR_DATA::beta

4.15.1.5 bool GCR_DATA::breakdown = false

4.15.1.6 std::vector<Matrix<double> > GCR_DATA::c

4.15.1.7 Matrix<double> GCR_DATA::c_temp

4.15.1.8 int GCR_DATA::iter_inner = 0

4.15.1.9 int GCR_DATA::iter_outer = 0

4.15.1.10 int GCR_DATA::maxit = 0

4.15.1.11 bool GCR_DATA::Output = true

4.15.1.12 Matrix<double> GCR_DATA::r

4.15.1.13 double GCR_DATA::relres

4.15.1.14 double GCR_DATA::relres_base

4.15.1.15 double GCR_DATA::res

4.15.1.16 int GCR_DATA::restart = -1

4.15.1.17 double GCR_DATA::tol_abs = 1e-6

4.15.1.18 double GCR_DATA::tol_rel = 1e-6

4.15.1.19 int GCR_DATA::total_iter = 0

4.15.1.20 OPTRANS_DATA GCR_DATA::transpose_dat

4.15.1.21 std::vector<Matrix<double> > GCR_DATA::u

4.15.1.22 Matrix<double> GCR_DATA::u_temp

4.15.1.23 Matrix<double> GCR_DATA::x

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

- lark.h

4.16 GMRESLP_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int restart = -1
- int maxit = 0
- int iter = 0
- int steps = 0
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x
- Matrix< double > bestx
- Matrix< double > r
- ARNOLDI_DATA arnoldi_dat

4.16.1 Member Data Documentation

4.16.1.1 ARNOLDI_DATA GMRESLP_DATA::arnoldi_dat

4.16.1.2 double GMRESLP_DATA::bestres

4.16.1.3 Matrix<double> GMRESLP_DATA::bestx

4.16.1.4 int GMRESLP_DATA::iter = 0

4.16.1.5 int GMRESLP_DATA::maxit = 0

4.16.1.6 bool GMRESLP_DATA::Output = true

4.16.1.7 Matrix<double> GMRESLP_DATA::r

4.16.1.8 double GMRESLP_DATA::relres

4.16.1.9 double GMRESLP_DATA::relres_base

4.16.1.10 double GMRESLP_DATA::res

4.16.1.11 int GMRESLP_DATA::restart = -1

4.16.1.12 int GMRESLP_DATA::steps = 0

4.16.1.13 double GMRESLP_DATA::tol_abs = 1e-6

4.16.1.14 double GMRESLP_DATA::tol_rel = 1e-6

4.16.1.15 Matrix<double> GMRESLP_DATA::x

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

- lark.h

4.17 GMRESR_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int gcr_restart = -1
- int gcr_maxit = 0
- int gmres_restart = -1
- int gmres_maxit = 1
- int N
- int total_iter
- int iter_outer
- int iter_inner
- bool GCR_Output = true
- bool GMRES_Output = false
- double gmres_tol = 0.1
- double gcr_rel_tol = 1e-6
- double gcr_abs_tol = 1e-6
- Matrix< double > arg
- GCR_DATA gcr_dat
- GMRESRP_DATA gmres_dat
- int(∗ matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)
- int(∗ terminal_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)
- const void ∗ matvec_data
- const void ∗ term_precon

4.17.1 Member Data Documentation

4.17.1.1 Matrix< double > GMRESR_DATA::arg

4.17.1.2 double GMRESR_DATA::gcr_abs_tol = 1e-6

4.17.1.3 GCR_DATA GMRESR_DATA::gcr_dat

4.17.1.4 int GMRESR_DATA::gcr_maxit = 0

4.17.1.5 bool GMRESR_DATA::GCR_Output = true

4.17.1.6 double GMRESR_DATA::gcr_rel_tol = 1e-6

4.17.1.7 int GMRESR_DATA::gcr_restart = -1

4.17.1.8 GMRESRP_DATA GMRESR_DATA::gmres_dat

4.17.1.9 int GMRESR_DATA::gmres_maxit = 1

4.17.1.10 bool GMRESR_DATA::GMRES_Output = false

4.17.1.11 int GMRESR_DATA::gmres_restart = -1

4.17.1.12 double GMRESR_DATA::gmres_tol = 0.1

4.17.1.13 int GMRESR_DATA::iter_inner

4.17.1.14 int GMRESR_DATA::iter_outer

4.17.1.15 int(∗ GMRESR_DATA::matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)

4.17.1.16 const void∗ GMRESR_DATA::matvec_data

4.17.1.17 int GMRESR_DATA::N

4.17.1.18 const void∗ GMRESR_DATA::term_precon

4.17.1.19 int(∗ GMRESR_DATA::terminal_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)

4.17.1.20 int GMRESR_DATA::total_iter

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

- lark.h

4.18 GMRESRP_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int restart = -1

- int maxit = 0
- int iter_outer = 0
- int iter_inner = 0
- int iter_total = 0
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x
- Matrix< double > bestx
- Matrix< double > r
- std::vector< Matrix< double > > Vk
- std::vector< std::vector
  < double > > H
- std::vector< std::vector
  < double > > H_bar
- std::vector< double > y
- std::vector< double > e0
- std::vector< double > e0_bar
- Matrix< double > w
- Matrix< double > v
- Matrix< double > sum

4.18.1 Member Data Documentation

4.18.1.1 double GMRESRP_DATA::bestres

4.18.1.2 Matrix<double> GMRESRP_DATA::bestx

4.18.1.3 std::vector< double > GMRESRP_DATA::e0

4.18.1.4 std::vector< double > GMRESRP_DATA::e0_bar

4.18.1.5 std::vector< std::vector< double > > GMRESRP_DATA::H

4.18.1.6 std::vector< std::vector< double > > GMRESRP_DATA::H_bar

4.18.1.7 int GMRESRP_DATA::iter_inner = 0

4.18.1.8 int GMRESRP_DATA::iter_outer = 0

4.18.1.9 int GMRESRP_DATA::iter_total = 0

4.18.1.10 int GMRESRP_DATA::maxit = 0

4.18.1.11 bool GMRESRP_DATA::Output = true

4.18.1.12 Matrix<double> GMRESRP_DATA::r

4.18.1.13 double GMRESRP_DATA::relres

4.18.1.14 double GMRESRP_DATA::relres_base

4.18.1.15 double GMRESRP_DATA::res

4.18.1.16 int GMRESRP_DATA::restart = -1

4.18.1.17 Matrix<double> GMRESRP_DATA::sum

4.18.1.18 double GMRESRP_DATA::tol_abs = 1e-6

4.18.1.19 double GMRESRP_DATA::tol_rel = 1e-6

4.18.1.20 Matrix<double> GMRESRP_DATA::v

4.18.1.21 std::vector< Matrix<double> > GMRESRP_DATA::Vk

4.18.1.22 Matrix<double> GMRESRP_DATA::w

4.18.1.23 Matrix<double> GMRESRP_DATA::x

4.18.1.24 std::vector< double > GMRESRP_DATA::y

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

- lark.h

4.19 GPAST_DATA Struct Reference

```
#include <magpie.h>
```

Public Attributes

- double x
- double y
- double He
- double q
- std::vector< double > gama_inf
- double qo
- double Plo
- std::vector< double > po
- double poi
- bool present

4.19.1 Member Data Documentation

4.19.1.1 std::vector<double> GPAST_DATA::gama_inf

4.19.1.2 double GPAST_DATA::He

4.19.1.3 double GPAST_DATA::Plo

4.19.1.4 std::vector<double> GPAST_DATA::po

4.19.1.5 double GPAST_DATA::poi

4.19.1.6 bool GPAST_DATA::present

4.19.1.7 double GPAST_DATA::q

4.19.1.8 double GPAST_DATA::qo

4.19.1.9 double GPAST_DATA::x

4.19.1.10 double GPAST_DATA::y

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

- magpie.h

4.20 GSTA_DATA Struct Reference

```
#include <magpie.h>
```

Public Attributes

- double qmax
- int m
- std::vector< double > dHo
- std::vector< double > dSo

4.20.1 Member Data Documentation

4.20.1.1 std::vector<double> GSTA_DATA::dHo

4.20.1.2 std::vector<double> GSTA_DATA::dSo

4.20.1.3 int GSTA_DATA::m

4.20.1.4 double GSTA_DATA::qmax

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

- magpie.h

4.21 GSTA_OPT_DATA Struct Reference

```
#include <gsta_opt.h>
```

Public Attributes

- int total_eval
- int n_par
- double qmax
- int iso
- std::vector< std::vector
< double > > Fobj

- std::vector< std::vector
  < double > > q
- std::vector< std::vector
  < double > > P
- std::vector< std::vector
  < double > > best_par
- std::vector< std::vector
  < double > > Kno
- std::vector< std::vector
  < std::vector< double > > > all_pars
- std::vector< std::vector
  < double > > norms
- std::vector< double > opt_qmax

4.21.1 Member Data Documentation

4.21.1.1 std::vector<std::vector<std::vector<double> > > GSTA_OPT_DATA::all_pars

4.21.1.2 std::vector<std::vector<double> > GSTA_OPT_DATA::best_par

4.21.1.3 std::vector<std::vector<double> > GSTA_OPT_DATA::Fobj

4.21.1.4 int GSTA_OPT_DATA::iso

4.21.1.5 std::vector<std::vector<double> > GSTA_OPT_DATA::Kno

4.21.1.6 int GSTA_OPT_DATA::n_par

4.21.1.7 std::vector<std::vector<double> > GSTA_OPT_DATA::norms

4.21.1.8 std::vector<double> GSTA_OPT_DATA::opt_qmax

4.21.1.9 std::vector<std::vector<double> > GSTA_OPT_DATA::P

4.21.1.10 std::vector<std::vector<double> > GSTA_OPT_DATA::q

4.21.1.11 double GSTA_OPT_DATA::qmax

4.21.1.12 int GSTA_OPT_DATA::total_eval

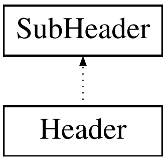
The documentation for this struct was generated from the following file:

- gsta_opt.h

4.22 Header Class Reference

```
#include <yaml_wrapper.h>
```

Inheritance diagram for Header:



Public Member Functions

- Header ()
- ∼Header ()
- Header (const Header &head)
- Header (std::string name)
- Header (const KeyValueMap &map)
- Header (std::string name, const KeyValueMap &map)
- Header (std::string key, const SubHeader &sub)
- Header & operator= (const Header &head)
- ValueTypePair & operator[] (const std::string key)
- ValueTypePair operator[] (const std::string key) const
- SubHeader & operator() (const std::string key)
- SubHeader operator() (const std::string key) const
- std::map< std::string,
  SubHeader > & getSubMap ()
- KeyValueMap & getDataMap ()
- SubHeader & getSubHeader (std::string key)
- std::map< std::string,
  SubHeader >::const_iterator end () const
- std::map< std::string,
  SubHeader >::iterator end ()
- std::map< std::string,
  SubHeader >::const_iterator begin () const
- std::map< std::string,
  SubHeader >::iterator begin ()
- void clear ()
- void resetKeys ()
- void changeKey (std::string oldKey, std::string newKey)
- void addPair (std::string key, std::string val)
- void addPair (std::string key, std::string val, int t)
- void setName (std::string name)
- void setAlias (std::string alias)
- void setNameAliasPair (std::string n, std::string a, int s)
- void setState (int state)
- void DisplayContents ()
- void addSubKey (std::string key)
- void copyAnchor2Alias (std::string alias, SubHeader &ref)
- int size ()
- std::string getName ()
- std::string getAlias ()
- int getState ()
- bool isAlias ()
- bool isAnchor ()
- SubHeader & getAnchoredSub (std::string alias)

Private Attributes

- std::map< std::string, SubHeader > Sub_Map

Additional Inherited Members

4.22.1 Constructor & Destructor Documentation

4.22.1.1 Header::Header ( )

4.22.1.2 Header::∼Header ( )

4.22.1.3 Header::Header (const Header & *head*)

4.22.1.4 Header::Header (std::string *name*)

4.22.1.5 Header::Header (const KeyValueMap & *map*)

4.22.1.6 Header::Header (std::string *name,* const KeyValueMap & *map*)

4.22.1.7 Header::Header (std::string *key,* const SubHeader & *sub*)

4.22.2 Member Function Documentation

4.22.2.1 void Header::addPair (std::string *key,* std::string *val*)

4.22.2.2 void Header::addPair (std::string *key,* std::string *val,* int *t*)

4.22.2.3 void Header::addSubKey (std::string *key*)

4.22.2.4 std::map< std::string, SubHeader >::const_iterator Header::begin ( ) const

4.22.2.5 std::map< std::string, SubHeader >::iterator Header::begin ( )

4.22.2.6 void Header::changeKey (std::string *oldKey,* std::string *newKey*)

4.22.2.7 void Header::clear ( )

4.22.2.8 void Header::copyAnchor2Alias (std::string *alias,* SubHeader & *ref*)

4.22.2.9 void Header::DisplayContents ( )

4.22.2.10 std::map< std::string, SubHeader >::const_iterator Header::end ( ) const

4.22.2.11 std::map< std::string, SubHeader >::iterator Header::end ( )

4.22.2.12 std::string Header::getAlias ( )

4.22.2.13 SubHeader & Header::getAnchoredSub (std::string *alias*)

4.22.2.14 KeyValueMap & Header::getDataMap ( )

4.22.2.15 std::string Header::getName ( )

4.22.2.16 int Header::getState ( )

4.22.2.17 SubHeader & Header::getSubHeader (std::string *key*)

4.22.2.18 std::map< std::string, SubHeader > & Header::getSubMap ( )

4.22.2.19 bool Header::isAlias ( )

4.22.2.20 bool Header::isAnchor ( )

4.22.2.21 SubHeader & Header::operator() (const std::string *key*)

4.22.2.22 SubHeader Header::operator() (const std::string *key*) const

4.22.2.23 Header & Header::operator= (const Header & *head*)

4.22.2.24 ValueTypePair & Header::operator[] (const std::string *key*)

4.22.2.25 ValueTypePair Header::operator[] (const std::string *key*) const

4.22.2.26 void Header::resetKeys ( )

4.22.2.27 void Header::setAlias (std::string *alias*)

4.22.2.28 void Header::setName (std::string *name*)

4.22.2.29 void Header::setNameAliasPair (std::string *n,* std::string *a,* int *s*)

4.22.2.30 void Header::setState (int *state*)

4.22.2.31 int Header::size ( )

4.22.3 Member Data Documentation

4.22.3.1 std::map<std::string, SubHeader> Header::Sub_Map [private]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.23 KeyValueMap Class Reference

```
#include <yaml_wrapper.h>
```

Public Member Functions

- KeyValueMap ()
- ∼KeyValueMap ()
- KeyValueMap (const std::map< std::string, std::string > &map)
- KeyValueMap (std::string key, std::string value)
- KeyValueMap (const KeyValueMap &map)
- KeyValueMap & operator= (const KeyValueMap &map)
- ValueTypePair & operator[] (const std::string key)
- ValueTypePair operator[] (const std::string key) const
- std::map< std::string,
  ValueTypePair > & getMap ()
- std::map< std::string,
  ValueTypePair >
  ::const_iterator end () const

- std::map< std::string,
  ValueTypePair >::iterator end ()
- std::map< std::string,
  ValueTypePair >
  ::const_iterator begin () const
- std::map< std::string,
  ValueTypePair >::iterator begin ()
- void clear ()
- void addKey (std::string key)
- void editValue4Key (std::string val, std::string key)
- void editValue4Key (std::string val, int type, std::string key)
- void addPair (std::string key, ValueTypePair val)
- void addPair (std::string key, std::string val)
- void addPair (std::string key, std::string val, int type)
- void findType (std::string key)
- void assertType (std::string key, int type)
- void findAllTypes ()
- void DisplayMap ()
- int size ()
- std::string getString (std::string key)
- bool getBool (std::string key)
- double getDouble (std::string key)
- int getInt (std::string key)
- std::string getValue (std::string key)
- int getType (std::string key)
- ValueTypePair & getPair (std::string key)

Private Attributes

- std::map< std::string,
  ValueTypePair > Key_Value

4.23.1 Constructor & Destructor Documentation

4.23.1.1 KeyValueMap::KeyValueMap ( )

4.23.1.2 KeyValueMap::∼KeyValueMap ( )

4.23.1.3 KeyValueMap::KeyValueMap (const std::map< std::string, std::string > & *map*)

4.23.1.4 KeyValueMap::KeyValueMap (std::string *key,* std::string *value*)

4.23.1.5 KeyValueMap::KeyValueMap (const KeyValueMap & *map*)

4.23.2 Member Function Documentation

4.23.2.1 void KeyValueMap::addKey (std::string *key*)

4.23.2.2 void KeyValueMap::addPair (std::string *key,* ValueTypePair *val*)

4.23.2.3 void KeyValueMap::addPair (std::string *key,* std::string *val*)

4.23.2.4 void KeyValueMap::addPair (std::string *key,* std::string *val,* int *type*)

4.23.2.5 void KeyValueMap::assertType (std::string *key,* int *type*)

4.23.2.6 std::map< std::string, **ValueTypePair** >::const_iterator KeyValueMap::begin ( ) const

4.23.2.7 std::map< std::string, **ValueTypePair** >::iterator KeyValueMap::begin ( )

4.23.2.8 void KeyValueMap::clear ( )

4.23.2.9 void KeyValueMap::DisplayMap ( )

4.23.2.10 void KeyValueMap::editValue4Key (std::string *val,* std::string *key*)

4.23.2.11 void KeyValueMap::editValue4Key (std::string *val,* int *type,* std::string *key*)

4.23.2.12 std::map< std::string, **ValueTypePair** >::const_iterator KeyValueMap::end ( ) const

4.23.2.13 std::map< std::string, **ValueTypePair** >::iterator KeyValueMap::end ( )

4.23.2.14 void KeyValueMap::findAllTypes ( )

4.23.2.15 void KeyValueMap::findType (std::string *key*)

4.23.2.16 bool KeyValueMap::getBool (std::string *key*)

4.23.2.17 double KeyValueMap::getDouble (std::string *key*)

4.23.2.18 int KeyValueMap::getInt (std::string *key*)

4.23.2.19 std::map< std::string, **ValueTypePair** > & KeyValueMap::getMap ( )

4.23.2.20 **ValueTypePair** & KeyValueMap::getPair (std::string *key*)

4.23.2.21 std::string KeyValueMap::getString (std::string *key*)

4.23.2.22 int KeyValueMap::getType (std::string *key*)

4.23.2.23 std::string KeyValueMap::getValue (std::string *key*)

4.23.2.24 **KeyValueMap** & KeyValueMap::operator= (const **KeyValueMap** & *map*)

4.23.2.25 **ValueTypePair** & KeyValueMap::operator[ ] (const std::string *key*)

4.23.2.26 **ValueTypePair** KeyValueMap::operator[ ] (const std::string *key*) const

4.23.2.27 int KeyValueMap::size ( )

4.23.3 Member Data Documentation

4.23.3.1 std::map<std::string, **ValueTypePair** > KeyValueMap::Key_Value `[private]`

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.24 MAGPIE_DATA Struct Reference

```
#include <magpie.h>
```

Public Attributes

- std::vector< GSTA_DATA > gsta_dat
- std::vector< mSPD_DATA > mspd_dat
- std::vector< GPAST_DATA > gpast_dat
- SYSTEM_DATA sys_dat

4.24.1 Member Data Documentation

4.24.1.1 std::vector<GPAST_DATA> MAGPIE_DATA::gpast_dat

4.24.1.2 std::vector<GSTA_DATA> MAGPIE_DATA::gsta_dat

4.24.1.3 std::vector<mSPD_DATA> MAGPIE_DATA::mspd_dat

4.24.1.4 SYSTEM_DATA MAGPIE_DATA::sys_dat

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

- magpie.h

4.25 MassBalance Class Reference

```
#include <shark.h>
```

Public Member Functions

- MassBalance ()
- ∼MassBalance ()
- void Initialize_List (MasterSpeciesList &List)
- void Display_Info ()
- void Set_Delta (int i, double v)
- void Set_TotalConcentration (double v)
- void Set_Name (std::string name)
- double Get_Delta (int i)
- double Sum_Delta ()
- double Get_TotalConcentration ()
- std::string Get_Name ()
- double Eval_Residual (const Matrix< double > &x)

Protected Attributes

- MasterSpeciesList ∗ List
- std::vector< double > Delta
- double TotalConcentration

Private Attributes

- std::string Name

4.25.1 Constructor & Destructor Documentation

4.25.1.1 MassBalance::MassBalance ( )

4.25.1.2 MassBalance::∼MassBalance ( )

4.25.2 Member Function Documentation

4.25.2.1 void MassBalance::Display_Info ( )

4.25.2.2 double MassBalance::Eval_Residual (const **Matrix**< double > & *x*)

4.25.2.3 double MassBalance::Get_Delta (int *i*)

4.25.2.4 std::string MassBalance::Get_Name ( )

4.25.2.5 double MassBalance::Get_TotalConcentration ( )

4.25.2.6 void MassBalance::Initialize_List (**MasterSpeciesList** & *List*)

4.25.2.7 void MassBalance::Set_Delta (int *i*, double *v*)

4.25.2.8 void MassBalance::Set_Name (std::string *name*)

4.25.2.9 void MassBalance::Set_TotalConcentration (double *v*)

4.25.2.10 double MassBalance::Sum_Delta ( )

4.25.3 Member Data Documentation

4.25.3.1 std::vector<double> MassBalance::Delta [protected]

4.25.3.2 MasterSpeciesList∗ MassBalance::List [protected]

4.25.3.3 std::string MassBalance::Name [private]

4.25.3.4 double MassBalance::TotalConcentration [protected]

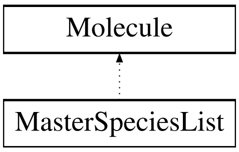
The documentation for this class was generated from the following files:

- shark.h
- shark.cpp

4.26 MasterSpeciesList Class Reference

```
#include <shark.h>
```

Inheritance diagram for MasterSpeciesList:



Public Member Functions

- MasterSpeciesList ()
- ∼MasterSpeciesList ()
- MasterSpeciesList (const MasterSpeciesList &msl)
- MasterSpeciesList & operator= (const MasterSpeciesList &msl)
- void set_list_size (int i)
- void set_species (int i, std::string formula)
- void set_species (int i, int charge, double enthalpy, double entropy, double energy, bool HS, bool G, std::string Phase, std::string Name, std::string Formula, std::string lin_formula)
- void DisplayInfo (int i)
- void DisplayAll ()
- void DisplayConcentrations (Matrix< double > &C)
- void set_alkalinity (double alk)
- int list_size ()
- Molecule & get_species (int i)
- int get_index (std::string name)
- double charge (int i)
- double alkalinity ()
- std::string speciesName (int i)
- double Eval_ChargeResidual (const Matrix< double > &x)

Protected Attributes

- int size
- std::vector< Molecule > species
- double residual_alkalinity

Additional Inherited Members

4.26.1 Constructor & Destructor Documentation

4.26.1.1 MasterSpeciesList::MasterSpeciesList ( )

4.26.1.2 MasterSpeciesList::∼MasterSpeciesList ( )

4.26.1.3 MasterSpeciesList::MasterSpeciesList (const MasterSpeciesList & *msl*)

4.26.2 Member Function Documentation

4.26.2.1 double MasterSpeciesList::alkalinity ( )

4.26.2.2 double MasterSpeciesList::charge (int *i*)

4.26.2.3 void MasterSpeciesList::DisplayAll ( )

4.26.2.4 void MasterSpeciesList::DisplayConcentrations (Matrix< double > & *C*)

4.26.2.5 void MasterSpeciesList::DisplayInfo (int *i*)

4.26.2.6 double MasterSpeciesList::Eval_ChargeResidual (const Matrix< double > & *x*)

4.26.2.7 int MasterSpeciesList::get_index (std::string *name*)

4.26.2.8 Molecule & MasterSpeciesList::get_species (int *i*)

4.26.2.9 int MasterSpeciesList::list_size ( )

4.26.2.10 MasterSpeciesList & MasterSpeciesList::operator= (const MasterSpeciesList & *msl*)

4.26.2.11 void MasterSpeciesList::set_alkalinity (double *alk*)

4.26.2.12 void MasterSpeciesList::set_list_size (int *i*)

4.26.2.13 void MasterSpeciesList::set_species (int *i,* std::string *formula*)

4.26.2.14 void MasterSpeciesList::set_species (int *i,* int *charge,* double *enthalpy,* double *entropy,* double *energy,* bool *HS,* bool *G,* std::string *Phase,* std::string *Name,* std::string *Formula,* std::string *lin_formula*)

4.26.2.15 std::string MasterSpeciesList::speciesName (int *i*)

4.26.3 Member Data Documentation

4.26.3.1 double MasterSpeciesList::residual_alkalinity [protected]

4.26.3.2 int MasterSpeciesList::size [protected]

4.26.3.3 std::vector<Molecule> MasterSpeciesList::species [protected]

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

- shark.h
- shark.cpp

4.27 Matrix< T > Class Template Reference

```
#include <macaw.h>
```

Public Member Functions

- Matrix (int rows, int columns)
- T & operator() (int i, int j)
- T operator() (int i, int j) const
- Matrix (const Matrix &M)
- Matrix & operator= (const Matrix &M)
- Matrix ()
- ∼Matrix ()
- void set_size (int i, int j)
- void zeros ()
- void edit (int i, int j, T value)

- int rows ()
- int columns ()
- T determinate ()
- T norm ()
- T sum ()
- T inner_product (const Matrix &x)
- Matrix & cofactor (const Matrix &M)
- Matrix operator+ (const Matrix &M)
- Matrix operator- (const Matrix &M)
- Matrix operator* (const T)
- Matrix operator/ (const T)
- Matrix operator* (const Matrix &M)
- Matrix & transpose (const Matrix &M)
- Matrix & transpose_multiply (const Matrix &MT, const Matrix &v)
- Matrix & adjoint (const Matrix &M)
- Matrix & inverse (const Matrix &M)
- void Display (const std::string Name)
- Matrix & tridiagonalSolve (const Matrix &A, const Matrix &b)
- Matrix & ladshawSolve (const Matrix &A, const Matrix &d)
- Matrix & tridiagonalFill (const T A, const T B, const T C, bool Spherical)
- Matrix & naturalLaplacian3D (int m)
- Matrix & sphericalBCFill (int node, const T coeff, T variable)
- Matrix & ConstantICFill (const T IC)
- Matrix & SolnTransform (const Matrix &A, bool Forward)
- T sphericalAvg (double radius, double dr, double bound, bool Dirichlet)
- T IntegralAvg (double radius, double dr, double bound, bool Dirichlet)
- T IntegralTotal (double dr, double bound, bool Dirichlet)
- Matrix & tridiagonalVectorFill (const std::vector< T > &A, const std::vector< T > &B, const std::vector< T > &C)
- Matrix & columnVectorFill (const std::vector< T > &A)
- Matrix & columnProjection (const Matrix &b, const Matrix &b_old, const double dt, const double dt_old)
- Matrix & dirichletBCFill (int node, const T coeff, T variable)
- Matrix & diagonalSolve (const Matrix &D, const Matrix &v)
- Matrix & upperTriangularSolve (const Matrix &U, const Matrix &v)
- Matrix & lowerTriangularSolve (const Matrix &L, const Matrix &v)
- Matrix & upperHessenberg2Triangular (Matrix &b)
- Matrix & lowerHessenberg2Triangular (Matrix &b)
- Matrix & upperHessenbergSolve (const Matrix &H, const Matrix &v)
- Matrix & lowerHessenbergSolve (const Matrix &H, const Matrix &v)
- Matrix & columnExtract (int j, const Matrix &M)
- Matrix & rowExtract (int i, const Matrix &M)
- Matrix & columnReplace (int j, const Matrix &v)
- Matrix & rowReplace (int i, const Matrix &v)
- void rowShrink ()
- void columnShrink ()
- void rowExtend (const Matrix &v)
- void columnExtend (const Matrix &v)

Protected Attributes

- int num_rows
- int num_cols
- std::vector< T > Data

4.27.1 Constructor & Destructor Documentation

4.27.1.1 template<class T > **Matrix**< T >::**Matrix** (int *rows,* int *columns*)

4.27.1.2 template<class T > **Matrix**< T >::**Matrix** (const **Matrix**< T > & *M*)

4.27.1.3 template<class T > **Matrix**< T >::**Matrix** ( )

4.27.1.4 template<class T > **Matrix**< T >::∼**Matrix** ( )

4.27.2 Member Function Documentation

4.27.2.1 template<class T > **Matrix**< T > & **Matrix**< T >::adjoint (const **Matrix**< T > & *M*)

4.27.2.2 template<class T > **Matrix**< T > & **Matrix**< T >::cofactor (const **Matrix**< T > & *M*)

4.27.2.3 template<class T > void **Matrix**< T >::columnExtend (const **Matrix**< T > & *v*)

4.27.2.4 template<class T > **Matrix**< T > & **Matrix**< T >::columnExtract (int *j,* const **Matrix**< T > & *M*)

4.27.2.5 template<class T > **Matrix**< T > & **Matrix**< T >::columnProjection (const **Matrix**< T > & *b,* const **Matrix**< T > & *b_old,* const double *dt,* const double *dt_old*)

4.27.2.6 template<class T > **Matrix**< T > & **Matrix**< T >::columnReplace (int *j,* const **Matrix**< T > & *v*)

4.27.2.7 template<class T > int **Matrix**< T >::columns ( )

4.27.2.8 template<class T > void **Matrix**< T >::columnShrink ( )

