Ecosystem

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Chapter 4

Class Documentation

4.1 ARNOLDI_DATA Struct Reference

Data structure for the construction of the Krylov subspaces for a linear system.

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

Public Attributes

- int k

  Desired size of the Krylov subspace.
- int iter

  Actual size of the Krylov subspace.
- double beta

  Normalization parameter.
- double hp1

  Additional row element of H (separate storage for holding)
- bool Output = true

  True = print messages to console.
- std::vector< Matrix< double > > Vk

  (N) x (k) orthonormal vector basis stored as a vector of column matrices
- Matrix< double > Hkp1

  (k+1) x (k) upper Hessenberg matrix
- Matrix< double > yk

  (k) x (1) vector search direction
- Matrix< double > e1

  (k) x (1) orthonormal vector with 1 in first position
- Matrix< double > w

  (N) x (1) interim result of the matrix_vector multiplication
- Matrix< double > v

  (N) x (1) holding cell for the column entries of Vk and other interims
- Matrix< double > sum

  (N) x (1) running sum of subspace vectors for use in altering w

4.1.1 Detailed Description

Data structure for the construction of the Krylov subspaces for a linear system.

C-style object used in conjunction with the Arnoldi algorithm to construct an orthonormal basis and upper Hessenberg representation of a given linear operator. This is used to solve a linear system both iteratively (i.e., in conjunction with GMRESLP) and directly (i.e., in conjunction with FOM). Alternatively, you can just store the factorized components for later use in another routine.

4.1.2 Member Data Documentation

4.1.2.1 int ARNOLDI_DATA::k

Desired size of the Krylov subspace.

4.1.2.2 int ARNOLDI_DATA::iter

Actual size of the Krylov subspace.

4.1.2.3 double ARNOLDI_DATA::beta

Normalization parameter.

4.1.2.4 double ARNOLDI_DATA::hp1

Additional row element of H (separate storage for holding)

4.1.2.5 bool ARNOLDI_DATA::Output = true

True = print messages to console.

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

(N) x (k) orthonormal vector basis stored as a vector of column matrices

4.1.2.7 Matrix<double> ARNOLDI_DATA::Hkp1

(k+1) x (k) upper Hessenberg matrix

4.1.2.8 Matrix<double> ARNOLDI_DATA::yk

(k) x (1) vector search direction

4.1.2.9 Matrix<double> ARNOLDI_DATA::e1

(k) x (1) orthonormal vector with 1 in first position

4.1.2.10 Matrix<double> ARNOLDI_DATA::w

(N) x (1) interim result of the matrix_vector multiplication

4.1.2.11 Matrix<double> ARNOLDI_DATA::v

(N) x (1) holding cell for the column entries of Vk and other interims

4.1.2.12 Matrix<double> ARNOLDI_DATA::sum

(N) x (1) running sum of subspace vectors for use in altering w

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

- lark.h

4.2 Atom Class Reference

Atom object to hold information about specific atoms in the periodic table (click Atom to go to function definitions)

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

Public Member Functions

- Atom ()
  Default Constructor.
- ∼Atom ()
  Default Destructor.
- Atom (std::string Name)
  Constructor by Atom Name.
- Atom (int number)
  Constructor by Atomic number.
- void Register (std::string Symbol)
  Register an atom object by symbol.
- void Register (int number)
  Register an atom object by number.
- void editAtomicWeight (double AW)
  Manually changes the atomic weight.
- void editOxidationState (int state)
  Manually changes the oxidation state.
- void editProtons (int proton)
  Manually changes the number of protons.
- void editNeutrons (int neutron)
  Manually changes the number of neutrons.
- void editElectrons (int electron)
  Manually changes the number of electrons.
- void editValence (int val)
  Manually changes the number of valence electrons.
- void removeProton ()
  Manually removes 1 proton and adjusts weight.
- void removeNeutron ()
  Manually removes 1 neutron and adjusts weight.
- void removeElectron ()
  Manually removes 1 electron from valence.
- double AtomicWeight ()

Returns the current atomic weight (g/mol)
- int OxidationState ()

    Returns the current oxidation state.
- int Protons ()

    Returns the current number of protons.
- int Neutrons ()

    Returns the current number of neutrons.
- int Electrons ()

    Returns the current number of electrons.
- int BondingElectrons ()

    Returns the number of electrons available for bonding.
- std::string AtomName ()

    Returns the name of the atom.
- std::string AtomSymbol ()

    Returns the symbol of the atom.
- std::string AtomCategory ()

    Returns the category of the atom.
- std::string AtomState ()

    Returns the state of the atom.
- int AtomicNumber ()

    Returns the atomic number of the atom.
- void DisplayInfo ()

    Displays Atom information to console.

Protected Attributes

- double atomic_weight

    Holds the atomic weight of the atom.
- int oxidation_state

    Holds the oxidation state of the atom.
- int protons

    Holds the number of protons in the atom.
- int neutrons

    Holds the number of neutrons in the atom.
- int electrons

    Holds the number of electrons in the atom.
- int valence_e

    Holds the number of valence electrons in the atom.

Private Attributes

- std::string Name

    Holds the name of the atom.
- std::string Symbol

    Holds the atomic symbol for the atom.
- std::string Category

    Holds the category of the atom (e.g., Alkali Metal)
- std::string NaturalState

    Holds the natural state of the atom (e.g., Gas)
- int atomic_number

    Holds the atomic number of the atom.

4.2.1 Detailed Description

Atom object to hold information about specific atoms in the periodic table (click Atom to go to function definitions)

C++ class object holding data and functions associated with atoms. Objects can be registered at the time of object construction, or after declaring an Atom object. Registration can be done via the atomic symbol or atomic number. Valid atoms go from Hydrogen (1) to Ununoctium (118).

4.2.2 Constructor & Destructor Documentation

4.2.2.1 Atom::Atom ( )

Default Constructor.

4.2.2.2 Atom::∼Atom ( )

Default Destructor.

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

Constructor by Atom Name.

4.2.2.4 Atom::Atom (int *number*)

Constructor by Atomic number.

4.2.3 Member Function Documentation

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

Register an atom object by symbol.

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

Register an atom object by number.

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

Manually changes the atomic weight.

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

Manually changes the oxidation state.

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

Manually changes the number of protons.

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

Manually changes the number of neutrons.

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

Manually changes the number of electrons.

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

Manually changes the number of valence electrons.

4.2.3.9 void Atom::removeProton ( )

Manually removes 1 proton and adjusts weight.

4.2.3.10 void Atom::removeNeutron ( )

Manually removes 1 neutron and adjusts weight.

4.2.3.11 void Atom::removeElectron ( )

Manually removes 1 electron from valence.

4.2.3.12 double Atom::AtomicWeight ( )

Returns the current atomic weight (g/mol)

4.2.3.13 int Atom::OxidationState ( )

Returns the current oxidation state.

4.2.3.14 int Atom::Protons ( )

Returns the current number of protons.

4.2.3.15 int Atom::Neutrons ( )

Returns the current number of neutrons.

4.2.3.16 int Atom::Electrons ( )

Returns the current number of electrons.

4.2.3.17 int Atom::BondingElectrons ( )

Returns the number of electrons available for bonding.

4.2.3.18 std::string Atom::AtomName ( )

Returns the name of the atom.

4.2.3.19 std::string Atom::AtomSymbol ( )

Returns the symbol of the atom.

4.2.3.20 std::string Atom::AtomCategory ( )

Returns the category of the atom.

4.2.3.21 std::string Atom::AtomState ( )

Returns the state of the atom.

4.2.3.22 int Atom::AtomicNumber ( )

Returns the atomic number of the atom.

4.2.3.23 void Atom::DisplayInfo ( )

Displays Atom information to console.

4.2.4 Member Data Documentation

4.2.4.1 double Atom::atomic_weight `[protected]`

Holds the atomic weight of the atom.

4.2.4.2 int Atom::oxidation_state `[protected]`

Holds the oxidation state of the atom.

4.2.4.3 int Atom::protons `[protected]`

Holds the number of protons in the atom.

4.2.4.4 int Atom::neutrons `[protected]`

Holds the number of neutrons in the atom.

4.2.4.5 int Atom::electrons `[protected]`

Holds the number of electrons in the atom.

4.2.4.6 int Atom::valence_e `[protected]`

Holds the number of valence electrons in the atom.

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

Holds the name of the atom.

4.2.4.8 std::string Atom::Symbol [private]

Holds the atomic symbol for the atom.

4.2.4.9 std::string Atom::Category [private]

Holds the category of the atom (e.g., Alkali Metal)

4.2.4.10 std::string Atom::NaturalState [private]

Holds the natural state of the atom (e.g., Gas)

4.2.4.11 int Atom::atomic_number [private]

Holds the atomic number of the atom.

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

- eel.h

4.3 BACKTRACK_DATA Struct Reference

Data structure for the implementation of Backtracking Linesearch.

`#include <lark.h>`

Public Attributes

- double alpha = 1e-4

    Scaling parameter for determination of search step size.
- double rho = 0.1

    Scaling parameter for to change step size by.
- double lambdaMin =DBL_EPSILON

    Smallest allowable step length.
- double normFkp1

    New residual norm of the Newton step.
- bool constRho = false

    True = use a constant value for rho.
- Matrix< double > Fk

    Old residual vector of the Newton step.
- Matrix< double > xk

    Old solution vector of the Newton step.

4.3.1 Detailed Description

Data structure for the implementation of Backtracking Linesearch.

C-style object used in conjunction with the Backtracking Linesearch algorithm to smooth out convergence of Netwon based iterative methods for non-linear systems of equations. The actual algorithm has been separated from the interior of the Newton method so that it can be included in any future Newton based iterative methods being developed.

4.3.2 Member Data Documentation

4.3.2.1 double BACKTRACK_DATA::alpha = 1e-4

Scaling parameter for determination of search step size.

4.3.2.2 double BACKTRACK_DATA::rho = 0.1

Scaling parameter for to change step size by.

4.3.2.3 double BACKTRACK_DATA::lambdaMin =DBL_EPSILON

Smallest allowable step length.

4.3.2.4 double BACKTRACK_DATA::normFkp1

New residual norm of the Newton step.

4.3.2.5 bool BACKTRACK_DATA::constRho = false

True = use a constant value for rho.

4.3.2.6 Matrix<double> BACKTRACK_DATA::Fk

Old residual vector of the Newton step.

4.3.2.7 Matrix<double> BACKTRACK_DATA::xk

Old solution vector of the Newton step.

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

- lark.h

4.4 BiCGSTAB_DATA Struct Reference

Data structure for the implementation of the BiCGSTAB algorithm for non-symmetric linear systems.

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

Public Attributes

- int maxit = 0

  *Maximum allowable iterations - default = min(2*vector_size,1000)*
- int iter = 0

  Actual number of iterations.
- bool breakdown

  Boolean to determine if the method broke down.
- double alpha

  Step size parameter for next solution.
- double beta

Step size parameter for search direction.
- double rho

  Scaling parameter for alpha and beta.
- double rho_old

  Previous scaling parameter for alpha and beta.
- double omega

  Scaling parameter and additional step length.
- double omega_old

  Previous scaling parameter and step length.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

  Absolution tolerance for convergence - default = 1e-6.
- double res

  Absolute residual norm.
- double relres

  Relative residual norm.
- double relres_base

  Initial residual norm.
- double bestres

  Best found residual norm.
- bool Output = true

  True = print messages to console.
- Matrix< double > x

  Current solution to the linear system.
- Matrix< double > bestx

  Best found solution to the linear system.
- Matrix< double > r

  Residual vector for the linear system.
- Matrix< double > r0

  Initial residual vector.
- Matrix< double > v

  Search direction for p.
- Matrix< double > p

  Search direction for updating.
- Matrix< double > y

  Preconditioned search direction.
- Matrix< double > s

  Residual updating vector.
- Matrix< double > z

  Preconditioned residual updating vector.
- Matrix< double > t

  Search direction for resdidual updates.

4.4.1 Detailed Description

Data structure for the implementation of the BiCGSTAB algorithm for non-symmetric linear systems.

C-style object used in conjunction with the Bi-Conjugate Gradient STABalized (BiCGSTAB) algorithm to solve a linear system of equations. This algorithm is generally more efficient than any GMRES or GCR variant, but may not always reduce the residual at each step. However, if used with preconditioning, then this algorithm is very efficient, especially when used for solving grid-based linear systems.

4.4.2 Member Data Documentation

4.4.2.1 int BiCGSTAB_DATA::maxit = 0

Maximum allowable iterations - default = min(2∗vector_size,1000)

4.4.2.2 int BiCGSTAB_DATA::iter = 0

Actual number of iterations.

4.4.2.3 bool BiCGSTAB_DATA::breakdown

Boolean to determine if the method broke down.

4.4.2.4 double BiCGSTAB_DATA::alpha

Step size parameter for next solution.

4.4.2.5 double BiCGSTAB_DATA::beta

Step size parameter for search direction.

4.4.2.6 double BiCGSTAB_DATA::rho

Scaling parameter for alpha and beta.

4.4.2.7 double BiCGSTAB_DATA::rho_old

Previous scaling parameter for alpha and beta.

4.4.2.8 double BiCGSTAB_DATA::omega

Scaling parameter and additional step length.

4.4.2.9 double BiCGSTAB_DATA::omega_old

Previous scaling parameter and step length.

4.4.2.10 double BiCGSTAB_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.4.2.11 double BiCGSTAB_DATA::tol_abs = 1e-6

Absolution tolerance for convergence - default = 1e-6.

4.4.2.12 double BiCGSTAB_DATA::res

Absolute residual norm.

4.4.2.13 double BiCGSTAB_DATA::relres

Relative residual norm.

4.4.2.14 double BiCGSTAB_DATA::relres_base

Initial residual norm.

4.4.2.15 double BiCGSTAB_DATA::bestres

Best found residual norm.

4.4.2.16 bool BiCGSTAB_DATA::Output = true

True = print messages to console.

4.4.2.17 Matrix<double> BiCGSTAB_DATA::x

Current solution to the linear system.

4.4.2.18 Matrix<double> BiCGSTAB_DATA::bestx

Best found solution to the linear system.

4.4.2.19 Matrix<double> BiCGSTAB_DATA::r

Residual vector for the linear system.

4.4.2.20 Matrix<double> BiCGSTAB_DATA::r0

Initial residual vector.

4.4.2.21 Matrix<double> BiCGSTAB_DATA::v

Search direction for p.

4.4.2.22 Matrix<double> BiCGSTAB_DATA::p

Search direction for updating.

4.4.2.23 Matrix<double> BiCGSTAB_DATA::y

Preconditioned search direction.

4.4.2.24 Matrix<double> BiCGSTAB_DATA::s

Residual updating vector.

4.4.2.25 Matrix<double> BiCGSTAB_DATA::z

Preconditioned residual updating vector.

4.4.2.26 Matrix<double> BiCGSTAB_DATA::t

Search direction for resdidual updates.

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

- lark.h

4.5 CGS_DATA Struct Reference

Data structure for the implementation of the CGS algorithm for non-symmetric linear systems.

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

Public Attributes

- int maxit = 0

  Maximum allowable iterations - default = min(2∗vector_size,1000)
- int iter = 0

  Actual number of iterations.
- bool breakdown

  Boolean to determine if the method broke down.
- double alpha

  Step size parameter for next solution.
- double beta

  Step size parameter for search direction.
- double rho

  Scaling parameter for alpha and beta.
- double sigma

  Scaling parameter and additional step length.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

  Absolution tolerance for convergence - default = 1e-6.
- double res

  Absolute residual norm.
- double relres

  Relative residual norm.
- double relres_base

  Initial residual norm.
- double bestres

  Best found residual norm.
- bool Output = true

  True = print messages to console.
- Matrix< double > x

  Current solution to the linear system.
- Matrix< double > bestx

Best found solution to the linear system.

- Matrix< double > r

  Residual vector for the linear system.
- Matrix< double > r0

  Initial residual vector.
- Matrix< double > u

  Search direction for v.
- Matrix< double > w

  Updates sigma and u.
- Matrix< double > v

  Search direction for x.
- Matrix< double > p

  Preconditioning result for w, z, and matvec for Ax.
- Matrix< double > c

  Holds the matvec result between A and p.
- Matrix< double > z

  Full search direction for x.

4.5.1 Detailed Description

Data structure for the implementation of the CGS algorithm for non-symmetric linear systems.

C-style object to be used in conjunction with the Conjugate Gradient Squared (CGS) algorithm to solve linear systems of equations. This algorithm is slightly less computational work than BiCGSTAB, but is much less stable. As a result, I do not recommend using this algorithm unless you also use some form of preconditioning.

4.5.2 Member Data Documentation

4.5.2.1 int CGS_DATA::maxit = 0

Maximum allowable iterations - default = min(2∗vector_size,1000)

4.5.2.2 int CGS_DATA::iter = 0

Actual number of iterations.

4.5.2.3 bool CGS_DATA::breakdown

Boolean to determine if the method broke down.

4.5.2.4 double CGS_DATA::alpha

Step size parameter for next solution.

4.5.2.5 double CGS_DATA::beta

Step size parameter for search direction.

4.5.2.6 double CGS_DATA::rho

Scaling parameter for alpha and beta.

4.5.2.7 double CGS_DATA::sigma

Scaling parameter and additional step length.

4.5.2.8 double CGS_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.5.2.9 double CGS_DATA::tol_abs = 1e-6

Absolution tolerance for convergence - default = 1e-6.

4.5.2.10 double CGS_DATA::res

Absolute residual norm.

4.5.2.11 double CGS_DATA::relres

Relative residual norm.

4.5.2.12 double CGS_DATA::relres_base

Initial residual norm.

4.5.2.13 double CGS_DATA::bestres

Best found residual norm.

4.5.2.14 bool CGS_DATA::Output = true

True = print messages to console.

4.5.2.15 Matrix<double> CGS_DATA::x

Current solution to the linear system.

4.5.2.16 Matrix<double> CGS_DATA::bestx

Best found solution to the linear system.