4.27.2.9 template<class T> **Matrix**< T > & **Matrix**< T >::columnVectorFill (const std::vector< T > & *A*)

4.27.2.10 template<class T> **Matrix**< T > & **Matrix**< T >::ConstantICFill (const T *IC*)

4.27.2.11 template<class T > T **Matrix**< T >::determinate ( )

4.27.2.12 template<class T > **Matrix**< T > & **Matrix**< T >::diagonalSolve (const **Matrix**< T > & *D,* const **Matrix**< T > & *v*)

4.27.2.13 template<class T> **Matrix**< T > & **Matrix**< T >::dirichletBCFill (int *node,* const T *coeff,* T *variable*)

4.27.2.14 template<class T > void **Matrix**< T >::Display (const std::string *Name*)

4.27.2.15 template<class T> void **Matrix**< T >::edit (int *i,* int *j,* T *value*)

4.27.2.16 template<class T > T **Matrix**< T >::inner_product (const **Matrix**< T > & *x*)

4.27.2.17 template<class T > T **Matrix**< T >::IntegralAvg (double *radius,* double *dr,* double *bound,* bool *Dirichlet*)

4.27.2.18 template<class T > T **Matrix**< T >::IntegralTotal (double *dr,* double *bound,* bool *Dirichlet*)

4.27.2.19 template<class T > **Matrix**< T > & **Matrix**< T >::inverse (const **Matrix**< T > & *M*)

4.27.2.20 template<class T > **Matrix**< T > & **Matrix**< T >::ladshawSolve (const **Matrix**< T > & *A,* const **Matrix**< T > & *d*)

4.27.2.21 template<class T > **Matrix**< T > & **Matrix**< T >::lowerHessenberg2Triangular (**Matrix**< T > & *b*)

4.27.2.22 template<class T > Matrix< T > & Matrix< T >::lowerHessenbergSolve (const Matrix< T > & *H*, const Matrix< T > & *v*)

4.27.2.23 template<class T > Matrix< T > & Matrix< T >::lowerTriangularSolve (const Matrix< T > & *L*, const Matrix< T > & *v*)

4.27.2.24 template<class T > Matrix< T > & Matrix< T >::naturalLaplacian3D (int *m*)

4.27.2.25 template<class T > T Matrix< T >::norm ( )

4.27.2.26 template<class T > T & Matrix< T >::operator() (int *i*, int *j*)

4.27.2.27 template<class T > T Matrix< T >::operator() (int *i*, int *j*) const

4.27.2.28 template<class T> Matrix< T > Matrix< T >::operator* (const T *a*)

4.27.2.29 template<class T> Matrix< T > Matrix< T >::operator* (const Matrix< T > & *M*)

4.27.2.30 template<class T > Matrix< T > Matrix< T >::operator+ (const Matrix< T > & *M*)

4.27.2.31 template<class T > Matrix< T > Matrix< T >::operator- (const Matrix< T > & *M*)

4.27.2.32 template<class T> Matrix< T > Matrix< T >::operator/ (const T *a*)

4.27.2.33 template<class T > Matrix< T > & Matrix< T >::operator= (const Matrix< T > & *M*)

4.27.2.34 template<class T > void Matrix< T >::rowExtend (const Matrix< T > & *v*)

4.27.2.35 template<class T > Matrix< T > & Matrix< T >::rowExtract (int *i*, const Matrix< T > & *M*)

4.27.2.36 template<class T > Matrix< T > & Matrix< T >::rowReplace (int *i*, const Matrix< T > & *v*)

4.27.2.37 template<class T > int Matrix< T >::rows ( )

4.27.2.38 template<class T > void Matrix< T >::rowShrink ( )

4.27.2.39 template<class T > void Matrix< T >::set_size (int *i*, int *j*)

4.27.2.40 template<class T > Matrix< T > & Matrix< T >::SolnTransform (const Matrix< T > & *A*, bool *Forward*)

4.27.2.41 template<class T > T Matrix< T >::sphericalAvg (double *radius*, double *dr*, double *bound*, bool *Dirichlet*)

4.27.2.42 template<class T> Matrix< T > & Matrix< T >::sphericalBCFill (int *node*, const T *coeff*, T *variable*)

4.27.2.43 template<class T > T Matrix< T >::sum ( )

4.27.2.44 template<class T > Matrix< T > & Matrix< T >::transpose (const Matrix< T > & *M*)

4.27.2.45 template<class T > Matrix< T > & Matrix< T >::transpose_multiply (const Matrix< T > & *MT*, const Matrix< T > & *v*)

4.27.2.46 template<class T> Matrix< T > & Matrix< T >::tridiagonalFill (const T *A*, const T *B*, const T *C*, bool *Spherical*)

4.27.2.47 template<class T > Matrix< T > & Matrix< T >::tridiagonalSolve (const Matrix< T > & *A*, const Matrix< T > & *b*)

4.27.2.48 template<class T> Matrix< T > & Matrix< T >::tridiagonalVectorFill (const std::vector< T > & *A*, const std::vector< T > & *B*, const std::vector< T > & *C*)

4.27.2.49 template<class T > Matrix< T > & Matrix< T >::upperHessenberg2Triangular (Matrix< T > & *b*)

4.27.2.50 template<class T > Matrix< T > & Matrix< T >::upperHessenbergSolve (const Matrix< T > & *H*, const Matrix< T > & *v*)

4.27.2.51 template<class T > Matrix< T > & Matrix< T >::upperTriangularSolve (const Matrix< T > & *U*, const Matrix< T > & *v*)

4.27.2.52 template<class T > void Matrix< T >::zeros ( )

4.27.3 Member Data Documentation

4.27.3.1 template<class T> std::vector<T> Matrix< T >::Data `[protected]`

4.27.3.2 template<class T> int Matrix< T >::num_cols `[protected]`

4.27.3.3 template<class T> int Matrix< T >::num_rows `[protected]`

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

- macaw.h

4.28 Mechanism Class Reference

`#include <shark.h>`

Protected Attributes

- MasterSpeciesList ∗ List
- std::vector< UnsteadyReaction > reactions
- std::vector< double > weight
- int species_index

4.28.1 Member Data Documentation

4.28.1.1 MasterSpeciesList∗ Mechanism::List `[protected]`

4.28.1.2 std::vector<UnsteadyReaction> Mechanism::reactions `[protected]`

4.28.1.3 int Mechanism::species_index `[protected]`

4.28.1.4 std::vector<double> Mechanism::weight `[protected]`

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

- shark.h

4.29 MIXED_GAS Struct Reference

`#include <egret.h>`

Public Attributes

- int N
- bool CheckMolefractions = true
- double total_pressure
- double gas_temperature
- double velocity
- double char_length
- std::vector< double > molefraction
- double total_density
- double total_dyn_vis
- double kinematic_viscosity
- double total_molecular_weight
- double total_specific_heat
- double Reynolds
- Matrix< double > binary_diffusion
- std::vector< PURE_GAS > species_dat

4.29.1 Member Data Documentation

4.29.1.1 Matrix<double> MIXED_GAS::binary_diffusion

4.29.1.2 double MIXED_GAS::char_length

4.29.1.3 bool MIXED_GAS::CheckMolefractions = true

4.29.1.4 double MIXED_GAS::gas_temperature

4.29.1.5 double MIXED_GAS::kinematic_viscosity

4.29.1.6 std::vector<double> MIXED_GAS::molefraction

4.29.1.7 int MIXED_GAS::N

4.29.1.8 double MIXED_GAS::Reynolds

4.29.1.9 std::vector<PURE_GAS> MIXED_GAS::species_dat

4.29.1.10 double MIXED_GAS::total_density

4.29.1.11 double MIXED_GAS::total_dyn_vis

4.29.1.12 double MIXED_GAS::total_molecular_weight

4.29.1.13 double MIXED_GAS::total_pressure

4.29.1.14 double MIXED_GAS::total_specific_heat

4.29.1.15 double MIXED_GAS::velocity

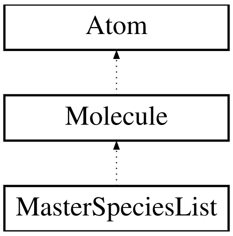
The documentation for this struct was generated from the following file:

- egret.h

4.30 Molecule Class Reference

```
#include <mola.h>
```

Inheritance diagram for Molecule:



Public Member Functions

- Molecule ()
- ∼Molecule ()
- Molecule (int charge, double enthalpy, double entropy, double energy, bool HS, bool G, std::string Phase, std::string Name, std::string Formula, std::string lin_formula)
- void Register (int charge, double enthalpy, double entropy, double energy, bool HS, bool G, std::string Phase, std::string Name, std::string Formula, std::string lin_formula)
- void Register (std::string formula)
- void setFormula (std::string form)
- void recalculateMolarWeight ()
- void setMolarWeigth (double mw)
- void editCharge (int c)
- void editOneOxidationState (int state, std::string Symbol)
- void editAllOxidationStates (int state, std::string Symbol)
- void calculateAvgOxiState (std::string Symbol)
- void editEnthalpy (double enthalpy)
- void editEntropy (double entropy)
- void editHS (double H, double S)
- void editEnergy (double energy)
- void removeOneAtom (std::string Symbol)
- void removeAllAtoms (std::string Symbol)
- int Charge ()
- double MolarWeight ()
- bool HaveHS ()
- bool HaveEnergy ()
- bool isRegistered ()
- double Enthalpy ()
- double Entropy ()
- double Energy ()
- std::string MoleculeName ()
- std::string MolecularFormula ()
- std::string MoleculePhase ()
- void DisplayInfo ()

Protected Attributes

- int charge
- double molar_weight
- double formation_enthalpy
- double formation_entropy
- double formation_energy
- std::string Phase
- std::vector< Atom > atoms

Private Attributes

- std::string Name
- std::string Formula
- bool haveG
- bool haveHS
- bool registered

Additional Inherited Members

4.30.1 Constructor & Destructor Documentation

4.30.1.1 Molecule::Molecule ( )

4.30.1.2 Molecule::∼Molecule ( )

4.30.1.3 Molecule::Molecule (int *charge*, double *enthalpy*, double *entropy*, double *energy*, bool *HS*, bool *G*, std::string *Phase*, std::string *Name*, std::string *Formula*, std::string *lin_formula*)

4.30.2 Member Function Documentation

4.30.2.1 void Molecule::calculateAvgOxiState (std::string *Symbol*)

4.30.2.2 int Molecule::Charge ( )

4.30.2.3 void Molecule::DisplayInfo ( )

4.30.2.4 void Molecule::editAllOxidationStates (int *state*, std::string *Symbol*)

4.30.2.5 void Molecule::editCharge (int *c*)

4.30.2.6 void Molecule::editEnergy (double *energy*)

4.30.2.7 void Molecule::editEnthalpy (double *enthalpy*)

4.30.2.8 void Molecule::editEntropy (double *entropy*)

4.30.2.9 void Molecule::editHS (double *H*, double *S*)

4.30.2.10 void Molecule::editOneOxidationState (int *state*, std::string *Symbol*)

4.30.2.11 double Molecule::Energy ( )

4.30.2.12 double Molecule::Enthalpy ( )

4.30.2.13 double Molecule::Entropy ( )

4.30.2.14 bool Molecule::HaveEnergy ( )

4.30.2.15 bool Molecule::HaveHS ( )

4.30.2.16 bool Molecule::isRegistered ( )

4.30.2.17 double Molecule::MolarWeight ( )

4.30.2.18 std::string Molecule::MolecularFormula ( )

4.30.2.19 std::string Molecule::MoleculeName ( )

4.30.2.20 std::string Molecule::MoleculePhase ( )

4.30.2.21 void Molecule::recalculateMolarWeight ( )

4.30.2.22 void Molecule::Register (int *charge*, double *enthalpy*, double *entropy*, double *energy*, bool *HS*, bool *G*, std::string *Phase*, std::string *Name*, std::string *Formula*, std::string *lin_formula*)

4.30.2.23 void Molecule::Register (std::string *formula*)

4.30.2.24 void Molecule::removeAllAtoms (std::string *Symbol*)

4.30.2.25 void Molecule::removeOneAtom (std::string *Symbol*)

4.30.2.26 void Molecule::setFormula (std::string *form*)

4.30.2.27 void Molecule::setMolarWeigth (double *mw*)

4.30.3 Member Data Documentation

4.30.3.1 std::vector<Atom> Molecule::atoms `[protected]`

4.30.3.2 int Molecule::charge `[protected]`

4.30.3.3 double Molecule::formation_energy `[protected]`

4.30.3.4 double Molecule::formation_enthalpy `[protected]`

4.30.3.5 double Molecule::formation_entropy `[protected]`

4.30.3.6 std::string Molecule::Formula `[private]`

4.30.3.7 bool Molecule::haveG `[private]`

4.30.3.8 bool Molecule::haveHS `[private]`

4.30.3.9 double Molecule::molar_weight `[protected]`

4.30.3.10 std::string Molecule::Name `[private]`

4.30.3.11 std::string Molecule::Phase `[protected]`

4.30.3.12 bool Molecule::registered [private]

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

- mola.h
- mola.cpp

4.31 MONKFISH_DATA Struct Reference

```
#include <monkfish.h>
```

Public Attributes

- unsigned long int total_steps = 0
- double time_old = 0.0
- double time = 0.0
- bool Print2File = true
- bool Print2Console = true
- bool DirichletBC = true
- bool NonLinear = false
- bool haveMinMax = false
- bool MultiScale = true
- int level = 2
- double t_counter = 0.0
- double t_print
- int NumComp
- double end_time
- double total_sorption_old
- double total_sorption
- double single_fiber_density
- double avg_fiber_density
- double max_fiber_density
- double min_fiber_density
- double max_porosity
- double min_porosity
- double domain_diameter
- FILE ∗ Output
- double(∗ eval_eps)(int i, int l, const void ∗user_data)
- double(∗ eval_rho)(int i, int l, const void ∗user_data)
- double(∗ eval_Dex)(int i, int l, const void ∗user_data)
- double(∗ eval_ads)(int i, int l, const void ∗user_data)
- double(∗ eval_Ret)(int i, int l, const void ∗user_data)
- double(∗ eval_Cex)(int i, const void ∗user_data)
- double(∗ eval_kf)(int i, const void ∗user_data)
- const void ∗ user_data
- std::vector< FINCH_DATA > finch_dat
- std::vector< MONKFISH_PARAM > param_dat
- std::vector< DOGFISH_DATA > dog_dat

4.31.1 Member Data Documentation

4.31.1.1 double MONKFISH_DATA::avg_fiber_density

4.31.1.2 bool MONKFISH_DATA::DirichletBC = true

4.31.1.3 std::vector<DOGFISH_DATA> MONKFISH_DATA::dog_dat

4.31.1.4 double MONKFISH_DATA::domain_diameter

4.31.1.5 double MONKFISH_DATA::end_time

4.31.1.6 double(∗ MONKFISH_DATA::eval_ads)(int i, int l, const void ∗user_data)

4.31.1.7 double(∗ MONKFISH_DATA::eval_Cex)(int i, const void ∗user_data)

4.31.1.8 double(∗ MONKFISH_DATA::eval_Dex)(int i, int l, const void ∗user_data)

4.31.1.9 double(∗ MONKFISH_DATA::eval_eps)(int i, int l, const void ∗user_data)

4.31.1.10 double(∗ MONKFISH_DATA::eval_kf)(int i, const void ∗user_data)

4.31.1.11 double(∗ MONKFISH_DATA::eval_Ret)(int i, int l, const void ∗user_data)

4.31.1.12 double(∗ MONKFISH_DATA::eval_rho)(int i, int l, const void ∗user_data)

4.31.1.13 std::vector<FINCH_DATA> MONKFISH_DATA::finch_dat

4.31.1.14 bool MONKFISH_DATA::haveMinMax = false

4.31.1.15 int MONKFISH_DATA::level = 2

4.31.1.16 double MONKFISH_DATA::max_fiber_density

4.31.1.17 double MONKFISH_DATA::max_porosity

4.31.1.18 double MONKFISH_DATA::min_fiber_density

4.31.1.19 double MONKFISH_DATA::min_porosity

4.31.1.20 bool MONKFISH_DATA::MultiScale = true

4.31.1.21 bool MONKFISH_DATA::NonLinear = false

4.31.1.22 int MONKFISH_DATA::NumComp

4.31.1.23 FILE∗ MONKFISH_DATA::Output

4.31.1.24 std::vector<MONKFISH_PARAM> MONKFISH_DATA::param_dat

4.31.1.25 bool MONKFISH_DATA::Print2Console = true

4.31.1.26 bool MONKFISH_DATA::Print2File = true

4.31.1.27 double MONKFISH_DATA::single_fiber_density

4.31.1.28 double MONKFISH_DATA::t_counter = 0.0

4.31.1.29 double MONKFISH_DATA::t_print

4.31.1.30 double MONKFISH_DATA::time = 0.0

4.31.1.31 double MONKFISH_DATA::time_old = 0.0

4.31.1.32 double MONKFISH_DATA::total_sorption

4.31.1.33 double MONKFISH_DATA::total_sorption_old

4.31.1.34 unsigned long int MONKFISH_DATA::total_steps = 0

4.31.1.35 const void* MONKFISH_DATA::user_data

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

- monkfish.h

4.32 MONKFISH_PARAM Struct Reference

```
#include <monkfish.h>
```

Public Attributes

- double interparticle_diffusion
- double exterior_concentration
- double exterior_transfer_coeff
- double sorbed_molefraction
- double initial_sorption
- double sorption_bc
- double intraparticle_diffusion
- double film_transfer_coeff
- Matrix< double > avg_sorption
- Matrix< double > avg_sorption_old
- Molecule species

4.32.1 Member Data Documentation

4.32.1.1 Matrix<double> MONKFISH_PARAM::avg_sorption

4.32.1.2 Matrix<double> MONKFISH_PARAM::avg_sorption_old

4.32.1.3 double MONKFISH_PARAM::exterior_concentration

4.32.1.4 double MONKFISH_PARAM::exterior_transfer_coeff

4.32.1.5 double MONKFISH_PARAM::film_transfer_coeff

4.32.1.6 double MONKFISH_PARAM::initial_sorption

4.32.1.7 double MONKFISH_PARAM::interparticle_diffusion

4.32.1.8 double MONKFISH_PARAM::intraparticle_diffusion

4.32.1.9 double MONKFISH_PARAM::sorbed_molefraction

4.32.1.10 double MONKFISH_PARAM::sorption_bc

4.32.1.11 Molecule MONKFISH_PARAM::species

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

- monkfish.h

4.33 mSPD_DATA Struct Reference

```
#include <magpie.h>
```

Public Attributes

- double s
- double v
- double eMax
- std::vector< double > eta
- double gama

4.33.1 Member Data Documentation

4.33.1.1 double mSPD_DATA::eMax

4.33.1.2 std::vector<double> mSPD_DATA::eta

4.33.1.3 double mSPD_DATA::gama

4.33.1.4 double mSPD_DATA::s

4.33.1.5 double mSPD_DATA::v

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

- magpie.h

4.34 NUM_JAC_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- double eps = sqrt(DBL_EPSILON)
- Matrix< double > Fx
- Matrix< double > Fxp
- Matrix< double > dxj

4.34.1 Member Data Documentation

4.34.1.1 Matrix<double> NUM_JAC_DATA::dxj

4.34.1.2 double NUM_JAC_DATA::eps = sqrt(DBL_EPSILON)

4.34.1.3 Matrix<double> NUM_JAC_DATA::Fx

4.34.1.4 Matrix<double> NUM_JAC_DATA::Fxp

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

- lark.h

4.35 OPTRANS_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- Matrix< double > Ii
- Matrix< double > Ai

4.35.1 Member Data Documentation

4.35.1.1 Matrix<double> OPTRANS_DATA::Ai

4.35.1.2 Matrix<double> OPTRANS_DATA::Ii

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

- lark.h

4.36 PCG_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int maxit = 0
- int iter = 0
- double alpha
- double beta
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x

- Matrix< double > bestx
- Matrix< double > r
- Matrix< double > r_old
- Matrix< double > z
- Matrix< double > z_old
- Matrix< double > p
- Matrix< double > Ap

4.36.1 Member Data Documentation

4.36.1.1 double PCG_DATA::alpha

4.36.1.2 Matrix<double> PCG_DATA::Ap

4.36.1.3 double PCG_DATA::bestres

4.36.1.4 Matrix<double> PCG_DATA::bestx

4.36.1.5 double PCG_DATA::beta

4.36.1.6 int PCG_DATA::iter = 0

4.36.1.7 int PCG_DATA::maxit = 0

4.36.1.8 bool PCG_DATA::Output = true

4.36.1.9 Matrix<double> PCG_DATA::p

4.36.1.10 Matrix<double> PCG_DATA::r

4.36.1.11 Matrix<double> PCG_DATA::r_old

4.36.1.12 double PCG_DATA::relres

4.36.1.13 double PCG_DATA::relres_base

4.36.1.14 double PCG_DATA::res

4.36.1.15 double PCG_DATA::tol_abs = 1e-6

4.36.1.16 double PCG_DATA::tol_rel = 1e-6

4.36.1.17 Matrix<double> PCG_DATA::x

4.36.1.18 Matrix<double> PCG_DATA::z

4.36.1.19 Matrix<double> PCG_DATA::z_old

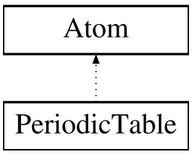
The documentation for this struct was generated from the following file:

- lark.h

4.37 PeriodicTable Class Reference

```
#include <eel.h>
```

Inheritance diagram for PeriodicTable:



Public Member Functions

- PeriodicTable ()
- ∼PeriodicTable ()
- PeriodicTable (int ∗n, int N)
- PeriodicTable (std::vector< std::string > &Symbol)
- PeriodicTable (std::vector< int > &n)
- void DisplayTable ()

Protected Attributes

- std::vector< Atom > Table

Private Attributes

- int number_elements

Additional Inherited Members

4.37.1 Constructor & Destructor Documentation

4.37.1.1 PeriodicTable::PeriodicTable ( )

4.37.1.2 PeriodicTable::∼PeriodicTable ( )

4.37.1.3 PeriodicTable::PeriodicTable (int ∗ *n*, int *N*)

4.37.1.4 PeriodicTable::PeriodicTable (std::vector< std::string > & *Symbol*)

4.37.1.5 PeriodicTable::PeriodicTable (std::vector< int > & *n*)

4.37.2 Member Function Documentation

4.37.2.1 void PeriodicTable::DisplayTable ( )

4.37.3 Member Data Documentation

4.37.3.1 int PeriodicTable::number_elements [private]

4.37.3.2 std::vector<Atom> PeriodicTable::Table [protected]

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

- eel.h
- eel.cpp

4.38 PICARD_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int maxit = 0
- int iter = 0
- double tol_rel = 1e-6
- double tol_abs = 1e-6
- double res
- double relres
- double relres_base
- double bestres
- bool Output = true
- Matrix< double > x0
- Matrix< double > bestx
- Matrix< double > r

4.38.1 Member Data Documentation

4.38.1.1 double PICARD_DATA::bestres

4.38.1.2 Matrix<double> PICARD_DATA::bestx

4.38.1.3 int PICARD_DATA::iter = 0

4.38.1.4 int PICARD_DATA::maxit = 0

4.38.1.5 bool PICARD_DATA::Output = true

4.38.1.6 Matrix<double> PICARD_DATA::r

4.38.1.7 double PICARD_DATA::relres

4.38.1.8 double PICARD_DATA::relres_base

4.38.1.9 double PICARD_DATA::res

4.38.1.10 double PICARD_DATA::tol_abs = 1e-6

4.38.1.11 double PICARD_DATA::tol_rel = 1e-6

4.38.1.12 Matrix<double> PICARD_DATA::x0

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

- lark.h

4.39 PJFNK_DATA Struct Reference

```
#include <lark.h>
```

Public Attributes

- int nl_iter = 0
- int l_iter = 0
- int nl_maxit = 0
- int linear_solver = -1
- double nl_tol_abs = 1e-6
- double nl_tol_rel = 1e-6
- double lin_tol_rel = 1e-6
- double lin_tol_abs = 1e-6
- double nl_res
- double nl_relres
- double nl_res_base
- double nl_bestres
- double eps =sqrt(DBL_EPSILON)
- bool NL_Output = true
- bool L_Output = false
- bool LineSearch = false
- bool Bounce = false
- Matrix< double > F
- Matrix< double > Fv
- Matrix< double > v
- Matrix< double > x
- Matrix< double > bestx
- GMRESLP_DATA gmreslp_dat
- PCG_DATA pcg_dat
- BiCGSTAB_DATA bicgstab_dat
- CGS_DATA cgs_dat
- GMRESRP_DATA gmresrp_dat
- GCR_DATA gcr_dat
- GMRESR_DATA gmresr_dat
- BACKTRACK_DATA backtrack_dat
- const void ∗ res_data
- const void ∗ precon_data
- int(∗ funeval)(const Matrix< double > &x, Matrix< double > &F, const void ∗res_data)
- int(∗ precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)

4.39.1 Member Data Documentation

4.39.1.1 BACKTRACK_DATA PJFNK_DATA::backtrack_dat

4.39.1.2 Matrix<double> PJFNK_DATA::bestx

4.39.1.3 BiCGSTAB_DATA PJFNK_DATA::bicgstab_dat

4.39.1.4 bool PJFNK_DATA::Bounce = false

4.39.1.5 CGS_DATA PJFNK_DATA::cgs_dat

4.39.1.6 double PJFNK_DATA::eps =sqrt(DBL_EPSILON)

4.39.1.7 Matrix<double> PJFNK_DATA::F

4.39.1.8 int(∗ PJFNK_DATA::funeval)(const Matrix< double > &x, Matrix< double > &F, const void ∗res_data)

4.39.1.9 Matrix<double> PJFNK_DATA::Fv

4.39.1.10 GCR_DATA PJFNK_DATA::gcr_dat

4.39.1.11 GMRESLP_DATA PJFNK_DATA::gmreslp_dat

4.39.1.12 GMRESR_DATA PJFNK_DATA::gmresr_dat

4.39.1.13 GMRESRP_DATA PJFNK_DATA::gmresrp_dat

4.39.1.14 int PJFNK_DATA::l_iter = 0

4.39.1.15 bool PJFNK_DATA::L_Output = false

4.39.1.16 double PJFNK_DATA::lin_tol_abs = 1e-6

4.39.1.17 double PJFNK_DATA::lin_tol_rel = 1e-6

4.39.1.18 int PJFNK_DATA::linear_solver = -1

4.39.1.19 bool PJFNK_DATA::LineSearch = false

4.39.1.20 double PJFNK_DATA::nl_bestres

4.39.1.21 int PJFNK_DATA::nl_iter = 0

4.39.1.22 int PJFNK_DATA::nl_maxit = 0

4.39.1.23 bool PJFNK_DATA::NL_Output = true

4.39.1.24 double PJFNK_DATA::nl_relres

4.39.1.25 double PJFNK_DATA::nl_res

4.39.1.26 double PJFNK_DATA::nl_res_base

4.39.1.27 double PJFNK_DATA::nl_tol_abs = 1e-6

4.39.1.28 double PJFNK_DATA::nl_tol_rel = 1e-6

4.39.1.29 PCG_DATA PJFNK_DATA::pcg_dat

4.39.1.30 int(∗ PJFNK_DATA::precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)

4.39.1.31 const void∗ PJFNK_DATA::precon_data

4.39.1.32 const void∗ PJFNK_DATA::res_data

4.39.1.33 Matrix<double> PJFNK_DATA::v

4.39.1.34 Matrix<double> PJFNK_DATA::x

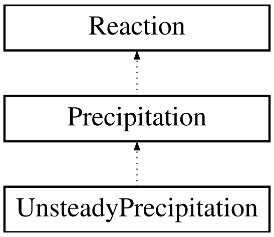
The documentation for this struct was generated from the following file:

- lark.h

4.40 Precipitation Class Reference

```
#include <shark.h>
```

Inheritance diagram for Precipitation:



Additional Inherited Members

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

- shark.h

4.41 PURE_GAS Struct Reference

```
#include <egret.h>
```

Public Attributes

- double molecular_weight
- double Sutherland_Temp
- double Sutherland_Const
- double Sutherland_Viscosity
- double specific_heat
- double molecular_diffusion
- double dynamic_viscosity
- double density
- double Schmidt

4.41.1 Member Data Documentation

4.41.1.1 double PURE_GAS::density

4.41.1.2 double PURE_GAS::dynamic_viscosity

4.41.1.3 double PURE_GAS::molecular_diffusion

4.41.1.4 double PURE_GAS::molecular_weight

4.41.1.5 double PURE_GAS::Schmidt

4.41.1.6 double PURE_GAS::specific_heat

4.41.1.7 double PURE_GAS::Sutherland_Const

4.41.1.8 double PURE_GAS::Sutherland_Temp

4.41.1.9 double PURE_GAS::Sutherland_Viscosity

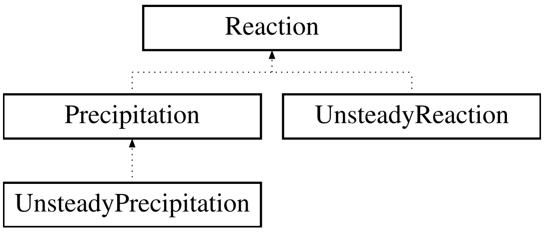
The documentation for this struct was generated from the following file:

- egret.h

4.42 Reaction Class Reference

```
#include <shark.h>
```

Inheritance diagram for Reaction:



Public Member Functions

- Reaction ()
- ∼Reaction ()
- void Initialize_List (MasterSpeciesList &List)
- void Display_Info ()
- void Set_Stoichiometric (int i, double v)
- void Set_Equilibrium (double v)
- void Set_Enthalpy (double H)
- void Set_Entropy (double S)
- void Set_EnthalpyANDEntropy (double H, double S)
- void Set_Energy (double G)
- void checkSpeciesEnergies ()
- void calculateEnergies ()
- void calculateEquilibrium (double T)
- bool haveEquilibrium ()
- double Get_Stoichiometric (int i)
- double Get_Equilibrium ()
- double Get_Enthalpy ()
- double Get_Entropy ()
- double Get_Energy ()
- double Eval_Residual (const Matrix< double > &x, const Matrix< double > &gama)

Protected Attributes

- MasterSpeciesList ∗ List
- std::vector< double > Stoichiometric
- double Equilibrium
- double enthalpy
- double entropy

- double energy
- bool CanCalcHS
- bool CanCalcG
- bool HaveHS
- bool HaveG
- bool HaveEquil

4.42.1 Constructor & Destructor Documentation

4.42.1.1 Reaction::Reaction ( )

4.42.1.2 Reaction::∼Reaction ( )

4.42.2 Member Function Documentation

4.42.2.1 void Reaction::calculateEnergies ( )

4.42.2.2 void Reaction::calculateEquilibrium (double *T*)

4.42.2.3 void Reaction::checkSpeciesEnergies ( )

4.42.2.4 void Reaction::Display_Info ( )

4.42.2.5 double Reaction::Eval_Residual (const Matrix< double > & *x*, const Matrix< double > & *gama*)

4.42.2.6 double Reaction::Get_Energy ( )

4.42.2.7 double Reaction::Get_Enthalpy ( )

4.42.2.8 double Reaction::Get_Entropy ( )

4.42.2.9 double Reaction::Get_Equilibrium ( )

4.42.2.10 double Reaction::Get_Stoichiometric (int *i*)

4.42.2.11 bool Reaction::haveEquilibrium ( )

4.42.2.12 void Reaction::Initialize_List (MasterSpeciesList & *List*)

4.42.2.13 void Reaction::Set_Energy (double *G*)

4.42.2.14 void Reaction::Set_Enthalpy (double *H*)

4.42.2.15 void Reaction::Set_EnthalpyANDEntropy (double *H*, double *S*)

4.42.2.16 void Reaction::Set_Entropy (double *S*)

4.42.2.17 void Reaction::Set_Equilibrium (double *v*)

4.42.2.18 void Reaction::Set_Stoichiometric (int *i*, double *v*)

4.42.3 Member Data Documentation

4.42.3.1 bool Reaction::CanCalcG [protected]

4.42.3.2 bool Reaction::CanCalcHS [protected]

4.42.3.3 double Reaction::energy [protected]

4.42.3.4 double Reaction::enthalpy [protected]

4.42.3.5 double Reaction::entropy [protected]

4.42.3.6 double Reaction::Equilibrium [protected]

4.42.3.7 bool Reaction::HaveEquil [protected]

4.42.3.8 bool Reaction::HaveG [protected]

4.42.3.9 bool Reaction::HaveHS [protected]

4.42.3.10 MasterSpeciesList* Reaction::List [protected]

4.42.3.11 std::vector<double> Reaction::Stoichiometric [protected]

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

- shark.h
- shark.cpp

4.43 SCOPSOWL_DATA Struct Reference

```
#include <scopsowl.h>
```

Public Attributes

- unsigned long int total_steps
- int coord_macro
- int coord_micro
- int level = 2
- double sim_time
- double t_old
- double t
- double t_counter = 0.0
- double t_print
- bool Print2File = true
- bool Print2Console = true
- bool SurfDiff = true
- bool Heterogeneous = true
- double gas_velocity
- double total_pressure
- double gas_temperature
- double pellet_radius
- double crystal_radius
- double char_macro
- double char_micro
- double binder_fraction
- double binder_porosity

- double binder_poresize
- double pellet_density
- bool DirichletBC = false
- bool NonLinear = true
- std::vector< double > y
- std::vector< double > tempy
- FILE ∗ OutputFile
- double(∗ eval_ads)(int i, int l, const void ∗user_data)
- double(∗ eval_retard)(int i, int l, const void ∗user_data)
- double(∗ eval_diff)(int i, int l, const void ∗user_data)
- double(∗ eval_surfDiff)(int i, int l, const void ∗user_data)
- double(∗ eval_kf)(int i, const void ∗user_data)
- const void ∗ user_data
- MIXED_GAS ∗ gas_dat
- MAGPIE_DATA magpie_dat
- std::vector< FINCH_DATA > finch_dat
- std::vector< SCOPSOWL_PARAM_DATA > param_dat
- std::vector< SKUA_DATA > skua_dat

4.43.1 Member Data Documentation

4.43.1.1 double SCOPSOWL_DATA::binder_fraction

4.43.1.2 double SCOPSOWL_DATA::binder_poresize

4.43.1.3 double SCOPSOWL_DATA::binder_porosity

4.43.1.4 double SCOPSOWL_DATA::char_macro

4.43.1.5 double SCOPSOWL_DATA::char_micro

4.43.1.6 int SCOPSOWL_DATA::coord_macro

4.43.1.7 int SCOPSOWL_DATA::coord_micro

4.43.1.8 double SCOPSOWL_DATA::crystal_radius

4.43.1.9 bool SCOPSOWL_DATA::DirichletBC = false

4.43.1.10 double(∗ SCOPSOWL_DATA::eval_ads)(int i, int l, const void ∗user_data)

4.43.1.11 double(∗ SCOPSOWL_DATA::eval_diff)(int i, int l, const void ∗user_data)

4.43.1.12 double(∗ SCOPSOWL_DATA::eval_kf)(int i, const void ∗user_data)

4.43.1.13 double(∗ SCOPSOWL_DATA::eval_retard)(int i, int l, const void ∗user_data)

4.43.1.14 double(∗ SCOPSOWL_DATA::eval_surfDiff)(int i, int l, const void ∗user_data)

4.43.1.15 std::vector<FINCH_DATA> SCOPSOWL_DATA::finch_dat

4.43.1.16 MIXED_GAS∗ SCOPSOWL_DATA::gas_dat

4.43.1.17 double SCOPSOWL_DATA::gas_temperature

4.43.1.18 double SCOPSOWL_DATA::gas_velocity

4.43.1.19 bool SCOPSOWL_DATA::Heterogeneous = true

4.43.1.20 int SCOPSOWL_DATA::level = 2

4.43.1.21 MAGPIE_DATA SCOPSOWL_DATA::magpie_dat

4.43.1.22 bool SCOPSOWL_DATA::NonLinear = true

4.43.1.23 FILE∗ SCOPSOWL_DATA::OutputFile

4.43.1.24 std::vector<SCOPSOWL_PARAM_DATA> SCOPSOWL_DATA::param_dat

4.43.1.25 double SCOPSOWL_DATA::pellet_density

4.43.1.26 double SCOPSOWL_DATA::pellet_radius

4.43.1.27 bool SCOPSOWL_DATA::Print2Console = true

4.43.1.28 bool SCOPSOWL_DATA::Print2File = true

4.43.1.29 double SCOPSOWL_DATA::sim_time

4.43.1.30 std::vector<SKUA_DATA> SCOPSOWL_DATA::skua_dat

4.43.1.31 bool SCOPSOWL_DATA::SurfDiff = true

4.43.1.32 double SCOPSOWL_DATA::t

4.43.1.33 double SCOPSOWL_DATA::t_counter = 0.0

4.43.1.34 double SCOPSOWL_DATA::t_old

4.43.1.35 double SCOPSOWL_DATA::t_print

4.43.1.36 std::vector<double> SCOPSOWL_DATA::tempy

4.43.1.37 double SCOPSOWL_DATA::total_pressure

4.43.1.38 unsigned long int SCOPSOWL_DATA::total_steps

4.43.1.39 const void∗ SCOPSOWL_DATA::user_data

4.43.1.40 std::vector<double> SCOPSOWL_DATA::y

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

- scopsowl.h

4.44 SCOPSOWL_OPT_DATA Struct Reference

```
#include <scopsowl_opt.h>
```

Public Attributes

- int num_curves
- int evaluation
- unsigned long int total_eval
- int current_points
- int num_params = 1
- int diffusion_type
- int adsorb_index
- int max_guess_iter = 20
- bool Optimize
- bool Rough
- double current_temp
- double current_press
- double current_equil
- double simulation_equil
- double max_bias
- double min_bias
- double e_norm
- double f_bias
- double e_norm_old
- double f_bias_old
- double param_guess
- double param_guess_old
- double rel_tol_norm = 0.01
- double abs_tol_bias = 1.0
- std::vector< double > y_base
- std::vector< double > q_data
- std::vector< double > q_sim
- std::vector< double > t
- FILE ∗ ParamFile
- FILE ∗ CompareFile
- SCOPSOWL_DATA owl_dat

4.44.1 Member Data Documentation

4.44.1.1 double SCOPSOWL_OPT_DATA::abs_tol_bias = 1.0

4.44.1.2 int SCOPSOWL_OPT_DATA::adsorb_index

4.44.1.3 FILE∗ SCOPSOWL_OPT_DATA::CompareFile

4.44.1.4 double SCOPSOWL_OPT_DATA::current_equil

4.44.1.5 int SCOPSOWL_OPT_DATA::current_points

4.44.1.6 double SCOPSOWL_OPT_DATA::current_press

4.44.1.7 double SCOPSOWL_OPT_DATA::current_temp

4.44.1.8 int SCOPSOWL_OPT_DATA::diffusion_type

4.44.1.9 double SCOPSOWL_OPT_DATA::e_norm

4.44.1.10 double SCOPSOWL_OPT_DATA::e_norm_old

4.44.1.11 int SCOPSOWL_OPT_DATA::evaluation

4.44.1.12 double SCOPSOWL_OPT_DATA::f_bias

4.44.1.13 double SCOPSOWL_OPT_DATA::f_bias_old

4.44.1.14 double SCOPSOWL_OPT_DATA::max_bias

4.44.1.15 int SCOPSOWL_OPT_DATA::max_guess_iter = 20

4.44.1.16 double SCOPSOWL_OPT_DATA::min_bias

4.44.1.17 int SCOPSOWL_OPT_DATA::num_curves

4.44.1.18 int SCOPSOWL_OPT_DATA::num_params = 1

4.44.1.19 bool SCOPSOWL_OPT_DATA::Optimize

4.44.1.20 SCOPSOWL_DATA SCOPSOWL_OPT_DATA::owl_dat

4.44.1.21 double SCOPSOWL_OPT_DATA::param_guess

4.44.1.22 double SCOPSOWL_OPT_DATA::param_guess_old

4.44.1.23 FILE* SCOPSOWL_OPT_DATA::ParamFile

4.44.1.24 std::vector<double> SCOPSOWL_OPT_DATA::q_data

4.44.1.25 std::vector<double> SCOPSOWL_OPT_DATA::q_sim

4.44.1.26 double SCOPSOWL_OPT_DATA::rel_tol_norm = 0.01

4.44.1.27 bool SCOPSOWL_OPT_DATA::Rough

4.44.1.28 double SCOPSOWL_OPT_DATA::simulation_equil

4.44.1.29 std::vector<double> SCOPSOWL_OPT_DATA::t

4.44.1.30 unsigned long int SCOPSOWL_OPT_DATA::total_eval

4.44.1.31 std::vector<double> SCOPSOWL_OPT_DATA::y_base

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

- scopsowl_opt.h

4.45 SCOPSOWL_PARAM_DATA Struct Reference

```
#include <scopsowl.h>
```

Public Attributes

- Matrix< double > qAvg

- Matrix< double > qAvg_old
- Matrix< double > Qst
- Matrix< double > Qst_old
- Matrix< double > dq_dc
- double xIC
- double qIntegralAvg
- double qIntegralAvg_old
- double QstAvg
- double QstAvg_old
- double qo
- double Qsto
- double dq_dco
- double pore_diffusion
- double film_transfer
- double activation_energy
- double ref_diffusion
- double ref_temperature
- double affinity
- double ref_pressure
- bool Adsorbable
- std::string speciesName

4.45.1 Member Data Documentation

4.45.1.1 double SCOPSOWL_PARAM_DATA::activation_energy

4.45.1.2 bool SCOPSOWL_PARAM_DATA::Adsorbable

4.45.1.3 double SCOPSOWL_PARAM_DATA::affinity

4.45.1.4 Matrix<double> SCOPSOWL_PARAM_DATA::dq_dc

4.45.1.5 double SCOPSOWL_PARAM_DATA::dq_dco

4.45.1.6 double SCOPSOWL_PARAM_DATA::film_transfer

4.45.1.7 double SCOPSOWL_PARAM_DATA::pore_diffusion

4.45.1.8 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg

4.45.1.9 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg_old

4.45.1.10 double SCOPSOWL_PARAM_DATA::qIntegralAvg

4.45.1.11 double SCOPSOWL_PARAM_DATA::qIntegralAvg_old

4.45.1.12 double SCOPSOWL_PARAM_DATA::qo

4.45.1.13 Matrix<double> SCOPSOWL_PARAM_DATA::Qst

4.45.1.14 Matrix<double> SCOPSOWL_PARAM_DATA::Qst_old

4.45.1.15 double SCOPSOWL_PARAM_DATA::QstAvg

4.45.1.16 double SCOPSOWL_PARAM_DATA::QstAvg_old

4.45.1.17 double SCOPSOWL_PARAM_DATA::Qsto

4.45.1.18 double SCOPSOWL_PARAM_DATA::ref_diffusion

4.45.1.19 double SCOPSOWL_PARAM_DATA::ref_pressure

4.45.1.20 double SCOPSOWL_PARAM_DATA::ref_temperature

4.45.1.21 std::string SCOPSOWL_PARAM_DATA::speciesName

4.45.1.22 double SCOPSOWL_PARAM_DATA::xIC

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

- scopsowl.h

4.46 SHARK_DATA Struct Reference

```
#include <shark.h>
```

Public Attributes

- MasterSpeciesList MasterList
- std::vector< Reaction > ReactionList
- std::vector< MassBalance > MassBalanceList
- std::vector< UnsteadyReaction > UnsteadyList
- std::vector< double(∗)(const
  Matrix< double > &x,
  SHARK_DATA ∗shark_dat, const
  void ∗data) > OtherList
- int numvar
- int num_ssr
- int num_mbe
- int num_usr
- int num_other = 0
- int act_fun = IDEAL
- int totalsteps = 0
- int timesteps = 0
- int pH_index = -1
- int pOH_index = -1
- double simulationtime = 0.0
- double dt = 0.1
- double dt_min = sqrt(DBL_EPSILON)
- double t_out = 0.0
- double t_count = 0.0
- double time = 0.0
- double time_old = 0.0
- double pH = 7.0
- double Norm = 0.0
- double dielectric_const = 78.325
- double temperature = 298.15

- bool steadystate = true
- bool TimeAdaptivity = false
- bool const_pH = false
- bool SpeciationCurve = false
- bool Console_Output = true
- bool File_Output = false
- bool Contains_pH = false
- bool Contains_pOH = false
- bool Converged = false
- Matrix< double > X_old
- Matrix< double > X_new
- Matrix< double > Conc_old
- Matrix< double > Conc_new
- Matrix< double > activity_new
- Matrix< double > activity_old
- int(∗ EvalActivity)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int(∗ Residual)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int(∗ lin_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗data)
- PJFNK_DATA Newton_data
- const void ∗ activity_data
- const void ∗ residual_data
- const void ∗ precon_data
- const void ∗ other_data
- FILE ∗ OutputFile
- yaml_cpp_class yaml_object

4.46.1 Member Data Documentation

4.46.1.1 int SHARK_DATA::act_fun = IDEAL

4.46.1.2 const void∗ SHARK_DATA::activity_data

4.46.1.3 Matrix<double> SHARK_DATA::activity_new

4.46.1.4 Matrix<double> SHARK_DATA::activity_old

4.46.1.5 Matrix<double> SHARK_DATA::Conc_new

4.46.1.6 Matrix<double> SHARK_DATA::Conc_old

4.46.1.7 bool SHARK_DATA::Console_Output = true

4.46.1.8 bool SHARK_DATA::const_pH = false

4.46.1.9 bool SHARK_DATA::Contains_pH = false

4.46.1.10 bool SHARK_DATA::Contains_pOH = false

4.46.1.11 bool SHARK_DATA::Converged = false

4.46.1.12 double SHARK_DATA::dielectric_const = 78.325

4.46.1.13 double SHARK_DATA::dt = 0.1

4.46.1.14 double SHARK_DATA::dt_min = sqrt(DBL_EPSILON)

4.46.1.15 int(∗ SHARK_DATA::EvalActivity)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)

4.46.1.16 bool SHARK_DATA::File_Output = false

4.46.1.17 int(∗ SHARK_DATA::lin_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗data)

4.46.1.18 std::vector<MassBalance> SHARK_DATA::MassBalanceList

4.46.1.19 MasterSpeciesList SHARK_DATA::MasterList

4.46.1.20 PJFNK_DATA SHARK_DATA::Newton_data

4.46.1.21 double SHARK_DATA::Norm = 0.0

4.46.1.22 int SHARK_DATA::num_mbe

4.46.1.23 int SHARK_DATA::num_other = 0

4.46.1.24 int SHARK_DATA::num_ssr

4.46.1.25 int SHARK_DATA::num_usr

4.46.1.26 int SHARK_DATA::numvar

4.46.1.27 const void∗ SHARK_DATA::other_data

4.46.1.28 std::vector< double (∗) (const Matrix<double> &x, SHARK_DATA ∗shark_dat, const void ∗data) > SHARK_DATA::OtherList

4.46.1.29 FILE∗ SHARK_DATA::OutputFile

4.46.1.30 double SHARK_DATA::pH = 7.0

4.46.1.31 int SHARK_DATA::pH_index = -1

4.46.1.32 int SHARK_DATA::pOH_index = -1

4.46.1.33 const void∗ SHARK_DATA::precon_data

4.46.1.34 std::vector<Reaction> SHARK_DATA::ReactionList

4.46.1.35 int(∗ SHARK_DATA::Residual)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)

4.46.1.36 const void∗ SHARK_DATA::residual_data

4.46.1.37 double SHARK_DATA::simulationtime = 0.0

4.46.1.38 bool SHARK_DATA::SpeciationCurve = false

4.46.1.39 bool SHARK_DATA::steadystate = true

4.46.1.40 double SHARK_DATA::t_count = 0.0

4.46.1.41 double SHARK_DATA::t_out = 0.0

4.46.1.42 double SHARK_DATA::temperature = 298.15

4.46.1.43 double SHARK_DATA::time = 0.0

4.46.1.44 double SHARK_DATA::time_old = 0.0

4.46.1.45 bool SHARK_DATA::TimeAdaptivity = false

4.46.1.46 int SHARK_DATA::timesteps = 0

4.46.1.47 int SHARK_DATA::totalsteps = 0

4.46.1.48 std::vector<UnsteadyReaction> SHARK_DATA::UnsteadyList

4.46.1.49 Matrix<double> SHARK_DATA::X_new

4.46.1.50 Matrix<double> SHARK_DATA::X_old

4.46.1.51 yaml_cpp_class SHARK_DATA::yaml_object

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

- shark.h

4.47 SKUA_DATA Struct Reference

```
#include <skua.h>
```

Public Attributes

- unsigned long int total_steps
- int coord
- double sim_time
- double t_old
- double t
- double t_counter = 0.0
- double t_print
- double qTn
- double qTnp1
- bool Print2File = true
- bool Print2Console = true
- double gas_velocity
- double pellet_radius
- double char_measure
- bool DirichletBC = true
- bool NonLinear = true
- std::vector< double > y
- FILE ∗ OutputFile
- double(∗ eval_diff)(int i, int l, const void ∗user_data)
- double(∗ eval_kf)(int i, const void ∗user_data)
- const void ∗ user_data
- MAGPIE_DATA magpie_dat
- MIXED_GAS ∗ gas_dat
- std::vector< FINCH_DATA > finch_dat
- std::vector< SKUA_PARAM > param_dat

4.47.1 Member Data Documentation

4.47.1.1 double SKUA_DATA::char_measure

4.47.1.2 int SKUA_DATA::coord

4.47.1.3 bool SKUA_DATA::DirichletBC = true

4.47.1.4 double(∗ SKUA_DATA::eval_diff)(int i, int l, const void ∗user_data)

4.47.1.5 double(∗ SKUA_DATA::eval_kf)(int i, const void ∗user_data)

4.47.1.6 std::vector<FINCH_DATA> SKUA_DATA::finch_dat

4.47.1.7 MIXED_GAS∗ SKUA_DATA::gas_dat

4.47.1.8 double SKUA_DATA::gas_velocity

4.47.1.9 MAGPIE_DATA SKUA_DATA::magpie_dat

4.47.1.10 bool SKUA_DATA::NonLinear = true

4.47.1.11 FILE∗ SKUA_DATA::OutputFile

4.47.1.12 std::vector<SKUA_PARAM> SKUA_DATA::param_dat

4.47.1.13 double SKUA_DATA::pellet_radius

4.47.1.14 bool SKUA_DATA::Print2Console = true

4.47.1.15 bool SKUA_DATA::Print2File = true

4.47.1.16 double SKUA_DATA::qTn

4.47.1.17 double SKUA_DATA::qTnp1

4.47.1.18 double SKUA_DATA::sim_time

4.47.1.19 double SKUA_DATA::t

4.47.1.20 double SKUA_DATA::t_counter = 0.0

4.47.1.21 double SKUA_DATA::t_old

4.47.1.22 double SKUA_DATA::t_print

4.47.1.23 unsigned long int SKUA_DATA::total_steps

4.47.1.24 const void∗ SKUA_DATA::user_data

4.47.1.25 std::vector<double> SKUA_DATA::y

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

- skua.h

4.48 SKUA_OPT_DATA Struct Reference

```
#include <skua_opt.h>
```

Public Attributes

- int num_curves
- int evaluation
- unsigned long int total_eval
- int current_points
- int num_params = 1
- int diffusion_type
- int adsorb_index
- int max_guess_iter = 20
- bool Optimize
- bool Rough
- double current_temp
- double current_press
- double current_equil
- double simulation_equil
- double max_bias
- double min_bias
- double e_norm
- double f_bias
- double e_norm_old
- double f_bias_old
- double param_guess
- double param_guess_old
- double rel_tol_norm = 0.1
- double abs_tol_bias = 0.1
- std::vector< double > y_base
- std::vector< double > q_data
- std::vector< double > q_sim
- std::vector< double > t
- FILE ∗ ParamFile
- FILE ∗ CompareFile
- SKUA_DATA skua_dat

4.48.1 Member Data Documentation

4.48.1.1 double SKUA_OPT_DATA::abs_tol_bias = 0.1

4.48.1.2 int SKUA_OPT_DATA::adsorb_index

4.48.1.3 FILE∗ SKUA_OPT_DATA::CompareFile

4.48.1.4 double SKUA_OPT_DATA::current_equil

4.48.1.5 int SKUA_OPT_DATA::current_points

4.48.1.6 double SKUA_OPT_DATA::current_press

4.48.1.7 double SKUA_OPT_DATA::current_temp

4.48.1.8 int SKUA_OPT_DATA::diffusion_type

4.48.1.9 double SKUA_OPT_DATA::e_norm

4.48.1.10 double SKUA_OPT_DATA::e_norm_old

4.48.1.11 int SKUA_OPT_DATA::evaluation

4.48.1.12 double SKUA_OPT_DATA::f_bias

4.48.1.13 double SKUA_OPT_DATA::f_bias_old

4.48.1.14 double SKUA_OPT_DATA::max_bias

4.48.1.15 int SKUA_OPT_DATA::max_guess_iter = 20

4.48.1.16 double SKUA_OPT_DATA::min_bias

4.48.1.17 int SKUA_OPT_DATA::num_curves

4.48.1.18 int SKUA_OPT_DATA::num_params = 1

4.48.1.19 bool SKUA_OPT_DATA::Optimize

4.48.1.20 double SKUA_OPT_DATA::param_guess

4.48.1.21 double SKUA_OPT_DATA::param_guess_old

4.48.1.22 FILE* SKUA_OPT_DATA::ParamFile

4.48.1.23 std::vector<double> SKUA_OPT_DATA::q_data

4.48.1.24 std::vector<double> SKUA_OPT_DATA::q_sim

4.48.1.25 double SKUA_OPT_DATA::rel_tol_norm = 0.1

4.48.1.26 bool SKUA_OPT_DATA::Rough

4.48.1.27 double SKUA_OPT_DATA::simulation_equil

4.48.1.28 SKUA_DATA SKUA_OPT_DATA::skua_dat

4.48.1.29 std::vector<double> SKUA_OPT_DATA::t

4.48.1.30 unsigned long int SKUA_OPT_DATA::total_eval

4.48.1.31 std::vector<double> SKUA_OPT_DATA::y_base

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

- skua_opt.h

4.49 SKUA_PARAM Struct Reference

```
#include <skua.h>
```

Public Attributes

- double activation_energy
- double ref_diffusion
- double ref_temperature
- double affinity
- double ref_pressure
- double film_transfer
- double xIC
- double y_eff
- double Qstn
- double Qstnp1
- double xn
- double xnp1
- bool Adsorbable
- std::string speciesName

4.49.1 Member Data Documentation

4.49.1.1 double SKUA_PARAM::activation_energy

4.49.1.2 bool SKUA_PARAM::Adsorbable

4.49.1.3 double SKUA_PARAM::affinity

4.49.1.4 double SKUA_PARAM::film_transfer

4.49.1.5 double SKUA_PARAM::Qstn

4.49.1.6 double SKUA_PARAM::Qstnp1

4.49.1.7 double SKUA_PARAM::ref_diffusion

4.49.1.8 double SKUA_PARAM::ref_pressure

4.49.1.9 double SKUA_PARAM::ref_temperature

4.49.1.10 std::string SKUA_PARAM::speciesName

4.49.1.11 double SKUA_PARAM::xIC

4.49.1.12 double SKUA_PARAM::xn

4.49.1.13 double SKUA_PARAM::xnp1

4.49.1.14 double SKUA_PARAM::y_eff

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

- skua.h

4.50 Speciation_Test01_Data Struct Reference

```
#include <sandbox.h>
```

Public Attributes

- int N = 4
- const double logKw = -14.0
- const double logKa1 = -6.35
- const double logKa2 = -10.33
- double CT = 0.1786
- double NaT = 0.1786
- std::vector< Molecule > x
- Matrix< double > Jacobian
- Matrix< double > NumJac
- Matrix< double > logC
- Matrix< double > C

4.50.1 Member Data Documentation

4.50.1.1 **Matrix**<double> Speciation_Test01_Data::C

4.50.1.2 double Speciation_Test01_Data::CT = 0.1786

4.50.1.3 **Matrix**<double> Speciation_Test01_Data::Jacobian

4.50.1.4 **Matrix**<double> Speciation_Test01_Data::logC

4.50.1.5 const double Speciation_Test01_Data::logKa1 = -6.35

4.50.1.6 const double Speciation_Test01_Data::logKa2 = -10.33

4.50.1.7 const double Speciation_Test01_Data::logKw = -14.0

4.50.1.8 int Speciation_Test01_Data::N = 4

4.50.1.9 double Speciation_Test01_Data::NaT = 0.1786

4.50.1.10 **Matrix**<double> Speciation_Test01_Data::NumJac

4.50.1.11 std::vector<**Molecule**> Speciation_Test01_Data::x

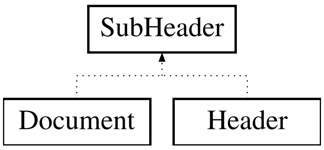
The documentation for this struct was generated from the following file:

- sandbox.h

4.51 SubHeader Class Reference

```
#include <yaml_wrapper.h>
```

Inheritance diagram for SubHeader:



Public Member Functions

- SubHeader ()
- ∼SubHeader ()
- SubHeader (const SubHeader &subheader)
- SubHeader (const KeyValueMap &map)
- SubHeader (std::string name)
- SubHeader (std::string name, const KeyValueMap &map)
- SubHeader & operator= (const SubHeader &sub)
- ValueTypePair & operator[] (const std::string key)
- ValueTypePair operator[] (const std::string key) const
- KeyValueMap & getMap ()
- void clear ()
- void addPair (std::string key, std::string val)
- void addPair (std::string key, std::string val, int type)
- void setName (std::string name)
- void setAlias (std::string alias)
- void setAlias (std::string alias, int state)
- void setNameAliasPair (std::string name, std::string alias, int state)
- void setState (int state)
- void DisplayContents ()
- std::string getName ()
- std::string getAlias ()
- bool isAlias ()
- bool isAnchor ()
- int getState ()

Protected Attributes

- KeyValueMap Data_Map
- std::string name
- std::string alias
- int state

4.51.1 Constructor & Destructor Documentation

4.51.1.1 SubHeader::SubHeader ( )

4.51.1.2 SubHeader::∼SubHeader ( )

4.51.1.3 SubHeader::SubHeader (const SubHeader & *subheader*)

4.51.1.4 SubHeader::SubHeader (const KeyValueMap & *map*)

4.51.1.5 SubHeader::SubHeader (std::string *name*)

4.51.1.6 SubHeader::SubHeader (std::string *name,* const KeyValueMap & *map*)

4.51.2 Member Function Documentation

4.51.2.1 void SubHeader::addPair (std::string *key,* std::string *val*)

4.51.2.2 void SubHeader::addPair (std::string *key,* std::string *val,* int *type*)