4.5.2.17 Matrix<double> CGS_DATA::r

Residual vector for the linear system.

4.5.2.18 Matrix<double> CGS_DATA::r0

Initial residual vector.

4.5.2.19 Matrix<double> CGS_DATA::u

Search direction for v.

4.5.2.20 Matrix<double> CGS_DATA::w

Updates sigma and u.

4.5.2.21 Matrix<double> CGS_DATA::v

Search direction for x.

4.5.2.22 Matrix<double> CGS_DATA::p

Preconditioning result for w, z, and matvec for Ax.

4.5.2.23 Matrix<double> CGS_DATA::c

Holds the matvec result between A and p.

4.5.2.24 Matrix<double> CGS_DATA::z

Full search direction for x.

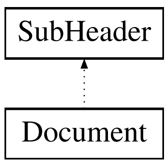
The documentation for this struct was generated from the following file:

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

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

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

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

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

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

4.6.2.7 KeyValueMap& Document::getDataMap ( )

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

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

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

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

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

4.6.2.13 void Document::clear ( )

4.6.2.14 void Document::resetKeys ( )

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

4.6.2.16 void Document::revalidateAllKeys ( )

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

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

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

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

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

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

4.6.2.23 void Document::DisplayContents ( )

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

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

4.6.2.26 int Document::size ( )

4.6.2.27 std::string Document::getName ( )

4.6.2.28 std::string Document::getAlias ( )

4.6.2.29 int Document::getState ( )

4.6.2.30 bool Document::isAlias ( )

4.6.2.31 bool Document::isAnchor ( )

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

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

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 file:

- yaml_wrapper.h

4.7 DOGFISH_DATA Struct Reference

Primary data structure for running the DOGFISH application.

`#include <dogfish.h>`

Public Attributes

- unsigned long int total_steps = 0

  Total number of solver steps taken.
- double time_old = 0.0

  Old value of time (hrs)
- double time = 0.0

  Current value of time (hrs)
- bool Print2File = true

  True = results to .txt; False = no printing.
- bool Print2Console = true

  True = results to console; False = no printing.
- bool DirichletBC = false

  False = uses film mass transfer for BC, True = Dirichlet BC.
- bool NonLinear = false

  False = Solve directly, True = Solve iteratively.
- double t_counter = 0.0

  Counter for the time output.
- double t_print

  Print output at every t_print time (hrs)
- int NumComp

  Number of species to track.

- double end_time

    Units: hours.
- double total_sorption_old

    Per mass or volume of single fiber.
- double total_sorption

    Per mass or volume of single fiber.
- double fiber_length

    Units: um.
- double fiber_diameter

    Units: um.
- FILE ∗ OutputFile

    Output file pointer to the output file for postprocesses and results.
- double(∗ eval_R)(int i, int l, const void ∗data)

    Function pointer to evaluate retardation coefficient.
- double(∗ eval_DI)(int i, int l, const void ∗data)

    Function pointer to evaluate intraparticle diffusivity.
- double(∗ eval_kf)(int i, const void ∗data)

    Function pointer to evaluate film mass transfer coefficient.
- double(∗ eval_qs)(int i, const void ∗data)

    Function pointer to evaluate fiber surface concentration.
- const void ∗ user_data

    Data structure for users info to calculate all parameters.
- std::vector< FINCH_DATA > finch_dat

    Data structure for FINCH_DATA objects.
- std::vector< DOGFISH_PARAM > param_dat

    Data structure for DOGFISH_PARAM objects.

4.7.1 Detailed Description

Primary data structure for running the DOGFISH application.

C-style object to hold information for the adsorption simulations. Contains function pointers and other data structures. This information is passed around to other functions used to simulate the fiber diffusion physics.

4.7.2 Member Data Documentation

4.7.2.1 unsigned long int DOGFISH_DATA::total_steps = 0

Total number of solver steps taken.

4.7.2.2 double DOGFISH_DATA::time_old = 0.0

Old value of time (hrs)

4.7.2.3 double DOGFISH_DATA::time = 0.0

Current value of time (hrs)

4.7.2.4 bool DOGFISH_DATA::Print2File = true

True = results to .txt; False = no printing.

4.7.2.5 bool DOGFISH_DATA::Print2Console = true

True = results to console; False = no printing.

4.7.2.6 bool DOGFISH_DATA::DirichletBC = false

False = uses film mass transfer for BC, True = Dirichlet BC.

4.7.2.7 bool DOGFISH_DATA::NonLinear = false

False = Solve directly, True = Solve iteratively.

4.7.2.8 double DOGFISH_DATA::t_counter = 0.0

Counter for the time output.

4.7.2.9 double DOGFISH_DATA::t_print

Print output at every t_print time (hrs)

4.7.2.10 int DOGFISH_DATA::NumComp

Number of species to track.

4.7.2.11 double DOGFISH_DATA::end_time

Units: hours.

4.7.2.12 double DOGFISH_DATA::total_sorption_old

Per mass or volume of single fiber.

4.7.2.13 double DOGFISH_DATA::total_sorption

Per mass or volume of single fiber.

4.7.2.14 double DOGFISH_DATA::fiber_length

Units: um.

4.7.2.15 double DOGFISH_DATA::fiber_diameter

Units: um.

4.7.2.16 FILE* DOGFISH_DATA::OutputFile

Output file pointer to the output file for postprocesses and results.

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

Function pointer to evaluate retardation coefficient.

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

Function pointer to evaluate intraparticle diffusivity.

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

Function pointer to evaluate film mass transfer coefficient.

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

Function pointer to evaluate fiber surface concentration.

4.7.2.21 const void∗ DOGFISH_DATA::user_data

Data structure for users info to calculate all parameters.

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

Data structure for FINCH_DATA objects.

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

Data structure for DOGFISH_PARAM objects.

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

- dogfish.h

4.8 DOGFISH_PARAM Struct Reference

Data structure for species-specific parameters.

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

Public Attributes

- double intraparticle_diffusion
  Units: um^2/hr.
- double film_transfer_coeff
  Units: um/hr.
- double surface_concentration
  Units: mg/g.
- double initial_sorption
  Units: mg/g.
- double sorbed_molefraction
  Molefraction of sorbed species.
- Molecule species
  Adsorbed species Molecule Object.

4.8.1 Detailed Description

Data structure for species-specific parameters.

C-style object to hold information on all adsorbing species. Parameters are given descriptive names to indicate what each is for.

4.8.2 Member Data Documentation

4.8.2.1 double DOGFISH_PARAM::intraparticle_diffusion

Units: um^2/hr.

4.8.2.2 double DOGFISH_PARAM::film_transfer_coeff

Units: um/hr.

4.8.2.3 double DOGFISH_PARAM::surface_concentration

Units: mg/g.

4.8.2.4 double DOGFISH_PARAM::initial_sorption

Units: mg/g.

4.8.2.5 double DOGFISH_PARAM::sorbed_molefraction

Molefraction of sorbed species.

4.8.2.6 Molecule DOGFISH_PARAM::species

Adsorbed species Molecule Object.

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

- dogfish.h

4.9 FINCH_DATA Struct Reference

Data structure for the FINCH object.

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

Public Attributes

- int d = 0

    Dimension of the problem: 0 = cartesian, 1 = cylindrical, 2 = spherical.
- double dt = 0.0125

    Time step.
- double dt_old = 0.0125

    Previous time step.

- double T = 1.0

  Total time.
- double dz = 0.1

  Space step.
- double L = 1.0

  Total space.
- double s = 1.0

  Char quantity (spherical = 1, cylindrical = length, cartesian = area)
- double t = 0.0

  Current Time.
- double t_old = 0.0

  Previous Time.
- double uT = 0.0

  Total amount of conserved quantity in domain.
- double uT_old = 0.0

  Old Total amount of conserved quantity.
- double uAvg = 0.0

  Average amount of conserved quantity in domain.
- double uAvg_old = 0.0

  Old Average amount of conserved quantity.
- double uIC = 0.0

  Initial condition of Conserved Quantity (if constant)
- double vIC = 1.0

  Initial condition of Velocity (if constant)
- double DIC = 1.0

  Initial condition of Dispersion (if constant)
- double kIC = 1.0

  Initial condition of Reaction (if constant)
- double RIC = 1.0

  Initial condition of the Time Coefficient (if constant)
- double uo = 1.0

  Boundary Value of Conserved Quantity.
- double vo = 1.0

  Boundary Value of Velocity.
- double Do = 1.0

  Boundary Value of Dispersion.
- double ko = 1.0

  Boundary Value of Reaction.
- double Ro = 1.0

  Boundary Value of Time Coefficient.
- double kfn = 1.0

  Film mass transfer coefficient Old.
- double kfnp1 = 1.0

  Film mass transfer coefficient New.
- double lambda_I

  Boundary Coefficient for Implicit Neumann (Calculated at Runtime)
- double lambda_E

  Boundary Coefficient for Explicit Neumann (Calculated at Runtime)
- int LN = 10

  Number of nodes.
- bool CN = true

True if Crank-Nicholson, false if Implicit, never use explicit.

- bool Update = false

  Flag to check if the system needs updating.
- bool Dirichlet = false

  Flag to indicate use of Dirichlet or Neumann starting boundary.
- bool CheckMass = false

  Flag to indicate whether or not mass is to be checked.
- bool ExplicitFlux = false

  Flag to indicate whether or not to use fully explicit flux limiters.
- bool Iterative = true

  Flag to indicate whether to solve directly, or iteratively.
- bool SteadyState = false

  Flag to determine whether or not to solve the steady-state problem.
- bool NormTrack = true

  Flag to determine whether or not to track the norms during simulation.
- double beta = 0.5

  Scheme type indicator: 0.5=CN & 1.0=Implicit; all else NULL.
- double tol_rel = 1e-6

  Relative Tolerance for Convergence.
- double tol_abs = 1e-6

  Absolute Tolerance for Convergence.
- int max_iter = 20

  Maximum number of iterations allowed.
- int total_iter = 0

  Total number of iterations made.
- int nl_method = FINCH_Picard

  Non-linear solution method - default = FINCH_Picard.
- std::vector< double > CL_I

  Left side, implicit coefficients (Calculated at Runtime)
- std::vector< double > CL_E

  Left side, explicit coefficients (Calculated at Runtime)
- std::vector< double > CC_I

  Centered, implicit coefficients (Calculated at Runtime)
- std::vector< double > CC_E

  Centered, explicit coefficients (Calculated at Runtime)
- std::vector< double > CR_I

  Right side, implicit coefficients (Calculated at Runtime)
- std::vector< double > CR_E

  Right side, explicit coefficients (Calculated at Runtime)
- std::vector< double > fL_I

  Left side, implicit fluxes (Calculated at Runtime)
- std::vector< double > fL_E

  Left side, explicit fluxes (Calculated at Runtime)
- std::vector< double > fC_I

  Centered, implicit fluxes (Calculated at Runtime)
- std::vector< double > fC_E

  Centered, explicit fluxes (Calculated at Runtime)
- std::vector< double > fR_I

  Right side, implicit fluxes (Calculated at Runtime)
- std::vector< double > fR_E

  Right side, explicit fluxes (Calculated at Runtime)

- std::vector< double > OI

  Implicit upper diagonal matrix elements (Calculated at Runtime)
- std::vector< double > OE

  Explicit upper diagonal matrix elements (Calculated at Runtime)
- std::vector< double > NI

  Implicit diagonal matrix elements (Calculated at Runtime)
- std::vector< double > NE

  Explicit diagonal matrix elements (Calculated at Runtime)
- std::vector< double > MI

  Implicit lower diagonal matrix elements (Calculated at Runtime)
- std::vector< double > ME

  Explicit lower diagonal matrix elements (Calculated at Runtime)
- std::vector< double > uz_l_I
- std::vector< double > uz_lm1_I
- std::vector< double > uz_lp1_I

  Implicit local slopes (Calculated at Runtime)
- std::vector< double > uz_l_E
- std::vector< double > uz_lm1_E
- std::vector< double > uz_lp1_E

  Explicit local slopes (Calculated at Runtime)
- Matrix< double > unm1

  Conserved Quantity Older.
- Matrix< double > un

  Conserved Quantity Old.
- Matrix< double > unp1

  Conserved Quantity New.
- Matrix< double > u_star

  Conserved Quantity Projected New.
- Matrix< double > ubest

  Best found solution if solving iteratively.
- Matrix< double > vn

  Velocity Old.
- Matrix< double > vnp1

  Velocity New.
- Matrix< double > Dn

  Dispersion Old.
- Matrix< double > Dnp1

  Dispersion New.
- Matrix< double > kn

  Reaction Old.
- Matrix< double > knp1

  Reaction New.
- Matrix< double > Sn

  Forcing Function Old.
- Matrix< double > Snp1

  Forcing Function New.
- Matrix< double > Rn

  Time Coeff Old.
- Matrix< double > Rnp1

  Time Coeff New.
- Matrix< double > Fn

Flux Limiter Old.
- Matrix< double > Fnp1

  Flux Limiter New.
- Matrix< double > gI

  Implicit Side Boundary Conditions.
- Matrix< double > gE

  Explicit Side Boundary Conditions.
- Matrix< double > res

  Current residual.
- Matrix< double > pres

  Current search direction.
- int(∗ callroutine)(const void ∗user_data)

  Function pointer to executioner (DEFAULT = default_execution)
- int(∗ setic)(const void ∗user_data)

  Function pointer to initial conditions (DEFAULT = default_ic)
- int(∗ settime)(const void ∗user_data)

  Function pointer to set time step (DEFAULT = default_timestep)
- int(∗ setpreprocess)(const void ∗user_data)

  Function pointer to preprocesses (DEFAULT = default_preprocess)
- int(∗ solve)(const void ∗user_data)

  Function pointer to the solver (DEFAULT = default_solve)
- int(∗ setparams)(const void ∗user_data)

  Function pointer to set parameters (DEFAULT = default_params)
- int(∗ discretize)(const void ∗user_data)

  Function pointer to discretization (DEFAULT = ospre_discretization)
- int(∗ setbcs)(const void ∗user_data)
- int(∗ evalres)(const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)

  Function pointer to the residual function (DEFAULT = default_res)
- int(∗ evalprecon)(const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)

  Function pointer to the preconditioning function (DEFAULT = default_precon)
- int(∗ setpostprocess)(const void ∗user_data)

  Function pointer to the postprocesses (DEFAULT = default_postprocess)
- int(∗ resettime)(const void ∗user_data)

  Function pointer to reset time (DEFAULT = default_reset)
- PICARD_DATA picard_dat

  Data structure for PICARD method (no need to use this)
- PJFNK_DATA pjfnk_dat

  Data structure for PJFNK method (more rigours method)
- const void ∗ param_data

  User's data structure used to evaluate the parameter function (Must override if setparams is overriden)

4.9.1 Detailed Description

Data structure for the FINCH object.

C-style object that holds data, functions, and other structures necessary to discretize and solve a FINCH problem. All of this information must be overriden or initialized prior to running a FINCH simulation. Many, many default functions are provided to make it easier to incorporate FINCH into other problems. The main function to override will be the setparams function. This will be a function that the user provides to tell the FINCH simulation how the parameters of the problem vary in time and space and whether or not they are coupled the the variable u. All functions are overridable and several can be skipped entirely, or called directly at different times in the execution of a particular routine. This make FINCH extremely flexible to the user.

Note

All parameters and dimensions do not carry any units with them. The user is required to keep track of all their own units in their particular problem and ensure that units will cancel and be consistent in their own physical model.

4.9.2 Member Data Documentation

4.9.2.1 int FINCH_DATA::d = 0

Dimension of the problem: 0 = cartesian, 1 = cylindrical, 2 = spherical.

4.9.2.2 double FINCH_DATA::dt = 0.0125

Time step.

4.9.2.3 double FINCH_DATA::dt_old = 0.0125

Previous time step.

4.9.2.4 double FINCH_DATA::T = 1.0

Total time.

4.9.2.5 double FINCH_DATA::dz = 0.1

Space step.

4.9.2.6 double FINCH_DATA::L = 1.0

Total space.

4.9.2.7 double FINCH_DATA::s = 1.0

Char quantity (spherical = 1, cylindrical = length, cartesian = area)

4.9.2.8 double FINCH_DATA::t = 0.0

Current Time.

4.9.2.9 double FINCH_DATA::t_old = 0.0

Previous Time.

4.9.2.10 double FINCH_DATA::uT = 0.0

Total amount of conserved quantity in domain.

4.9.2.11 double FINCH_DATA::uT_old = 0.0

Old Total amount of conserved quantity.

4.9.2.12 double FINCH_DATA::uAvg = 0.0

Average amount of conserved quantity in domain.

4.9.2.13 double FINCH_DATA::uAvg_old = 0.0

Old Average amount of conserved quantity.

4.9.2.14 double FINCH_DATA::uIC = 0.0

Initial condition of Conserved Quantity (if constant)

4.9.2.15 double FINCH_DATA::vIC = 1.0

Initial condition of Velocity (if constant)

4.9.2.16 double FINCH_DATA::DIC = 1.0

Initial condition of Dispersion (if constant)

4.9.2.17 double FINCH_DATA::kIC = 1.0

Initial condition of Reaction (if constant)

4.9.2.18 double FINCH_DATA::RIC = 1.0

Initial condition of the Time Coefficient (if constant)

4.9.2.19 double FINCH_DATA::uo = 1.0

Boundary Value of Conserved Quantity.

4.9.2.20 double FINCH_DATA::vo = 1.0

Boundary Value of Velocity.

4.9.2.21 double FINCH_DATA::Do = 1.0

Boundary Value of Dispersion.

4.9.2.22 double FINCH_DATA::ko = 1.0

Boundary Value of Reaction.

4.9.2.23 double FINCH_DATA::Ro = 1.0

Boundary Value of Time Coefficient.

4.9.2.24 double FINCH_DATA::kfn = 1.0

Film mass transfer coefficient Old.

4.9.2.25 double FINCH_DATA::kfnp1 = 1.0

Film mass transfer coefficient New.