4.51.2.3 void SubHeader::clear ( )

4.51.2.4 void SubHeader::DisplayContents ( )

4.51.2.5 std::string SubHeader::getAlias ( )

4.51.2.6 KeyValueMap & SubHeader::getMap ( )

4.51.2.7 std::string SubHeader::getName ( )

4.51.2.8 int SubHeader::getState ( )

4.51.2.9 bool SubHeader::isAlias ( )

4.51.2.10 bool SubHeader::isAnchor ( )

4.51.2.11 SubHeader & SubHeader::operator= (const SubHeader & *sub*)

4.51.2.12 ValueTypePair & SubHeader::operator[] (const std::string *key*)

4.51.2.13 ValueTypePair SubHeader::operator[] (const std::string *key*) const

4.51.2.14 void SubHeader::setAlias (std::string *alias*)

4.51.2.15 void SubHeader::setAlias (std::string *alias,* int *state*)

4.51.2.16 void SubHeader::setName (std::string *name*)

4.51.2.17 void SubHeader::setNameAliasPair (std::string *name,* std::string *alias,* int *state*)

4.51.2.18 void SubHeader::setState (int *state*)

4.51.3 Member Data Documentation

4.51.3.1 std::string SubHeader::alias [protected]

4.51.3.2 KeyValueMap SubHeader::Data_Map [protected]

4.51.3.3 std::string SubHeader::name [protected]

4.51.3.4 int SubHeader::state [protected]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.52 SYSTEM_DATA Struct Reference

```
#include <magpie.h>
```

Public Attributes

- double T

- double PT
- double qT
- double PI
- double pi
- double As
- int N
- int I
- int J
- int K
- unsigned long int total_eval
- double avg_norm
- double max_norm
- int Sys
- int Par
- bool Recover
- bool Carrier
- bool Ideal
- bool Output

4.52.1 Member Data Documentation

4.52.1.1 double SYSTEM_DATA::As

4.52.1.2 double SYSTEM_DATA::avg_norm

4.52.1.3 bool SYSTEM_DATA::Carrier

4.52.1.4 int SYSTEM_DATA::I

4.52.1.5 bool SYSTEM_DATA::Ideal

4.52.1.6 int SYSTEM_DATA::J

4.52.1.7 int SYSTEM_DATA::K

4.52.1.8 double SYSTEM_DATA::max_norm

4.52.1.9 int SYSTEM_DATA::N

4.52.1.10 bool SYSTEM_DATA::Output

4.52.1.11 int SYSTEM_DATA::Par

4.52.1.12 double SYSTEM_DATA::PI

4.52.1.13 double SYSTEM_DATA::pi

4.52.1.14 double SYSTEM_DATA::PT

4.52.1.15 double SYSTEM_DATA::qT

4.52.1.16 bool SYSTEM_DATA::Recover

4.52.1.17 int SYSTEM_DATA::Sys

4.52.1.18 double SYSTEM_DATA::T

4.52.1.19 unsigned long int SYSTEM_DATA::total_eval

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

- magpie.h

4.53 TRAJECTORY_DATA Struct Reference

```
#include <Trajectory.h>
```

Public Attributes

- double mu_0 = 12.57e-7
- double rho_f = 1000.0
- double eta = 0.001
- double Hamaker = 1.3e-21
- double Temp = 298
- double k = 1.38e-23
- double Rs = 0.0026925
- double L = 0.0611
- double porosity = 0.8979
- double V_separator
- double a = 33.0e-6
- double V_wire
- double L_wire
- double A_separator
- double A_wire
- double B0 = 1.0
- double H0
- double Ms = 0.6
- double b = 0.25e-6
- double chi_p = 3.87e-6
- double rho_p = 8700.0
- double Q_in
- double V0
- double Y_initial = 20.0
- double dt
- double M
- double mp
- double beta
- double q_bar
- double sigma_v
- double sigma_vz
- double sigma_z
- double sigma_n
- double sigma_m
- double n_rand
- double m_rand
- double s_rand
- double t_rand
- Matrix< double > POL

- Matrix< double > H
- Matrix< double > dX
- Matrix< double > dY
- Matrix< double > X
- Matrix< double > Y
- Matrix< int > Cap

4.53.1 Member Data Documentation

4.53.1.1 double TRAJECTORY_DATA::a = 33.0e-6

4.53.1.2 double TRAJECTORY_DATA::A_separator

4.53.1.3 double TRAJECTORY_DATA::A_wire

4.53.1.4 double TRAJECTORY_DATA::b = 0.25e-6

4.53.1.5 double TRAJECTORY_DATA::B0 = 1.0

4.53.1.6 double TRAJECTORY_DATA::beta

4.53.1.7 Matrix<int> TRAJECTORY_DATA::Cap

4.53.1.8 double TRAJECTORY_DATA::chi_p = 3.87e-6

4.53.1.9 double TRAJECTORY_DATA::dt

4.53.1.10 Matrix<double> TRAJECTORY_DATA::dX

4.53.1.11 Matrix<double> TRAJECTORY_DATA::dY

4.53.1.12 double TRAJECTORY_DATA::eta = 0.001

4.53.1.13 Matrix<double> TRAJECTORY_DATA::H

4.53.1.14 double TRAJECTORY_DATA::H0

4.53.1.15 double TRAJECTORY_DATA::Hamaker = 1.3e-21

4.53.1.16 double TRAJECTORY_DATA::k = 1.38e-23

4.53.1.17 double TRAJECTORY_DATA::L = 0.0611

4.53.1.18 double TRAJECTORY_DATA::L_wire

4.53.1.19 double TRAJECTORY_DATA::M

4.53.1.20 double TRAJECTORY_DATA::m_rand

4.53.1.21 double TRAJECTORY_DATA::mp

4.53.1.22 double TRAJECTORY_DATA::Ms = 0.6

4.53.1.23 double TRAJECTORY_DATA::mu_0 = 12.57e-7

4.53.1.24 double TRAJECTORY_DATA::n_rand

4.53.1.25 Matrix<double> TRAJECTORY_DATA::POL

4.53.1.26 double TRAJECTORY_DATA::porosity = 0.8979

4.53.1.27 double TRAJECTORY_DATA::q_bar

4.53.1.28 double TRAJECTORY_DATA::Q_in

4.53.1.29 double TRAJECTORY_DATA::rho_f = 1000.0

4.53.1.30 double TRAJECTORY_DATA::rho_p = 8700.0

4.53.1.31 double TRAJECTORY_DATA::Rs = 0.0026925

4.53.1.32 double TRAJECTORY_DATA::s_rand

4.53.1.33 double TRAJECTORY_DATA::sigma_m

4.53.1.34 double TRAJECTORY_DATA::sigma_n

4.53.1.35 double TRAJECTORY_DATA::sigma_v

4.53.1.36 double TRAJECTORY_DATA::sigma_vz

4.53.1.37 double TRAJECTORY_DATA::sigma_z

4.53.1.38 double TRAJECTORY_DATA::t_rand

4.53.1.39 double TRAJECTORY_DATA::Temp = 298

4.53.1.40 double TRAJECTORY_DATA::V0

4.53.1.41 double TRAJECTORY_DATA::V_separator

4.53.1.42 double TRAJECTORY_DATA::V_wire

4.53.1.43 Matrix<double> TRAJECTORY_DATA::X

4.53.1.44 Matrix<double> TRAJECTORY_DATA::Y

4.53.1.45 double TRAJECTORY_DATA::Y_initial = 20.0

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

- Trajectory.h

4.54 UI_DATA Struct Reference

```
#include <ui.h>
```

Public Attributes

- ValueTypePair value_type

- std::vector< std::string > user_input
- std::vector< std::string > input_files
- std::string path
- int count = 0
- int max = 3
- int option
- bool Path = false
- bool Files = false
- bool MissingArg = true
- bool BasicUI = true
- int argc
- const char ∗ argv []

4.54.1 Member Data Documentation

4.54.1.1 int UI_DATA::argc

4.54.1.2 const char∗ UI_DATA::argv[ ]

4.54.1.3 bool UI_DATA::BasicUI = true

4.54.1.4 int UI_DATA::count = 0

4.54.1.5 bool UI_DATA::Files = false

4.54.1.6 std::vector<std::string> UI_DATA::input_files

4.54.1.7 int UI_DATA::max = 3

4.54.1.8 bool UI_DATA::MissingArg = true

4.54.1.9 int UI_DATA::option

4.54.1.10 std::string UI_DATA::path

4.54.1.11 bool UI_DATA::Path = false

4.54.1.12 std::vector<std::string> UI_DATA::user_input

4.54.1.13 ValueTypePair UI_DATA::value_type

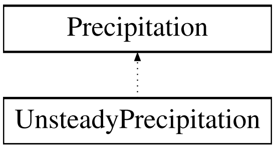
The documentation for this struct was generated from the following file:

- ui.h

4.55 UnsteadyPrecipitation Class Reference

```
#include <shark.h>
```

Inheritance diagram for UnsteadyPrecipitation:



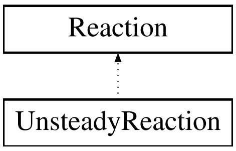
The documentation for this class was generated from the following file:

- shark.h

4.56 UnsteadyReaction Class Reference

```
#include <shark.h>
```

Inheritance diagram for UnsteadyReaction:



Public Member Functions

- UnsteadyReaction ()
- ∼UnsteadyReaction ()
- void Initialize_List (MasterSpeciesList &List)
- void Display_Info ()
- void Set_Species_Index (int i)
- void Set_Species_Index (std::string formula)
- void Set_Stoichiometric (int i, double v)
- void Set_Equilibrium (double v)
- void Set_Enthalpy (double H)
- void Set_Entropy (double S)
- void Set_EnthalpyANDEntropy (double H, double S)
- void Set_Energy (double G)
- void Set_InitialValue (double ic)
- void Set_MaximumValue (double max)
- void Set_Forward (double forward)
- void Set_Reverse (double reverse)
- void Set_ForwardRef (double Fref)
- void Set_ReverseRef (double Rref)
- void Set_ActivationEnergy (double E)
- void Set_Affinity (double b)
- void Set_TimeStep (double dt)
- void checkSpeciesEnergies ()
- void calculateEnergies ()
- void calculateEquilibrium (double T)
- void calculateRate (double T)
- bool haveEquilibrium ()
- bool haveRate ()
- int Get_Species_Index ()

- double Get_Stoichiometric (int i)
- double Get_Equilibrium ()
- double Get_Enthalpy ()
- double Get_Entropy ()
- double Get_Energy ()
- double Get_InitialValue ()
- double Get_MaximumValue ()
- double Get_Forward ()
- double Get_Reverse ()
- double Get_ForwardRef ()
- double Get_ReverseRef ()
- double Get_ActivationEnergy ()
- double Get_Affinity ()
- double Get_TimeStep ()
- double Eval_ReactionRate (const Matrix< double > &x, const Matrix< double > &gama)
- double Eval_Residual (const Matrix< double > &x_new, const Matrix< double > &x_old, const Matrix< double > &gama_new, const Matrix< double > &gama_old)
- double Eval_Residual (const Matrix< double > &x, const Matrix< double > &gama)
- double Eval_IC_Residual (const Matrix< double > &x)
- double Explicit_Eval (const Matrix< double > &x, const Matrix< double > &gama)

Protected Attributes

- double initial_value
- double max_value
- double forward_rate
- double reverse_rate
- double forward_ref_rate
- double reverse_ref_rate
- double activation_energy
- double temperature_affinity
- double time_step
- bool HaveForward
- bool HaveReverse
- bool HaveForRef
- bool HaveRevRef
- int species_index

Additional Inherited Members

4.56.1 Constructor & Destructor Documentation

4.56.1.1 UnsteadyReaction::UnsteadyReaction ( )

4.56.1.2 UnsteadyReaction::∼UnsteadyReaction ( )

4.56.2 Member Function Documentation

4.56.2.1 void UnsteadyReaction::calculateEnergies ( )

4.56.2.2 void UnsteadyReaction::calculateEquilibrium (double *T*)

4.56.2.3 void UnsteadyReaction::calculateRate (double *T*)

4.56.2.4 void UnsteadyReaction::checkSpeciesEnergies ( )

4.56.2.5 void UnsteadyReaction::Display_Info ( )

4.56.2.6 double UnsteadyReaction::Eval_IC_Residual (const **Matrix**< double > & *x*)

4.56.2.7 double UnsteadyReaction::Eval_ReactionRate (const **Matrix**< double > & *x,* const **Matrix**< double > & *gama*)

4.56.2.8 double UnsteadyReaction::Eval_Residual (const **Matrix**< double > & *x_new,* const **Matrix**< double > & *x_old,* const **Matrix**< double > & *gama_new,* const **Matrix**< double > & *gama_old*)

4.56.2.9 double UnsteadyReaction::Eval_Residual (const **Matrix**< double > & *x,* const **Matrix**< double > & *gama*)

4.56.2.10 double UnsteadyReaction::Explicit_Eval (const **Matrix**< double > & *x,* const **Matrix**< double > & *gama*)

4.56.2.11 double UnsteadyReaction::Get_ActivationEnergy ( )

4.56.2.12 double UnsteadyReaction::Get_Affinity ( )

4.56.2.13 double UnsteadyReaction::Get_Energy ( )

4.56.2.14 double UnsteadyReaction::Get_Enthalpy ( )

4.56.2.15 double UnsteadyReaction::Get_Entropy ( )

4.56.2.16 double UnsteadyReaction::Get_Equilibrium ( )

4.56.2.17 double UnsteadyReaction::Get_Forward ( )

4.56.2.18 double UnsteadyReaction::Get_ForwardRef ( )

4.56.2.19 double UnsteadyReaction::Get_InitialValue ( )

4.56.2.20 double UnsteadyReaction::Get_MaximumValue ( )

4.56.2.21 double UnsteadyReaction::Get_Reverse ( )

4.56.2.22 double UnsteadyReaction::Get_ReverseRef ( )

4.56.2.23 int UnsteadyReaction::Get_Species_Index ( )

4.56.2.24 double UnsteadyReaction::Get_Stoichiometric (int *i*)

4.56.2.25 double UnsteadyReaction::Get_TimeStep ( )

4.56.2.26 bool UnsteadyReaction::haveEquilibrium ( )

4.56.2.27 bool UnsteadyReaction::haveRate ( )

4.56.2.28 void UnsteadyReaction::Initialize_List (**MasterSpeciesList** & *List*)

4.56.2.29 void UnsteadyReaction::Set_ActivationEnergy (double *E*)

4.56.2.30 void UnsteadyReaction::Set_Affinity (double *b*)

4.56.2.31 void UnsteadyReaction::Set_Energy (double *G*)

4.56.2.32 void UnsteadyReaction::Set_Enthalpy (double *H*)

4.56.2.33 void UnsteadyReaction::Set_EnthalpyANDEntropy (double *H,* double *S*)

4.56.2.34 void UnsteadyReaction::Set_Entropy (double *S*)

4.56.2.35 void UnsteadyReaction::Set_Equilibrium (double *v*)

4.56.2.36 void UnsteadyReaction::Set_Forward (double *forward*)

4.56.2.37 void UnsteadyReaction::Set_ForwardRef (double *Fref*)

4.56.2.38 void UnsteadyReaction::Set_InitialValue (double *ic*)

4.56.2.39 void UnsteadyReaction::Set_MaximumValue (double *max*)

4.56.2.40 void UnsteadyReaction::Set_Reverse (double *reverse*)

4.56.2.41 void UnsteadyReaction::Set_ReverseRef (double *Rref*)

4.56.2.42 void UnsteadyReaction::Set_Species_Index (int *i*)

4.56.2.43 void UnsteadyReaction::Set_Species_Index (std::string *formula*)

4.56.2.44 void UnsteadyReaction::Set_Stoichiometric (int *i,* double *v*)

4.56.2.45 void UnsteadyReaction::Set_TimeStep (double *dt*)

4.56.3 Member Data Documentation

4.56.3.1 double UnsteadyReaction::activation_energy `[protected]`

4.56.3.2 double UnsteadyReaction::forward_rate `[protected]`

4.56.3.3 double UnsteadyReaction::forward_ref_rate `[protected]`

4.56.3.4 bool UnsteadyReaction::HaveForRef `[protected]`

4.56.3.5 bool UnsteadyReaction::HaveForward `[protected]`

4.56.3.6 bool UnsteadyReaction::HaveReverse `[protected]`

4.56.3.7 bool UnsteadyReaction::HaveRevRef `[protected]`

4.56.3.8 double UnsteadyReaction::initial_value `[protected]`

4.56.3.9 double UnsteadyReaction::max_value `[protected]`

4.56.3.10 double UnsteadyReaction::reverse_rate `[protected]`

4.56.3.11 double UnsteadyReaction::reverse_ref_rate `[protected]`

4.56.3.12 int UnsteadyReaction::species_index `[protected]`

4.56.3.13 double UnsteadyReaction::temperature_affinity `[protected]`

4.56.3.14 double UnsteadyReaction::time_step [protected]

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

- shark.h
- shark.cpp

4.57 ValueTypePair Class Reference

```
#include <yaml_wrapper.h>
```

Public Member Functions

- ValueTypePair ()
- ∼ValueTypePair ()
- ValueTypePair (const std::pair< std::string, int > &vt)
- ValueTypePair (std::string value, int type)
- ValueTypePair (const ValueTypePair &vt)
- ValueTypePair & operator= (const ValueTypePair &vt)
- void editValue (std::string value)
- void editPair (std::string value, int type)
- void findType ()
- void assertType (int type)
- void DisplayPair ()
- std::string getString ()
- bool getBool ()
- double getDouble ()
- int getInt ()
- std::string getValue ()
- int getType ()
- std::pair< std::string, int > & getPair ()

Private Attributes

- std::pair< std::string, int > Value_Type
- int type

4.57.1 Constructor & Destructor Documentation

4.57.1.1 ValueTypePair::ValueTypePair ( )

4.57.1.2 ValueTypePair::∼ValueTypePair ( )

4.57.1.3 ValueTypePair::ValueTypePair (const std::pair< std::string, int > & *vt*)

4.57.1.4 ValueTypePair::ValueTypePair (std::string *value,* int *type*)

4.57.1.5 ValueTypePair::ValueTypePair (const ValueTypePair & *vt*)

4.57.2 Member Function Documentation

4.57.2.1 void ValueTypePair::assertType (int *type*)

4.57.2.2 void ValueTypePair::DisplayPair ( )

4.57.2.3 void ValueTypePair::editPair (std::string *value,* int *type*)

4.57.2.4 void ValueTypePair::editValue (std::string *value*)

4.57.2.5 void ValueTypePair::findType ( )

4.57.2.6 bool ValueTypePair::getBool ( )

4.57.2.7 double ValueTypePair::getDouble ( )

4.57.2.8 int ValueTypePair::getInt ( )

4.57.2.9 std::pair< std::string, int > & ValueTypePair::getPair ( )

4.57.2.10 std::string ValueTypePair::getString ( )

4.57.2.11 int ValueTypePair::getType ( )

4.57.2.12 std::string ValueTypePair::getValue ( )

4.57.2.13 ValueTypePair & ValueTypePair::operator= (const ValueTypePair & *vt*)

4.57.3 Member Data Documentation

4.57.3.1 int ValueTypePair::type [private]

4.57.3.2 std::pair<std::string,int> ValueTypePair::Value_Type [private]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.58 yaml_cpp_class Class Reference

```
#include <yaml_wrapper.h>
```

Public Member Functions

- yaml_cpp_class ()
- ∼yaml_cpp_class ()
- int setInputFile (const char ∗file)
- int readInputFile ()
- int cleanup ()
- int executeYamlRead (const char ∗file)
- YamlWrapper & getYamlWrapper ()
- void DisplayContents ()

Private Attributes

- YamlWrapper yaml_wrapper
- FILE ∗ input_file
- const char ∗ file_name
- yaml_parser_t token_parser
- yaml_token_t current_token
- yaml_token_t previous_token

4.58.1 Constructor & Destructor Documentation

4.58.1.1 yaml_cpp_class::yaml_cpp_class ( )

4.58.1.2 yaml_cpp_class::∼yaml_cpp_class ( )

4.58.2 Member Function Documentation

4.58.2.1 int yaml_cpp_class::cleanup ( )

4.58.2.2 void yaml_cpp_class::DisplayContents ( )

4.58.2.3 int yaml_cpp_class::executeYamlRead (const char ∗ *file*)

4.58.2.4 YamlWrapper & yaml_cpp_class::getYamlWrapper ( )

4.58.2.5 int yaml_cpp_class::readInputFile ( )

4.58.2.6 int yaml_cpp_class::setInputFile (const char ∗ *file*)

4.58.3 Member Data Documentation

4.58.3.1 yaml_token_t yaml_cpp_class::current_token [private]

4.58.3.2 const char∗ yaml_cpp_class::file_name [private]

4.58.3.3 FILE∗ yaml_cpp_class::input_file [private]

4.58.3.4 yaml_token_t yaml_cpp_class::previous_token [private]

4.58.3.5 yaml_parser_t yaml_cpp_class::token_parser [private]

4.58.3.6 YamlWrapper yaml_cpp_class::yaml_wrapper [private]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

4.59 YamlWrapper Class Reference

```
#include <yaml_wrapper.h>
```

Public Member Functions

- YamlWrapper ()
- ∼YamlWrapper ()
- YamlWrapper (const YamlWrapper &yaml)
- YamlWrapper (std::string key, const Document &doc)
- YamlWrapper & operator= (const YamlWrapper &yaml)
- Document & operator() (const std::string key)
- Document operator() (const std::string key) const
- std::map< std::string, Document > & getDocMap ()
- Document & getDocument (std::string key)
- std::map< std::string,
  Document >::const_iterator end () const
- std::map< std::string,
  Document >::iterator end ()
- std::map< std::string,
  Document >::const_iterator begin () const
- std::map< std::string,
  Document >::iterator begin ()
- void clear ()
- void resetKeys ()
- void changeKey (std::string oldKey, std::string newKey)
- void revalidateAllKeys ()
- void DisplayContents ()
- void addDocKey (std::string key)
- void copyAnchor2Alias (std::string alias, Document &ref)
- int size ()
- Document & getAnchoredDoc (std::string alias)
- Document & getDocFromHeadAlias (std::string alias)
- Document & getDocFromSubAlias (std::string alias)

Private Attributes

- std::map< std::string, Document > Doc_Map

4.59.1 Constructor & Destructor Documentation

4.59.1.1 YamlWrapper::YamlWrapper ( )

4.59.1.2 YamlWrapper::∼YamlWrapper ( )

4.59.1.3 YamlWrapper::YamlWrapper (const YamlWrapper & *yaml*)

4.59.1.4 YamlWrapper::YamlWrapper (std::string *key,* const Document & *doc*)

4.59.2 Member Function Documentation

4.59.2.1 void YamlWrapper::addDocKey (std::string *key*)

4.59.2.2 std::map< std::string, Document >::const_iterator YamlWrapper::begin ( ) const

4.59.2.3 std::map< std::string, Document >::iterator YamlWrapper::begin ( )

4.59.2.4 void YamlWrapper::changeKey (std::string *oldKey,* std::string *newKey*)

4.59.2.5 void YamlWrapper::clear ( )

4.59.2.6 void YamlWrapper::copyAnchor2Alias (std::string *alias,* Document & *ref*)

4.59.2.7 void YamlWrapper::DisplayContents ( )

4.59.2.8 std::map< std::string, Document >::const_iterator YamlWrapper::end ( ) const

4.59.2.9 std::map< std::string, Document >::iterator YamlWrapper::end ( )

4.59.2.10 Document & YamlWrapper::getAnchoredDoc (std::string *alias*)

4.59.2.11 Document & YamlWrapper::getDocFromHeadAlias (std::string *alias*)

4.59.2.12 Document & YamlWrapper::getDocFromSubAlias (std::string *alias*)

4.59.2.13 std::map< std::string, Document > & YamlWrapper::getDocMap ( )

4.59.2.14 Document & YamlWrapper::getDocument (std::string *key*)

4.59.2.15 Document & YamlWrapper::operator() (const std::string *key*)

4.59.2.16 Document YamlWrapper::operator() (const std::string *key*) const

4.59.2.17 YamlWrapper & YamlWrapper::operator= (const YamlWrapper & *yaml*)

4.59.2.18 void YamlWrapper::resetKeys ( )

4.59.2.19 void YamlWrapper::revalidateAllKeys ( )

4.59.2.20 int YamlWrapper::size ( )

4.59.3 Member Data Documentation

4.59.3.1 std::map<std::string, Document> YamlWrapper::Doc_Map [private]

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

- yaml_wrapper.h
- yaml_wrapper.cpp

Chapter 5

File Documentation

5.1 dogfish.cpp File Reference

```
#include "dogfish.h"
```

Functions

- void print2file_species_header (FILE ∗Output, DOGFISH_DATA ∗dog_dat, int i)
- void print2file_DOGFISH_header (DOGFISH_DATA ∗dog_dat)
- void print2file_DOGFISH_result_old (DOGFISH_DATA ∗dog_dat)
- void print2file_DOGFISH_result_new (DOGFISH_DATA ∗dog_dat)
- double default_Retardation (int i, int l, const void ∗data)
- double default_IntraDiffusion (int i, int l, const void ∗data)
- double default_FilmMTCoeff (int i, const void ∗data)
- double default_SurfaceConcentration (int i, const void ∗data)
- int setup_DOGFISH_DATA (FILE ∗file, double(∗eval_R)(int i, int l, const void ∗user_data), double(∗eval_DI)(int i, int l, const void ∗user_data), double(∗eval_kf)(int i, const void ∗user_data), double(∗eval_qs)(int i, const void ∗user_data), const void ∗user_data, DOGFISH_DATA ∗dog_dat)
- int DOGFISH_Executioner (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_ICs (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_timestep (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_preprocesses (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_params (const void ∗user_data)
- int DOGFISH_postprocesses (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_reset (DOGFISH_DATA ∗dog_dat)
- int DOGFISH (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_TESTS ()

5.1.1 Function Documentation

5.1.1.1 double default_FilmMTCoeff (int *i*, const void ∗ *data*)

5.1.1.2 double default_IntraDiffusion (int *i*, int *l*, const void ∗ *data*)

5.1.1.3 double default_Retardation (int *i*, int *l*, const void ∗ *data*)

5.1.1.4 double default_SurfaceConcentration (int *i*, const void ∗ *data*)

5.1.1.5 int DOGFISH (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.6 int DOGFISH_Executioner (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.7 int DOGFISH_postprocesses (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.8 int DOGFISH_preprocesses (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.9 int DOGFISH_reset (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.10 int DOGFISH_TESTS ( )

5.1.1.11 void print2file_DOGFISH_header (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.12 void print2file_DOGFISH_result_new (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.13 void print2file_DOGFISH_result_old (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.14 void print2file_species_header (FILE ∗ *Output,* DOGFISH_DATA ∗ *dog_dat,* int *i*)

5.1.1.15 int set_DOGFISH_ICs (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.16 int set_DOGFISH_params (const void ∗ *user_data*)

5.1.1.17 int set_DOGFISH_timestep (DOGFISH_DATA ∗ *dog_dat*)

5.1.1.18 int setup_DOGFISH_DATA (FILE ∗ *file,* double(∗)(int i, int l, const void ∗user_data) *eval_R,* double(∗)(int i, int l, const void ∗user_data) *eval_DI,* double(∗)(int i, const void ∗user_data) *eval_kf,* double(∗)(int i, const void ∗user_data) *eval_qs,* const void ∗ *user_data,* DOGFISH_DATA ∗ *dog_dat*)

5.2 dogfish.h File Reference

```
#include "finch.h"
#include "mola.h"
```

Classes

- struct DOGFISH_PARAM
- struct DOGFISH_DATA

Functions

- void print2file_species_header (FILE ∗Output, DOGFISH_DATA ∗dog_dat, int i)
- void print2file_DOGFISH_header (DOGFISH_DATA ∗dog_dat)
- void print2file_DOGFISH_result_old (DOGFISH_DATA ∗dog_dat)
- void print2file_DOGFISH_result_new (DOGFISH_DATA ∗dog_dat)
- double default_Retardation (int i, int l, const void ∗data)
- double default_IntraDiffusion (int i, int l, const void ∗data)
- double default_FilmMTCoeff (int i, const void ∗data)
- double default_SurfaceConcentration (int i, const void ∗data)
- int setup_DOGFISH_DATA (FILE ∗file, double(∗eval_R)(int i, int l, const void ∗user_data), double(∗eval_DI)(int i, int l, const void ∗user_data), double(∗eval_kf)(int i, const void ∗user_data), double(∗eval_qs)(int i, const void ∗user_data), const void ∗user_data, DOGFISH_DATA ∗dog_dat)

- int DOGFISH_Executioner (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_ICs (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_timestep (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_preprocesses (DOGFISH_DATA ∗dog_dat)
- int set_DOGFISH_params (const void ∗user_data)
- int DOGFISH_postprocesses (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_reset (DOGFISH_DATA ∗dog_dat)
- int DOGFISH (DOGFISH_DATA ∗dog_dat)
- int DOGFISH_TESTS ()

5.2.1 Function Documentation

5.2.1.1 double default_FilmMTCoeff (int *i*, const void ∗ *data*)

5.2.1.2 double default_IntraDiffusion (int *i*, int *l*, const void ∗ *data*)

5.2.1.3 double default_Retardation (int *i*, int *l*, const void ∗ *data*)

5.2.1.4 double default_SurfaceConcentration (int *i*, const void ∗ *data*)

5.2.1.5 int DOGFISH (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.6 int DOGFISH_Executioner (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.7 int DOGFISH_postprocesses (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.8 int DOGFISH_preprocesses (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.9 int DOGFISH_reset (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.10 int DOGFISH_TESTS ( )

5.2.1.11 void print2file_DOGFISH_header (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.12 void print2file_DOGFISH_result_new (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.13 void print2file_DOGFISH_result_old (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.14 void print2file_species_header (FILE ∗ *Output*, DOGFISH_DATA ∗ *dog_dat*, int *i*)

5.2.1.15 int set_DOGFISH_ICs (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.16 int set_DOGFISH_params (const void ∗ *user_data*)

5.2.1.17 int set_DOGFISH_timestep (DOGFISH_DATA ∗ *dog_dat*)

5.2.1.18 int setup_DOGFISH_DATA (FILE ∗ *file*, double(∗)(int i, int l, const void ∗user_data) *eval_R*, double(∗)(int i, int l, const void ∗user_data) *eval_DI*, double(∗)(int i, const void ∗user_data) *eval_kf*, double(∗)(int i, const void ∗user_data) *eval_qs*, const void ∗ *user_data*, DOGFISH_DATA ∗ *dog_dat*)

5.3 eel.cpp File Reference

```
#include "eel.h"
```

Functions

- int EEL_TESTS ()

5.3.1 Function Documentation

5.3.1.1 int EEL_TESTS ( )

5.4 eel.h File Reference

```
#include <stdio.h>
#include <math.h>
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <vector>
#include <time.h>
#include <float.h>
#include <string>
#include "error.h"
```

Classes

- class Atom
- class PeriodicTable

Functions

- int EEL_TESTS ()

5.4.1 Function Documentation

5.4.1.1 int EEL_TESTS ( )

5.5 egret.cpp File Reference

```
#include "egret.h"
```

Functions

- int initialize_data (int N, MIXED_GAS *gas_dat)
- int set_variables (double PT, double T, double us, double L, std::vector< double > &y, MIXED_GAS *gas_dat)
- int calculate_properties (MIXED_GAS *gas_dat)
- int EGRET_TESTS ()

5.5.1 Function Documentation

5.5.1.1 int calculate_properties (**MIXED_GAS** * *gas_dat*)

5.5.1.2 int EGRET_TESTS ( )

5.5.1.3 int initialize_data (int *N*, MIXED_GAS ∗ *gas_dat*)

5.5.1.4 int set_variables (double *PT*, double *T*, double *us*, double *L*, std::vector< double > & *y*, MIXED_GAS ∗ *gas_dat*)

5.6 egret.h File Reference

```
#include "macaw.h"
```

Classes

- struct PURE_GAS
- struct MIXED_GAS

Macros

- #define Rstd 8.3144621
- #define RE3 8.3144621E+3
- #define Po 100.0
- #define Cstd(p, T) ((p)/(Rstd∗T))
- #define CE3(p, T) ((p)/(RE3∗T))
- #define Pstd(c, T) ((c)∗Rstd∗T)
- #define PE3(c, T) ((c)∗RE3∗T)
- #define Nu(mu, rho) ((mu)/(rho))
- #define PSI(T) (0.873143 + (0.000072375∗T))
- #define Dp_ij(Dij, PT) ((PT∗Dij)/Po)
- #define D_ij(MWi, MWj, rhoi, rhoj, mui, muj) ((4.0 / sqrt(2.0)) ∗ pow(((1/MWi)+(1/MWj)),0.5)) / pow((pow((pow((rhoi/(1.385∗mui)),2.0)/MWi),0.25)+ pow((pow((rhoj/(1.385∗muj)),2.0)/MWj),0.25)),2.0)
- #define Mu(muo, To, C, T) (muo ∗ ((To + C)/(T + C)) ∗ pow((T/To),1.5))
- #define D_ii(rhoi, mui) (1.385∗mui/rhoi)
- #define ReNum(u, L, nu) (u∗L/nu)
- #define ScNum(nu, D) (nu/D)
- #define FilmMTCoeff(D, L, Re, Sc) ((D/L)∗(2.0 + (1.1∗pow(Re,0.6)∗pow(Sc,0.3))))

Functions

- int initialize_data (int N, MIXED_GAS ∗gas_dat)
- int set_variables (double PT, double T, double us, double L, std::vector< double > &y, MIXED_GAS ∗gas_dat)
- int calculate_properties (MIXED_GAS ∗gas_dat)
- int EGRET_TESTS ()

5.6.1 Macro Definition Documentation

5.6.1.1 #define CE3(*p*, *T*) ((p)/(RE3∗T))

5.6.1.2 #define Cstd(*p*, *T*) ((p)/(Rstd∗T))

5.6.1.3 #define D_ii(*rhoi*, *mui*) (1.385∗mui/rhoi)

5.6.1.4 #define D_ij(*MWi, MWj, rhoi, rhoj, mui, muj*) ((4.0 / sqrt(2.0)) ∗ pow(((1/MWi)+(1/MWj)),0.5)) / pow((pow((pow((rhoi/(1.385∗mui)),2.0)/MWi),0.25)+ pow((pow((rhoj/(1.385∗muj)),2.0)/MWj),0.25)),2.0)

5.6.1.5 #define Dp_ij(*Dij, PT*) ((PT∗Dij)/Po)

5.6.1.6 #define FilmMTCoeff(*D, L, Re, Sc*) ((D/L)∗(2.0 + (1.1∗pow(Re,0.6)∗pow(Sc,0.3))))

5.6.1.7 #define Mu(*muo, To, C, T*) (muo ∗ ((To + C)/(T + C)) ∗ pow((T/To),1.5))

5.6.1.8 #define Nu(*mu, rho*) ((mu)/(rho))

5.6.1.9 #define PE3(*c, T*) ((c)∗RE3∗T)

5.6.1.10 #define Po 100.0

5.6.1.11 #define PSI(*T*) (0.873143 + (0.000072375∗T))

5.6.1.12 #define Pstd(*c, T*) ((c)∗Rstd∗T)

5.6.1.13 #define RE3 8.3144621E+3

5.6.1.14 #define ReNum(*u, L, nu*) (u∗L/nu)

5.6.1.15 #define Rstd 8.3144621

5.6.1.16 #define ScNum(*nu, D*) (nu/D)

5.6.2 Function Documentation

5.6.2.1 int calculate_properties (MIXED_GAS ∗ *gas_dat*)

5.6.2.2 int EGRET_TESTS ( )

5.6.2.3 int initialize_data (int *N*, MIXED_GAS ∗ *gas_dat*)

5.6.2.4 int set_variables (double *PT*, double *T*, double *us*, double *L*, std::vector< double > & *y*, MIXED_GAS ∗ *gas_dat*)

5.7 error.cpp File Reference

```
#include "error.h"
```

Functions

- void error (int flag)

5.7.1 Function Documentation

5.7.1.1 void error (int *flag*)

5.8 error.h File Reference

```
#include <iostream>
```

Macros

- #define mError(i)

Enumerations

- enum error_type {
  generic_error, file_dne, indexing_error, magpie_reverse_error,
  simulation_fail, invalid_components, invalid_boolean, invalid_molefraction,
  invalid_gas_sum, invalid_solid_sum, scenario_fail, out_of_bounds,
  non_square_matrix, dim_mis_match, empty_matrix, opt_no_support,
  invalid_fraction, ortho_check_fail, unstable_matrix, no_diffusion,
  negative_mass, negative_time, matvec_mis_match, arg_matrix_same,
  singular_matrix, matrix_too_small, invalid_size, nullptr_func,
  invalid_norm, vector_out_of_bounds, zero_vector, tensor_out_of_bounds,
  non_real_edge, nullptr_error, invalid_atom, invalid_proton,
  invalid_neutron, invalid_electron, invalid_valence, string_parse_error,
  unregistered_name, rxn_rate_error, invalid_species, duplicate_variable,
  missing_information, invalid_type, key_not_found, anchor_alias_dne,
  initial_error, not_a_token, read_error, invalid_console_input }

Functions

- void error (int flag)

5.8.1 Macro Definition Documentation

5.8.1.1 #define mError(i)

Value:

```
{error(i);          \
std::cout << "Source: " << __FILE__ << "\nLine: " << __LINE__ << std::endl;}
```

5.8.2 Enumeration Type Documentation

5.8.2.1 enum error_type

Enumerator

generic_error

file_dne

indexing_error

magpie_reverse_error

simulation_fail

invalid_components

invalid_boolean

invalid_molefraction

invalid_gas_sum

invalid_solid_sum

scenario_fail

out_of_bounds

non_square_matrix

dim_mis_match

empty_matrix

opt_no_support

invalid_fraction

ortho_check_fail

unstable_matrix

no_diffusion

negative_mass

negative_time

matvec_mis_match

arg_matrix_same

singular_matrix

matrix_too_small

invalid_size

nullptr_func

invalid_norm

vector_out_of_bounds

zero_vector

tensor_out_of_bounds

non_real_edge

nullptr_error

invalid_atom

invalid_proton

invalid_neutron

invalid_electron

invalid_valence

string_parse_error

unregistered_name

rxn_rate_error

invalid_species

duplicate_variable

missing_information

invalid_type

key_not_found

anchor_alias_dne

initial_error

not_a_token

read_error

invalid_console_input

5.8.3 Function Documentation

5.8.3.1 void error (int *flag*)

5.9 finch.cpp File Reference

```
#include "finch.h"
```

Functions

- double max (std::vector< double > &values)
- double min (std::vector< double > &values)
- double minmod (std::vector< double > &values)
- int uTotal (FINCH_DATA ∗dat)
- int uAverage (FINCH_DATA ∗dat)
- int check_Mass (FINCH_DATA ∗dat)
- int l_direct (FINCH_DATA ∗dat)
- int lark_picard_step (const Matrix< double > &x, Matrix< double > &G, const void ∗data)
- int nl_picard (FINCH_DATA ∗dat)
- int setup_FINCH_DATA (int(∗user_callroutine)(const void ∗user_data), int(∗user_setic)(const void ∗user_data), int(∗user_timestep)(const void ∗user_data), int(∗user_preprocess)(const void ∗user_data), int(∗user_solve)(const void ∗user_data), int(∗user_setparams)(const void ∗user_data), int(∗user_discretize)(const void ∗user_data), int(∗user_bcs)(const void ∗user_data), int(∗user_res)(const Matrix< double > &x, Matrix< double > &res, const void ∗user_data), int(∗user_precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗user_data), int(∗user_postprocess)(const void ∗user_data), int(∗user_reset)(const void ∗user_data), FINCH_DATA ∗dat, const void ∗param_data)
- void print2file_dim_header (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_time_header (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_result_old (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_result_new (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_newline (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_tab (FILE ∗Output, FINCH_DATA ∗dat)
- int default_execution (const void ∗user_data)
- int default_ic (const void ∗user_data)
- int default_timestep (const void ∗user_data)
- int default_preprocess (const void ∗user_data)
- int default_solve (const void ∗user_data)
- int default_params (const void ∗user_data)
- int minmod_discretization (const void ∗user_data)
- int vanAlbada_discretization (const void ∗user_data)
- int ospre_discretization (const void ∗user_data)
- int default_bcs (const void ∗user_data)
- int default_res (const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)
- int default_precon (const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)
- int default_postprocess (const void ∗user_data)
- int default_reset (const void ∗user_data)
- int buckley_leverett_ic (const void ∗user_data)
- int buckley_leverett_params (const void ∗user_data)
- int burgers_ic (const void ∗user_data)
- int burgers_params (const void ∗user_data)
- int burgers_bcs (const void ∗user_data)
- int FINCH_TESTS ()

5.9.1 Function Documentation

5.9.1.1 int buckley_leverett_ic (const void ∗ *user_data*)

5.9.1.2 int buckley_leverett_params (const void ∗ *user_data*)

5.9.1.3 int burgers_bcs (const void ∗ *user_data*)

5.9.1.4 int burgers_ic (const void ∗ *user_data*)

5.9.1.5 int burgers_params (const void * *user_data*)

5.9.1.6 int check_Mass (FINCH_DATA * *dat*)

5.9.1.7 int default_bcs (const void * *user_data*)

5.9.1.8 int default_execution (const void * *user_data*)

5.9.1.9 int default_ic (const void * *user_data*)

5.9.1.10 int default_params (const void * *user_data*)

5.9.1.11 int default_postprocess (const void * *user_data*)

5.9.1.12 int default_precon (const Matrix< double > & *b,* Matrix< double > & *p,* const void * *user_data*)

5.9.1.13 int default_preprocess (const void * *user_data*)

5.9.1.14 int default_res (const Matrix< double > & *x,* Matrix< double > & *res,* const void * *user_data*)

5.9.1.15 int default_reset (const void * *user_data*)

5.9.1.16 int default_solve (const void * *user_data*)

5.9.1.17 int default_timestep (const void * *user_data*)

5.9.1.18 int FINCH_TESTS ( )

5.9.1.19 int l_direct (FINCH_DATA * *dat*)

5.9.1.20 int lark_picard_step (const Matrix< double > & *x,* Matrix< double > & *G,* const void * *data*)

5.9.1.21 double max (std::vector< double > & *values*)

5.9.1.22 double min (std::vector< double > & *values*)

5.9.1.23 double minmod (std::vector< double > & *values*)

5.9.1.24 int minmod_discretization (const void * *user_data*)

5.9.1.25 int nl_picard (FINCH_DATA * *dat*)

5.9.1.26 int ospre_discretization (const void * *user_data*)

5.9.1.27 void print2file_dim_header (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.28 void print2file_newline (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.29 void print2file_result_new (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.30 void print2file_result_old (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.31 void print2file_tab (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.32 void print2file_time_header (FILE * *Output,* FINCH_DATA * *dat*)

5.9.1.33 int setup_FINCH_DATA (int(∗)(const void ∗user_data) *user_callroutine,* int(∗)(const void ∗user_data) *user_setic,* int(∗)(const void ∗user_data) *user_timestep,* int(∗)(const void ∗user_data) *user_preprocess,* int(∗)(const void ∗user_data) *user_solve,* int(∗)(const void ∗user_data) *user_setparams,* int(∗)(const void ∗user_data) *user_discretize,* int(∗)(const void ∗user_data) *user_bcs,* int(∗)(const **Matrix**< double > &x, **Matrix**< double > &res, const void ∗user_data) *user_res,* int(∗)(const **Matrix**< double > &b, **Matrix**< double > &p, const void ∗user_data) *user_precon,* int(∗)(const void ∗user_data) *user_postprocess,* int(∗)(const void ∗user_data) *user_reset,* **FINCH_DATA** ∗ *dat,* const void ∗ *param_data*)

5.9.1.34 int uAverage (**FINCH_DATA** ∗ *dat*)

5.9.1.35 int uTotal (**FINCH_DATA** ∗ *dat*)

5.9.1.36 int vanAlbada_discretization (const void ∗ *user_data*)

5.10 finch.h File Reference

```
#include "macaw.h"
#include "lark.h"
```

Classes

- struct FINCH_DATA

Macros

- #define FINCH_Picard 0
- #define LARK_Picard 1
- #define LARK_PJFNK 2
- #define Cartesian 0
- #define Cylindrical 1
- #define Spherical 2

Functions

- double max (std::vector< double > &values)
- double min (std::vector< double > &values)
- double minmod (std::vector< double > &values)
- int uTotal (FINCH_DATA ∗dat)
- int uAverage (FINCH_DATA ∗dat)
- int check_Mass (FINCH_DATA ∗dat)
- int l_direct (FINCH_DATA ∗dat)
- int lark_picard_step (const Matrix< double > &x, Matrix< double > &G, const void ∗data)
- int nl_picard (FINCH_DATA ∗dat)
- int setup_FINCH_DATA (int(∗user_callroutine)(const void ∗user_data), int(∗user_setic)(const void ∗user_data), int(∗user_timestep)(const void ∗user_data), int(∗user_preprocess)(const void ∗user_data), int(∗user_solve)(const void ∗user_data), int(∗user_setparams)(const void ∗user_data), int(∗user_discretize)(const void ∗user_data), int(∗user_bcs)(const void ∗user_data), int(∗user_res)(const Matrix< double > &x, Matrix< double > &res, const void ∗user_data), int(∗user_precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗user_data), int(∗user_postprocess)(const void ∗user_data), int(∗user_reset)(const void ∗user_data), FINCH_DATA ∗dat, const void ∗param_data)
- void print2file_dim_header (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_time_header (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_result_old (FILE ∗Output, FINCH_DATA ∗dat)

- void print2file_result_new (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_newline (FILE ∗Output, FINCH_DATA ∗dat)
- void print2file_tab (FILE ∗Output, FINCH_DATA ∗dat)
- int default_execution (const void ∗user_data)
- int default_ic (const void ∗user_data)
- int default_timestep (const void ∗user_data)
- int default_preprocess (const void ∗user_data)
- int default_solve (const void ∗user_data)
- int default_params (const void ∗user_data)
- int minmod_discretization (const void ∗user_data)
- int vanAlbada_discretization (const void ∗user_data)
- int ospre_discretization (const void ∗user_data)
- int default_bcs (const void ∗user_data)
- int default_res (const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)
- int default_precon (const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)
- int default_postprocess (const void ∗user_data)
- int default_reset (const void ∗user_data)
- int buckley_leverett_ic (const void ∗user_data)
- int buckley_leverett_params (const void ∗user_data)
- int burgers_ic (const void ∗user_data)
- int burgers_params (const void ∗user_data)
- int burgers_bcs (const void ∗user_data)
- int FINCH_TESTS ()

5.10.1 Macro Definition Documentation

5.10.1.1 #define Cartesian 0

5.10.1.2 #define Cylindrical 1

5.10.1.3 #define FINCH_Picard 0

5.10.1.4 #define LARK_Picard 1

5.10.1.5 #define LARK_PJFNK 2

5.10.1.6 #define Spherical 2

5.10.2 Function Documentation

5.10.2.1 int buckley_leverett_ic (const void ∗ *user_data*)

5.10.2.2 int buckley_leverett_params (const void ∗ *user_data*)

5.10.2.3 int burgers_bcs (const void ∗ *user_data*)

5.10.2.4 int burgers_ic (const void ∗ *user_data*)

5.10.2.5 int burgers_params (const void ∗ *user_data*)

5.10.2.6 int check_Mass (FINCH_DATA ∗ *dat*)

5.10.2.7 int default_bcs (const void ∗ *user_data*)

5.10.2.8 int default_execution (const void $*$ *user_data*)

5.10.2.9 int default_ic (const void $*$ *user_data*)

5.10.2.10 int default_params (const void $*$ *user_data*)

5.10.2.11 int default_postprocess (const void $*$ *user_data*)

5.10.2.12 int default_precon (const Matrix< double > & *b*, Matrix< double > & *p*, const void $*$ *user_data*)

5.10.2.13 int default_preprocess (const void $*$ *user_data*)

5.10.2.14 int default_res (const Matrix< double > & *x*, Matrix< double > & *res*, const void $*$ *user_data*)

5.10.2.15 int default_reset (const void $*$ *user_data*)

5.10.2.16 int default_solve (const void $*$ *user_data*)

5.10.2.17 int default_timestep (const void $*$ *user_data*)

5.10.2.18 int FINCH_TESTS ( )

5.10.2.19 int l_direct (FINCH_DATA $*$ *dat*)

5.10.2.20 int lark_picard_step (const Matrix< double > & *x*, Matrix< double > & *G*, const void $*$ *data*)

5.10.2.21 double max (std::vector< double > & *values*)

5.10.2.22 double min (std::vector< double > & *values*)

5.10.2.23 double minmod (std::vector< double > & *values*)

5.10.2.24 int minmod_discretization (const void $*$ *user_data*)

5.10.2.25 int nl_picard (FINCH_DATA $*$ *dat*)

5.10.2.26 int ospre_discretization (const void $*$ *user_data*)

5.10.2.27 void print2file_dim_header (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.28 void print2file_newline (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.29 void print2file_result_new (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.30 void print2file_result_old (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.31 void print2file_tab (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.32 void print2file_time_header (FILE $*$ *Output*, FINCH_DATA $*$ *dat*)

5.10.2.33 int setup_FINCH_DATA (int(∗)(const void ∗user_data) *user_callroutine,* int(∗)(const void ∗user_data) *user_setic,* int(∗)(const void ∗user_data) *user_timestep,* int(∗)(const void ∗user_data) *user_preprocess,* int(∗)(const void ∗user_data) *user_solve,* int(∗)(const void ∗user_data) *user_setparams,* int(∗)(const void ∗user_data) *user_discretize,* int(∗)(const void ∗user_data) *user_bcs,* int(∗)(const **Matrix**< double > &x, **Matrix**< double > &res, const void ∗user_data) *user_res,* int(∗)(const **Matrix**< double > &b, **Matrix**< double > &p, const void ∗user_data) *user_precon,* int(∗)(const void ∗user_data) *user_postprocess,* int(∗)(const void ∗user_data) *user_reset,* **FINCH_DATA** ∗ *dat,* const void ∗ *param_data*)

5.10.2.34 int uAverage (**FINCH_DATA** ∗ *dat*)

5.10.2.35 int uTotal (**FINCH_DATA** ∗ *dat*)

5.10.2.36 int vanAlbada_discretization (const void ∗ *user_data*)

5.11 flock.h File Reference

```
#include "macaw.h"
#include "egret.h"
#include "finch.h"
#include "lark.h"
#include "skua.h"
#include "scopsowl.h"
#include "gsta_opt.h"
#include "magpie.h"
#include "skua_opt.h"
#include "scopsowl_opt.h"
#include "yaml_wrapper.h"
```

5.12 gsta_opt.cpp File Reference

```
#include "gsta_opt.h"
```

Functions

- int roundIt (double d)
- int twoFifths (int m)
- int orderMag (double x)
- int minValue (std::vector< int > array)
- int minIndex (std::vector< double > array)
- int avgPar (std::vector< int > array)
- double avgValue (std::vector< double > array)
- double weightedAvg (double ∗enorm, double ∗x, int n)
- double rSq (double ∗x, double ∗y, double slope, double vint, int m_dat)
- bool isSmooth (double ∗par, void ∗data)
- void orthoLinReg (double ∗x, double ∗y, double ∗par, int m_dat, int n_par)
- void eduGuess (double ∗P, double ∗q, double ∗par, int k, int m_dat, void ∗data)
- double gstaFunc (double p, const double ∗K, double qmax, int n_par)
- double gstaObjFunc (double ∗t, double ∗y, double ∗par, int m_dat, void ∗data)
- void eval_GSTA (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int gsta_optimize (const char ∗fileName)

5.12.1 Function Documentation

5.12.1.1 int avgPar (std::vector< int > *array*)

5.12.1.2 double avgValue (std::vector< double > *array*)

5.12.1.3 void eduGuess (double * *P,* double * *q,* double * *par,* int *k,* int *m_dat,* void * *data*)

5.12.1.4 void eval_GSTA (const double * *par,* int *m_dat,* const void * *data,* double * *fvec,* int * *info*)

5.12.1.5 int gsta_optimize (const char * *fileName*)

5.12.1.6 double gstaFunc (double *p,* const double * *K,* double *qmax,* int *n_par*)

5.12.1.7 double gstaObjFunc (double * *t,* double * *y,* double * *par,* int *m_dat,* void * *data*)

5.12.1.8 bool isSmooth (double * *par,* void * *data*)

5.12.1.9 int minIndex (std::vector< double > *array*)

5.12.1.10 int minValue (std::vector< int > *array*)

5.12.1.11 int orderMag (double *x*)

5.12.1.12 void orthoLinReg (double * *x,* double * *y,* double * *par,* int *m_dat,* int *n_par*)

5.12.1.13 int roundIt (double *d*)

5.12.1.14 double rSq (double * *x,* double * *y,* double *slope,* double *vint,* int *m_dat*)

5.12.1.15 int twoFifths (int *m*)

5.12.1.16 double weightedAvg (double * *enorm,* double * *x,* int *n*)

5.13 gsta_opt.h File Reference

```
#include "lmcurve.h"
#include <stdio.h>
#include <math.h>
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <vector>
#include <time.h>
#include <float.h>
#include <string>
#include "error.h"
```

Classes

- struct GSTA_OPT_DATA

Macros

- #define Po 100.0
- #define R 8.3144621
- #define Na 6.0221413E+23

Functions

- void error ()
- int roundIt (double d)
- int twoFifths (int m)
- int orderMag (double x)
- int minValue (std::vector< int > array)
- int minIndex (std::vector< double > array)
- int avgPar (std::vector< int > array)
- double avgValue (std::vector< double > array)
- double weightedAvg (double ∗enorm, double ∗x, int n)
- double rSq (double ∗x, double ∗y, double slope, double vint, int m_dat)
- bool isSmooth (double ∗par, void ∗data)
- void orthoLinReg (double ∗x, double ∗y, double ∗par, int m_dat, int n_par)
- void eduGuess (double ∗P, double ∗q, double ∗par, int k, int m_dat, void ∗data)
- double gstaFunc (double p, const double ∗K, double qmax, int n_par)
- double gstaObjFunc (double ∗t, double ∗y, double ∗par, int m_dat, void ∗data)
- void eval_GSTA (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int gsta_optimize (const char ∗fileName)

5.13.1 Macro Definition Documentation

5.13.1.1 #define Na 6.0221413E+23

5.13.1.2 #define Po 100.0

5.13.1.3 #define R 8.3144621

5.13.2 Function Documentation

5.13.2.1 int avgPar (std::vector< int > *array*)

5.13.2.2 double avgValue (std::vector< double > *array*)

5.13.2.3 void eduGuess (double ∗ *P,* double ∗ *q,* double ∗ *par,* int *k,* int *m_dat,* void ∗ *data*)

5.13.2.4 void error ( )

5.13.2.5 void eval_GSTA (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.13.2.6 int gsta_optimize (const char ∗ *fileName*)

5.13.2.7 double gstaFunc (double *p,* const double ∗ *K,* double *qmax,* int *n_par*)

5.13.2.8 double gstaObjFunc (double ∗ *t,* double ∗ *y,* double ∗ *par,* int *m_dat,* void ∗ *data*)

5.13.2.9 bool isSmooth (double ∗ *par,* void ∗ *data*)

5.13.2.10 int minIndex (std::vector< double > *array*)

5.13.2.11 int minValue (std::vector< int > *array*)

5.13.2.12 int orderMag (double *x*)

5.13.2.13 void orthoLinReg (double ∗ *x,* double ∗ *y,* double ∗ *par,* int *m_dat,* int *n_par*)

5.13.2.14 int roundIt (double *d*)

5.13.2.15 double rSq (double ∗ *x,* double ∗ *y,* double *slope,* double *vint,* int *m_dat*)

5.13.2.16 int twoFifths (int *m*)

5.13.2.17 double weightedAvg (double ∗ *enorm,* double ∗ *x,* int *n*)

5.14 lark.cpp File Reference

```
#include "lark.h"
```

Functions

- int matvec_ex01 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex01 (const Matrix< double > &b, Matrix< double > &p, const void ∗data)
- int matvec_ex02 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int matvec_ex04 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex04 (const Matrix< double > &b, Matrix< double > &p, const void ∗data)
- int evalx_ex09 (const Matrix< double > &x, Matrix< double > &G, const void ∗data)
- int funeval_ex09 (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int funeval_ex10 (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int precon_ex10 (const Matrix< double > &r, Matrix< double > &p, const void ∗data)
- int matvec_ex15 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex15 (const Matrix< double > &w, Matrix< double > &p, const void ∗data)
- int update_arnoldi_solution (Matrix< double > &x, Matrix< double > &x0, ARNOLDI_DATA ∗arnoldi_dat)
- int arnoldi (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &r0, ARNOLDI_DATA ∗arnoldi_dat, const void ∗matvec_data, const void ∗precon_data)
- int gmresLeftPreconditioned (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &P, const void ∗data), Matrix< double > &b, GMRESLP_DATA ∗gmreslp_dat, const void ∗matvec_data, const void ∗precon_data)
- int fom (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &P, const void ∗data), Matrix< double > &b, GMRESLP_DATA ∗gmreslp_dat, const void ∗matvec_data, const void ∗precon_data)
- int gmresRightPreconditioned (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &b, GMRESRP_DATA ∗gmresrp_dat, const void ∗matvec_data, const void ∗precon_data)
- int pcg (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, PCG_DATA ∗pcg_dat, const void ∗matvec_data, const void ∗precon_data)
- int bicgstab (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, BiCGSTAB_DATA ∗bicg_dat, const void ∗matvec_data, const void ∗precon_data)

- int cgs (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, CGS_DATA ∗cgs_dat, const void ∗matvec_data, const void ∗precon_data)
- int operatorTranspose (int(∗matvec)(const Matrix< double > &v, Matrix< double > &Av, const void ∗data), Matrix< double > &r, Matrix< double > &u, OPTRANS_DATA ∗transpose_dat, const void ∗matvec_data)
- int gcr (int(∗matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data), Matrix< double > &b, GCR_DATA ∗gcr_dat, const void ∗matvec_data, const void ∗precon_data)
- int gmresPreconditioner (const Matrix< double > &r, Matrix< double > &Mr, const void ∗data)
- int gmresr (int(∗matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data), int(∗terminal_precon)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data), Matrix< double > &b, GMRESR_DATA ∗gmresr_dat, const void ∗matvec_data, const void ∗term_precon_data)
- int picard (int(∗res)(const Matrix< double > &x, Matrix< double > &r, const void ∗data), int(∗evalx)(const Matrix< double > &x0, Matrix< double > &x, const void ∗data), Matrix< double > &x, PICARD_DATA ∗picard_dat, const void ∗res_data, const void ∗evalx_data)
- int jacvec (const Matrix< double > &v, Matrix< double > &Jv, const void ∗data)
- int backtrackLineSearch (int(∗feval)(const Matrix< double > &x, Matrix< double > &F, const void ∗data), Matrix< double > &Fkp1, Matrix< double > &xkp1, Matrix< double > &pk, double normFk, BACKTRACK_DATA ∗backtrack_dat, const void ∗feval_data)
- int pjfnk (int(∗res)(const Matrix< double > &x, Matrix< double > &F, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗data), Matrix< double > &x, PJFNK_DATA ∗pjfnk_dat, const void ∗res_data, const void ∗precon_data)
- int NumericalJacobian (int(∗Func)(const Matrix< double > &x, Matrix< double > &F, const void ∗user_data), const Matrix< double > &x, Matrix< double > &J, int Nx, int Nf, NUM_JAC_DATA ∗jac_dat, const void ∗user_data)
- int LARK_TESTS ()