4.9.2.26 double FINCH_DATA::lambda_I

Boundary Coefficient for Implicit Neumann (Calculated at Runtime)

4.9.2.27 double FINCH_DATA::lambda_E

Boundary Coefficient for Explicit Neumann (Calculated at Runtime)

4.9.2.28 int FINCH_DATA::LN = 10

Number of nodes.

4.9.2.29 bool FINCH_DATA::CN = true

True if Crank-Nicholson, false if Implicit, never use explicit.

4.9.2.30 bool FINCH_DATA::Update = false

Flag to check if the system needs updating.

4.9.2.31 bool FINCH_DATA::Dirichlet = false

Flag to indicate use of Dirichlet or Neumann starting boundary.

4.9.2.32 bool FINCH_DATA::CheckMass = false

Flag to indicate whether or not mass is to be checked.

4.9.2.33 bool FINCH_DATA::ExplicitFlux = false

Flag to indicate whether or not to use fully explicit flux limiters.

4.9.2.34 bool FINCH_DATA::Iterative = true

Flag to indicate whether to solve directly, or iteratively.

4.9.2.35 bool FINCH_DATA::SteadyState = false

Flag to determine whether or not to solve the steady-state problem.

4.9.2.36 bool FINCH_DATA::NormTrack = true

Flag to determine whether or not to track the norms during simulation.

4.9.2.37 double FINCH_DATA::beta = 0.5

Scheme type indicator: 0.5=CN & 1.0=Implicit; all else NULL.

4.9.2.38 double FINCH_DATA::tol_rel = 1e-6

Relative Tolerance for Convergence.

4.9.2.39 double FINCH_DATA::tol_abs = 1e-6

Absolute Tolerance for Convergence.

4.9.2.40 int FINCH_DATA::max_iter = 20

Maximum number of iterations allowed.

4.9.2.41 int FINCH_DATA::total_iter = 0

Total number of iterations made.

4.9.2.42 int FINCH_DATA::nl_method = FINCH_Picard

Non-linear solution method - default = FINCH_Picard.

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

Left side, implicit coefficients (Calculated at Runtime)

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

Left side, explicit coefficients (Calculated at Runtime)

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

Centered, implicit coefficients (Calculated at Runtime)

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

Centered, explicit coefficients (Calculated at Runtime)

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

Right side, implicit coefficients (Calculated at Runtime)

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

Right side, explicit coefficients (Calculated at Runtime)

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

Left side, implicit fluxes (Calculated at Runtime)

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

Left side, explicit fluxes (Calculated at Runtime)

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

Centered, implicit fluxes (Calculated at Runtime)

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

Centered, explicit fluxes (Calculated at Runtime)

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

Right side, implicit fluxes (Calculated at Runtime)

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

Right side, explicit fluxes (Calculated at Runtime)

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

Implicit upper diagonal matrix elements (Calculated at Runtime)

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

Explicit upper diagonal matrix elements (Calculated at Runtime)

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

Implicit diagonal matrix elements (Calculated at Runtime)

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

Explicit diagonal matrix elements (Calculated at Runtime)

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

Implicit lower diagonal matrix elements (Calculated at Runtime)

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

Explicit lower diagonal matrix elements (Calculated at Runtime)

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

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

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

Implicit local slopes (Calculated at Runtime)

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

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

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

Explicit local slopes (Calculated at Runtime)

4.9.2.67 Matrix<double> FINCH_DATA::unm1

Conserved Quantity Older.

4.9.2.68 Matrix<double> FINCH_DATA::un

Conserved Quantity Old.

4.9.2.69 Matrix<double> FINCH_DATA::unp1

Conserved Quantity New.

4.9.2.70 Matrix<double> FINCH_DATA::u_star

Conserved Quantity Projected New.

4.9.2.71 Matrix<double> FINCH_DATA::ubest

Best found solution if solving iteratively.

4.9.2.72 Matrix<double> FINCH_DATA::vn

Velocity Old.

4.9.2.73 Matrix<double> FINCH_DATA::vnp1

Velocity New.

4.9.2.74 Matrix<double> FINCH_DATA::Dn

Dispersion Old.

4.9.2.75 Matrix<double> FINCH_DATA::Dnp1

Dispersion New.

4.9.2.76 Matrix<double> FINCH_DATA::kn

Reaction Old.

4.9.2.77 Matrix<double> FINCH_DATA::knp1

Reaction New.

4.9.2.78 Matrix<double> FINCH_DATA::Sn

Forcing Function Old.

4.9.2.79 Matrix<double> FINCH_DATA::Snp1

Forcing Function New.

4.9.2.80 Matrix<double> FINCH_DATA::Rn

Time Coeff Old.

4.9.2.81 Matrix<double> FINCH_DATA::Rnp1

Time Coeff New.

4.9.2.82 Matrix<double> FINCH_DATA::Fn

Flux Limiter Old.

4.9.2.83 Matrix<double> FINCH_DATA::Fnp1

Flux Limiter New.

4.9.2.84 Matrix<double> FINCH_DATA::gI

Implicit Side Boundary Conditions.

4.9.2.85 Matrix<double> FINCH_DATA::gE

Explicit Side Boundary Conditions.

4.9.2.86 Matrix<double> FINCH_DATA::res

Current residual.

4.9.2.87 Matrix<double> FINCH_DATA::pres

Current search direction.

4.9.2.88 int(* FINCH_DATA::callroutine)(const void *user_data)

Function pointer to executioner (DEFAULT = default_execution)

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

Function pointer to initial conditions (DEFAULT = default_ic)

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

Function pointer to set time step (DEFAULT = default_timestep)

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

Function pointer to preprocesses (DEFAULT = default_preprocess)

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

Function pointer to the solver (DEFAULT = default_solve)

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

Function pointer to set parameters (DEFAULT = default_params)

4.9.2.94 int(* FINCH_DATA::discretize)(const void *user_data)

Function pointer to discretization (DEFAULT = ospre_discretization)

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

Function pointer to set boundary conditions (DEFAULT = default_bcs)

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

Function pointer to the residual function (DEFAULT = default_res)

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

Function pointer to the preconditioning function (DEFAULT = default_precon)

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

Function pointer to the postprocesses (DEFAULT = default_postprocess)

4.9.2.99 int(∗ FINCH_DATA::resettime)(const void ∗user_data)

Function pointer to reset time (DEFAULT = default_reset)

4.9.2.100 PICARD_DATA FINCH_DATA::picard_dat

Data structure for PICARD method (no need to use this)

4.9.2.101 PJFNK_DATA FINCH_DATA::pjfnk_dat

Data structure for PJFNK method (more rigours method)

4.9.2.102 const void∗ FINCH_DATA::param_data

User's data structure used to evaluate the parameter function (Must override if setparams is overriden)

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

- finch.h

4.10 GCR_DATA Struct Reference

Data structure for the implementation of the GCR algorithm for non-symmetric linear systems.

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

Public Attributes

- int restart = -1

  Restart parameter for outer iterations - default = 20.
- int maxit = 0

  Maximum allowable outer iterations.
- int iter_outer = 0

  Number of outer iterations taken.
- int iter_inner = 0

  Number of inner iterations taken.
- int total_iter = 0

  Total number of iterations taken.
- bool breakdown = false

  Boolean to determine if a step has failed.
- double alpha

  Inner iteration step size.
- double beta

  Outer iteration step size.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

  Absolute tolerance for convergence - default = 1e-6.
- double res

  Absolute residual norm for linear system.
- double relres

Relative residual norm for linear system.
- double relres_base

  Initial residual norm of the linear system.
- double bestres

  Best found residual norm of the linear system.
- bool Output = true

  True = print messages to the console.
- Matrix< double > x

  Current solution to the linear system.
- Matrix< double > bestx

  Best found solution to the linear system.
- Matrix< double > r

  Residual Vector.
- Matrix< double > c_temp

  Temporary c vector to be updated.
- Matrix< double > u_temp

  Temporary u vector to be updated.
- std::vector< Matrix< double > > u

  Vector span for updating x.
- std::vector< Matrix< double > > c

  Vector span for updating r.
- OPTRANS_DATA transpose_dat

  Data structure for Operator Transposition.

4.10.1 Detailed Description

Data structure for the implementation of the GCR algorithm for non-symmetric linear systems.

C-style object used in conjunction with the Generalized Conjugate Residual (GCR) algorithm for solving a non-symmetric linear system of equations. When the linear system in question has a positive-definite-symmetric component to it, then this algorithm is equivalent to GMRESRP. However, it is generally less efficient than GMRESRP and can suffer breakdowns.

4.10.2 Member Data Documentation

4.10.2.1 int GCR_DATA::restart = -1

Restart parameter for outer iterations - default = 20.

4.10.2.2 int GCR_DATA::maxit = 0

Maximum allowable outer iterations.

4.10.2.3 int GCR_DATA::iter_outer = 0

Number of outer iterations taken.

4.10.2.4 int GCR_DATA::iter_inner = 0

Number of inner iterations taken.

4.10.2.5 int GCR_DATA::total_iter = 0

Total number of iterations taken.

4.10.2.6 bool GCR_DATA::breakdown = false

Boolean to determine if a step has failed.

4.10.2.7 double GCR_DATA::alpha

Inner iteration step size.

4.10.2.8 double GCR_DATA::beta

Outer iteration step size.

4.10.2.9 double GCR_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.10.2.10 double GCR_DATA::tol_abs = 1e-6

Absolute tolerance for convergence - default = 1e-6.

4.10.2.11 double GCR_DATA::res

Absolute residual norm for linear system.

4.10.2.12 double GCR_DATA::relres

Relative residual norm for linear system.

4.10.2.13 double GCR_DATA::relres_base

Initial residual norm of the linear system.

4.10.2.14 double GCR_DATA::bestres

Best found residual norm of the linear system.

4.10.2.15 bool GCR_DATA::Output = true

True = print messages to the console.

4.10.2.16 Matrix<double> GCR_DATA::x

Current solution to the linear system.

4.10.2.17 Matrix<double> GCR_DATA::bestx

Best found solution to the linear system.

4.10.2.18 Matrix<double> GCR_DATA::r

Residual Vector.

4.10.2.19 Matrix<double> GCR_DATA::c_temp

Temporary c vector to be updated.

4.10.2.20 Matrix<double> GCR_DATA::u_temp

Temporary u vector to be updated.

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

Vector span for updating x.

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

Vector span for updating r.

4.10.2.23 OPTRANS_DATA GCR_DATA::transpose_dat

Data structure for Operator Transposition.

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

- lark.h

4.11 GMRESLP_DATA Struct Reference

Data structure for implementation of the Restarted GMRES algorithm with Left Preconditioning.

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

Public Attributes

- int restart = -1

  Restart parameter - default = min(vector_size,20)
- int maxit = 0

  Maximum allowable iterations - default = min(vector_size,1000)
- int iter = 0

  Number of iterations needed for convergence.
- int steps = 0

  Total number of gmres iterations and krylov iterations.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.

- double tol_abs = 1e-6

  Absolution tolerance for convergence - default = 1e-6.
- double res

  Absolution redisual norm of the linear system.
- double relres

  Relative residual norm of the linear system.
- double relres_base

  Initial residual norm of the linear system.
- double bestres

  Best found residual norm of the linear system.
- bool Output = true

  True = print messages to console.
- Matrix< double > x

  Current solution to the linear system.
- Matrix< double > bestx

  Best found solution to the linear system.
- Matrix< double > r

  Residual vector for the linear system.
- ARNOLDI_DATA arnoldi_dat

  Data structure for the kyrlov subspace.

4.11.1 Detailed Description

Data structure for implementation of the Restarted GMRES algorithm with Left Preconditioning.

C-style object used in conjunction with Generalized Minimum RESidual Left-Precondtioned (GMRESLP) and Full Orthogonalization Method (FOM) algorithms to iteratively or directly solve a linear system of equations. When using with GMRESLP, you can only check/observe the linear residuals before a restart or after the Arnoldi space is constructed. This is because this object uses Left-side Preconditioning. A faster routine may be GMRESRP, which is able to construct residuals after each Arnoldi iteration.

4.11.2 Member Data Documentation

4.11.2.1 int GMRESLP_DATA::restart = -1

Restart parameter - default = min(vector_size,20)

4.11.2.2 int GMRESLP_DATA::maxit = 0

Maximum allowable iterations - default = min(vector_size,1000)

4.11.2.3 int GMRESLP_DATA::iter = 0

Number of iterations needed for convergence.

4.11.2.4 int GMRESLP_DATA::steps = 0

Total number of gmres iterations and krylov iterations.

4.11.2.5 double GMRESLP_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.11.2.6 double GMRESLP_DATA::tol_abs = 1e-6

Absolution tolerance for convergence - default = 1e-6.

4.11.2.7 double GMRESLP_DATA::res

Absolution redisual norm of the linear system.

4.11.2.8 double GMRESLP_DATA::relres

Relative residual norm of the linear system.

4.11.2.9 double GMRESLP_DATA::relres_base

Initial residual norm of the linear system.

4.11.2.10 double GMRESLP_DATA::bestres

Best found residual norm of the linear system.

4.11.2.11 bool GMRESLP_DATA::Output = true

True = print messages to console.

4.11.2.12 Matrix<double> GMRESLP_DATA::x

Current solution to the linear system.

4.11.2.13 Matrix<double> GMRESLP_DATA::bestx

Best found solution to the linear system.

4.11.2.14 Matrix<double> GMRESLP_DATA::r

Residual vector for the linear system.

4.11.2.15 ARNOLDI_DATA GMRESLP_DATA::arnoldi_dat

Data structure for the kyrlov subspace.

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

- lark.h

4.12 GMRESR_DATA Struct Reference

Data structure for the implementation of GCR with Nested GMRES preconditioning (i.e., GMRESR)

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

Public Attributes

- int gcr_restart = -1

  Number of GCR restarts (default = 20, max = N)
- int gcr_maxit = 0

  Number of GCR iterations.
- int gmres_restart = -1

  Number of GMRES restarts (max = 20)
- int gmres_maxit = 1

  Number of GMRES iterations (max = 5, default = 1)
- int N

  Dimension of the linear system.
- int total_iter

  Total GMRES and GCR iterations.
- int iter_outer

  Total GCR iterations.
- int iter_inner

  Total GMRES iterations.
- bool GCR_Output = true

  True = print GCR messages.
- bool GMRES_Output = false

  True = print GMRES messages.
- double gmres_tol = 0.1

  Tolerance relative to GCR iterations.
- double gcr_rel_tol = 1e-6

  Relative outer residual tolerance.
- double gcr_abs_tol = 1e-6

  Absolute outer residual tolerance.
- Matrix< double > arg

  Argument matrix passed between preconditioner and iterator.
- GCR_DATA gcr_dat

  Data structure for the outer GCR steps.
- GMRESRP_DATA gmres_dat

  Data structure for the inner GMRES steps.
- int(∗ matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)

  User supplied matrix-vector product function.
- int(∗ terminal_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)

  Optional user supplied terminal preconditioner.
- const void ∗ matvec_data

  Data structure for the user's matvec function.
- const void ∗ term_precon

  Data structure for the user's terminal preconditioner.

4.12.1 Detailed Description

Data structure for the implementation of GCR with Nested GMRES preconditioning (i.e., GMRESR)

C-style object to be used in conjunction with the Generalized Minimum RESidual Recurive (GMRESR) algorithm. Although the name suggests that this method used GMRES recursively, what it is actually doing is nesting GMRESRP iterations inside the GCR method to form a preconditioner for GCR. The name GMRESR came from literature (Vorst and Vuik, "GMRESR: A family of nested GMRES methods", 1991).

4.12.2 Member Data Documentation

4.12.2.1 int GMRESR_DATA::gcr_restart = -1

Number of GCR restarts (default = 20, max = N)

4.12.2.2 int GMRESR_DATA::gcr_maxit = 0

Number of GCR iterations.

4.12.2.3 int GMRESR_DATA::gmres_restart = -1

Number of GMRES restarts (max = 20)

4.12.2.4 int GMRESR_DATA::gmres_maxit = 1

Number of GMRES iterations (max = 5, default = 1)

4.12.2.5 int GMRESR_DATA::N

Dimension of the linear system.

4.12.2.6 int GMRESR_DATA::total_iter

Total GMRES and GCR iterations.

4.12.2.7 int GMRESR_DATA::iter_outer

Total GCR iterations.

4.12.2.8 int GMRESR_DATA::iter_inner

Total GMRES iterations.

4.12.2.9 bool GMRESR_DATA::GCR_Output = true

True = print GCR messages.

4.12.2.10 bool GMRESR_DATA::GMRES_Output = false

True = print GMRES messages.

4.12.2.11 double GMRESR_DATA::gmres_tol = 0.1

Tolerance relative to GCR iterations.

4.12.2.12 double GMRESR_DATA::gcr_rel_tol = 1e-6

Relative outer residual tolerance.

4.12.2.13 double GMRESR_DATA::gcr_abs_tol = 1e-6

Absolute outer residual tolerance.

4.12.2.14 Matrix<double> GMRESR_DATA::arg

Argument matrix passed between preconditioner and iterator.

4.12.2.15 GCR_DATA GMRESR_DATA::gcr_dat

Data structure for the outer GCR steps.

4.12.2.16 GMRESRP_DATA GMRESR_DATA::gmres_dat

Data structure for the inner GMRES steps.

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

User supplied matrix-vector product function.

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

Optional user supplied terminal preconditioner.

4.12.2.19 const void∗ GMRESR_DATA::matvec_data

Data structure for the user's matvec function.

4.12.2.20 const void∗ GMRESR_DATA::term_precon

Data structure for the user's terminal preconditioner.

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

- lark.h

4.13 GMRESRP_DATA Struct Reference

Data structure for the Restarted GMRES algorithm with Right Preconditioning.

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

Public Attributes

- int restart = -1

    Restart parameter - default = min(20,vector_size)
- int maxit = 0

    Maximum allowable outer iterations.
- int iter_outer = 0

Total number of outer iterations.