5.14.1 Function Documentation

5.14.1.1 int arnoldi (int(∗)(const **Matrix**< double > &v, **Matrix**< double > &w, const void ∗data) *matvec,* int(∗)(const **Matrix**< double > &b, **Matrix**< double > &p, const void ∗data) *precon,* **Matrix**< double > & *r0,* **ARNOLDI_DATA** ∗ *arnoldi_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.2 int backtrackLineSearch (int(∗)(const **Matrix**< double > &x, **Matrix**< double > &F, const void ∗data) *feval,* **Matrix**< double > & *Fkp1,* **Matrix**< double > & *xkp1,* **Matrix**< double > & *pk,* double *normFk,* **BACKTRACK_DATA** ∗ *backtrack_dat,* const void ∗ *feval_data*)

5.14.1.3 int bicgstab (int(∗)(const **Matrix**< double > &p, **Matrix**< double > &Ap, const void ∗data) *matvec,* int(∗)(const **Matrix**< double > &r, **Matrix**< double > &z, const void ∗data) *precon,* **Matrix**< double > & *b,* **BiCGSTAB_DATA** ∗ *bicg_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.4 int cgs (int(∗)(const **Matrix**< double > &p, **Matrix**< double > &Ap, const void ∗data) *matvec,* int(∗)(const **Matrix**< double > &r, **Matrix**< double > &z, const void ∗data) *precon,* **Matrix**< double > & *b,* **CGS_DATA** ∗ *cgs_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.5 int evalx_ex09 (const **Matrix**< double > & *x,* **Matrix**< double > & *G,* const void ∗ *data*)

5.14.1.6 int fom (int(∗)(const **Matrix**< double > &v, **Matrix**< double > &w, const void ∗data) *matvec,* int(∗)(const **Matrix**< double > &b, **Matrix**< double > &P, const void ∗data) *precon,* **Matrix**< double > & *b,* **GMRESLP_DATA** ∗ *gmreslp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.7 int funeval_ex09 (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void ∗ *data*)

5.14.1.8 int funeval_ex10 (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void ∗ *data*)

5.14.1.9 int gcr (int(∗)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data) *precon,* Matrix< double > & *b,* GCR_DATA ∗ *gcr_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.10 int gmresLeftPreconditioned (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &P, const void ∗data) *precon,* Matrix< double > & *b,* GMRESLP_DATA ∗ *gmreslp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.11 int gmresPreconditioner (const Matrix< double > & *r,* Matrix< double > & *Mr,* const void ∗ *data*)

5.14.1.12 int gmresr (int(∗)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data) *terminal_precon,* Matrix< double > & *b,* GMRESR_DATA ∗ *gmresr_dat,* const void ∗ *matvec_data,* const void ∗ *term_precon_data*)

5.14.1.13 int gmresRightPreconditioned (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *b,* GMRESRP_DATA ∗ *gmresrp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.14 int jacvec (const Matrix< double > & *v,* Matrix< double > & *Jv,* const void ∗ *data*)

5.14.1.15 int LARK_TESTS ( )

5.14.1.16 int matvec_ex01 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.14.1.17 int matvec_ex02 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.14.1.18 int matvec_ex04 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.14.1.19 int matvec_ex15 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.14.1.20 int NumericalJacobian (int(∗)(const Matrix< double > &x, Matrix< double > &F, const void ∗user_data) *Func,* const Matrix< double > & *x,* Matrix< double > & *J,* int *Nx,* int *Nf,* NUM_JAC_DATA ∗ *jac_dat,* const void ∗ *user_data*)

5.14.1.21 int operatorTranspose (int(∗)(const Matrix< double > &v, Matrix< double > &Av, const void ∗data) *matvec,* Matrix< double > & *r,* Matrix< double > & *u,* OPTRANS_DATA ∗ *transpose_dat,* const void ∗ *matvec_data*)

5.14.1.22 int pcg (int(∗)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &z, const void ∗data) *precon,* Matrix< double > & *b,* PCG_DATA ∗ *pcg_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.14.1.23 int picard (int(∗)(const Matrix< double > &x, Matrix< double > &r, const void ∗data) *res,* int(∗)(const Matrix< double > &x0, Matrix< double > &x, const void ∗data) *evalx,* Matrix< double > & *x,* PICARD_DATA ∗ *picard_dat,* const void ∗ *res_data,* const void ∗ *evalx_data*)

5.14.1.24 int pjfnk (int(∗)(const Matrix< double > &x, Matrix< double > &F, const void ∗data) *res,* int(∗)(const Matrix< double > &r, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *x,* PJFNK_DATA ∗ *pjfnk_dat,* const void ∗ *res_data,* const void ∗ *precon_data*)

5.14.1.25 int precon_ex01 (const Matrix< double > & *b,* Matrix< double > & *p,* const void ∗ *data*)

5.14.1.26 int precon_ex04 (const Matrix< double > & *b,* Matrix< double > & *p,* const void ∗ *data*)

5.14.1.27 int precon_ex10 (const Matrix< double > & *r,* Matrix< double > & *p,* const void ∗ *data*)

5.14.1.28 int precon_ex15 (const Matrix< double > & *w,* Matrix< double > & *p,* const void ∗ *data*)

5.14.1.29 int update_arnoldi_solution (**Matrix**< double > & *x*, **Matrix**< double > & *x0*, **ARNOLDI_DATA** ∗ *arnoldi_dat*)

5.15 lark.h File Reference

```
#include "macaw.h"
#include <float.h>
```

Classes

- struct ARNOLDI_DATA
- struct GMRESLP_DATA
- struct GMRESRP_DATA
- struct PCG_DATA
- struct BiCGSTAB_DATA
- struct CGS_DATA
- struct OPTRANS_DATA
- struct GCR_DATA
- struct GMRESR_DATA
- struct PICARD_DATA
- struct BACKTRACK_DATA
- struct PJFNK_DATA
- struct NUM_JAC_DATA
- struct EX01_DATA
- struct EX02_DATA
- struct EX04_DATA
- struct EX09_DATA
- struct EX15_DATA

Enumerations

- enum krylov_method {
  GMRESLP, PCG, BiCGSTAB, CGS,
  FOM, GMRESRP, GCR, GMRESR }

Functions

- int matvec_ex01 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex01 (const Matrix< double > &b, Matrix< double > &p, const void ∗data)
- int matvec_ex02 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int matvec_ex04 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex04 (const Matrix< double > &b, Matrix< double > &p, const void ∗data)
- int evalx_ex09 (const Matrix< double > &x, Matrix< double > &G, const void ∗data)
- int funeval_ex09 (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int funeval_ex10 (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int precon_ex10 (const Matrix< double > &r, Matrix< double > &p, const void ∗data)
- int matvec_ex15 (const Matrix< double > &v, Matrix< double > &w, const void ∗data)
- int precon_ex15 (const Matrix< double > &w, Matrix< double > &p, const void ∗data)
- int update_arnoldi_solution (Matrix< double > &x, Matrix< double > &x0, ARNOLDI_DATA ∗arnoldi_dat)
- int arnoldi (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &r0, ARNOLDI_DATA ∗arnoldi_dat, const void ∗matvec_data, const void ∗precon_data)

- int gmresLeftPreconditioned (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &b, GMRESLP_DATA ∗gmreslp_dat, const void ∗matvec_data, const void ∗precon_data)
- int fom (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &b, GMRESLP_DATA ∗gmreslp_dat, const void ∗matvec_data, const void ∗precon_data)
- int gmresRightPreconditioned (int(∗matvec)(const Matrix< double > &v, Matrix< double > &w, const void ∗data), int(∗precon)(const Matrix< double > &b, Matrix< double > &p, const void ∗data), Matrix< double > &b, GMRESRP_DATA ∗gmresrp_dat, const void ∗matvec_data, const void ∗precon_data)
- int pcg (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, PCG_DATA ∗pcg_dat, const void ∗matvec_data, const void ∗precon_data)
- int bicgstab (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, BiCGSTAB_DATA ∗bicg_dat, const void ∗matvec_data, const void ∗precon_data)
- int cgs (int(∗matvec)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &z, const void ∗data), Matrix< double > &b, CGS_DATA ∗cgs_dat, const void ∗matvec_data, const void ∗precon_data)
- int operatorTranspose (int(∗matvec)(const Matrix< double > &v, Matrix< double > &Av, const void ∗data), Matrix< double > &r, Matrix< double > &u, OPTRANS_DATA ∗transpose_dat, const void ∗matvec_data)
- int gcr (int(∗matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data), Matrix< double > &b, GCR_DATA ∗gcr_dat, const void ∗matvec_data, const void ∗precon_data)
- int gmresPreconditioner (const Matrix< double > &r, Matrix< double > &Mr, const void ∗data)
- int gmresr (int(∗matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data), int(∗terminal_precon)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data), Matrix< double > &b, GMRESR_DATA ∗gmresr_dat, const void ∗matvec_data, const void ∗term_precon_data)
- int picard (int(∗res)(const Matrix< double > &x, Matrix< double > &r, const void ∗data), int(∗evalx)(const Matrix< double > &x0, Matrix< double > &x, const void ∗data), Matrix< double > &x, PICARD_DATA ∗picard_dat, const void ∗res_data, const void ∗evalx_data)
- int jacvec (const Matrix< double > &v, Matrix< double > &Jv, const void ∗data)
- int backtrackLineSearch (int(∗feval)(const Matrix< double > &x, Matrix< double > &F, const void ∗data), Matrix< double > &Fkp1, Matrix< double > &xkp1, Matrix< double > &pk, double normFk, BACKTRACK_DATA ∗backtrack_dat, const void ∗feval_data)
- int pjfnk (int(∗res)(const Matrix< double > &x, Matrix< double > &F, const void ∗data), int(∗precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗data), Matrix< double > &x, PJFNK_DATA ∗pjfnk_dat, const void ∗res_data, const void ∗precon_data)
- int NumericalJacobian (int(∗Func)(const Matrix< double > &x, Matrix< double > &F, const void ∗user_data), const Matrix< double > &x, Matrix< double > &J, int Nx, int Nf, NUM_JAC_DATA ∗jac_dat, const void ∗user_data)
- int LARK_TESTS ()

5.15.1 Enumeration Type Documentation

5.15.1.1 enum krylov_method

Enumerator

GMRESLP

PCG

BiCGSTAB

CGS

FOM

GMRESRP

GCR

GMRESR

5.15.2 Function Documentation

5.15.2.1 int arnoldi (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *r0,* ARNOLDI_DATA ∗ *arnoldi_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.2 int backtrackLineSearch (int(∗)(const Matrix< double > &x, Matrix< double > &F, const void ∗data) *feval,* Matrix< double > & *Fkp1,* Matrix< double > & *xkp1,* Matrix< double > & *pk,* double *normFk,* BACKTRACK_DATA ∗ *backtrack_dat,* const void ∗ *feval_data*)

5.15.2.3 int bicgstab (int(∗)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &z, const void ∗data) *precon,* Matrix< double > & *b,* BiCGSTAB_DATA ∗ *bicg_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.4 int cgs (int(∗)(const Matrix< double > &p, Matrix< double > &Ap, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &z, const void ∗data) *precon,* Matrix< double > & *b,* CGS_DATA ∗ *cgs_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.5 int evalx_ex09 (const Matrix< double > & *x,* Matrix< double > & *G,* const void ∗ *data*)

5.15.2.6 int fom (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *b,* GMRESLP_DATA ∗ *gmreslp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.7 int funeval_ex09 (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.15.2.8 int funeval_ex10 (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.15.2.9 int gcr (int(∗)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data) *precon,* Matrix< double > & *b,* GCR_DATA ∗ *gcr_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.10 int gmresLeftPreconditioned (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *b,* GMRESLP_DATA ∗ *gmreslp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.11 int gmresPreconditioner (const Matrix< double > & *r,* Matrix< double > & *Mr,* const void ∗ *data*)

5.15.2.12 int gmresr (int(∗)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗data) *matvec,* int(∗)(const Matrix< double > &r, Matrix< double > &Mr, const void ∗data) *terminal_precon,* Matrix< double > & *b,* GMRESR_DATA ∗ *gmresr_dat,* const void ∗ *matvec_data,* const void ∗ *term_precon_data*)

5.15.2.13 int gmresRightPreconditioned (int(∗)(const Matrix< double > &v, Matrix< double > &w, const void ∗data) *matvec,* int(∗)(const Matrix< double > &b, Matrix< double > &p, const void ∗data) *precon,* Matrix< double > & *b,* GMRESRP_DATA ∗ *gmresrp_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.14 int jacvec (const Matrix< double > & *v,* Matrix< double > & *Jv,* const void ∗ *data*)

5.15.2.15 int LARK_TESTS ( )

5.15.2.16 int matvec_ex01 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.15.2.17 int matvec_ex02 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.15.2.18 int matvec_ex04 (const Matrix< double > & *v,* Matrix< double > & *w,* const void ∗ *data*)

5.15.2.19 int matvec_ex15 (const **Matrix**< double > & *v,* **Matrix**< double > & *w,* const void ∗ *data*)

5.15.2.20 int NumericalJacobian (int(∗)(const **Matrix**< double > &x, **Matrix**< double > &F, const void ∗user_data) *Func,* const **Matrix**< double > & *x,* **Matrix**< double > & *J,* int *Nx,* int *Nf,* **NUM_JAC_DATA** ∗ *jac_dat,* const void ∗ *user_data*)

5.15.2.21 int operatorTranspose (int(∗)(const **Matrix**< double > &v, **Matrix**< double > &Av, const void ∗data) *matvec,* **Matrix**< double > & *r,* **Matrix**< double > & *u,* **OPTRANS_DATA** ∗ *transpose_dat,* const void ∗ *matvec_data*)

5.15.2.22 int pcg (int(∗)(const **Matrix**< double > &p, **Matrix**< double > &Ap, const void ∗data) *matvec,* int(∗)(const **Matrix**< double > &r, **Matrix**< double > &z, const void ∗data) *precon,* **Matrix**< double > & *b,* **PCG_DATA** ∗ *pcg_dat,* const void ∗ *matvec_data,* const void ∗ *precon_data*)

5.15.2.23 int picard (int(∗)(const **Matrix**< double > &x, **Matrix**< double > &r, const void ∗data) *res,* int(∗)(const **Matrix**< double > &x0, **Matrix**< double > &x, const void ∗data) *evalx,* **Matrix**< double > & *x,* **PICARD_DATA** ∗ *picard_dat,* const void ∗ *res_data,* const void ∗ *evalx_data*)

5.15.2.24 int pjfnk (int(∗)(const **Matrix**< double > &x, **Matrix**< double > &F, const void ∗data) *res,* int(∗)(const **Matrix**< double > &r, **Matrix**< double > &p, const void ∗data) *precon,* **Matrix**< double > & *x,* **PJFNK_DATA** ∗ *pjfnk_dat,* const void ∗ *res_data,* const void ∗ *precon_data*)

5.15.2.25 int precon_ex01 (const **Matrix**< double > & *b,* **Matrix**< double > & *p,* const void ∗ *data*)

5.15.2.26 int precon_ex04 (const **Matrix**< double > & *b,* **Matrix**< double > & *p,* const void ∗ *data*)

5.15.2.27 int precon_ex10 (const **Matrix**< double > & *r,* **Matrix**< double > & *p,* const void ∗ *data*)

5.15.2.28 int precon_ex15 (const **Matrix**< double > & *w,* **Matrix**< double > & *p,* const void ∗ *data*)

5.15.2.29 int update_arnoldi_solution (**Matrix**< double > & *x,* **Matrix**< double > & *x0,* **ARNOLDI_DATA** ∗ *arnoldi_dat*)

5.16 macaw.cpp File Reference

```
#include "macaw.h"
```

Functions

- int MACAW_TESTS ()

5.16.1 Function Documentation

5.16.1.1 int MACAW_TESTS ( )

5.17 macaw.h File Reference

```
#include <stdio.h>
```

```
#include <math.h>
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <vector>
#include <time.h>
#include <float.h>
#include <string>
#include <exception>
#include "error.h"
```

Classes

- class Matrix< T >

Macros

- #define M_PI 3.14159265358979323846264338327950288 /∗ pi ∗/

Functions

- int MACAW_TESTS ()

5.17.1 Macro Definition Documentation

5.17.1.1 #define M_PI 3.14159265358979323846264338327950288 /∗ pi ∗/

5.17.2 Function Documentation

5.17.2.1 int MACAW_TESTS ( )

5.18 magpie.cpp File Reference

```
#include "magpie.h"
```

Functions

- double qo (double po, const void ∗data, int i)
- double dq_dp (double p, const void ∗data, int i)
- double q_p (double p, const void ∗data, int i)
- double PI (double po, const void ∗data, int i)
- double eMax (const void ∗data, int i)
- double Qst (double po, const void ∗data, int i)
- double lnact_mSPD (const double ∗par, const void ∗data, int i, volatile double PI)
- double grad_mSPD (const double ∗par, const void ∗data, int i)
- double qT (const double ∗par, const void ∗data)
- void initialGuess_mSPD (double ∗par, const void ∗data)
- void eval_po_PI (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_po_qo (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_po (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

- void eval_eta (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_GPAST (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int MAGPIE (const void ∗data)
- int MAGPIE_SCENARIOS (const char ∗inputFileName, const char ∗sceneFileName)

5.18.1 Function Documentation

5.18.1.1 double dq_dp (double *p*, const void ∗ *data*, int *i*)

5.18.1.2 double eMax (const void ∗ *data*, int *i*)

5.18.1.3 void eval_eta (const double ∗ *par*, int *m_dat*, const void ∗ *data*, double ∗ *fvec*, int ∗ *info*)

5.18.1.4 void eval_GPAST (const double ∗ *par*, int *m_dat*, const void ∗ *data*, double ∗ *fvec*, int ∗ *info*)

5.18.1.5 void eval_po (const double ∗ *par*, int *m_dat*, const void ∗ *data*, double ∗ *fvec*, int ∗ *info*)

5.18.1.6 void eval_po_PI (const double ∗ *par*, int *m_dat*, const void ∗ *data*, double ∗ *fvec*, int ∗ *info*)

5.18.1.7 void eval_po_qo (const double ∗ *par*, int *m_dat*, const void ∗ *data*, double ∗ *fvec*, int ∗ *info*)

5.18.1.8 double grad_mSPD (const double ∗ *par*, const void ∗ *data*, int *i*)

5.18.1.9 void initialGuess_mSPD (double ∗ *par*, const void ∗ *data*)

5.18.1.10 double lnact_mSPD (const double ∗ *par*, const void ∗ *data*, int *i*, volatile double *PI*)

5.18.1.11 int MAGPIE (const void ∗ *data*)

5.18.1.12 int MAGPIE_SCENARIOS (const char ∗ *inputFileName*, const char ∗ *sceneFileName*)

5.18.1.13 double PI (double *po*, const void ∗ *data*, int *i*)

5.18.1.14 double q_p (double *p*, const void ∗ *data*, int *i*)

5.18.1.15 double qo (double *po*, const void ∗ *data*, int *i*)

5.18.1.16 double Qst (double *po*, const void ∗ *data*, int *i*)

5.18.1.17 double qT (const double ∗ *par*, const void ∗ *data*)

5.19 magpie.h File Reference

```
#include "lmcurve.h"
#include <stdio.h>
#include <math.h>
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <vector>
#include <time.h>
#include <float.h>
#include <string>
#include "error.h"
```

Classes

- struct GSTA_DATA
- struct mSPD_DATA
- struct GPAST_DATA
- struct SYSTEM_DATA
- struct MAGPIE_DATA

Macros

- #define DBL_EPSILON 2.2204460492503131e-016
- #define Z 10.0
- #define A 3.13E+09
- #define V 18.92
- #define Po 100.0
- #define R 8.3144621
- #define Na 6.0221413E+23
- #define kB 1.3806488E-23
- #define shapeFactor(v_i) (((Z - 2) ∗ v_i) / (Z ∗ V)) + (2 / Z)
- #define lnKo(H, S, T) -(H / (R ∗ T)) + (S / R)
- #define He(qm, K1, m) (qm ∗ K1) / (m ∗ Po)

Functions

- double qo (double po, const void ∗data, int i)
- double dq_dp (double p, const void ∗data, int i)
- double q_p (double p, const void ∗data, int i)
- double PI (double po, const void ∗data, int i)
- double Qst (double po, const void ∗data, int i)
- double eMax (const void ∗data, int i)
- double lnact_mSPD (const double ∗par, const void ∗data, int i, volatile double PI)
- double grad_mSPD (const double ∗par, const void ∗data, int i)
- double qT (const double ∗par, const void ∗data)
- void initialGuess_mSPD (double ∗par, const void ∗data)
- void eval_po_PI (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_po_qo (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_po (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_eta (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- void eval_GPAST (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int MAGPIE (const void ∗data)
- int MAGPIE_SCENARIOS (const char ∗inputFileName, const char ∗sceneFileName)

5.19.1 Macro Definition Documentation

5.19.1.1 #define A 3.13E+09

5.19.1.2 #define DBL_EPSILON 2.2204460492503131e-016

5.19.1.3 #define He(*qm*, *K1*, *m*) (qm ∗ K1) / (m ∗ Po)

5.19.1.4 #define kB 1.3806488E-23

5.19.1.5 #define lnKo(*H*, *S*, *T*) -(H / (R ∗ T)) + (S / R)

5.19.1.6 #define Na 6.0221413E+23

5.19.1.7 #define Po 100.0

5.19.1.8 #define R 8.3144621

5.19.1.9 #define shapeFactor(*v_i*) (((Z - 2) ∗ v_i) / (Z ∗ V)) + (2 / Z)

5.19.1.10 #define V 18.92

5.19.1.11 #define Z 10.0

5.19.2 Function Documentation

5.19.2.1 double dq_dp (double *p,* const void ∗ *data,* int *i*)

5.19.2.2 double eMax (const void ∗ *data,* int *i*)

5.19.2.3 void eval_eta (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.2.4 void eval_GPAST (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.2.5 void eval_po (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.2.6 void eval_po_PI (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.2.7 void eval_po_qo (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.2.8 double grad_mSPD (const double ∗ *par,* const void ∗ *data,* int *i*)

5.19.2.9 void initialGuess_mSPD (double ∗ *par,* const void ∗ *data*)

5.19.2.10 double lnact_mSPD (const double ∗ *par,* const void ∗ *data,* int *i,* volatile double *PI*)

5.19.2.11 int MAGPIE (const void ∗ *data*)

5.19.2.12 int MAGPIE_SCENARIOS (const char ∗ *inputFileName,* const char ∗ *sceneFileName*)

5.19.2.13 double PI (double *po,* const void ∗ *data,* int *i*)

5.19.2.14 double q_p (double *p,* const void ∗ *data,* int *i*)

5.19.2.15 double qo (double *po,* const void ∗ *data,* int *i*)

5.19.2.16 double Qst (double *po,* const void ∗ *data,* int *i*)

5.19.2.17 double qT (const double ∗ *par,* const void ∗ *data*)

5.20 main.cpp File Reference

```
#include "ui.h"
```

Functions

- int main (int argc, const char ∗argv[])

5.20.1 Function Documentation

5.20.1.1 int main (int *argc,* const char ∗ *argv[]*)

5.21 mola.cpp File Reference

```
#include "mola.h"
```

Functions

- int MOLA_TESTS ()

5.21.1 Function Documentation

5.21.1.1 int MOLA_TESTS ( )

5.22 mola.h File Reference

```
#include <ctype.h>
#include "eel.h"
```

Classes

- class Molecule

Functions

- int MOLA_TESTS ()

5.22.1 Function Documentation

5.22.1.1 int MOLA_TESTS ( )

5.23 monkfish.cpp File Reference

```
#include "monkfish.h"
```

Functions

- double default_porosity (int i, int l, const void ∗user_data)
- double default_density (int i, int l, const void ∗user_data)
- double default_interparticle_diffusion (int i, int l, const void ∗user_data)

- double default_monk_adsorption (int i, int l, const void ∗user_data)
- double default_monk_equilibrium (int i, int l, const void ∗user_data)
- double default_monkfish_retardation (int i, int l, const void ∗user_data)
- double default_exterior_concentration (int i, const void ∗user_data)
- double default_film_transfer (int i, const void ∗user_data)
- int MONKFISH_TESTS ()

5.23.1 Function Documentation

5.23.1.1 double default_density (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.2 double default_exterior_concentration (int *i,* const void ∗ *user_data*)

5.23.1.3 double default_film_transfer (int *i,* const void ∗ *user_data*)

5.23.1.4 double default_interparticle_diffusion (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.5 double default_monk_adsorption (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.6 double default_monk_equilibrium (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.7 double default_monkfish_retardation (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.8 double default_porosity (int *i,* int *l,* const void ∗ *user_data*)

5.23.1.9 int MONKFISH_TESTS ( )

5.24 monkfish.h File Reference

```
#include "dogfish.h"
```

Classes

- struct MONKFISH_PARAM
- struct MONKFISH_DATA

Functions

- double default_porosity (int i, int l, const void ∗user_data)
- double default_density (int i, int l, const void ∗user_data)
- double default_interparticle_diffusion (int i, int l, const void ∗user_data)
- double default_monk_adsorption (int i, int l, const void ∗user_data)
- double default_monk_equilibrium (int i, int l, const void ∗user_data)
- double default_monkfish_retardation (int i, int l, const void ∗user_data)
- double default_exterior_concentration (int i, const void ∗user_data)
- double default_film_transfer (int i, const void ∗user_data)
- int setup_MONKFISH_DATA (FILE ∗file, double(∗eval_porosity)(int i, int l, const void ∗user_data), double(∗eval_density)(int i, int l, const void ∗user_data), double(∗eval_ext_diff)(int i, int l, const void ∗user_data), double(∗eval_adsorb)(int i, int l, const void ∗user_data), double(∗eval_retard)(int i, int l, const void ∗user_data), double(∗eval_ext_conc)(int i, const void ∗user_data), double(∗eval_ext_film)(int i, const void ∗user_data), double(∗dog_diffusion)(int i, int l, const void ∗user_data), double(∗dog_ext_film)(int i, const void ∗user_data), double(∗dog_surf_conc)(int i, const void ∗user_data), const void ∗user_data, MONKFISH_DATA ∗monk_dat)
- int MONKFISH_TESTS ()

5.24.1 Function Documentation

5.24.1.1 double default_density (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.2 double default_exterior_concentration (int *i*, const void ∗ *user_data*)

5.24.1.3 double default_film_transfer (int *i*, const void ∗ *user_data*)

5.24.1.4 double default_interparticle_diffusion (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.5 double default_monk_adsorption (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.6 double default_monk_equilibrium (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.7 double default_monkfish_retardation (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.8 double default_porosity (int *i*, int *l*, const void ∗ *user_data*)

5.24.1.9 int MONKFISH_TESTS ( )

5.24.1.10 int setup_MONKFISH_DATA (FILE ∗ *file*, double(∗)(int i, int l, const void ∗user_data) *eval_porosity*, double(∗)(int i, int l, const void ∗user_data) *eval_density*, double(∗)(int i, int l, const void ∗user_data) *eval_ext_diff*, double(∗)(int i, int l, const void ∗user_data) *eval_adsorb*, double(∗)(int i, int l, const void ∗user_data) *eval_retard*, double(∗)(int i, const void ∗user_data) *eval_ext_conc*, double(∗)(int i, const void ∗user_data) *eval_ext_film*, double(∗)(int i, int l, const void ∗user_data) *dog_diffusion*, double(∗)(int i, const void ∗user_data) *dog_ext_film*, double(∗)(int i, const void ∗user_data) *dog_surf_conc*, const void ∗ *user_data*, MONKFISH_DATA ∗ *monk_dat*)

5.25 sandbox.cpp File Reference

```
#include "sandbox.h"
```

Functions

- int Speciation_Test01_Function (const Matrix< double > &x, Matrix< double > &F, const void ∗res_data)
- int Speciation_Test01_Jacobian (const Matrix< double > &x, Matrix< double > &J, const void ∗precon_data)
- int Speciation_Test01_Guess (const void ∗user_data)
- int Speciation_Test01_MatVec (const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)
- int RUN_SANDBOX ()

5.25.1 Function Documentation

5.25.1.1 int RUN_SANDBOX ( )

5.25.1.2 int Speciation_Test01_Function (const Matrix< double > & *x*, Matrix< double > & *F*, const void ∗ *res_data*)

5.25.1.3 int Speciation_Test01_Guess (const void ∗ *user_data*)

5.25.1.4 int Speciation_Test01_Jacobian (const Matrix< double > & *x*, Matrix< double > & *J*, const void ∗ *precon_data*)