- int iter_inner = 0

  Total number of inner iterations.
- int iter_total = 0

  Total number of overall iterations.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

  Absolute tolerance for convergence - default = 1e-6.
- double res

  Absolute residual norm for linear system.
- double relres

  Relative residual norm for linear system.
- double relres_base

  Initial residual norm of the linear system.
- double bestres

  Best found residual norm of the linear system.
- bool Output = true

  True = print messages to console.
- Matrix< double > x

  Current solution to the linear system.
- Matrix< double > bestx

  Best found solution to the linear system.
- Matrix< double > r

  Residual vector for the linear system.
- std::vector< Matrix< double > > Vk

  (N x k) orthonormal vector basis
- std::vector< Matrix< double > > Zk

  (N x k) preconditioned vector set
- std::vector< std::vector
  < double > > H

  (k+1 x k) upper Hessenberg storage matrix
- std::vector< std::vector
  < double > > H_bar

  (k+1 x k) Factorized matrix
- std::vector< double > y

  (k x 1) Vector search direction
- std::vector< double > e0

  (k+1 x 1) Normalized vector with residual info
- std::vector< double > e0_bar

  (k+1 x 1) Factorized normal vector
- Matrix< double > w

  (N) x (1) interim result of the matrix_vector multiplication
- Matrix< double > v

  (N) x (1) holding cell for the column entries of Vk and other interims
- Matrix< double > sum

  (N) x (1) running sum of subspace vectors for use in altering w

4.13.1 Detailed Description

Data structure for the Restarted GMRES algorithm with Right Preconditioning.

C-style object used in conjunction with Generalized Minimum RESidual Right Preconditioned (GMRESRP) algorithm to iteratively solve a linear system of equations. Unlike GMRESLP, the GMRESRP method is capable of checking linear residuals at both the inner and outer steps. As a result, this algorithm may terminate earlier than GMRESLP if it has found a suitable solution during one of the inner steps.

4.13.2 Member Data Documentation

4.13.2.1 int GMRESRP_DATA::restart = -1

Restart parameter - default = min(20,vector_size)

4.13.2.2 int GMRESRP_DATA::maxit = 0

Maximum allowable outer iterations.

4.13.2.3 int GMRESRP_DATA::iter_outer = 0

Total number of outer iterations.

4.13.2.4 int GMRESRP_DATA::iter_inner = 0

Total number of inner iterations.

4.13.2.5 int GMRESRP_DATA::iter_total = 0

Total number of overall iterations.

4.13.2.6 double GMRESRP_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.13.2.7 double GMRESRP_DATA::tol_abs = 1e-6

Absolute tolerance for convergence - default = 1e-6.

4.13.2.8 double GMRESRP_DATA::res

Absolute residual norm for linear system.

4.13.2.9 double GMRESRP_DATA::relres

Relative residual norm for linear system.

4.13.2.10 double GMRESRP_DATA::relres_base

Initial residual norm of the linear system.

4.13.2.11 double GMRESRP_DATA::bestres

Best found residual norm of the linear system.

4.13.2.12 bool GMRESRP_DATA::Output = true

True = print messages to console.

4.13.2.13 Matrix<double> GMRESRP_DATA::x

Current solution to the linear system.

4.13.2.14 Matrix<double> GMRESRP_DATA::bestx

Best found solution to the linear system.

4.13.2.15 Matrix<double> GMRESRP_DATA::r

Residual vector for the linear system.

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

(N x k) orthonormal vector basis

4.13.2.17 std::vector< Matrix<double> > GMRESRP_DATA::Zk

(N x k) preconditioned vector set

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

(k+1 x k) upper Hessenberg storage matrix

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

(k+1 x k) Factorized matrix

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

(k x 1) Vector search direction

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

(k+1 x 1) Normalized vector with residual info

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

(k+1 x 1) Factorized normal vector

4.13.2.23 Matrix<double> GMRESRP_DATA::w

(N) x (1) interim result of the matrix_vector multiplication

4.13.2.24 Matrix<double> GMRESRP_DATA::v

(N) x (1) holding cell for the column entries of Vk and other interims

4.13.2.25 Matrix<double> GMRESRP_DATA::sum

(N) x (1) running sum of subspace vectors for use in altering w

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

- lark.h

4.14 GPAST_DATA Struct Reference

GPAST Data Structure.

`#include <magpie.h>`

Public Attributes

- double x

  Adsorbed mole fraction.
- double y

  Gas phase mole fraction.
- double He

  Henry's Coefficient (mol/kg/kPa)
- double q

  Amount adsorbed for each component (mol/kg)
- std::vector< double > gama_inf

  Infinite dilution activities.
- double qo

  Pure component capacities (mol/kg)
- double PIo

  Pure component spreading pressures (mol/kg)
- std::vector< double > po

  Pure component reference state pressures (kPa)
- double poi

  Reference state pressures solved for using Recover eval GPAST.
- bool present

  If true, then the component is present; if false, then the component is not present.

4.14.1 Detailed Description

GPAST Data Structure.

C-style object holding all parameter information associated with the Generalized Predictive Adsorbed Solution Theory (GPAST) system of equations. Each species in the gas phase will have one of these objects.

4.14.2 Member Data Documentation

4.14.2.1 double GPAST_DATA::x

Adsorbed mole fraction.

4.14.2.2 double GPAST_DATA::y

Gas phase mole fraction.

4.14.2.3 double GPAST_DATA::He

Henry's Coefficient (mol/kg/kPa)

4.14.2.4 double GPAST_DATA::q

Amount adsorbed for each component (mol/kg)

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

Infinite dilution activities.

4.14.2.6 double GPAST_DATA::qo

Pure component capacities (mol/kg)

4.14.2.7 double GPAST_DATA::PIo

Pure component spreading pressures (mol/kg)

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

Pure component reference state pressures (kPa)

4.14.2.9 double GPAST_DATA::poi

Reference state pressures solved for using Recover eval GPAST.

4.14.2.10 bool GPAST_DATA::present

If true, then the component is present; if false, then the component is not present.

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

- magpie.h

4.15 GSTA_DATA Struct Reference

GSTA Data Structure.

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

Public Attributes

- double qmax
  Theoretical maximum capacity of adsorbate-adsorbent pair (mol/kg)
- int m
  Number of parameters in the GSTA isotherm.
- std::vector< double > dHo
  Enthalpies for each site (J/mol)
- std::vector< double > dSo
  Entropies for each site (J/(K∗mol))

4.15.1 Detailed Description

GSTA Data Structure.

C-style object holding all parameter information associated with the Generalized Statistical Thermodynamic Adsorption (GSTA) isotherm model. Each species in the gas phase will have one of these objects.

4.15.2 Member Data Documentation

4.15.2.1 double GSTA_DATA::qmax

Theoretical maximum capacity of adsorbate-adsorbent pair (mol/kg)

4.15.2.2 int GSTA_DATA::m

Number of parameters in the GSTA isotherm.

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

Enthalpies for each site (J/mol)

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

Entropies for each site (J/(K∗mol))

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

- magpie.h

4.16 GSTA_OPT_DATA Struct Reference

Data structure used in the GSTA optimization routines.

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

Public Attributes

- int total_eval
  Keeps track of the total number of function evaluations.
- int n_par

Number of parameters being optimized for.

- double qmax

  Maximum theoretical adsorption capacity (M/M) (0 if unknown)
- int iso

  Keeps isotherm that is currently being optimized.
- std::vector< std::vector
  < double > > Fobj

  Creates a dynamic array to store all Fobj values.
- std::vector< std::vector
  < double > > q
- std::vector< std::vector
  < double > > P

  Creates a dynamic array for q and P data pairs.
- std::vector< std::vector
  < double > > best_par

  Used to store the values of the parameters of best fit.
- std::vector< std::vector
  < double > > Kno

  Dimensionless parameters determined from best_par.
- std::vector< std::vector
  < std::vector< double > > > all_pars

  Used to create a ragged array of all parameters.
- std::vector< std::vector
  < double > > norms

  Used to store the values of all the calculated norms.
- std::vector< double > opt_qmax

  If qmax is unknown, this vector holds it's optimized values.

4.16.1 Detailed Description

Data structure used in the GSTA optimization routines.

C-style structure that keeps track of all infomation during the optimization routine. All solutions and parameters to the GSTA isotherm are held in order to find the best solution with the fewest parameters.

4.16.2 Member Data Documentation

4.16.2.1 int GSTA_OPT_DATA::total_eval

Keeps track of the total number of function evaluations.

4.16.2.2 int GSTA_OPT_DATA::n_par

Number of parameters being optimized for.

4.16.2.3 double GSTA_OPT_DATA::qmax

Maximum theoretical adsorption capacity (M/M) (0 if unknown)

4.16.2.4 int GSTA_OPT_DATA::iso

Keeps isotherm that is currently being optimized.

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

Creates a dynamic array to store all Fobj values.

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

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

Creates a dynamic array for q and P data pairs.

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

Used to store the values of the parameters of best fit.

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

Dimensionless parameters determined from best_par.

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

Used to create a ragged array of all parameters.

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

Used to store the values of all the calculated norms.

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

If qmax is unknown, this vector holds it's optimized values.

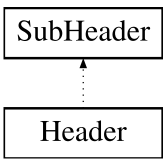
The documentation for this struct was generated from the following file:

- gsta_opt.h

4.17 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

4.17.1 Constructor & Destructor Documentation

4.17.1.1 Header::Header ( )

4.17.1.2 Header::~Header ( )

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

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

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

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

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

4.17.2 Member Function Documentation

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

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

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

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

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

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

4.17.2.7 KeyValueMap& Header::getDataMap ( )

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

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

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

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

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

4.17.2.13 void Header::clear ( )

4.17.2.14 void Header::resetKeys ( )

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

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

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

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

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

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

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

4.17.2.22 void Header::DisplayContents ( )

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

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

4.17.2.25 int Header::size ( )

4.17.2.26 std::string Header::getName ( )

4.17.2.27 std::string Header::getAlias ( )

4.17.2.28 int Header::getState ( )

4.17.2.29 bool Header::isAlias ( )

4.17.2.30 bool Header::isAnchor ( )

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

4.17.3 Member Data Documentation

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

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

- yaml_wrapper.h

4.18 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

4.18.1 Constructor & Destructor Documentation

4.18.1.1 KeyValueMap::KeyValueMap ( )

4.18.1.2 KeyValueMap::~KeyValueMap ( )

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

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

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

4.18.2 Member Function Documentation

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

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

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

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

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

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

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

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

4.18.2.9 void KeyValueMap::clear ( )

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

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

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

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

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

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

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

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

4.18.2.18 void KeyValueMap::findAllTypes ( )

4.18.2.19 void KeyValueMap::DisplayMap ( )

4.18.2.20 int KeyValueMap::size ( )

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

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

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

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

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

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

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

4.18.3 Member Data Documentation

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

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

- yaml_wrapper.h

4.19 KMS_DATA Struct Reference

Data structure for the implemenation of the Krylov Multi-Space (KMS) Method.

`#include <lark.h>`

Public Attributes

- int level = 0

  Current level in the recursion.
- int max_level = 0

Maximum allowable recursion levels (Default = 0 -> GMRES, Max = 5)
- int restart = -1

  Restart parameter for the outer iterates (Default = 20, Max = N)
- int maxit = 0

  Maximum allowable iterations for the outer steps.
- int inner_iter = 0

  Number of inner steps taken.
- int outer_iter = 0

  Number of outer steps taken.
- int total_iter = 0

  Total number of iterations in all steps.
- double outer_reltol = 1e-6

  Relative residual tolerance for outer steps (Default = 1e-6)
- double outer_abstol = 1e-6

  Absolute residual tolerance for outer steps (Default = 1e-6)
- double inner_reltol = 0.1

  Residual tolerance for inner steps made relative to outer steps (Default = 0.1)
- bool Output_out = true

  True = Print the outer steps residuals.
- bool Output_in = false

  True = Print the inner steps residuals.
- GMRESRP_DATA gmres_out

  Data structure for the outer steps.
- std::vector< GMRESRP_DATA > gmres_in

  Data structures for each recursion level.
- int(∗ matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void ∗matvec_data)

  User supplied matrix-vector product function.
- int(∗ terminal_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗precon_data)

  Optional user supplied terminal preconditioner.
- const void ∗ matvec_data

  Data structure for the user's matvec function.
- const void ∗ term_precon

  Data structure for the user's terminal preconditioner.

4.19.1 Detailed Description

Data structure for the implemenation of the Krylov Multi-Space (KMS) Method.

C-style object to be used in conjunction with the Krylov Multi-Space (KMS) Algorithm to iteratively solve non-symmetric, indefinite linear systems. This method was inspired by the Flexible GMRES (FGMRES) and Recursive GMRES (GMRESR) methods proposed by Saad (1993) and Vorst and Vuik (1991), respectively. The idea behind this method is to recursively call FGMRES to solve a linear system with pregressively smaller Krylov Subspaces built by a Right-Preconditioned GMRES algorithm. Thus creating a "V-cycle" of iteration similar to that seen in Multi-Grid algorithms.

4.19.2 Member Data Documentation

4.19.2.1 int KMS_DATA::level = 0

Current level in the recursion.

4.19.2.2 int KMS_DATA::max_level = 0

Maximum allowable recursion levels (Default = 0 -> GMRES, Max = 5)

4.19.2.3 int KMS_DATA::restart = -1

Restart parameter for the outer iterates (Default = 20, Max = N)

4.19.2.4 int KMS_DATA::maxit = 0

Maximum allowable iterations for the outer steps.

4.19.2.5 int KMS_DATA::inner_iter = 0

Number of inner steps taken.

4.19.2.6 int KMS_DATA::outer_iter = 0

Number of outer steps taken.

4.19.2.7 int KMS_DATA::total_iter = 0

Total number of iterations in all steps.

4.19.2.8 double KMS_DATA::outer_reltol = 1e-6

Relative residual tolerance for outer steps (Default = 1e-6)

4.19.2.9 double KMS_DATA::outer_abstol = 1e-6

Absolute residual tolerance for outer steps (Default = 1e-6)

4.19.2.10 double KMS_DATA::inner_reltol = 0.1

Residual tolerance for inner steps made relative to outer steps (Default = 0.1)

4.19.2.11 bool KMS_DATA::Output_out = true

True = Print the outer steps residuals.

4.19.2.12 bool KMS_DATA::Output_in = false

True = Print the inner steps residuals.

4.19.2.13 GMRESRP_DATA KMS_DATA::gmres_out

Data structure for the outer steps.

4.19.2.14 std::vector< GMRESRP_DATA > KMS_DATA::gmres_in

Data structures for each recursion level.

4.19.2.15 int(* KMS_DATA::matvec)(const Matrix< double > &x, Matrix< double > &Ax, const void *matvec_data)

User supplied matrix-vector product function.

4.19.2.16 int(* KMS_DATA::terminal_precon)(const Matrix< double > &r, Matrix< double > &p, const void *precon_data)

Optional user supplied terminal preconditioner.

4.19.2.17 const void* KMS_DATA::matvec_data

Data structure for the user's matvec function.

4.19.2.18 const void* KMS_DATA::term_precon

Data structure for the user's terminal preconditioner.

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

- lark.h

4.20 MAGPIE_DATA Struct Reference

MAGPIE Data Structure.

```
#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

4.20.1 Detailed Description

MAGPIE Data Structure.

C-style object holding all information necessary to run a MAGPIE simulation. This is the data structure that will be used in other sub-routines when a mixed gas adsorption simulation needs to be run.

4.20.2 Member Data Documentation

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

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

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

4.20.2.4 SYSTEM_DATA MAGPIE_DATA::sys_dat

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

- magpie.h

4.21 MassBalance Class Reference

Mass Balance Object.

`#include <shark.h>`

Public Member Functions

- MassBalance ()
  Default Constructor.
- ∼MassBalance ()
  Default Destructor.
- void Initialize_List (MasterSpeciesList &List)
  Function to initialize the MassBalance object from the MasterSpeciesList.
- void Display_Info ()
  Display the mass balance information.
- void Set_Delta (int i, double v)
  Function to set the ith weight (delta) for the mass balance.
- void Set_TotalConcentration (double v)
  Set the total concentration of the mass balance to v (mol/L)
- void Set_Name (std::string name)
  Set the name of the mass balance (i.e., Uranium, Carbonate, etc.)
- double Get_Delta (int i)
  Fetch the ith weight (i.e., delta) value.
- double Sum_Delta ()
  Sums up the delta values and returns the total (should never be zero)
- double Get_TotalConcentration ()
  Fetch the total concentration (mol/L)
- std::string Get_Name ()
  Return name of mass balance object.
- double Eval_Residual (const Matrix< double > &x)
  Evaluate the residual for the mass balance object given the log(C) concentrations.

Protected Attributes

- MasterSpeciesList ∗ List
  Pointer to a master species object.
- std::vector< double > Delta
  Vector of weights (i.e., deltas) used in the mass balance.
- double TotalConcentration
  Total concentration of specific object (mol/L)

Private Attributes

- std::string Name

  Name designation used in mass balance.

4.21.1 Detailed Description

Mass Balance Object.

C++ style object that holds data and functions associated with mass balances of primary species in a system. The mass balances involve a total concentration (in mol/L) and a vector of weighted contributions to that total concentration from each species in the MasterSpeciesList. This object only considers mass balances in a batch type of system (i.e., not input or output of mass). However, one could inherit from this object to create mass balances for flow systems as well.

4.21.2 Constructor & Destructor Documentation

4.21.2.1 MassBalance::MassBalance ( )

Default Constructor.

4.21.2.2 MassBalance::∼MassBalance ( )

Default Destructor.

4.21.3 Member Function Documentation

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

Function to initialize the MassBalance object from the MasterSpeciesList.

4.21.3.2 void MassBalance::Display_Info ( )

Display the mass balance information.

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

Function to set the ith weight (delta) for the mass balance.

This function sets the weight (i.e., delta value) of the ith species in the list to the value of v. That value represents the weighting of that species in the determination of the total mass for the primary species set.

Parameters

i	index of the species in the MasterSpeciesList
v	value of the weigth (or delta) applied to the mass balance

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

Set the total concentration of the mass balance to v (mol/L)

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

Set the name of the mass balance (i.e., Uranium, Carbonate, etc.)

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

Fetch the ith weight (i.e., delta) value.

4.21.3.7 double MassBalance::Sum_Delta ( )

Sums up the delta values and returns the total (should never be zero)

4.21.3.8 double MassBalance::Get_TotalConcentration ( )

Fetch the total concentration (mol/L)

4.21.3.9 std::string MassBalance::Get_Name ( )

Return name of mass balance object.

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

Evaluate the residual for the mass balance object given the log(C) concentrations.

This function calculates and provides the residual for this mass balance object based on the total concentration in the system and the weighted contributions from each species. Concentrations are given as the log(C) values.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step

4.21.4 Member Data Documentation

4.21.4.1 **MasterSpeciesList**∗ MassBalance::List [protected]

Pointer to a master species object.

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

Vector of weights (i.e., deltas) used in the mass balance.

4.21.4.3 double MassBalance::TotalConcentration [protected]

Total concentration of specific object (mol/L)

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

Name designation used in mass balance.

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

- shark.h

4.22 MasterSpeciesList Class Reference

Master Species List Object.

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

Public Member Functions

- MasterSpeciesList ()

  Default constructor.
- ∼MasterSpeciesList ()

  Default destructor.
- MasterSpeciesList (const MasterSpeciesList &msl)

  Copy Constructor.
- MasterSpeciesList & operator= (const MasterSpeciesList &msl)

  Equals operator.
- void set_list_size (int i)

  Function to initialize the size of the list.
- void set_species (int i, std::string formula)

  Function to register the ith species in the list based on a registered molecular formula (see mola.h)
- 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)

  Function to register the ith species in the list based on custom molecule information (see mola.h)
- void DisplayInfo (int i)

  Function to display information of ith object.
- void DisplayAll ()

  Function to display all information of list.
- void DisplayConcentrations (Matrix< double > &C)

  Function to display the concentrations of species in list.
- void set_alkalinity (double alk)

  Set the alkalinity of the solution (Default = 0 M)
- int list_size ()

  Returns size of list.
- Molecule & get_species (int i)

  Returns a reference to the ith species in master list.
- int get_index (std::string name)

  Returns an integer representing location of the named species in the list.
- double charge (int i)

  Fetch and return charge of ith species in list.
- double alkalinity ()

  Fetch the value of alkalinity of the solution (mol/L)
- std::string speciesName (int i)

  Function to return the name of the ith species.
- double Eval_ChargeResidual (const Matrix< double > &x)

  Calculate charge balance residual for the electroneutrality constraint.

Protected Attributes

- int size

  Size of the list.
- std::vector< Molecule > species

  List of Molecule Objects.
- double residual_alkalinity

  Conc of strong base - conc of strong acid in solution (mol/L)

4.22.1 Detailed Description

Master Species List Object.

C++ style object that holds data and function associated with solving multi-species problems. This object contains a vector of Molecule objects from mola.h and uses those objects to help setup speciation problems that need to be solved. One of the primary functions in this object is the contribution of electroneutrality (Eval_ChargeResidual). However, we only need this constraint if the pH of our aqueous system is unknown.

4.22.2 Constructor & Destructor Documentation

4.22.2.1 MasterSpeciesList::MasterSpeciesList ( )

Default constructor.

4.22.2.2 MasterSpeciesList::∼MasterSpeciesList ( )

Default destructor.

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

Copy Constructor.

4.22.3 Member Function Documentation

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

Equals operator.

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

Function to initialize the size of the list.

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

Function to register the ith species in the list based on a registered molecular formula (see mola.h)

4.22.3.4 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*)

Function to register the ith species in the list based on custom molecule information (see mola.h)

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

Function to display information of ith object.

4.22.3.6 void MasterSpeciesList::DisplayAll ( )

Function to display all information of list.

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

Function to display the concentrations of species in list.

This function will print to the console the species list in order with each species associated concentration from the matrix C. The concentrations and species list MUST be in the same order and the units of C are assumed to be mol/L.

Parameters

C	matrix of concentrations of species in the list in mol/L

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

Set the alkalinity of the solution (Default = 0 M)

This function is used to set the value of residual alkalinity used in the electroneutrality calculations. Typically, this value will be 0 M (mol/L) if all species in the system are present as variables. However, occasionally, one may want to set the alkalinity of the solution to a constant in order to restrict the pH of the solution.

Parameters

alk	Residual alkalinity in M (mol/L)

4.22.3.9 int MasterSpeciesList::list_size ( )

Returns size of list.

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

Returns a reference to the ith species in master list.

This function will return a Molecule object for the ith species in the list of molecules. Once returned, the user then can operate on that molecule using the functions define in mola.h.

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

Returns an integer representing location of the named species in the list.

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

Fetch and return charge of ith species in list.

4.22.3.13 double MasterSpeciesList::alkalinity ( )

Fetch the value of alkalinity of the solution (mol/L)

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

Function to return the name of the ith species.

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

Calculate charge balance residual for the electroneutrality constraint.

This function returns the value of the residual for the electroneutrality equation in the system. Electroneutrality is based on the concentrations and charges of each species in the system so the charges of each molecule must be appropriately set. Concentrations of those species are fed into this function via the argument x, but come in as the log(C) values (i.e., x = log(C)).

Parameters

x	matrix of the log(C) concentration values at the current non-linear step

4.22.4 Member Data Documentation

4.22.4.1 int MasterSpeciesList::size [protected]

Size of the list.

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

List of Molecule Objects.

4.22.4.3 double MasterSpeciesList::residual_alkalinity [protected]

Conc of strong base - conc of strong acid in solution (mol/L)

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

- shark.h

4.23 Matrix< T > Class Template Reference

Templated C++ Matrix Class Object (click Matrix to go to function definitions)

`#include <macaw.h>`

Public Member Functions

- Matrix (int rows, int columns)

    Constructor for matrix with given number of rows and columns.
- T & operator() (int i, int j)

    Access operator for the matrix element at row i and column j (e.g., aij = A(i,j))
- T operator() (int i, int j) const

    Constant access operator for the the matrix element at row i and column j.

- Matrix (const Matrix &M)

  Copy constructor for constructing a matrix as a copy of another matrix.
- Matrix & operator= (const Matrix &M)

  Equals operator for setting one matrix equal to another matrix.
- Matrix ()

  Default constructor for creating an empty matrix.
- ∼Matrix ()

  Default destructor for clearing out memory.
- void set_size (int i, int j)

  Function to set/change the size of a matrix to i rows and j columns.
- void zeros ()

  Function to set/change all values in a matrix to zeros.
- void edit (int i, int j, T value)

  Function to set/change the element of a matrix at row i and column j to given value.
- int rows ()

  Function to return the number of rows in a given matrix.
- int columns ()

  Function to return the number of columns in a matrix.
- T determinate ()

  Function to compute the determinate of a matrix and return that value.
- T norm ()

  Function to compute the L2-norm of a matrix and return that value.
- T sum ()

  Function to compute the sum of all elements in a matrix and return that value.
- T inner_product (const Matrix &x)

  Function to compute the inner product between this matrix and matrix x.
- Matrix & cofactor (const Matrix &M)

  Function to convert this matrix to a cofactor matrix of the given matrix M.
- Matrix operator+ (const Matrix &M)

  Operator to add this matrix and matrix M and return the new matrix result.
- Matrix operator- (const Matrix &M)

  Operator to subtract this matrix and matrix M and return the new matrix result.
- Matrix operator∗ (const T)

  Operator to multiply this matrix by a scalar T return the new matrix result.
- Matrix operator/ (const T)

  Operator to divide this matrix by a scalar T and return the new matrix result.
- Matrix operator∗ (const Matrix &M)

  Operator to multiply this matrix and matrix M and return the new matrix result.
- Matrix & transpose (const Matrix &M)

  Function to convert this matrix to the transpose of the given matrix M.
- Matrix & transpose_multiply (const Matrix &MT, const Matrix &v)

  Function to convert this matrix into the result of the given matrix M transposed and multiplied by the other given matrix v.
- Matrix & adjoint (const Matrix &M)

  Function to convert this matrix to the adjoint of the given matrix.
- Matrix & inverse (const Matrix &M)

  Function to convert this matrix to the inverse of the given matrix.
- void Display (const std::string Name)

  Function to display the contents of this matrix given a Name for the matrix.
- Matrix & tridiagonalSolve (const Matrix &A, const Matrix &b)

  Function to solve Ax=b for x if A is symmetric, tridiagonal (this->x)

- Matrix & ladshawSolve (const Matrix &A, const Matrix &d)

  Function to solve Ax=d for x if A is non-symmetric, tridiagonal (this->x)
- Matrix & tridiagonalFill (const T A, const T B, const T C, bool Spherical)

  Function to fill in this matrix with coefficients A, B, and C to form a tridiagonal matrix.
- Matrix & naturalLaplacian3D (int m)

  Function to fill out this matrix with coefficients from a 3D Laplacian function.
- Matrix & sphericalBCFill (int node, const T coeff, T variable)

  Function to fill out a column matrix with spherical specific boundary conditions.
- Matrix & ConstantICFill (const T IC)

  Function to set all values in a column matrix to a given constant.
- Matrix & SolnTransform (const Matrix &A, bool Forward)

  Function to transform the values in a column matrix from cartesian to spherical coordinates.
- T sphericalAvg (double radius, double dr, double bound, bool Dirichlet)

  Function to compute a spatial average of this column matrix in spherical coordinates.
- T IntegralAvg (double radius, double dr, double bound, bool Dirichlet)

  Function to compute a spatial average of this column matrix in spherical coordinates.
- T IntegralTotal (double dr, double bound, bool Dirichlet)

  Function to compute a spatial total of this column matrix in spherical coordinates.
- Matrix & tridiagonalVectorFill (const std::vector< T > &A, const std::vector< T > &B, const std::vector< T > &C)

  Function to fill in this matrix, in tridiagonal fashion, using the vectors of coefficients.
- Matrix & columnVectorFill (const std::vector< T > &A)

  Function to fill in a column matrix with the values of the given vector object.
- Matrix & columnProjection (const Matrix &b, const Matrix &b_old, const double dt, const double dt_old)

  Function to project a column matrix solution in time based on older state vectors.
- Matrix & dirichletBCFill (int node, const T coeff, T variable)

  Function to fill in a column matrix with all zeros except at the given node.
- Matrix & diagonalSolve (const Matrix &D, const Matrix &v)

  Function to solve the system Dx=v for x given that D is diagonal (this->x)
- Matrix & upperTriangularSolve (const Matrix &U, const Matrix &v)

  Function to solve the system Ux=v for x given that U is upper Triagular (this->x)
- Matrix & lowerTriangularSolve (const Matrix &L, const Matrix &v)

  Function to solve the system Lx=v for x given that L is lower Triagular (this->x)
- Matrix & upperHessenberg2Triangular (Matrix &b)

  Function to convert this square matrix to upper Triangular (assuming this is upper Hessenberg)
- Matrix & lowerHessenberg2Triangular (Matrix &b)

  Function to convert this square matrix to lower Triangular (assuming this is lower Hessenberg)
- Matrix & upperHessenbergSolve (const Matrix &H, const Matrix &v)

  Function to solve the system Hx=v for x given that H is upper Hessenberg (this->x)
- Matrix & lowerHessenbergSolve (const Matrix &H, const Matrix &v)

  Function to solve the system Hx=v for x given that H is lower Hessenberg (this->x)
- Matrix & columnExtract (int j, const Matrix &M)

  Function to set this column matrix to the jth column of the given matrix M.
- Matrix & rowExtract (int i, const Matrix &M)

  Function to set this row matrix to the ith row of the given matrix M.
- Matrix & columnReplace (int j, const Matrix &v)

  Function to this matrices' jth column with the given column matrix v.
- Matrix & rowReplace (int i, const Matrix &v)

  Function to this matrices' ith row with the given row matrix v.
- void rowShrink ()

  Function to delete the last row of this matrix.

- void columnShrink ()

    Function to delete the last column of this matrix.
- void rowExtend (const Matrix &v)

    Function to add the row matrix v to the end of this matrix.
- void columnExtend (const Matrix &v)

    Function to add the column matrix v to the end of this matrix.

Protected Attributes

- int num_rows

    Number of rows of the matrix.
- int num_cols

    Number of columns of the matrix.
- std::vector< T > Data

    Storage vector for the elements of the matrix.

4.23.1 Detailed Description

template<class T>class Matrix< T >

Templated C++ Matrix Class Object (click Matrix to go to function definitions)

C++ templated class object containing many different functions, actions, and solver routines associated with Dense Matrices. Operator overloads are also provided to give the user a more natural way of operating matrices on other matrices or scalars. These operator overloads are especially useful for reducing the amount of code needed to be written when working with matrix-based problems.

4.23.2 Constructor & Destructor Documentation

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

Constructor for matrix with given number of rows and columns.

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

Copy constructor for constructing a matrix as a copy of another matrix.

4.23.2.3 template<class T > Matrix< T >::Matrix ( )

Default constructor for creating an empty matrix.

4.23.2.4 template<class T > Matrix< T >::~Matrix ( )

Default destructor for clearing out memory.

4.23.3 Member Function Documentation

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

Access operator for the matrix element at row i and column j (e.g., aij = A(i,j))

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

Constant access operator for the the matrix element at row i and column j.

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

Equals operator for setting one matrix equal to another matrix.

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

Function to set/change the size of a matrix to i rows and j columns.

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

Function to set/change all values in a matrix to zeros.

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

Function to set/change the element of a matrix at row i and column j to given value.

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

Function to return the number of rows in a given matrix.

4.23.3.8 template<class T > int Matrix< T >::columns ( )

Function to return the number of columns in a matrix.

4.23.3.9 template<class T > T Matrix< T >::determinate ( )

Function to compute the determinate of a matrix and return that value.

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

Function to compute the L2-norm of a matrix and return that value.

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

Function to compute the sum of all elements in a matrix and return that value.

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

Function to compute the inner product between this matrix and matrix x.

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

Function to convert this matrix to a cofactor matrix of the given matrix M.