5.25.1.5 int Speciation_Test01_MatVec (const Matrix< double > & *x*, Matrix< double > & *Ax*, const void ∗ *matvec_data*)

5.26 sandbox.h File Reference

```
#include "flock.h"
#include "school.h"
```

Classes

- struct Speciation_Test01_Data

Functions

- int Speciation_Test01_Function (const Matrix< double > &x, Matrix< double > &F, const void ∗res_data)
- int Speciation_Test01_Jacobian (const Matrix< double > &x, Matrix< double > &J, const void ∗precon_data)
- int Speciation_Test01_Guess (const void ∗user_data)
- int Speciation_Test01_MatVec (const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)
- int RUN_SANDBOX ()

5.26.1 Function Documentation

5.26.1.1 int RUN_SANDBOX ( )

5.26.1.2 int Speciation_Test01_Function (const **Matrix**< double > & *x*, **Matrix**< double > & *F*, const void ∗ *res_data*)

5.26.1.3 int Speciation_Test01_Guess (const void ∗ *user_data*)

5.26.1.4 int Speciation_Test01_Jacobian (const **Matrix**< double > & *x*, **Matrix**< double > & *J*, const void ∗ *precon_data*)

5.26.1.5 int Speciation_Test01_MatVec (const **Matrix**< double > & *x*, **Matrix**< double > & *Ax*, const void ∗ *matvec_data*)

5.27 school.h File Reference

```
#include "eel.h"
#include "mola.h"
#include "shark.h"
#include "dogfish.h"
#include "monkfish.h"
#include "yaml_wrapper.h"
```

5.28 scopsowl.cpp File Reference

```
#include "scopsowl.h"
```

Functions

- void print2file_species_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)
- void print2file_SCOPSOWL_time_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)
- void print2file_SCOPSOWL_header (SCOPSOWL_DATA ∗owl_dat)

- void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA ∗owl_dat)
- void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA ∗owl_dat)
- double default_adsorption (int i, int l, const void ∗user_data)
- double default_retardation (int i, int l, const void ∗user_data)
- double default_pore_diffusion (int i, int l, const void ∗user_data)
- double default_surf_diffusion (int i, int l, const void ∗user_data)
- double default_effective_diffusion (int i, int l, const void ∗user_data)
- double const_pore_diffusion (int i, int l, const void ∗user_data)
- double default_filmMassTransfer (int i, const void ∗user_data)
- double const_filmMassTransfer (int i, const void ∗user_data)
- int setup_SCOPSOWL_DATA (FILE ∗file, double(∗eval_sorption)(int i, int l, const void ∗user_data), double(∗eval_retardation)(int i, int l, const void ∗user_data), double(∗eval_pore_diff)(int i, int l, const void ∗user_data), double(∗eval_filmMT)(int i, const void ∗user_data), double(∗eval_surface_diff)(int i, int l, const void ∗user_data), const void ∗user_data, MIXED_GAS ∗gas_data, SCOPSOWL_DATA ∗owl_data)
- int SCOPSOWL_Executioner (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_ICs (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_timestep (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_preprocesses (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_params (const void ∗user_data)
- int SCOPSOWL_postprocesses (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_reset (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL (SCOPSOWL_DATA ∗owl_dat)
- int LARGE_CYCLE_TEST01 (SCOPSOWL_DATA ∗owl_dat)
- int SMALL_CYCLE_TEST02 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST03 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST04 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST05 (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_SCENARIOS (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate)
- int SCOPSOWL_TESTS ()

5.28.1 Function Documentation

5.28.1.1 double const_filmMassTransfer (int *i*, const void ∗ *user_data*)

5.28.1.2 double const_pore_diffusion (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.3 int CURVE_TEST03 (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.4 int CURVE_TEST04 (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.5 int CURVE_TEST05 (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.6 double default_adsorption (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.7 double default_effective_diffusion (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.8 double default_filmMassTransfer (int *i*, const void ∗ *user_data*)

5.28.1.9 double default_pore_diffusion (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.10 double default_retardation (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.11 double default_surf_diffusion (int *i*, int *l*, const void ∗ *user_data*)

5.28.1.12 int LARGE_CYCLE_TEST01 (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.13 void print2file_SCOPSOWL_header (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.14 void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.15 void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.16 void print2file_SCOPSOWL_time_header (FILE ∗ *Output,* SCOPSOWL_DATA ∗ *owl_dat,* int *i*)

5.28.1.17 void print2file_species_header (FILE ∗ *Output,* SCOPSOWL_DATA ∗ *owl_dat,* int *i*)

5.28.1.18 int SCOPSOWL (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.19 int SCOPSOWL_Executioner (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.20 int SCOPSOWL_postprocesses (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.21 int SCOPSOWL_preprocesses (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.22 int SCOPSOWL_reset (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.23 int SCOPSOWL_SCENARIOS (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate*)

5.28.1.24 int SCOPSOWL_TESTS ( )

5.28.1.25 int set_SCOPSOWL_ICs (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.26 int set_SCOPSOWL_params (const void ∗ *user_data*)

5.28.1.27 int set_SCOPSOWL_timestep (SCOPSOWL_DATA ∗ *owl_dat*)

5.28.1.28 int setup_SCOPSOWL_DATA (FILE ∗ *file,* double(∗)(int i, int l, const void ∗user_data) *eval_sorption,* double(∗)(int i, int l, const void ∗user_data) *eval_retardation,* double(∗)(int i, int l, const void ∗user_data) *eval_pore_diff,* double(∗)(int i, const void ∗user_data) *eval_filmMT,* double(∗)(int i, int l, const void ∗user_data) *eval_surface_diff,* const void ∗ *user_data,* MIXED_GAS ∗ *gas_data,* SCOPSOWL_DATA ∗ *owl_data*)

5.28.1.29 int SMALL_CYCLE_TEST02 (SCOPSOWL_DATA ∗ *owl_dat*)

5.29 scopsowl.h File Reference

```
#include "egret.h"
#include "skua.h"
```

Classes

- struct SCOPSOWL_PARAM_DATA
- struct SCOPSOWL_DATA

Macros

- #define SCOPSOWL_HPP_
- #define Dp(Dm, ep) (ep∗ep∗Dm)

- #define Dk(rp, T, MW) (9700.0∗rp∗pow((T/MW),0.5))
- #define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)),-1.0))

Functions

- void print2file_species_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)
- void print2file_SCOPSOWL_time_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)
- void print2file_SCOPSOWL_header (SCOPSOWL_DATA ∗owl_dat)
- void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA ∗owl_dat)
- void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA ∗owl_dat)
- double default_adsorption (int i, int l, const void ∗user_data)
- double default_retardation (int i, int l, const void ∗user_data)
- double default_pore_diffusion (int i, int l, const void ∗user_data)
- double default_surf_diffusion (int i, int l, const void ∗user_data)
- double default_effective_diffusion (int i, int l, const void ∗user_data)
- double const_pore_diffusion (int i, int l, const void ∗user_data)
- double default_filmMassTransfer (int i, const void ∗user_data)
- double const_filmMassTransfer (int i, const void ∗user_data)
- int setup_SCOPSOWL_DATA (FILE ∗file, double(∗eval_sorption)(int i, int l, const void ∗user_data), double(∗eval_retardation)(int i, int l, const void ∗user_data), double(∗eval_pore_diff)(int i, int l, const void ∗user_data), double(∗eval_filmMT)(int i, const void ∗user_data), double(∗eval_surface_diff)(int i, int l, const void ∗user_data), const void ∗user_data, MIXED_GAS ∗gas_data, SCOPSOWL_DATA ∗owl_data)
- int SCOPSOWL_Executioner (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_ICs (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_timestep (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_preprocesses (SCOPSOWL_DATA ∗owl_dat)
- int set_SCOPSOWL_params (const void ∗user_data)
- int SCOPSOWL_postprocesses (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_reset (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL (SCOPSOWL_DATA ∗owl_dat)
- int LARGE_CYCLE_TEST01 (SCOPSOWL_DATA ∗owl_dat)
- int SMALL_CYCLE_TEST02 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST03 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST04 (SCOPSOWL_DATA ∗owl_dat)
- int CURVE_TEST05 (SCOPSOWL_DATA ∗owl_dat)
- int SCOPSOWL_SCENARIOS (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate)
- int SCOPSOWL_TESTS ()

5.29.1 Macro Definition Documentation

5.29.1.1 #define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)),-1.0))

5.29.1.2 #define Dk(*rp*, *T*, *MW*) (9700.0∗rp∗pow((T/MW),0.5))

5.29.1.3 #define Dp(*Dm*, *ep*) (ep∗ep∗Dm)

5.29.1.4 #define SCOPSOWL_HPP_

5.29.2 Function Documentation

5.29.2.1 double const_filmMassTransfer (int *i*, const void ∗ *user_data*)

5.29.2.2 double const_pore_diffusion (int *i,* int *l,* const void * *user_data*)

5.29.2.3 int CURVE_TEST03 (SCOPSOWL_DATA * *owl_dat*)

5.29.2.4 int CURVE_TEST04 (SCOPSOWL_DATA * *owl_dat*)

5.29.2.5 int CURVE_TEST05 (SCOPSOWL_DATA * *owl_dat*)

5.29.2.6 double default_adsorption (int *i,* int *l,* const void * *user_data*)

5.29.2.7 double default_effective_diffusion (int *i,* int *l,* const void * *user_data*)

5.29.2.8 double default_filmMassTransfer (int *i,* const void * *user_data*)

5.29.2.9 double default_pore_diffusion (int *i,* int *l,* const void * *user_data*)

5.29.2.10 double default_retardation (int *i,* int *l,* const void * *user_data*)

5.29.2.11 double default_surf_diffusion (int *i,* int *l,* const void * *user_data*)

5.29.2.12 int LARGE_CYCLE_TEST01 (SCOPSOWL_DATA * *owl_dat*)

5.29.2.13 void print2file_SCOPSOWL_header (SCOPSOWL_DATA * *owl_dat*)

5.29.2.14 void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA * *owl_dat*)

5.29.2.15 void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA * *owl_dat*)

5.29.2.16 void print2file_SCOPSOWL_time_header (FILE * *Output,* SCOPSOWL_DATA * *owl_dat,* int *i*)

5.29.2.17 void print2file_species_header (FILE * *Output,* SCOPSOWL_DATA * *owl_dat,* int *i*)

5.29.2.18 int SCOPSOWL (SCOPSOWL_DATA * *owl_dat*)

5.29.2.19 int SCOPSOWL_Executioner (SCOPSOWL_DATA * *owl_dat*)

5.29.2.20 int SCOPSOWL_postprocesses (SCOPSOWL_DATA * *owl_dat*)

5.29.2.21 int SCOPSOWL_preprocesses (SCOPSOWL_DATA * *owl_dat*)

5.29.2.22 int SCOPSOWL_reset (SCOPSOWL_DATA * *owl_dat*)

5.29.2.23 int SCOPSOWL_SCENARIOS (const char * *scene,* const char * *sorbent,* const char * *comp,* const char * *sorbate*)

5.29.2.24 int SCOPSOWL_TESTS ( )

5.29.2.25 int set_SCOPSOWL_ICs (SCOPSOWL_DATA * *owl_dat*)

5.29.2.26 int set_SCOPSOWL_params (const void * *user_data*)

5.29.2.27 int set_SCOPSOWL_timestep (SCOPSOWL_DATA * *owl_dat*)

5.29.2.28 int setup_SCOPSOWL_DATA (FILE * *file,* double(*)(int i, int l, const void *user_data) *eval_sorption,* double(*)(int i, int l, const void *user_data) *eval_retardation,* double(*)(int i, int l, const void *user_data) *eval_pore_diff,* double(*)(int i, const void *user_data) *eval_filmMT,* double(*)(int i, int l, const void *user_data) *eval_surface_diff,* const void * *user_data,* MIXED_GAS * *gas_data,* SCOPSOWL_DATA * *owl_data*)

5.29.2.29 int SMALL_CYCLE_TEST02 (SCOPSOWL_DATA ∗ *owl_dat*)

5.30 scopsowl_opt.cpp File Reference

```
#include "scopsowl_opt.h"
```

Functions

- int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA ∗owl_opt)
- int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA ∗owl_opt)
- void eval_SCOPSOWL_Uptake (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int SCOPSOWL_OPTIMIZE (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate, const char ∗data)

5.30.1 Function Documentation

5.30.1.1 void eval_SCOPSOWL_Uptake (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.30.1.2 int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA ∗ *owl_opt*)

5.30.1.3 int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA ∗ *owl_opt*)

5.30.1.4 int SCOPSOWL_OPTIMIZE (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate,* const char ∗ *data*)

5.31 scopsowl_opt.h File Reference

```
#include "scopsowl.h"
```

Classes

- struct SCOPSOWL_OPT_DATA

Functions

- int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA ∗owl_opt)
- int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA ∗owl_opt)
- void eval_SCOPSOWL_Uptake (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int SCOPSOWL_OPTIMIZE (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate, const char ∗data)

5.31.1 Function Documentation

5.31.1.1 void eval_SCOPSOWL_Uptake (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.31.1.2 int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA ∗ *owl_opt*)

5.31.1.3 int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA ∗ *owl_opt*)

5.31.1.4 int SCOPSOWL_OPTIMIZE (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate,* const char ∗ *data*)

5.32 shark.cpp File Reference

```
#include "shark.h"
```

Functions

- void print2file_shark_info (SHARK_DATA ∗shark_dat)
- void print2file_shark_header (SHARK_DATA ∗shark_dat)
- void print2file_shark_results_new (SHARK_DATA ∗shark_dat)
- void print2file_shark_results_old (SHARK_DATA ∗shark_dat)
- int ideal_solution (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int Davies_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int DebyeHuckel_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int DaviesLadshaw_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int act_choice (const std::string &input)
- bool linesearch_choice (const std::string &input)
- int linearsolve_choice (const std::string &input)
- int Convert2LogConcentration (const Matrix< double > &x, Matrix< double > &logx)
- int Convert2Concentration (const Matrix< double > &logx, Matrix< double > &x)
- int read_scenario (SHARK_DATA ∗shark_dat)
- int read_options (SHARK_DATA ∗shark_dat)
- int read_species (SHARK_DATA ∗shark_dat)
- int read_massbalance (SHARK_DATA ∗shark_dat)
- int read_equilrxn (SHARK_DATA ∗shark_dat)
- int read_unsteadyrxn (SHARK_DATA ∗shark_dat)
- int setup_SHARK_DATA (FILE ∗file, int(∗residual)(const Matrix< double > &x, Matrix< double > &res, const void ∗data), int(∗activity)(const Matrix< double > &x, Matrix< double > &gama, const void ∗data), int(∗precond)(const Matrix< double > &r, Matrix< double > &p, const void ∗data), SHARK_DATA ∗dat, const void ∗activity_data, const void ∗residual_data, const void ∗precon_data, const void ∗other_data)
- int shark_add_customResidual (int i, double(∗other_res)(const Matrix< double > &x, SHARK_DATA ∗shark_dat, const void ∗other_data), SHARK_DATA ∗shark_dat)
- int shark_parameter_check (SHARK_DATA ∗shark_dat)
- int shark_energy_calculations (SHARK_DATA ∗shark_dat)
- int shark_temperature_calculations (SHARK_DATA ∗shark_dat)
- int shark_pH_finder (SHARK_DATA ∗shark_dat)
- int shark_guess (SHARK_DATA ∗shark_dat)
- int shark_initial_conditions (SHARK_DATA ∗shark_dat)
- int shark_executioner (SHARK_DATA ∗shark_dat)
- int shark_timestep_const (SHARK_DATA ∗shark_dat)
- int shark_timestep_adapt (SHARK_DATA ∗shark_dat)
- int shark_preprocesses (SHARK_DATA ∗shark_dat)
- int shark_solver (SHARK_DATA ∗shark_dat)
- int shark_postprocesses (SHARK_DATA ∗shark_dat)
- int shark_reset (SHARK_DATA ∗shark_dat)
- int shark_residual (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int SHARK (SHARK_DATA ∗shark_dat)
- int SHARK_SCENARIO (const char ∗yaml_input)
- int SHARK_TESTS ()

5.32.1 Function Documentation

5.32.1.1 int act_choice (const std::string & *input*)

5.32.1.2 int Convert2Concentration (const **Matrix**< double > & *logx,* **Matrix**< double > & *x*)

5.32.1.3 int Convert2LogConcentration (const **Matrix**< double > & *x,* **Matrix**< double > & *logx*)

5.32.1.4 int Davies_equation (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void * *data*)

5.32.1.5 int DaviesLadshaw_equation (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void * *data*)

5.32.1.6 int DebyeHuckel_equation (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void * *data*)

5.32.1.7 int ideal_solution (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void * *data*)

5.32.1.8 int linearsolve_choice (const std::string & *input*)

5.32.1.9 bool linesearch_choice (const std::string & *input*)

5.32.1.10 void print2file_shark_header (**SHARK_DATA** * *shark_dat*)

5.32.1.11 void print2file_shark_info (**SHARK_DATA** * *shark_dat*)

5.32.1.12 void print2file_shark_results_new (**SHARK_DATA** * *shark_dat*)

5.32.1.13 void print2file_shark_results_old (**SHARK_DATA** * *shark_dat*)

5.32.1.14 int read_equilrxn (**SHARK_DATA** * *shark_dat*)

5.32.1.15 int read_massbalance (**SHARK_DATA** * *shark_dat*)

5.32.1.16 int read_options (**SHARK_DATA** * *shark_dat*)

5.32.1.17 int read_scenario (**SHARK_DATA** * *shark_dat*)

5.32.1.18 int read_species (**SHARK_DATA** * *shark_dat*)

5.32.1.19 int read_unsteadyrxn (**SHARK_DATA** * *shark_dat*)

5.32.1.20 int setup_SHARK_DATA (FILE * *file,* int(*)(const **Matrix**< double > &x, **Matrix**< double > &res, const void *data) *residual,* int(*)(const **Matrix**< double > &x, **Matrix**< double > &gama, const void *data) *activity,* int(*)(const **Matrix**< double > &r, **Matrix**< double > &p, const void *data) *precond,* **SHARK_DATA** * *dat,* const void * *activity_data,* const void * *residual_data,* const void * *precon_data,* const void * *other_data*)

5.32.1.21 int SHARK (**SHARK_DATA** * *shark_dat*)

5.32.1.22 int shark_add_customResidual (int *i,* double(*)(const **Matrix**< double > &x, **SHARK_DATA** *shark_dat, const void *other_data) *other_res,* **SHARK_DATA** * *shark_dat*)

5.32.1.23 int shark_energy_calculations (**SHARK_DATA** * *shark_dat*)

5.32.1.24 int shark_executioner (**SHARK_DATA** * *shark_dat*)

5.32.1.25 int shark_guess (**SHARK_DATA** * *shark_dat*)

5.32.1.26 int shark_initial_conditions (SHARK_DATA ∗ *shark_dat*)

5.32.1.27 int shark_parameter_check (SHARK_DATA ∗ *shark_dat*)

5.32.1.28 int shark_pH_finder (SHARK_DATA ∗ *shark_dat*)

5.32.1.29 int shark_postprocesses (SHARK_DATA ∗ *shark_dat*)

5.32.1.30 int shark_preprocesses (SHARK_DATA ∗ *shark_dat*)

5.32.1.31 int shark_reset (SHARK_DATA ∗ *shark_dat*)

5.32.1.32 int shark_residual (const Matrix< double > & *x*, Matrix< double > & *F*, const void ∗ *data*)

5.32.1.33 int SHARK_SCENARIO (const char ∗ *yaml_input*)

5.32.1.34 int shark_solver (SHARK_DATA ∗ *shark_dat*)

5.32.1.35 int shark_temperature_calculations (SHARK_DATA ∗ *shark_dat*)

5.32.1.36 int SHARK_TESTS ( )

5.32.1.37 int shark_timestep_adapt (SHARK_DATA ∗ *shark_dat*)

5.32.1.38 int shark_timestep_const (SHARK_DATA ∗ *shark_dat*)

5.33 shark.h File Reference

```
#include "mola.h"
#include "macaw.h"
#include "lark.h"
#include "yaml_wrapper.h"
```

Classes

- class MasterSpeciesList
- class Reaction
- class MassBalance
- class UnsteadyReaction
- class Mechanism
- class Precipitation
- class UnsteadyPrecipitation
- struct SHARK_DATA

Macros

- #define Rstd 8.3144621

Typedefs

- typedef struct SHARK_DATA SHARK_DATA

Enumerations

- enum valid_act {
  IDEAL, DAVIES, DEBYE_HUCKEL, DAVIES_LADSHAW,
  SIT, PITZER }

Functions

- void print2file_shark_info (SHARK_DATA ∗shark_dat)
- void print2file_shark_header (SHARK_DATA ∗shark_dat)
- void print2file_shark_results_new (SHARK_DATA ∗shark_dat)
- void print2file_shark_results_old (SHARK_DATA ∗shark_dat)
- int ideal_solution (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int Davies_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int DebyeHuckel_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int DaviesLadshaw_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int act_choice (const std::string &input)
- bool linesearch_choice (const std::string &input)
- int linearsolve_choice (const std::string &input)
- int Convert2LogConcentration (const Matrix< double > &x, Matrix< double > &logx)
- int Convert2Concentration (const Matrix< double > &logx, Matrix< double > &x)
- int read_scenario (SHARK_DATA ∗shark_dat)
- int read_options (SHARK_DATA ∗shark_dat)
- int read_species (SHARK_DATA ∗shark_dat)
- int read_massbalance (SHARK_DATA ∗shark_dat)
- int read_equilrxn (SHARK_DATA ∗shark_dat)
- int read_unsteadyrxn (SHARK_DATA ∗shark_dat)
- int setup_SHARK_DATA (FILE ∗file, int(∗residual)(const Matrix< double > &x, Matrix< double > &res, const void ∗data), int(∗activity)(const Matrix< double > &x, Matrix< double > &gama, const void ∗data), int(∗precond)(const Matrix< double > &r, Matrix< double > &p, const void ∗data), SHARK_DATA ∗dat, const void ∗activity_data, const void ∗residual_data, const void ∗precon_data, const void ∗other_data)
- int shark_add_customResidual (int i, double(∗other_res)(const Matrix< double > &x, SHARK_DATA ∗shark_dat, const void ∗other_data), SHARK_DATA ∗shark_dat)
- int shark_parameter_check (SHARK_DATA ∗shark_dat)
- int shark_energy_calculations (SHARK_DATA ∗shark_dat)
- int shark_temperature_calculations (SHARK_DATA ∗shark_dat)
- int shark_pH_finder (SHARK_DATA ∗shark_dat)
- int shark_guess (SHARK_DATA ∗shark_dat)
- int shark_initial_conditions (SHARK_DATA ∗shark_dat)
- int shark_executioner (SHARK_DATA ∗shark_dat)
- int shark_timestep_const (SHARK_DATA ∗shark_dat)
- int shark_timestep_adapt (SHARK_DATA ∗shark_dat)
- int shark_preprocesses (SHARK_DATA ∗shark_dat)
- int shark_solver (SHARK_DATA ∗shark_dat)
- int shark_postprocesses (SHARK_DATA ∗shark_dat)
- int shark_reset (SHARK_DATA ∗shark_dat)
- int shark_residual (const Matrix< double > &x, Matrix< double > &F, const void ∗data)
- int SHARK (SHARK_DATA ∗shark_dat)
- int SHARK_SCENARIO (const char ∗yaml_input)
- int SHARK_TESTS ()

5.33.1 Macro Definition Documentation

5.33.1.1 #define Rstd 8.3144621

5.33.2 Typedef Documentation

5.33.2.1 typedef struct SHARK_DATA SHARK_DATA

5.33.3 Enumeration Type Documentation

5.33.3.1 enum valid_act

Enumerator

IDEAL

DAVIES

DEBYE_HUCKEL

DAVIES_LADSHAW

SIT

PITZER

5.33.4 Function Documentation

5.33.4.1 int act_choice (const std::string & *input*)

5.33.4.2 int Convert2Concentration (const Matrix< double > & *logx,* Matrix< double > & *x*)

5.33.4.3 int Convert2LogConcentration (const Matrix< double > & *x,* Matrix< double > & *logx*)

5.33.4.4 int Davies_equation (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.33.4.5 int DaviesLadshaw_equation (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.33.4.6 int DebyeHuckel_equation (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.33.4.7 int ideal_solution (const Matrix< double > & *x,* Matrix< double > & *F,* const void ∗ *data*)

5.33.4.8 int linearsolve_choice (const std::string & *input*)

5.33.4.9 bool linesearch_choice (const std::string & *input*)

5.33.4.10 void print2file_shark_header (SHARK_DATA ∗ *shark_dat*)

5.33.4.11 void print2file_shark_info (SHARK_DATA ∗ *shark_dat*)

5.33.4.12 void print2file_shark_results_new (SHARK_DATA ∗ *shark_dat*)

5.33.4.13 void print2file_shark_results_old (SHARK_DATA ∗ *shark_dat*)

5.33.4.14 int read_equilrxn (SHARK_DATA ∗ *shark_dat*)

5.33.4.15 int read_massbalance (SHARK_DATA ∗ *shark_dat*)

5.33.4.16 int read_options (SHARK_DATA ∗ *shark_dat*)

5.33.4.17 int read_scenario (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.18 int read_species (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.19 int read_unsteadyrxn (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.20 int setup_SHARK_DATA (FILE ∗ *file,* int(∗)(const **Matrix**< double > &x, **Matrix**< double > &res, const void ∗data) *residual,* int(∗)(const **Matrix**< double > &x, **Matrix**< double > &gama, const void ∗data) *activity,* int(∗)(const **Matrix**< double > &r, **Matrix**< double > &p, const void ∗data) *precond,* **SHARK_DATA** ∗ *dat,* const void ∗ *activity_data,* const void ∗ *residual_data,* const void ∗ *precon_data,* const void ∗ *other_data*)

5.33.4.21 int SHARK (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.22 int shark_add_customResidual (int *i,* double(∗)(const **Matrix**< double > &x, **SHARK_DATA** ∗shark_dat, const void ∗other_data) *other_res,* **SHARK_DATA** ∗ *shark_dat*)

5.33.4.23 int shark_energy_calculations (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.24 int shark_executioner (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.25 int shark_guess (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.26 int shark_initial_conditions (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.27 int shark_parameter_check (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.28 int shark_pH_finder (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.29 int shark_postprocesses (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.30 int shark_preprocesses (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.31 int shark_reset (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.32 int shark_residual (const **Matrix**< double > & *x,* **Matrix**< double > & *F,* const void ∗ *data*)

5.33.4.33 int SHARK_SCENARIO (const char ∗ *yaml_input*)

5.33.4.34 int shark_solver (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.35 int shark_temperature_calculations (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.36 int SHARK_TESTS ( )

5.33.4.37 int shark_timestep_adapt (**SHARK_DATA** ∗ *shark_dat*)

5.33.4.38 int shark_timestep_const (**SHARK_DATA** ∗ *shark_dat*)

5.34 skua.cpp File Reference

```
#include "skua.h"
```

Functions

- void print2file_species_header (FILE ∗Output, SKUA_DATA ∗skua_dat, int i)
- void print2file_SKUA_time_header (FILE ∗Output, SKUA_DATA ∗skua_dat, int i)
- void print2file_SKUA_header (SKUA_DATA ∗skua_dat)
- void print2file_SKUA_results_old (SKUA_DATA ∗skua_dat)
- void print2file_SKUA_results_new (SKUA_DATA ∗skua_dat)
- double default_Dc (int i, int l, const void ∗data)
- double default_kf (int i, const void ∗data)
- double const_Dc (int i, int l, const void ∗data)
- double simple_darken_Dc (int i, int l, const void ∗data)
- double theoretical_darken_Dc (int i, int l, const void ∗data)
- double empirical_kf (int i, const void ∗data)
- double const_kf (int i, const void ∗data)
- int molefractionCheck (SKUA_DATA ∗skua_dat)
- int setup_SKUA_DATA (FILE ∗file, double(∗eval_Dc)(int i, int l, const void ∗user_data), double(∗eval_Kf)(int i, const void ∗user_data), const void ∗user_data, MIXED_GAS ∗gas_data, SKUA_DATA ∗skua_dat)
- int SKUA_Executioner (SKUA_DATA ∗skua_dat)
- int set_SKUA_ICs (SKUA_DATA ∗skua_dat)
- int set_SKUA_timestep (SKUA_DATA ∗skua_dat)
- int SKUA_preprocesses (SKUA_DATA ∗skua_dat)
- int set_SKUA_params (const void ∗user_data)
- int SKUA_postprocesses (SKUA_DATA ∗skua_dat)
- int SKUA_reset (SKUA_DATA ∗skua_dat)
- int SKUA (SKUA_DATA ∗skua_dat)
- int SKUA_CYCLE_TEST01 (SKUA_DATA ∗skua_dat)
- int SKUA_CYCLE_TEST02 (SKUA_DATA ∗skua_dat)
- int SKUA_LOW_TEST03 (SKUA_DATA ∗skua_dat)
- int SKUA_MID_TEST04 (SKUA_DATA ∗skua_dat)
- int SKUA_SCENARIOS (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate)
- int SKUA_TESTS ()

5.34.1 Function Documentation

5.34.1.1 double const_Dc (int *i*, int *l*, const void ∗ *data*)

5.34.1.2 double const_kf (int *i*, const void ∗ *data*)

5.34.1.3 double default_Dc (int *i*, int *l*, const void ∗ *data*)

5.34.1.4 double default_kf (int *i*, const void ∗ *data*)

5.34.1.5 double empirical_kf (int *i*, const void ∗ *data*)