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

Operator to add this matrix and matrix M and return the new matrix result.

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

Operator to subtract this matrix and matrix M and return the new matrix result.

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

Operator to multiply this matrix by a scalar T return the new matrix result.

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

Operator to divide this matrix by a scalar T and return the new matrix result.

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

Operator to multiply this matrix and matrix M and return the new matrix result.

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

Function to convert this matrix to the transpose of the given matrix M.

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

Function to convert this matrix into the result of the given matrix M transposed and multiplied by the other given matrix v.

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

Function to convert this matrix to the adjoint of the given matrix.

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

Function to convert this matrix to the inverse of the given matrix.

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

Function to display the contents of this matrix given a Name for the matrix.

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

Function to solve Ax=b for x if A is symmetric, tridiagonal (this->x)

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

Function to solve Ax=d for x if A is non-symmetric, tridiagonal (this->x)

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

Function to fill in this matrix with coefficients A, B, and C to form a tridiagonal matrix.

This function fills in the diagonal elements of a square matrix with coefficient B, upper diagonal with C, and lower diagonal with A. The boolean will apply a transformation to those coefficients, if the problem happens to stem from 1-D diffusion in spherical coordinates.

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

Function to fill out this matrix with coefficients from a 3D Laplacian function.

This function will fill out the coefficients of the matrix with the coefficients that stem from discretizing a 3D Laplacian on a natural grid with 2nd order finite differences.

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

Function to fill out a column matrix with spherical specific boundary conditions.

This function will fille out a column matrix with zeros at all nodes expect for the node indicated. That node's value will be the product of the node id with the coeff and variable values given.

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

Function to set all values in a column matrix to a given constant.

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

Function to transform the values in a column matrix from cartesian to spherical coordinates.

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

Function to compute a spatial average of this column matrix in spherical coordinates.

This function is used to compute an average value of a variable, represented in this column matrix, by integrating over the domain of the sphere. (Assumes you have variable value at center node)

Parameters

radius	radius of the sphere
dr	space between each node
bound	value of the variable at the boundary
Dirichlet	True if problem has a Dirichlet BC, False if Neumann

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

Function to compute a spatial average of this column matrix in spherical coordinates.

This function is used to compute an average value of a variable, represented in this column matrix, by integrating over the domain of the sphere. (Assumes you DO NOT have variable value at center node)

Parameters

radius	radius of the sphere
dr	space between each node
bound	value of the variable at the boundary
Dirichlet	True if problem has a Dirichlet BC, False if Neumann

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

Function to compute a spatial total of this column matrix in spherical coordinates.

This function is used to compute an average value of a variable, represented in this column matrix, by integrating over the domain of the sphere. (Assumes you DO NOT have variable value at center node)

Parameters

dr	space between each node
bound	value of the variable at the boundary
Dirichlet	True if problem has a Dirichlet BC, False if Neumann

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

Function to fill in this matrix, in tridiagonal fashion, using the vectors of coefficients.

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

Function to fill in a column matrix with the values of the given vector object.

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

Function to project a column matrix solution in time based on older state vectors.

This function is used in finch.h to form Matrix u_star. It uses the size of the current step and old step, dt and dt_old respectively, to form an approximation for the next state. The current state and olde state of the variables are passed as b and b_old respectively.

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

Function to fill in a column matrix with all zeros except at the given node.

Similar to sphericalBCFill, this function will set the values of all elements in the column matrix to zero except at the given node, where the value is set to the product of coeff and variable. This is often used to set BCs in finch.h or other related files/simulations.

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

Function to solve the system Dx=v for x given that D is diagonal (this->x)

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

Function to solve the system Ux=v for x given that U is upper Triagular (this->x)

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

Function to solve the system Lx=v for x given that L is lower Triagular (this->x)

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

Function to convert this square matrix to upper Triangular (assuming this is upper Hessenberg)

During this transformation, a column vector (b) is also being transformed to represent the BCs in a linear system. This algorithm uses Givens Rotations to efficiently convert the upper Hessenberg matrix to an upper triangular matrix.

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

Function to convert this square matrix to lower Triangular (assuming this is lower Hessenberg)

During this transformation, a column vector (b) is also being transformed to represent the BCs in a linear system. This algorithm uses Givens Rotations to efficiently convert the lower Hessenberg matrix to an lower triangular matrix.

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

Function to solve the system Hx=v for x given that H is upper Hessenberg (this->x)

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

Function to solve the system Hx=v for x given that H is lower Hessenberg (this->x)

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

Function to set this column matrix to the jth column of the given matrix M.

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

Function to set this row matrix to the ith row of the given matrix M.

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

Function to this matrices' jth column with the given column matrix v.

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

Function to this matrices' ith row with the given row matrix v.

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

Function to delete the last row of this matrix.

4.23.3.50 template< class T > void Matrix< T >::columnShrink ( )

Function to delete the last column of this matrix.

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

Function to add the row matrix v to the end of this matrix.

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

Function to add the column matrix v to the end of this matrix.

4.23.4 Member Data Documentation

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

Number of rows of the matrix.

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

Number of columns of the matrix.

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

Storage vector for the elements of the matrix.

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

- macaw.h

4.24 MIXED_GAS Struct Reference

Data structure holding information necessary for computing mixed gas properties.

`#include <egret.h>`

Public Attributes

- int N

  Given: Total number of gas species.
- bool CheckMolefractions = true

  Given: True = Check Molefractions for errors.
- double total_pressure

  Given: Total gas pressure (kPa)
- double gas_temperature

  Given: Gas temperature (K)

- double velocity

  Given: Gas phase velocity (cm/s)
- double char_length

  Given: Characteristic Length (cm)
- std::vector< double > molefraction

  Given: Gas molefractions of each species (-)
- double total_density

  Calculated: Total gas density (g/cm^3) {use RE3}.
- double total_dyn_vis

  Calculated: Total dynamic viscosity (g/cm/s)
- double kinematic_viscosity

  Calculated: Kinematic viscosity (cm^2/s)
- double total_molecular_weight

  Calculated: Total molecular weight (g/mol)
- double total_specific_heat

  Calculated: Total specific heat (J/g/K)
- double Reynolds

  Calculated: Value of the Reynold's number (-)
- Matrix< double > binary_diffusion

  Calculated: Tensor matrix of binary gas diffusivities (cm^2/s)
- std::vector< PURE_GAS > species_dat

  Vector of the pure gas info of all species.

4.24.1 Detailed Description

Data structure holding information necessary for computing mixed gas properties.

C-style object holding the mixed gas information necessary for performing gas dynamic simulations. This object works in conjunction with the calculate_variables function and uses the kinetic theory of gases to estimate mixed gas properties.

4.24.2 Member Data Documentation

4.24.2.1 int MIXED_GAS::N

Given: Total number of gas species.

4.24.2.2 bool MIXED_GAS::CheckMolefractions = true

Given: True = Check Molefractions for errors.

4.24.2.3 double MIXED_GAS::total_pressure

Given: Total gas pressure (kPa)

4.24.2.4 double MIXED_GAS::gas_temperature

Given: Gas temperature (K)

4.24.2.5 double MIXED_GAS::velocity

Given: Gas phase velocity (cm/s)

4.24.2.6 double MIXED_GAS::char_length

Given: Characteristic Length (cm)

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

Given: Gas molefractions of each species (-)

4.24.2.8 double MIXED_GAS::total_density

Calculated: Total gas density (g/cm^3) {use RE3}.

4.24.2.9 double MIXED_GAS::total_dyn_vis

Calculated: Total dynamic viscosity (g/cm/s)

4.24.2.10 double MIXED_GAS::kinematic_viscosity

Calculated: Kinematic viscosity (cm^2/s)

4.24.2.11 double MIXED_GAS::total_molecular_weight

Calculated: Total molecular weight (g/mol)

4.24.2.12 double MIXED_GAS::total_specific_heat

Calculated: Total specific heat (J/g/K)

4.24.2.13 double MIXED_GAS::Reynolds

Calculated: Value of the Reynold's number (-)

4.24.2.14 Matrix<double> MIXED_GAS::binary_diffusion

Calculated: Tensor matrix of binary gas diffusivities (cm^2/s)

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

Vector of the pure gas info of all species.

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

- egret.h

4.25 Molecule Class Reference

C++ Molecule Object built from Atom Objects (click Molecule to go to function definitions)

`#include <mola.h>`

Public Member Functions

- Molecule ()

  Default Constructor (builds an empty molecule object)
- ∼Molecule ()

  Default Destructor (clears out memory)
- 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)

  Construct any molecule from the available information.
- 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)

  Function to register this molecule from the available information.
- void Register (std::string formula)

  Function to register this molecule based on the given formula (if formula is in library)
- void setFormula (std::string form)

  Sets the formula for a molecule.
- void recalculateMolarWeight ()

  Forces molecule to recalculate its molar weight.
- void setMolarWeigth (double mw)

  Set the molar weight of species to a constant.
- void editCharge (int c)

  Change the ionic charge of a molecule.
- void editOneOxidationState (int state, std::string Symbol)

  Change oxidation state of one of the given atoms (always first match found)
- void editAllOxidationStates (int state, std::string Symbol)

  Change oxidation state of all of the given atoms.
- void calculateAvgOxiState (std::string Symbol)

  Function to calculate the average oxidation state of the atoms.
- void editEnthalpy (double enthalpy)

  Edit the molecules formation enthalpy (J/mol)
- void editEntropy (double entropy)

  Edit the molecules formation entropy (J/K/mol)
- void editHS (double H, double S)

  Edit both formation enthalpy and entropy.
- void editEnergy (double energy)

  Edit Gibb's formation energy.
- void removeOneAtom (std::string Symbol)

  Removes one atom of the symbol given (always the first atom found)
- void removeAllAtoms (std::string Symbol)

  Removes all atoms of the symbol given.
- int Charge ()

  Return the charge of the molecule.
- double MolarWeight ()

  Return the molar weight of the molecule.
- bool HaveHS ()

Returns true if enthalpy and entropy are known.

- bool HaveEnergy ()

  Returns true if the Gibb's energy is known.
- bool isRegistered ()

  Returns true if the molecule has been registered.
- double Enthalpy ()

  Return the formation enthalpy of the molecule.
- double Entropy ()

  Return the formation entropy of the molecule.
- double Energy ()

  Return the Gibb's formation energy of the molecule.
- std::string MoleculeName ()

  Return the common name of the molecule.
- std::string MolecularFormula ()

  Return the molecular formula of the molecule.
- std::string MoleculePhase ()

  Return the phase of the molecule.
- void DisplayInfo ()

  Function to display molecule information.

Protected Attributes

- int charge

  Ionic charge of the molecule - specified.
- double molar_weight

  Molar weight of the molecule (g/mol) - determined from atoms or specified.
- double formation_enthalpy

  Enthalpy of formation of the molecule (J/mol) - constant.
- double formation_entropy

  Entropy of formation of the molecule (J/K/mol) - constant.
- double formation_energy

  Gibb's energy of formation (J/mol) - given.
- std::string Phase

  Phase of the molecule (i.e. Solid, Liquid, Aqueous, Gas...)
- std::vector$<$ Atom $>$ atoms

  Atoms which make up the molecule - based on Formula.

Private Attributes

- std::string Name

  Name of the Molecule - Common Name (i.e. H2O = Water)
- std::string Formula

  Formula for the molecule - specified (i.e. H2O)
- bool haveG

  True = given Gibb's energy of formation.
- bool haveHS

  True = give enthalpy and entropy of formation.
- bool registered

  True = the object was registered.

4.25.1 Detailed Description

C++ Molecule Object built from Atom Objects (click Molecule to go to function definitions)

C++ Class Object that stores information and certain operations associated with molecules. Registered molecules are built up from their respective atoms so that the molecule can keep track of information such as molecular weigth and oxidation states. Primarily, this object is used in conjunction with shark.h to formulate the system of equations necessary for solving speciation type problems in aqueous systems. However, this object is generalized enough to be of use in RedOx calculations, reaction formulation, and molecular transformations.

All information for a molecule should be initialized prior to performing operations with or on the object. There are several molecules already defined for construction by the formulas listed at the top of this section.

4.25.2 Constructor & Destructor Documentation

4.25.2.1 Molecule::Molecule ( )

Default Constructor (builds an empty molecule object)

4.25.2.2 Molecule::∼Molecule ( )

Default Destructor (clears out memory)

4.25.2.3 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*)

Construct any molecule from the available information.

This constructor will build a user defined custom molecule.

Parameters

charge	the ionic charge of the molecule
enthalpy	the standard formation enthalpy of the molecule (J/mol)
entropy	the standard formation entropy of the molecule (J/K/mol)
energy	the standard Gibb's Free Energy of formation of the molecule (J/mol)
HS	boolean to be set to true if enthalpy and entropy were given
G	boolean to be set to true if the energy was given
Phase	string denoting molecule's phase (i.e., Liquid, Aqueous, Gas, Solid)
Name	string denoting the common name of the molecule (i.e., H2O -> Water)
Formula	string denoting the formula by which the molecule is referened (i.e., Cl - (aq))
lin_formula	string denoting all the atoms in the molecule (i.e., UO2(OH)2 -> UO4H2)

4.25.3 Member Function Documentation

4.25.3.1 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*)

Function to register this molecule from the available information.

This function will build a user defined custom molecule.

Parameters

charge	the ionic charge of the molecule
enthalpy	the standard formation enthalpy of the molecule (J/mol)
entropy	the standard formation entropy of the molecule (J/K/mol)
energy	the standard Gibb's Free Energy of formation of the molecule (J/mol)

HS	boolean to be set to true if enthalpy and entropy were given
G	boolean to be set to true if the energy was given
Phase	string denoting molecule's phase (i.e., Liquid, Aqueous, Gas, Solid)
Name	string denoting the common name of the molecule (i.e., H2O -> Water)
Formula	string denoting the formula by which the molecule is referened (i.e., Cl - (aq))
lin_formula	string denoting all the atoms in the molecule (i.e., UO2(OH)2 -> UO4H2)

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

Function to register this molecule based on the given formula (if formula is in library)

This function will create this molecule object from the given formula, but only if that formula is already registered in the library. See the top of this class section for a list of all currently registered formulas.

Note

The formula is checked against a known set of molecules inside of the registration function If the formula is unknown, an error will print to the screen. Unknown molecules should be registered using the full registration function from above. The library can only be added to by a going in and editing the source code of the mola.cpp file. However, this is a relatively simple task.

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

Sets the formula for a molecule.

4.25.3.4 void Molecule::recalculateMolarWeight ( )

Forces molecule to recalculate its molar weight.

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

Set the molar weight of species to a constant.

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

Change the ionic charge of a molecule.

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

Change oxidation state of one of the given atoms (always first match found)

This function will search the list of Atoms that make up the Molecule for the given atomic Symbol. It will change the oxidation state of the first found matching atom with the given state.

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

Change oxidation state of all of the given atoms.

This function will search the list of Atoms that make up the Molecule for the given atomic Symbol. It will change the oxidation state of all found matching atoms with the given state.

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

Function to calculate the average oxidation state of the atoms.

This function search the atoms in the molecule for the matching atomic Symbol. It then looks at all oxidation states of that atom in the molecule and then sets all the oxidation states of that atom to the average value calculated.

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

Edit the molecules formation enthalpy (J/mol)

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

Edit the molecules formation entropy (J/K/mol)

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

Edit both formation enthalpy and entropy.

This function will change or set the values for formation enthalpy (J/mol) and formation entropy (J/K/mol) based on the given values.

Parameters

H	formation enthalpy (J/mol)
S	formation entropy (J/K/mol)

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

Edit Gibb's formation energy.

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

Removes one atom of the symbol given (always the first atom found)

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

Removes all atoms of the symbol given.

4.25.3.16 int Molecule::Charge ( )

Return the charge of the molecule.

4.25.3.17 double Molecule::MolarWeight ( )

Return the molar weight of the molecule.

4.25.3.18 bool Molecule::HaveHS ( )

Returns true if enthalpy and entropy are known.

4.25.3.19 bool Molecule::HaveEnergy ( )

Returns true if the Gibb's energy is known.

4.25.3.20 bool Molecule::isRegistered ( )

Returns true if the molecule has been registered.

4.25.3.21 double Molecule::Enthalpy ( )

Return the formation enthalpy of the molecule.

4.25.3.22 double Molecule::Entropy ( )

Return the formation entropy of the molecule.

4.25.3.23 double Molecule::Energy ( )

Return the Gibb's formation energy of the molecule.

4.25.3.24 std::string Molecule::MoleculeName ( )

Return the common name of the molecule.

4.25.3.25 std::string Molecule::MolecularFormula ( )

Return the molecular formula of the molecule.

4.25.3.26 std::string Molecule::MoleculePhase ( )

Return the phase of the molecule.

4.25.3.27 void Molecule::DisplayInfo ( )

Function to display molecule information.

4.25.4 Member Data Documentation

4.25.4.1 int Molecule::charge `[protected]`

Ionic charge of the molecule - specified.

4.25.4.2 double Molecule::molar_weight `[protected]`

Molar weight of the molecule (g/mol) - determined from atoms or specified.

4.25.4.3 double Molecule::formation_enthalpy `[protected]`

Enthalpy of formation of the molecule (J/mol) - constant.

4.25.4.4 double Molecule::formation_entropy [protected]

Entropy of formation of the molecule (J/K/mol) - constant.

4.25.4.5 double Molecule::formation_energy [protected]

Gibb's energy of formation (J/mol) - given.

4.25.4.6 std::string Molecule::Phase [protected]

Phase of the molecule (i.e. Solid, Liquid, Aqueous, Gas...)

4.25.4.7 std::vector<Atom> Molecule::atoms [protected]

Atoms which make up the molecule - based on Formula.

4.25.4.8 std::string Molecule::Name [private]

Name of the Molecule - Common Name (i.e. H2O = Water)

4.25.4.9 std::string Molecule::Formula [private]

Formula for the molecule - specified (i.e. H2O)

4.25.4.10 bool Molecule::haveG [private]

True = given Gibb's energy of formation.

4.25.4.11 bool Molecule::haveHS [private]

True = give enthalpy and entropy of formation.

4.25.4.12 bool Molecule::registered [private]

True = the object was registered.

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

- mola.h

4.26 MONKFISH_DATA Struct Reference

Primary data structure for running MONKFISH.

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

Public Attributes

- unsigned long int total_steps = 0

    Total number of steps taken by the algorithm (iterations and time steps)

- double time_old = 0.0

  Old value of time in the simulation (hrs)
- double time = 0.0

  Current value of time in the simulation (hrs)
- bool Print2File = true

  True = results to .txt; False = no printing.
- bool Print2Console = true

  True = results to console; False = no printing.
- bool DirichletBC = true

  False = uses film mass transfer for BC, True = Dirichlet BC.
- bool NonLinear = false

  False = Solve directly, True = Solve iteratively.
- bool haveMinMax = false

  True = know min and max fiber density, False = only know avg density (Used in ICs)
- bool MultiScale = true

  True = solve single fiber model at nodes, False = solve equilibrium at nodes.
- int level = 2

  Level of coupling between multiple scales (default = 2)
- double t_counter = 0.0

  Counter for the time output.
- double t_print

  Print output at every t_print time (hrs)
- int NumComp

  Number of species to track.
- double end_time

  Units: hours.
- double total_sorption_old

  Old total adsorption per mass of woven nest (mg/g)
- double total_sorption

  Current total adsorption per mass woven nest (mg/g)
- double single_fiber_density

  Units: g/L.
- double avg_fiber_density

  Units: g/L (Used in ICs)
- double max_fiber_density

  Units: g/L (Used in ICs)
- double min_fiber_density

  Units: g/L (Used in ICs)
- double max_porosity

  Units: -.
- double min_porosity

  Units: -.
- double domain_diameter

  Nominal diameter of the woven fiber ball - Units: cm.
- FILE ∗ Output

  Output file pointer for printing to text file.
- double(∗ eval_eps)(int i, int l, const void ∗user_data)

  Function pointer to evaluate the porosity of the woven bundle of fibers.
- double(∗ eval_rho)(int i, int l, const void ∗user_data)

  Function pointer to evaluate the fiber density in the domain.
- double(∗ eval_Dex)(int i, int l, const void ∗user_data)

Function pointer to evaluate the interparticle diffusivity.

- double(∗ eval_ads)(int i, int l, const void ∗user_data)

  Function pointer to evaluate the adsorption strength for the macro-scale.

- double(∗ eval_Ret)(int i, int l, const void ∗user_data)

  Function pointer to evaluate the retardation coefficient for the macro-scale.

- double(∗ eval_Cex)(int i, const void ∗user_data)

  Function pointer to evaluate the exterior concentration for the domain.

- double(∗ eval_kf)(int i, const void ∗user_data)

  Function pointer to evalutate the film mass transfer coefficient for the macro-scale.

- const void ∗ user_data

  User supplied data function to evaluate the function pointers (Default = MONKFISH_DATA)

- std::vector< FINCH_DATA > finch_dat

  FINCH data structures to solve each species interparticle diffusion equation.

- std::vector< MONKFISH_PARAM > param_dat

  MONKFISH parameter data structure for each species adsorbing.

- std::vector< DOGFISH_DATA > dog_dat

  DOGFISH data structures for each node in the macro-scale problem.

4.26.1 Detailed Description

Primary data structure for running MONKFISH.

C-style object holding simulation information for MONKFISH as well as common system parameters like fiber density, fiber diameter, fiber length, etc. This object also contains function pointers to different parameter evaluation functions that can be changed to suit a particular problem. Default functions will be given, so not every user needs to override these functions. This structure also contains vectors of other objects including FINCH and DOGFISH objects to resolve the diffusion physics at both the macro- and micro-scale.

4.26.2 Member Data Documentation

4.26.2.1 unsigned long int MONKFISH_DATA::total_steps = 0

Total number of steps taken by the algorithm (iterations and time steps)

4.26.2.2 double MONKFISH_DATA::time_old = 0.0

Old value of time in the simulation (hrs)

4.26.2.3 double MONKFISH_DATA::time = 0.0

Current value of time in the simulation (hrs)

4.26.2.4 bool MONKFISH_DATA::Print2File = true

True = results to .txt; False = no printing.

4.26.2.5 bool MONKFISH_DATA::Print2Console = true

True = results to console; False = no printing.

4.26.2.6 bool MONKFISH_DATA::DirichletBC = true

False = uses film mass transfer for BC, True = Dirichlet BC.

4.26.2.7 bool MONKFISH_DATA::NonLinear = false

False = Solve directly, True = Solve iteratively.

4.26.2.8 bool MONKFISH_DATA::haveMinMax = false

True = know min and max fiber density, False = only know avg density (Used in ICs)

4.26.2.9 bool MONKFISH_DATA::MultiScale = true

True = solve single fiber model at nodes, False = solve equilibrium at nodes.

4.26.2.10 int MONKFISH_DATA::level = 2

Level of coupling between multiple scales (default = 2)

4.26.2.11 double MONKFISH_DATA::t_counter = 0.0

Counter for the time output.

4.26.2.12 double MONKFISH_DATA::t_print

Print output at every t_print time (hrs)

4.26.2.13 int MONKFISH_DATA::NumComp

Number of species to track.

4.26.2.14 double MONKFISH_DATA::end_time

Units: hours.

4.26.2.15 double MONKFISH_DATA::total_sorption_old

Old total adsorption per mass of woven nest (mg/g)

4.26.2.16 double MONKFISH_DATA::total_sorption

Current total adsorption per mass woven nest (mg/g)

4.26.2.17 double MONKFISH_DATA::single_fiber_density

Units: g/L.

4.26.2.18 double MONKFISH_DATA::avg_fiber_density

Units: g/L (Used in ICs)

4.26.2.19 double MONKFISH_DATA::max_fiber_density

Units: g/L (Used in ICs)

4.26.2.20 double MONKFISH_DATA::min_fiber_density

Units: g/L (Used in ICs)

4.26.2.21 double MONKFISH_DATA::max_porosity

Units: -.

4.26.2.22 double MONKFISH_DATA::min_porosity

Units: -.

4.26.2.23 double MONKFISH_DATA::domain_diameter

Nominal diameter of the woven fiber ball - Units: cm.

4.26.2.24 FILE* MONKFISH_DATA::Output

Output file pointer for printing to text file.

4.26.2.25 double(* MONKFISH_DATA::eval_eps)(int i, int l, const void *user_data)

Function pointer to evaluate the porosity of the woven bundle of fibers.

4.26.2.26 double(* MONKFISH_DATA::eval_rho)(int i, int l, const void *user_data)

Function pointer to evaluate the fiber density in the domain.

4.26.2.27 double(* MONKFISH_DATA::eval_Dex)(int i, int l, const void *user_data)

Function pointer to evaluate the interparticle diffusivity.

4.26.2.28 double(* MONKFISH_DATA::eval_ads)(int i, int l, const void *user_data)

Function pointer to evaluate the adsorption strength for the macro-scale.

4.26.2.29 double(* MONKFISH_DATA::eval_Ret)(int i, int l, const void *user_data)

Function pointer to evaluate the retardation coefficient for the macro-scale.

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

Function pointer to evaluate the exterior concentration for the domain.

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

Function pointer to evalutate the film mass transfer coefficient for the macro-scale.

4.26.2.32 const void∗ MONKFISH_DATA::user_data

User supplied data function to evaluate the function pointers (Default = MONKFISH_DATA)

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

FINCH data structures to solve each species interparticle diffusion equation.

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

MONKFISH parameter data structure for each species adsorbing.

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

DOGFISH data structures for each node in the macro-scale problem.

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

- monkfish.h

4.27 MONKFISH_PARAM Struct Reference

Data structure for species specific information and parameters.

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

Public Attributes

- double interparticle_diffusion

    Units: cm^2/hr.
- double exterior_concentration

    Units: mol/L.
- double exterior_transfer_coeff

    Units: cm/hr.
- double sorbed_molefraction

    Units: -.
- double initial_sorption

    Units: mg/g.
- double sorption_bc

    Units: mg/g.
- double intraparticle_diffusion

    Units: um^2/hr.

- double film_transfer_coeff

  Units: um/hr.
- Matrix< double > avg_sorption

  Units: mg/g.
- Matrix< double > avg_sorption_old

  Units: mg/g.
- Molecule species

  Species in the liquid phase.

4.27.1 Detailed Description

Data structure for species specific information and parameters.

C-style object to hold information associated with the different species present in the interparticle diffusion problem. Each species may have different diffusivities, mass transfer coefficients, etc. Average adsorption for each species will be held in matrix objects.

4.27.2 Member Data Documentation

4.27.2.1 double MONKFISH_PARAM::interparticle_diffusion

Units: cm^2/hr.

4.27.2.2 double MONKFISH_PARAM::exterior_concentration

Units: mol/L.

4.27.2.3 double MONKFISH_PARAM::exterior_transfer_coeff

Units: cm/hr.

4.27.2.4 double MONKFISH_PARAM::sorbed_molefraction

Units: -.

4.27.2.5 double MONKFISH_PARAM::initial_sorption

Units: mg/g.

4.27.2.6 double MONKFISH_PARAM::sorption_bc

Units: mg/g.

4.27.2.7 double MONKFISH_PARAM::intraparticle_diffusion

Units: um^2/hr.

4.27.2.8 double MONKFISH_PARAM::film_transfer_coeff

Units: um/hr.

4.27.2.9 Matrix<double> MONKFISH_PARAM::avg_sorption

Units: mg/g.

4.27.2.10 Matrix<double> MONKFISH_PARAM::avg_sorption_old

Units: mg/g.

4.27.2.11 Molecule MONKFISH_PARAM::species

Species in the liquid phase.

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

- monkfish.h

4.28 mSPD_DATA Struct Reference

MSPD Data Structure.

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

Public Attributes

- double s

  Area shape factor.
- double v

  van der Waals Volume (cm^3/mol)
- double eMax

  Maximum lateral interaction energy (J/mol)
- std::vector< double > eta

  Binary interaction parameter matrix (i,j)
- double gama

  Activity coefficient calculated from mSPD.

4.28.1 Detailed Description

MSPD Data Structure.

C-Style object holding all parameter information associated with the Modified Spreading Pressure Dependent (SPD) activity model. Each species in the gas phase will have one of these objects.

4.28.2 Member Data Documentation

4.28.2.1 double mSPD_DATA::s

Area shape factor.

4.28.2.2 double mSPD_DATA::v

van der Waals Volume (cm^3/mol)

4.28.2.3 double mSPD_DATA::eMax

Maximum lateral interaction energy (J/mol)

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

Binary interaction parameter matrix (i,j)

4.28.2.5 double mSPD_DATA::gama

Activity coefficient calculated from mSPD.

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

- magpie.h

4.29 NUM_JAC_DATA Struct Reference

Data structure to form a numerical jacobian matrix with finite differences.

`#include <lark.h>`

Public Attributes

- double eps = sqrt(DBL_EPSILON)

  Perturbation value.
- Matrix< double > Fx

  Vector of function evaluations at x.
- Matrix< double > Fxp

  Vector of function evaluations at x+eps.
- Matrix< double > dxj

  Vector of perturbed x values.

4.29.1 Detailed Description

Data structure to form a numerical jacobian matrix with finite differences.

C-style object to be used in conjunction with the Numerical Jacobian algorithm. This algorithm will used double-precision finite-differences to formulate an approximate Jacobian matrix at the given variable state for the given residual/non-linear function.

4.29.2 Member Data Documentation

4.29.2.1 double NUM_JAC_DATA::eps = sqrt(DBL_EPSILON)

Perturbation value.

4.29.2.2 Matrix<double> NUM_JAC_DATA::Fx

Vector of function evaluations at x.

4.29.2.3 Matrix<double> NUM_JAC_DATA::Fxp

Vector of function evaluations at x+eps.

4.29.2.4 Matrix<double> NUM_JAC_DATA::dxj

Vector of perturbed x values.

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

- lark.h

4.30 OPTRANS_DATA Struct Reference

Data structure for implementation of linear operator transposition.

`#include <lark.h>`

Public Attributes

- Matrix< double > Ii

    The ith column vector of the identity operator.
- Matrix< double > Ai

    The ith column vector of the user's linear operator.

4.30.1 Detailed Description

Data structure for implementation of linear operator transposition.

C-style object used in conjunction with the Operator Transpose algorithm to form an action of A^T*r when A is only available as a linear operator and not a matrix. This is a sub-routine required by GCR and GMRESR to stabilize the outer iterations.

4.30.2 Member Data Documentation

4.30.2.1 Matrix<double> OPTRANS_DATA::Ii

The ith column vector of the identity operator.

4.30.2.2 Matrix<double> OPTRANS_DATA::Ai

The ith column vector of the user's linear operator.

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

- lark.h

4.31 PCG_DATA Struct Reference

Data structure for implementation of the PCG algorithms for symmetric linear systems.

`#include <lark.h>`

Public Attributes

- int maxit = 0

    Maximum allowable iterations - default = min(vector_size,1000)
- int iter = 0

    Actual number of iterations taken.
- double alpha

    Step size for new solution.
- double beta

    Step size for new search direction.
- double tol_rel = 1e-6

    Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

    Absolution tolerance for convergence - default = 1e-6.
- double res

    Absolute residual norm.
- double relres

    Relative residual norm.
- double relres_base

    Initial residual norm.
- double bestres

    Best found residual norm.
- bool Output = true

    True = print messages to console.
- Matrix< double > x

    Current solution to the linear system.
- Matrix< double > bestx

    Best found solution to the linear system.
- Matrix< double > r

    Residual vector for the linear system.
- Matrix< double > r_old

    Previous residual vector.
- Matrix< double > z

    Preconditioned residual vector (result of precon function)
- Matrix< double > z_old

    Previous preconditioned residual vector.
- Matrix< double > p

    Search direction.
- Matrix< double > Ap

    Result of matrix-vector multiplication.

4.31.1 Detailed Description

Data structure for implementation of the PCG algorithms for symmetric linear systems.

C-style object used in conjunction with the Preconditioned Conjugate Gradient (PCG) algorithm to iteratively solve a symmetric linear system of equations. This algorithm is optimal if your linear system is symmetric, but will not work at all if your system is asymmetric. For asymmetric systems, use one of the other linear methods.

4.31.2 Member Data Documentation

4.31.2.1 int PCG_DATA::maxit = 0

Maximum allowable iterations - default = min(vector_size,1000)

4.31.2.2 int PCG_DATA::iter = 0

Actual number of iterations taken.

4.31.2.3 double PCG_DATA::alpha

Step size for new solution.

4.31.2.4 double PCG_DATA::beta

Step size for new search direction.

4.31.2.5 double PCG_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.31.2.6 double PCG_DATA::tol_abs = 1e-6

Absolution tolerance for convergence - default = 1e-6.

4.31.2.7 double PCG_DATA::res

Absolute residual norm.

4.31.2.8 double PCG_DATA::relres

Relative residual norm.

4.31.2.9 double PCG_DATA::relres_base

Initial residual norm.

4.31.2.10 double PCG_DATA::bestres

Best found residual norm.

4.31.2.11 bool PCG_DATA::Output = true

True = print messages to console.

4.31.2.12 Matrix<double> PCG_DATA::x

Current solution to the linear system.

4.31.2.13 Matrix<double> PCG_DATA::bestx

Best found solution to the linear system.

4.31.2.14 Matrix<double> PCG_DATA::r

Residual vector for the linear system.

4.31.2.15 Matrix<double> PCG_DATA::r_old

Previous residual vector.

4.31.2.16 Matrix<double> PCG_DATA::z

Preconditioned residual vector (result of precon function)

4.31.2.17 Matrix<double> PCG_DATA::z_old

Previous preconditioned residual vector.

4.31.2.18 Matrix<double> PCG_DATA::p

Search direction.

4.31.2.19 Matrix<double> PCG_DATA::Ap

Result of matrix-vector multiplication.

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

- lark.h

4.32 PeriodicTable Class Reference

Class object that store a digitial copy of all Atom objects.

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

Public Member Functions

- PeriodicTable ()
  Default Constructor - Build Perodic Table.
- ∼PeriodicTable ()
  Default Destructor - Destroy the table.
- PeriodicTable (int ∗n, int N)
  Construct a partial table from a list of atomic numbers.
- PeriodicTable (std::vector< std::string > &Symbol)
  Construct a partial table from a vector of atom symbols.
- PeriodicTable (std::vector< int > &n)
  Construct a partial table from a vector of atomic numbers.
- void DisplayTable ()
  Displays the periodic table via symbols.

Protected Attributes

- std::vector< Atom > Table

    Storage vector for all atoms in the table.

Private Attributes

- int number_elements

    Number of atom objects being stored.

4.32.1 Detailed Description

Class object that store a digitial copy of all Atom objects.

C++ class object to hold digitally registered Atom objects. All registered atoms (Hydrogen to Ununoctium) are stored as in a vector. Currently, this object is unused, but could be modified to be explorable and used as a constant referece for all atoms in the table.

4.32.2 Constructor & Destructor Documentation

4.32.2.1 PeriodicTable::PeriodicTable ( )

Default Constructor - Build Perodic Table.

4.32.2.2 PeriodicTable::∼PeriodicTable ( )

Default Destructor - Destroy the table.

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

Construct a partial table from a list of atomic numbers.

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

Construct a partial table from a vector of atom symbols.

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

Construct a partial table from a vector of atomic numbers.

4.32.3 Member Function Documentation

4.32.3.1 void PeriodicTable::DisplayTable ( )

Displays the periodic table via symbols.

4.32.4 Member Data Documentation

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

Storage vector for all atoms in the table.

4.32.4.2 int PeriodicTable::number_elements [private]

Number of atom objects being stored.

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

- eel.h

4.33 PICARD_DATA Struct Reference

Data structure for the implementation of a Picard or Fixed-Point iteration for non-linear systems.

`#include <lark.h>`

Public Attributes

- int maxit = 0

  Maximum allowable iterations - default = min(3∗vec_size,1000)
- int iter = 0

  Actual number of iterations.
- double tol_rel = 1e-6

  Relative tolerance for convergence - default = 1e-6.
- double tol_abs = 1e-6

  Absolution tolerance for convergence - default = 1e-6.
- double res

  Residual norm of the iterate.
- double relres

  Relative residual norm of the iterate.
- double relres_base

  Initial residual norm.
- double bestres

  Best found residual norm.
- bool Output = true

  True = print messages to console.
- Matrix< double > x0

  Previous iterate solution vector.
- Matrix< double > bestx

  Best found solution vector.
- Matrix< double > r

  Residual of the non-linear system.

4.33.1 Detailed Description

Data structure for the implementation of a Picard or Fixed-Point iteration for non-linear systems.