5.34.1.6 int molefractionCheck (SKUA_DATA ∗ *skua_dat*)

5.34.1.7 void print2file_SKUA_header (SKUA_DATA ∗ *skua_dat*)

5.34.1.8 void print2file_SKUA_results_new (SKUA_DATA ∗ *skua_dat*)

5.34.1.9 void print2file_SKUA_results_old (SKUA_DATA ∗ *skua_dat*)

5.34.1.10 void print2file_SKUA_time_header (FILE ∗ *Output*, SKUA_DATA ∗ *skua_dat*, int *i*)

5.34.1.11 void print2file_species_header (FILE ∗ *Output,* SKUA_DATA ∗ *skua_dat,* int *i*)

5.34.1.12 int set_SKUA_ICs (SKUA_DATA ∗ *skua_dat*)

5.34.1.13 int set_SKUA_params (const void ∗ *user_data*)

5.34.1.14 int set_SKUA_timestep (SKUA_DATA ∗ *skua_dat*)

5.34.1.15 int setup_SKUA_DATA (FILE ∗ *file,* double(∗)(int i, int l, const void ∗user_data) *eval_Dc,* double(∗)(int i, const void ∗user_data) *eval_Kf,* const void ∗ *user_data,* MIXED_GAS ∗ *gas_data,* SKUA_DATA ∗ *skua_dat*)

5.34.1.16 double simple_darken_Dc (int *i,* int *l,* const void ∗ *data*)

5.34.1.17 int SKUA (SKUA_DATA ∗ *skua_dat*)

5.34.1.18 int SKUA_CYCLE_TEST01 (SKUA_DATA ∗ *skua_dat*)

5.34.1.19 int SKUA_CYCLE_TEST02 (SKUA_DATA ∗ *skua_dat*)

5.34.1.20 int SKUA_Executioner (SKUA_DATA ∗ *skua_dat*)

5.34.1.21 int SKUA_LOW_TEST03 (SKUA_DATA ∗ *skua_dat*)

5.34.1.22 int SKUA_MID_TEST04 (SKUA_DATA ∗ *skua_dat*)

5.34.1.23 int SKUA_postprocesses (SKUA_DATA ∗ *skua_dat*)

5.34.1.24 int SKUA_preprocesses (SKUA_DATA ∗ *skua_dat*)

5.34.1.25 int SKUA_reset (SKUA_DATA ∗ *skua_dat*)

5.34.1.26 int SKUA_SCENARIOS (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate*)

5.34.1.27 int SKUA_TESTS ( )

5.34.1.28 double theoretical_darken_Dc (int *i,* int *l,* const void ∗ *data*)

5.35 skua.h File Reference

```
#include "finch.h"
#include "magpie.h"
#include "egret.h"
```

Classes

- struct SKUA_PARAM
- struct SKUA_DATA

Macros

- #define SKUA_HPP_
- #define D_inf(Dref, Tref, B, p, T) (Dref ∗ pow(p+sqrt(DBL_EPSILON),(Tref/T)-B))
- #define D_o(Diff, E, T) (Diff ∗ exp(-E/(Rstd∗T)))
- #define D_c(Diff, phi) (Diff ∗ (1.0/((1.0+1.1E-6)-phi)))

Functions

- void print2file_species_header (FILE ∗Output, SKUA_DATA ∗skua_dat, int i)
- void print2file_SKUA_time_header (FILE ∗Output, SKUA_DATA ∗skua_dat, int i)
- void print2file_SKUA_header (SKUA_DATA ∗skua_dat)
- void print2file_SKUA_results_old (SKUA_DATA ∗skua_dat)
- void print2file_SKUA_results_new (SKUA_DATA ∗skua_dat)
- double default_Dc (int i, int l, const void ∗data)
- double default_kf (int i, const void ∗data)
- double const_Dc (int i, int l, const void ∗data)
- double simple_darken_Dc (int i, int l, const void ∗data)
- double theoretical_darken_Dc (int i, int l, const void ∗data)
- double empirical_kf (int i, const void ∗data)
- double const_kf (int i, const void ∗data)
- int molefractionCheck (SKUA_DATA ∗skua_dat)
- int setup_SKUA_DATA (FILE ∗file, double(∗eval_Dc)(int i, int l, const void ∗user_data), double(∗eval_Kf)(int i, const void ∗user_data), const void ∗user_data, MIXED_GAS ∗gas_data, SKUA_DATA ∗skua_dat)
- int SKUA_Executioner (SKUA_DATA ∗skua_dat)
- int set_SKUA_ICs (SKUA_DATA ∗skua_dat)
- int set_SKUA_timestep (SKUA_DATA ∗skua_dat)
- int SKUA_preprocesses (SKUA_DATA ∗skua_dat)
- int set_SKUA_params (const void ∗user_data)
- int SKUA_postprocesses (SKUA_DATA ∗skua_dat)
- int SKUA_reset (SKUA_DATA ∗skua_dat)
- int SKUA (SKUA_DATA ∗skua_dat)
- int SKUA_CYCLE_TEST01 (SKUA_DATA ∗skua_dat)
- int SKUA_CYCLE_TEST02 (SKUA_DATA ∗skua_dat)
- int SKUA_LOW_TEST03 (SKUA_DATA ∗skua_dat)
- int SKUA_MID_TEST04 (SKUA_DATA ∗skua_dat)
- int SKUA_SCENARIOS (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate)
- int SKUA_TESTS ()

5.35.1 Macro Definition Documentation

5.35.1.1 #define D_c(*Diff, phi*) (Diff ∗ (1.0/((1.0+1.1E-6)-phi)))

5.35.1.2 #define D_inf(*Dref, Tref, B, p, T*) (Dref ∗ pow(p+sqrt(DBL_EPSILON),(Tref/T)-B))

5.35.1.3 #define D_o(*Diff, E, T*) (Diff ∗ exp(-E/(Rstd∗T)))

5.35.1.4 #define SKUA_HPP_

5.35.2 Function Documentation

5.35.2.1 double const_Dc (int *i*, int *l*, const void ∗ *data*)

5.35.2.2 double const_kf (int *i*, const void ∗ *data*)

5.35.2.3 double default_Dc (int *i*, int *l*, const void ∗ *data*)

5.35.2.4 double default_kf (int *i*, const void ∗ *data*)

5.35.2.5 double empirical_kf (int *i*, const void ∗ *data*)

5.35.2.6 int molefractionCheck (SKUA_DATA ∗ *skua_dat*)

5.35.2.7 void print2file_SKUA_header (SKUA_DATA ∗ *skua_dat*)

5.35.2.8 void print2file_SKUA_results_new (SKUA_DATA ∗ *skua_dat*)

5.35.2.9 void print2file_SKUA_results_old (SKUA_DATA ∗ *skua_dat*)

5.35.2.10 void print2file_SKUA_time_header (FILE ∗ *Output,* SKUA_DATA ∗ *skua_dat,* int *i*)

5.35.2.11 void print2file_species_header (FILE ∗ *Output,* SKUA_DATA ∗ *skua_dat,* int *i*)

5.35.2.12 int set_SKUA_ICs (SKUA_DATA ∗ *skua_dat*)

5.35.2.13 int set_SKUA_params (const void ∗ *user_data*)

5.35.2.14 int set_SKUA_timestep (SKUA_DATA ∗ *skua_dat*)

5.35.2.15 int setup_SKUA_DATA (FILE ∗ *file,* double(∗)(int i, int l, const void ∗user_data) *eval_Dc,* double(∗)(int i, const void ∗user_data) *eval_Kf,* const void ∗ *user_data,* MIXED_GAS ∗ *gas_data,* SKUA_DATA ∗ *skua_dat*)

5.35.2.16 double simple_darken_Dc (int *i,* int *l,* const void ∗ *data*)

5.35.2.17 int SKUA (SKUA_DATA ∗ *skua_dat*)

5.35.2.18 int SKUA_CYCLE_TEST01 (SKUA_DATA ∗ *skua_dat*)

5.35.2.19 int SKUA_CYCLE_TEST02 (SKUA_DATA ∗ *skua_dat*)

5.35.2.20 int SKUA_Executioner (SKUA_DATA ∗ *skua_dat*)

5.35.2.21 int SKUA_LOW_TEST03 (SKUA_DATA ∗ *skua_dat*)

5.35.2.22 int SKUA_MID_TEST04 (SKUA_DATA ∗ *skua_dat*)

5.35.2.23 int SKUA_postprocesses (SKUA_DATA ∗ *skua_dat*)

5.35.2.24 int SKUA_preprocesses (SKUA_DATA ∗ *skua_dat*)

5.35.2.25 int SKUA_reset (SKUA_DATA ∗ *skua_dat*)

5.35.2.26 int SKUA_SCENARIOS (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate*)

5.35.2.27 int SKUA_TESTS ( )

5.35.2.28 double theoretical_darken_Dc (int *i,* int *l,* const void ∗ *data*)

5.36 skua_opt.cpp File Reference

```
#include "skua_opt.h"
```

Functions

- int SKUA_OPT_set_y (SKUA_OPT_DATA ∗skua_opt)

- int initial_guess_SKUA (SKUA_OPT_DATA ∗skua_opt)
- void eval_SKUA_Uptake (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int SKUA_OPTIMIZE (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate, const char ∗data)

5.36.1 Function Documentation

5.36.1.1 void eval_SKUA_Uptake (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.36.1.2 int initial_guess_SKUA (SKUA_OPT_DATA ∗ *skua_opt*)

5.36.1.3 int SKUA_OPT_set_y (SKUA_OPT_DATA ∗ *skua_opt*)

5.36.1.4 int SKUA_OPTIMIZE (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate,* const char ∗ *data*)

5.37 skua_opt.h File Reference

```
#include "skua.h"
```

Classes

- struct SKUA_OPT_DATA

Functions

- int SKUA_OPT_set_y (SKUA_OPT_DATA ∗skua_opt)
- int initial_guess_SKUA (SKUA_OPT_DATA ∗skua_opt)
- void eval_SKUA_Uptake (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)
- int SKUA_OPTIMIZE (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate, const char ∗data)

5.37.1 Function Documentation

5.37.1.1 void eval_SKUA_Uptake (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.37.1.2 int initial_guess_SKUA (SKUA_OPT_DATA ∗ *skua_opt*)

5.37.1.3 int SKUA_OPT_set_y (SKUA_OPT_DATA ∗ *skua_opt*)

5.37.1.4 int SKUA_OPTIMIZE (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate,* const char ∗ *data*)

5.38 Trajectory.cpp File Reference

```
#include "Trajectory.h"
```

Functions

- double Magnetic_R (const Matrix< double > &dX, const Matrix< double > &dY, int i, double b, double mu_0, double chi_p, double M, double H0, double a)
- double Magnetic_T (const Matrix< double > &dX, const Matrix< double > &dY, int i, double b, double mu_0, double chi_p, double M, double H0, double a)
- double Grav_R (const Matrix< double > &dX, int i, double b, double rho_p, double rho_f)
- double Grav_T (const Matrix< double > &dX, int i, double b, double rho_p, double rho_f)
- double Van_R (const Matrix< double > &dX, const Matrix< double > &dY, int i, double Hamaker, double b, double a)
- double V_RAD (const Matrix< double > &dX, const Matrix< double > &dY, int i, double V0, double rho_f, double a, double eta)
- double V_THETA (const Matrix< double > &dX, const Matrix< double > &dY, int i, double V0, double rho_f, double a, double eta)
- double Brown_RAD (double n_rand, double m_rand, double sigma_n, double sigma_m)
- double Brown_THETA (double s_rand, double t_rand, double sigma_n, double sigma_m)
- int POLAR (Matrix< double > &POL, const Matrix< double > &dX, const Matrix< double > &dY, const void ∗data, int i)
- double RADIAL_FORCE (const Matrix< double > &POL, double eta, double b, double mp, double t, double a)
- double TANGENTIAL_FORCE (const Matrix< double > &POL, const Matrix< double > &dY, double eta, double b, double mp, double t, double a, int i)
- int CARTESIAN (const Matrix< double > &POL, Matrix< double > &H, const Matrix< double > &dY, double i, const void ∗data)
- int DISPLACEMENT (Matrix< double > &dX, Matrix< double > &dY, const Matrix< double > &H, int i)
- int LOCATION (const Matrix< double > &dY, const Matrix< double > &dX, Matrix< double > &X, Matrix< double > &Y, int i)
- double Removal_Efficiency (double Sum_Cap, const void ∗data)
- int Trajectory_SetupConstants (TRAJECTORY_DATA ∗dat)
- int Number_Generator (TRAJECTORY_DATA ∗dat)
- int Run_Trajectory ()

5.38.1 Function Documentation

5.38.1.1 double Brown_RAD (double *n_rand*, double *m_rand*, double *sigma_n*, double *sigma_m*)

5.38.1.2 double Brown_THETA (double *s_rand*, double *t_rand*, double *sigma_n*, double *sigma_m*)

5.38.1.3 int CARTESIAN (const Matrix< double > & *POL*, Matrix< double > & *H*, const Matrix< double > & *dY*, double *i*, const void ∗ *data*)

5.38.1.4 int DISPLACEMENT (Matrix< double > & *dX*, Matrix< double > & *dY*, const Matrix< double > & *H*, int *i*)

5.38.1.5 double Grav_R (const Matrix< double > & *dX*, int *i*, double *b*, double *rho_p*, double *rho_f*)

5.38.1.6 double Grav_T (const Matrix< double > & *dX*, int *i*, double *b*, double *rho_p*, double *rho_f*)

5.38.1.7 int LOCATION (const Matrix< double > & *dY*, const Matrix< double > & *dX*, Matrix< double > & *X*, Matrix< double > & *Y*, int *i*)

5.38.1.8 double Magnetic_R (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *b*, double *mu_0*, double *chi_p*, double *M*, double *H0*, double *a*)

5.38.1.9 double Magnetic_T (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *b*, double *mu_0*, double *chi_p*, double *M*, double *H0*, double *a*)

5.38.1.10 int Number_Generator (TRAJECTORY_DATA ∗ *dat*)

5.38.1.11 int POLAR (Matrix< double > & *POL*, const Matrix< double > & *dX*, const Matrix< double > & *dY*, const void ∗ *data*, int *i*)

5.38.1.12 double RADIAL_FORCE (const Matrix< double > & *POL*, double *eta*, double *b*, double *mp*, double *t*, double *a*)

5.38.1.13 double Removal_Efficiency (double *Sum_Cap*, const void ∗ *data*)

5.38.1.14 int Run_Trajectory ( )

5.38.1.15 double TANGENTIAL_FORCE (const Matrix< double > & *POL*, const Matrix< double > & *dY*, double *eta*, double *b*, double *mp*, double *t*, double *a*, int *i*)

5.38.1.16 int Trajectory_SetupConstants (TRAJECTORY_DATA ∗ *dat*)

5.38.1.17 double V_RAD (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *V0*, double *rho_f*, double *a*, double *eta*)

5.38.1.18 double V_THETA (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *V0*, double *rho_f*, double *a*, double *eta*)

5.38.1.19 double Van_R (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *Hamaker*, double *b*, double *a*)

5.39 Trajectory.h File Reference

```
#include "macaw.h"
#include <random>
#include <chrono>
```

Classes

- struct TRAJECTORY_DATA

Functions

- double Magnetic_R (const Matrix< double > &dX, const Matrix< double > &dY, int i, double b, double mu_0, double chi_p, double M, double H0, double a)
- double Magnetic_T (const Matrix< double > &dX, const Matrix< double > &dY, int i, double b, double mu_0, double chi_p, double M, double H0, double a)
- double Grav_R (const Matrix< double > &dX, int i, double b, double rho_p, double rho_f)
- double Grav_T (const Matrix< double > &dX, int i, double b, double rho_p, double rho_f)
- double Van_R (const Matrix< double > &dX, const Matrix< double > &dY, int i, double Hamaker, double b, double a)
- double V_RAD (const Matrix< double > &dX, const Matrix< double > &dY, int i, double V0, double rho_f, double a, double eta)
- double V_THETA (const Matrix< double > &dX, const Matrix< double > &dY, int i, double V0, double rho_f, double a, double eta)
- double Brown_RAD (double n_rand, double m_rand, double sigma_n, double sigma_m)
- double Brown_THETA (double s_rand, double t_rand, double sigma_n, double sigma_m)
- int POLAR (Matrix< double > &POL, const Matrix< double > &dX, const Matrix< double > &dY, const void ∗data, int i)

- double RADIAL_FORCE (const Matrix< double > &POL, double eta, double b, double mp, double t, double a)
- double TANGENTIAL_FORCE (const Matrix< double > &POL, const Matrix< double > &dY, double eta, double b, double mp, double t, double a, int i)
- int CARTESIAN (const Matrix< double > &POL, Matrix< double > &H, const Matrix< double > &dY, double i, const void ∗data)
- int DISPLACEMENT (Matrix< double > &dX, Matrix< double > &dY, const Matrix< double > &H, int i)
- int LOCATION (const Matrix< double > &dY, const Matrix< double > &dX, Matrix< double > &X, Matrix< double > &Y, int i)
- double Removal_Efficiency (double Sum_Cap, const void ∗data)
- int Trajectory_SetupConstants (TRAJECTORY_DATA ∗dat)
- int Number_Generator (TRAJECTORY_DATA ∗dat)
- int Run_Trajectory ()

5.39.1 Function Documentation

5.39.1.1 double Brown_RAD (double *n_rand,* double *m_rand,* double *sigma_n,* double *sigma_m*)

5.39.1.2 double Brown_THETA (double *s_rand,* double *t_rand,* double *sigma_n,* double *sigma_m*)

5.39.1.3 int CARTESIAN (const Matrix< double > & *POL,* Matrix< double > & *H,* const Matrix< double > & *dY,* double *i,* const void ∗ *data*)

5.39.1.4 int DISPLACEMENT (Matrix< double > & *dX,* Matrix< double > & *dY,* const Matrix< double > & *H,* int *i*)

5.39.1.5 double Grav_R (const Matrix< double > & *dX,* int *i,* double *b,* double *rho_p,* double *rho_f*)

5.39.1.6 double Grav_T (const Matrix< double > & *dX,* int *i,* double *b,* double *rho_p,* double *rho_f*)

5.39.1.7 int LOCATION (const Matrix< double > & *dY,* const Matrix< double > & *dX,* Matrix< double > & *X,* Matrix< double > & *Y,* int *i*)

5.39.1.8 double Magnetic_R (const Matrix< double > & *dX,* const Matrix< double > & *dY,* int *i,* double *b,* double *mu_0,* double *chi_p,* double *M,* double *H0,* double *a*)

5.39.1.9 double Magnetic_T (const Matrix< double > & *dX,* const Matrix< double > & *dY,* int *i,* double *b,* double *mu_0,* double *chi_p,* double *M,* double *H0,* double *a*)

5.39.1.10 int Number_Generator (TRAJECTORY_DATA ∗ *dat*)

5.39.1.11 int POLAR (Matrix< double > & *POL,* const Matrix< double > & *dX,* const Matrix< double > & *dY,* const void ∗ *data,* int *i*)

5.39.1.12 double RADIAL_FORCE (const Matrix< double > & *POL,* double *eta,* double *b,* double *mp,* double *t,* double *a*)

5.39.1.13 double Removal_Efficiency (double *Sum_Cap,* const void ∗ *data*)

5.39.1.14 int Run_Trajectory ( )

5.39.1.15 double TANGENTIAL_FORCE (const Matrix< double > & *POL,* const Matrix< double > & *dY,* double *eta,* double *b,* double *mp,* double *t,* double *a,* int *i*)

5.39.1.16 int Trajectory_SetupConstants (TRAJECTORY_DATA ∗ *dat*)

5.39.1.17 double V_RAD (const Matrix< double > & *dX,* const Matrix< double > & *dY,* int *i,* double *V0,* double *rho_f,* double *a,* double *eta*)

5.39.1.18 double V_THETA (const Matrix< double > & *dX,* const Matrix< double > & *dY,* int *i,* double *V0,* double *rho_f,* double *a,* double *eta*)

5.39.1.19 double Van_R (const Matrix< double > & *dX,* const Matrix< double > & *dY,* int *i,* double *Hamaker,* double *b,* double *a*)

5.40 ui.cpp File Reference

```
#include "ui.h"
```

Functions

- void aui_help ()
- void bui_help ()
- std::string allLower (const std::string &input)
- bool exit (const std::string &input)
- bool help (const std::string &input)
- bool version (const std::string &input)
- bool test (const std::string &input)
- bool exec (const std::string &input)
- bool path (const std::string &input)
- bool input (const std::string &input)
- bool valid_test_string (const std::string &input, UI_DATA ∗ui_dat)
- bool valid_exec_string (const std::string &input, UI_DATA ∗ui_dat)
- int number_files (UI_DATA ∗ui_dat)
- bool valid_addon_options (UI_DATA ∗ui_dat)
- void display_help (UI_DATA ∗ui_dat)
- void display_version (UI_DATA ∗ui_dat)
- int invalid_input (int count, int max)
- bool valid_input_main (UI_DATA ∗ui_dat)
- bool valid_input_tests (UI_DATA ∗ui_dat)
- bool valid_input_execute (UI_DATA ∗ui_dat)
- int test_loop (UI_DATA ∗ui_dat)
- int exec_loop (UI_DATA ∗ui_dat)
- int run_test (UI_DATA ∗ui_dat)
- int run_exec (UI_DATA ∗ui_dat)
- int run_executable (int argc, const char ∗argv[])

5.40.1 Function Documentation

5.40.1.1 std::string allLower (const std::string & *input*)

5.40.1.2 void aui_help ( )

5.40.1.3 void bui_help ( )

5.40.1.4 void display_help (UI_DATA ∗ *ui_dat*)

5.40.1.5 void display_version (UI_DATA ∗ *ui_dat*)

5.40.1.6 bool exec (const std::string & *input*)

5.40.1.7 int exec_loop (UI_DATA ∗ *ui_dat*)

5.40.1.8 bool exit (const std::string & *input*)

5.40.1.9 bool help (const std::string & *input*)

5.40.1.10 bool input (const std::string & *input*)

5.40.1.11 int invalid_input (int *count,* int *max*)

5.40.1.12 int number_files (UI_DATA ∗ *ui_dat*)

5.40.1.13 bool path (const std::string & *input*)

5.40.1.14 int run_exec (UI_DATA ∗ *ui_dat*)

5.40.1.15 int run_executable (int *argc,* const char ∗ *argv[ ]*)

5.40.1.16 int run_test (UI_DATA ∗ *ui_dat*)

5.40.1.17 bool test (const std::string & *input*)

5.40.1.18 int test_loop (UI_DATA ∗ *ui_dat*)

5.40.1.19 bool valid_addon_options (UI_DATA ∗ *ui_dat*)

5.40.1.20 bool valid_exec_string (const std::string & *input,* UI_DATA ∗ *ui_dat*)

5.40.1.21 bool valid_input_execute (UI_DATA ∗ *ui_dat*)

5.40.1.22 bool valid_input_main (UI_DATA ∗ *ui_dat*)

5.40.1.23 bool valid_input_tests (UI_DATA ∗ *ui_dat*)

5.40.1.24 bool valid_test_string (const std::string & *input,* UI_DATA ∗ *ui_dat*)

5.40.1.25 bool version (const std::string & *input*)

5.41 ui.h File Reference

```
#include <fstream>
#include <string>
#include <iostream>
#include "error.h"
#include "yaml_wrapper.h"
#include "flock.h"
#include "school.h"
#include "sandbox.h"
#include "Trajectory.h"
```

Classes

- struct UI_DATA

Macros

- #define UI_HPP_
- #define ECO_VERSION "0.0 alpha"
- #define ECO_EXECUTABLE "eco0"

Enumerations

- enum valid_options {
  TEST, EXECUTE, EXIT, CONTINUE,
  HELP, dogfish, eel, egret,
  finch, lark, macaw, mola,
  monkfish, sandbox, scopsowl, shark,
  skua, gsta_opt, magpie, scops_opt,
  skua_opt, trajectory }

Functions

- void aui_help ()
- void bui_help ()
- std::string allLower (const std::string &input)
- bool exit (const std::string &input)
- bool help (const std::string &input)
- bool version (const std::string &input)
- bool test (const std::string &input)
- bool exec (const std::string &input)
- bool path (const std::string &input)
- bool input (const std::string &input)
- bool valid_test_string (const std::string &input, UI_DATA ∗ui_dat)
- bool valid_exec_string (const std::string &input, UI_DATA ∗ui_dat)
- int number_files (UI_DATA ∗ui_dat)
- bool valid_addon_options (UI_DATA ∗ui_dat)
- void exec_option (UI_DATA ∗ui_dat)
- void display_help (UI_DATA ∗ui_dat)
- void display_version (UI_DATA ∗ui_dat)
- int invalid_input (int count, int max)
- bool valid_input_main (UI_DATA ∗ui_dat)
- bool valid_input_tests (UI_DATA ∗ui_dat)
- bool valid_input_execute (UI_DATA ∗ui_dat)
- int test_loop (UI_DATA ∗ui_dat)
- int exec_loop (UI_DATA ∗ui_dat)
- int run_test (UI_DATA ∗ui_dat)
- int run_exec (UI_DATA ∗ui_dat)
- int run_executable (int argc, const char ∗argv[ ])

5.41.1 Macro Definition Documentation

5.41.1.1 #define ECO_EXECUTABLE ”eco0”

5.41.1.2 #define ECO_VERSION ”0.0 alpha”

5.41.1.3 #define UI_HPP_

5.41.2 Enumeration Type Documentation

5.41.2.1 enum valid_options

Enumerator

- ***TEST***
- ***EXECUTE***
- ***EXIT***
- ***CONTINUE***
- ***HELP***
- ***dogfish***
- ***eel***
- ***egret***
- ***finch***
- ***lark***
- ***macaw***
- ***mola***
- ***monkfish***
- ***sandbox***
- ***scopsowl***
- ***shark***
- ***skua***
- ***gsta_opt***
- ***magpie***
- ***scops_opt***
- ***skua_opt***
- ***trajectory***

5.41.3 Function Documentation

5.41.3.1 std::string allLower (const std::string & *input*)

5.41.3.2 void aui_help ( )

5.41.3.3 void bui_help ( )

5.41.3.4 void display_help (UI_DATA ∗ *ui_dat*)

5.41.3.5 void display_version (UI_DATA ∗ *ui_dat*)

5.41.3.6 bool exec (const std::string & *input*)

5.41.3.7 int exec_loop (UI_DATA ∗ *ui_dat*)

5.41.3.8 void exec_option (UI_DATA ∗ *ui_dat*)

5.41.3.9 bool exit (const std::string & *input*)

5.41.3.10 bool help (const std::string & *input*)

5.41.3.11 bool input (const std::string & *input*)

5.41.3.12 int invalid_input (int *count,* int *max*)

5.41.3.13 int number_files (UI_DATA ∗ *ui_dat*)

5.41.3.14 bool path (const std::string & *input*)

5.41.3.15 int run_exec (UI_DATA ∗ *ui_dat*)

5.41.3.16 int run_executable (int *argc,* const char ∗ *argv[ ]*)

5.41.3.17 int run_test (UI_DATA ∗ *ui_dat*)

5.41.3.18 bool test (const std::string & *input*)

5.41.3.19 int test_loop (UI_DATA ∗ *ui_dat*)

5.41.3.20 bool valid_addon_options (UI_DATA ∗ *ui_dat*)

5.41.3.21 bool valid_exec_string (const std::string & *input,* UI_DATA ∗ *ui_dat*)

5.41.3.22 bool valid_input_execute (UI_DATA ∗ *ui_dat*)

5.41.3.23 bool valid_input_main (UI_DATA ∗ *ui_dat*)

5.41.3.24 bool valid_input_tests (UI_DATA ∗ *ui_dat*)

5.41.3.25 bool valid_test_string (const std::string & *input,* UI_DATA ∗ *ui_dat*)

5.41.3.26 bool version (const std::string & *input*)

5.42 yaml_wrapper.cpp File Reference

```
#include "yaml_wrapper.h"
```

Functions

- int YAML_WRAPPER_TESTS ()
- int YAML_CPP_TEST (const char ∗file)

5.42.1 Function Documentation

5.42.1.1 int YAML_CPP_TEST (const char ∗ *file*)

5.42.1.2 int YAML_WRAPPER_TESTS ( )

5.43 yaml_wrapper.h File Reference

```
#include "yaml.h"
#include "error.h"
#include <map>
#include <string>
#include <iostream>
#include <utility>
#include <stdexcept>
```

Classes

- class ValueTypePair
- class KeyValueMap
- class SubHeader
- class Header
- class Document
- class YamlWrapper
- class yaml_cpp_class

Typedefs

- typedef enum data_type data_type
- typedef enum header_state header_state

Enumerations

- enum data_type {
  STRING, BOOLEAN, DOUBLE, INT,
  UNKNOWN }
- enum header_state { ANCHOR, ALIAS, NONE }

Functions

- int YAML_WRAPPER_TESTS ()
- int YAML_CPP_TEST (const char ∗file)

5.43.1 Typedef Documentation

5.43.1.1 typedef enum data_type data_type

5.43.1.2 typedef enum header_state header_state

5.43.2 Enumeration Type Documentation

5.43.2.1 enum data_type

Enumerator

STRING

BOOLEAN

DOUBLE

INT

UNKNOWN

5.43.2.2 enum header_state

Enumerator

ANCHOR

ALIAS

NONE

5.43.3 Function Documentation

5.43.3.1 int YAML_CPP_TEST (const char ∗ *file*)

5.43.3.2 int YAML_WRAPPER_TESTS ( )

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