C-style object used in conjunction with the Picard algorithm for solving a non-linear system of equations. This is an extradorinarily simple iterative method by which a weak or loose form of the non-linear system is solved based on an initial guess. User must supplied a residual function for the non-linear system and a function representing the weak solution. Generally, this method is less efficient than Newton methods, but is significantly cheaper.

4.33.2 Member Data Documentation

4.33.2.1 int PICARD_DATA::maxit = 0

Maximum allowable iterations - default = min(3∗vec_size,1000)

4.33.2.2 int PICARD_DATA::iter = 0

Actual number of iterations.

4.33.2.3 double PICARD_DATA::tol_rel = 1e-6

Relative tolerance for convergence - default = 1e-6.

4.33.2.4 double PICARD_DATA::tol_abs = 1e-6

Absolution tolerance for convergence - default = 1e-6.

4.33.2.5 double PICARD_DATA::res

Residual norm of the iterate.

4.33.2.6 double PICARD_DATA::relres

Relative residual norm of the iterate.

4.33.2.7 double PICARD_DATA::relres_base

Initial residual norm.

4.33.2.8 double PICARD_DATA::bestres

Best found residual norm.

4.33.2.9 bool PICARD_DATA::Output = true

True = print messages to console.

4.33.2.10 Matrix<double> PICARD_DATA::x0

Previous iterate solution vector.

4.33.2.11 Matrix<double> PICARD_DATA::bestx

Best found solution vector.

4.33.2.12 Matrix<double> PICARD_DATA::r

Residual of the non-linear system.

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

- lark.h

4.34 PJFNK_DATA Struct Reference

Data structure for the implementation of the PJFNK algorithm for non-linear systems.

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

Public Attributes

- int nl_iter = 0

  Number of non-linear iterations.
- int l_iter = 0

  Number of linear iterations.
- int nl_maxit = 0

  Maximum allowable non-linear steps.
- int linear_solver = -1

  Flag to denote which linear solver to use - default = PJFNK Chooses.
- double nl_tol_abs = 1e-6

  Absolute Convergence tolerance for non-linear system - default = 1e-6.
- double nl_tol_rel = 1e-6

  Relative Convergence tol for the non-linear system - default = 1e-6.
- double lin_tol_rel = 1e-6

  Relative tolerance of the linear solver - default = 1e-6.
- double lin_tol_abs = 1e-6

  Absolute tolerance of the linear solver - default = 1e-6.
- double nl_res

  Absolute redidual norm for the non-linear system.
- double nl_relres

  Relative residual for the non-linear system.
- double nl_res_base

  Initial residual norm for the non-linear system.
- double nl_bestres

  Best found residual norm.
- double eps =sqrt(DBL_EPSILON)

  Value of epsilon used jacvec - default = sqrt(DBL_EPSILON)
- bool NL_Output = true

  True = print PJFNK messages to console.
- bool L_Output = false

  True = print Linear messages to console.
- bool LineSearch = false

  True = use Backtracking Linesearch for global convergence.
- bool Bounce = false

  True = allow Linesearch to go outside local well, False = Strict local convergence.
- Matrix< double > F

Stored fuction evaluation at x (also the residual)

- Matrix< double > Fv

  Stored function evaluation at x+eps∗v.

- Matrix< double > v

  Stored vector of x+eps∗v.

- Matrix< double > x

  Current solution vector for the non-linear system.

- Matrix< double > bestx

  Best found solution vector to the non-linear system.

- GMRESLP_DATA gmreslp_dat

  Data structure for the GMRESLP method.

- PCG_DATA pcg_dat

  Data structure for the PCG method.

- BiCGSTAB_DATA bicgstab_dat

  Data structure for the BiCGSTAB method.

- CGS_DATA cgs_dat

  Data structure for the CGS method.

- GMRESRP_DATA gmresrp_dat

  Data structure for the GMRESRP method.

- GCR_DATA gcr_dat

  Data structure for the GCR method.

- GMRESR_DATA gmresr_dat

  Data structure for the GMRESR method.

- BACKTRACK_DATA backtrack_dat

  Data structure for the Backtracking Linesearch algorithm.

- const void ∗ res_data

  Data structure pointer for user's residual data.

- const void ∗ precon_data

  Data structure pointer for user's preconditioning data.

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

  Function pointer for the user's function F(x) using there data.

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

  Function pointer for the user's preconditioning function for the linear system.

4.34.1 Detailed Description

Data structure for the implementation of the PJFNK algorithm for non-linear systems.

C-style object to be used in conjunction with the Preconditioned Jacobian-Free Newton-Krylov (PJFNK) method for solving a non-linear system of equations. You can use any of the Krylov methods listed in the krylov_method enum to solve the linear sub-problem. When FOM is specified as the Krylov method, this algorithm becomes equivalent to an exact Newton method. If no Krylov method is specified, then the algorithm will try to pick a method based on the problem size and availability of preconditioning.

4.34.2 Member Data Documentation

4.34.2.1 int PJFNK_DATA::nl_iter = 0

Number of non-linear iterations.

4.34.2.2 int PJFNK_DATA::l_iter = 0

Number of linear iterations.

4.34.2.3 int PJFNK_DATA::nl_maxit = 0

Maximum allowable non-linear steps.

4.34.2.4 int PJFNK_DATA::linear_solver = -1

Flag to denote which linear solver to use - default = PJFNK Chooses.

4.34.2.5 double PJFNK_DATA::nl_tol_abs = 1e-6

Absolute Convergence tolerance for non-linear system - default = 1e-6.

4.34.2.6 double PJFNK_DATA::nl_tol_rel = 1e-6

Relative Convergence tol for the non-linear system - default = 1e-6.

4.34.2.7 double PJFNK_DATA::lin_tol_rel = 1e-6

Relative tolerance of the linear solver - default = 1e-6.

4.34.2.8 double PJFNK_DATA::lin_tol_abs = 1e-6

Absolute tolerance of the linear solver - default = 1e-6.

4.34.2.9 double PJFNK_DATA::nl_res

Absolute redidual norm for the non-linear system.

4.34.2.10 double PJFNK_DATA::nl_relres

Relative residual for the non-linear system.

4.34.2.11 double PJFNK_DATA::nl_res_base

Initial residual norm for the non-linear system.

4.34.2.12 double PJFNK_DATA::nl_bestres

Best found residual norm.

4.34.2.13 double PJFNK_DATA::eps =sqrt(DBL_EPSILON)

Value of epsilon used jacvec - default = sqrt(DBL_EPSILON)

4.34.2.14 bool PJFNK_DATA::NL_Output = true

True = print PJFNK messages to console.

4.34.2.15 bool PJFNK_DATA::L_Output = false

True = print Linear messages to console.

4.34.2.16 bool PJFNK_DATA::LineSearch = false

True = use Backtracking Linesearch for global convergence.

4.34.2.17 bool PJFNK_DATA::Bounce = false

True = allow Linesearch to go outside local well, False = Strict local convergence.

4.34.2.18 Matrix<double> PJFNK_DATA::F

Stored fuction evaluation at x (also the residual)

4.34.2.19 Matrix<double> PJFNK_DATA::Fv

Stored function evaluation at x+eps∗v.

4.34.2.20 Matrix<double> PJFNK_DATA::v

Stored vector of x+eps∗v.

4.34.2.21 Matrix<double> PJFNK_DATA::x

Current solution vector for the non-linear system.

4.34.2.22 Matrix<double> PJFNK_DATA::bestx

Best found solution vector to the non-linear system.

4.34.2.23 GMRESLP_DATA PJFNK_DATA::gmreslp_dat

Data structure for the GMRESLP method.

4.34.2.24 PCG_DATA PJFNK_DATA::pcg_dat

Data structure for the PCG method.

4.34.2.25 BiCGSTAB_DATA PJFNK_DATA::bicgstab_dat

Data structure for the BiCGSTAB method.

4.34.2.26 CGS_DATA PJFNK_DATA::cgs_dat

Data structure for the CGS method.

4.34.2.27 GMRESRP_DATA PJFNK_DATA::gmresrp_dat

Data structure for the GMRESRP method.

4.34.2.28 GCR_DATA PJFNK_DATA::gcr_dat

Data structure for the GCR method.

4.34.2.29 GMRESR_DATA PJFNK_DATA::gmresr_dat

Data structure for the GMRESR method.

4.34.2.30 BACKTRACK_DATA PJFNK_DATA::backtrack_dat

Data structure for the Backtracking Linesearch algorithm.

4.34.2.31 const void* PJFNK_DATA::res_data

Data structure pointer for user's residual data.

4.34.2.32 const void* PJFNK_DATA::precon_data

Data structure pointer for user's preconditioning data.

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

Function pointer for the user's function F(x) using there data.

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

Function pointer for the user's preconditioning function for the linear system.

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

- lark.h

4.35 PURE_GAS Struct Reference

Data structure holding all the parameters for each pure gas spieces.

`#include <egret.h>`

Public Attributes

- double molecular_weight
  Given: molecular weights (g/mol)

- double Sutherland_Temp

  Given: Sutherland's Reference Temperature (K)
- double Sutherland_Const

  Given: Sutherland's Constant (K)
- double Sutherland_Viscosity

  Given: Sutherland's Reference Viscosity (g/cm/s)
- double specific_heat

  Given: Specific heat of the gas (J/g/K)
- double molecular_diffusion

  Calculated: molecular diffusivities (cm^2/s)
- double dynamic_viscosity

  Calculated: dynamic viscosities (g/cm/s)
- double density

  Calculated: gas densities (g/cm^3) {use RE3}.
- double Schmidt

  Calculated: Value of the Schmidt number (-)

4.35.1 Detailed Description

Data structure holding all the parameters for each pure gas spieces.

C-style object that holds the constants and parameters associated with each pure gas species in the overall mixture. This information is used in conjunction with the kinetic theory of gases to produce approximations to many different gas properties needed in simulating gas dynamics, mobility of a gas through porous media, as well as some kinetic adsorption parameters such as diffusivities.

4.35.2 Member Data Documentation

4.35.2.1 double PURE_GAS::molecular_weight

Given: molecular weights (g/mol)

4.35.2.2 double PURE_GAS::Sutherland_Temp

Given: Sutherland's Reference Temperature (K)

4.35.2.3 double PURE_GAS::Sutherland_Const

Given: Sutherland's Constant (K)

4.35.2.4 double PURE_GAS::Sutherland_Viscosity

Given: Sutherland's Reference Viscosity (g/cm/s)

4.35.2.5 double PURE_GAS::specific_heat

Given: Specific heat of the gas (J/g/K)

4.35.2.6 double PURE_GAS::molecular_diffusion

Calculated: molecular diffusivities (cm^2/s)

4.35.2.7 double PURE_GAS::dynamic_viscosity

Calculated: dynamic viscosities (g/cm/s)

4.35.2.8 double PURE_GAS::density

Calculated: gas densities (g/cm^3) {use RE3}.

4.35.2.9 double PURE_GAS::Schmidt

Calculated: Value of the Schmidt number (-)

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

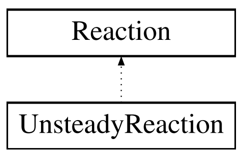
- egret.h

4.36 Reaction Class Reference

Reaction Object.

#include <shark.h>

Inheritance diagram for Reaction:



Public Member Functions

- Reaction ()
  Default constructor.
- ∼Reaction ()
  Default destructor.
- void Initialize_List (MasterSpeciesList &List)
  Function to initialize the Reaction object from the MasterSpeciesList.
- void Display_Info ()
  Display the reaction information.
- void Set_Stoichiometric (int i, double v)
  Set the ith stoichiometric value.
- void Set_Equilibrium (double logK)
  Set the equilibrium constant in log(K) units.
- void Set_Enthalpy (double H)
  Set the enthalpy of the reaction (J/mol)
- void Set_Entropy (double S)
  Set the entropy of the reaction (J/K/mol)
- void Set_EnthalpyANDEntropy (double H, double S)
  Set both the enthalpy and entropy (J/mol) & (J/K/mol)
- void Set_Energy (double G)
  Set the Gibb's free energy of reaction (J/mol)

- void checkSpeciesEnergies ()

  Function to check MasterList Reference for species energy info.
- void calculateEnergies ()
- void calculateEquilibrium (double T)

  Function to calculate the equilibrium constant based on temperature in K.
- bool haveEquilibrium ()

  Function to return true if equilibrium constant is given or can be calculated.
- double Get_Stoichiometric (int i)

  Fetch the ith stoichiometric value.
- double Get_Equilibrium ()

  Fetch the equilibrium constant (logK)
- double Get_Enthalpy ()

  Fetch the enthalpy of the reaction (J/mol)
- double Get_Entropy ()

  Fetch the entropy of the reaction (J/K/mol)
- double Get_Energy ()

  Fetch the energy of the reaction (J/mol)
- double Eval_Residual (const Matrix< double > &x, const Matrix< double > &gama)

Protected Attributes

- MasterSpeciesList ∗ List

  Pointer to a master species object.
- std::vector< double > Stoichiometric

  Vector of stoichiometric constants corresponding to species list.
- double Equilibrium

  Equilibrium constant for the reaction (logK)
- double enthalpy

  Reaction enthalpy (J/mol)
- double entropy

  Reaction entropy (J/K/mol)
- double energy

  Gibb's Free energy of reaction (J/mol)
- bool CanCalcHS

  True if all molecular info is avaiable to calculate dH and dS.
- bool CanCalcG

  True if all molecular info is available to calculate dG.
- bool HaveHS

  True if dH and dS is given, or can be calculated.
- bool HaveG

  True if dG is given, or can be calculated.
- bool HaveEquil

  True as long as Equilibrium is given, or can be calculated.

4.36.1 Detailed Description

Reaction Object.

C++ style object that holds data and functions associated with standard chemical reactions...

i.e., aA + bB <=> cC + dD

These reactions are assumed steady state and are characterized by stoichiometry coefficients and equilibrium/stability constants. Types of reactions that these are valid for would be acid/base reactions, metal-ligand complexation reactions, oxidation-reduction reactions, Henry's Law phase changes, and more. Reactions that this may not be suitable for include mechanisms, adsorption, and precipitation. Those types of reactions would be better handled by more specific objects that inherit from this object.

If all species in the reaction are registered and known species in mola.h AND have known formation energies, then the equilibrium constants for that particular reaction will be calculated based on the species involved in the reaction. However, if using some custom molecule objects, then the reaction equilibrium may not be able to be automatically formed by the routine. In this case, you would need to also supply the equilibrium constant for the particular reaction.

4.36.2 Constructor & Destructor Documentation

4.36.2.1 Reaction::Reaction ( )

Default constructor.

4.36.2.2 Reaction::∼Reaction ( )

Default destructor.

4.36.3 Member Function Documentation

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

Function to initialize the Reaction object from the MasterSpeciesList.

4.36.3.2 void Reaction::Display_Info ( )

Display the reaction information.

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

Set the ith stoichiometric value.

This function will set the stoichiometric constant of the ith species in the master list to the given value of v. All values of v are set to zero unless overriden by this function.

Parameters

i	index of the species in the MasterSpeciesList
v	value of the stoichiometric constant for that species in the reaction

4.36.3.4 void Reaction::Set_Equilibrium (double *logK*)

Set the equilibrium constant in log(K) units.

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

Set the enthalpy of the reaction (J/mol)

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

Set the entropy of the reaction (J/K/mol)

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

Set both the enthalpy and entropy (J/mol) & (J/K/mol)

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

Set the Gibb's free energy of reaction (J/mol)

4.36.3.9 void Reaction::checkSpeciesEnergies ( )

Function to check MasterList Reference for species energy info.

This function will go through the stoichiometry of this reaction and check the molecules in the MasterSpeciesList that correspond to the species present in this reaction for the existance of their formation energies. Based on the states of those energies, it will note internally whether or not it can determine the equilibrium constants based soley on individual species information. If it cannot, then the user must provide either the reaction energies to form the equilibrium constant or the equilibrium constant itself. Function to calculate and set the energy of the reaction

4.36.3.10 void Reaction::calculateEnergies ( )

If the energies of the reaction can be determined from the individual species in the reaction, then this function uses that information. Otherwise, it sets the energies equal to the constants given to the object by the user.

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

Function to calculate the equilibrium constant based on temperature in K.

4.36.3.12 bool Reaction::haveEquilibrium ( )

Function to return true if equilibrium constant is given or can be calculated.

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

Fetch the ith stoichiometric value.

4.36.3.14 double Reaction::Get_Equilibrium ( )

Fetch the equilibrium constant (logK)

4.36.3.15 double Reaction::Get_Enthalpy ( )

Fetch the enthalpy of the reaction (J/mol)

4.36.3.16 double Reaction::Get_Entropy ( )

Fetch the entropy of the reaction (J/K/mol)

4.36.3.17 double Reaction::Get_Energy ( )

Fetch the energy of the reaction (J/mol)

Evaluate a residual for the reaction given variable x=log(C) and activity coefficients gama

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

This function will calculate the reaction residual from this object's stoichiometry, equilibrium constant, log(C) concentrations, and activity coefficients.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
gama	matrix of activity coefficients for each species at the current non-linear step

4.36.4 Member Data Documentation

4.36.4.1 **MasterSpeciesList**∗ Reaction::List [protected]

Pointer to a master species object.

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

Vector of stoichiometric constants corresponding to species list.

4.36.4.3 double Reaction::Equilibrium [protected]

Equilibrium constant for the reaction (logK)

4.36.4.4 double Reaction::enthalpy [protected]

Reaction enthalpy (J/mol)

4.36.4.5 double Reaction::entropy [protected]

Reaction entropy (J/K/mol)

4.36.4.6 double Reaction::energy [protected]

Gibb's Free energy of reaction (J/mol)

4.36.4.7 bool Reaction::CanCalcHS [protected]

True if all molecular info is avaiable to calculate dH and dS.

4.36.4.8 bool Reaction::CanCalcG [protected]

True if all molecular info is available to calculate dG.

4.36.4.9 bool Reaction::HaveHS [protected]

True if dH and dS is given, or can be calculated.

4.36.4.10 bool Reaction::HaveG [protected]

True if dG is given, or can be calculated.

4.36.4.11 bool Reaction::HaveEquil [protected]

True as long as Equilibrium is given, or can be calculated.

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

- shark.h

4.37 SCOPSOWL_DATA Struct Reference

Primary data structure for SCOPSOWL simulations.

`#include <scopsowl.h>`

Public Attributes

- unsigned long int total_steps

  Running total of all calculation steps.
- int coord_macro

  Coordinate system for large pellet.
- int coord_micro

  Coordinate system for small crystal (if any)
- int level = 2

  Level of coupling between the different scales (default = 2)
- double sim_time

  Stopping time for the simulation (hrs)
- double t_old

  Old time of the simulations (hrs)
- double t

  Current time of the simulations (hrs)
- double t_counter = 0.0

  Counter for the time output.
- double t_print

  Print output at every t_print time (hrs)
- bool Print2File = true

  True = results to .txt; False = no printing.
- bool Print2Console = true

  True = results to console; False = no printing.
- bool SurfDiff = true

True = includes SKUA simulation if Heterogeneous; False = only uses MAGPIE.

- bool Heterogeneous = true

  True = pellet is made of binder and crystals, False = all one phase.

- double gas_velocity

  Superficial Gas Velocity arount pellet (cm/s)

- double total_pressure

  Gas phase total pressure (kPa)

- double gas_temperature

  Gas phase temperature (K)

- double pellet_radius

  Nominal radius of the pellet - macroscale domain (cm)

- double crystal_radius

  Nominal radius of the crystal - microscale domain (um)

- double char_macro

  Characteristic size for macro scale (cm or cm^2) - only if pellet is not spherical.

- double char_micro

  Characteristic size for micro scale (um or um^2) - only if crystal is not spherical.

- double binder_fraction

  Volume of binder per total volume of pellet (-)

- double binder_porosity

  Volume of pores per volume of binder (-)

- double binder_poresize

  Nominal radius of the binder pores (cm)

- double pellet_density

  Mass of the pellet per volume of pellet (kg/L)

- bool DirichletBC = false

  True = Dirichlet BC; False = Neumann BC.

- bool NonLinear = true

  True = Non-linear solver; False = Linear solver.

- std::vector< double > y

  Outside mole fractions of each component (-)

- std::vector< double > tempy

  Temporary place holder for gas mole fractions in other locations (-)

- FILE * OutputFile

  Output file pointer to the output file for postprocesses.

- double(* eval_ads)(int i, int l, const void *user_data)

  Function pointer for evaluating adsorption (mol/kg)

- double(* eval_retard)(int i, int l, const void *user_data)

  Function pointer for evaluating retardation (-)

- double(* eval_diff)(int i, int l, const void *user_data)

  Function pointer for evaluating pore diffusion (cm^2/hr)

- double(* eval_surfDiff)(int i, int l, const void *user_data)

  Function pointer for evaluating surface diffusion (um^2/hr)

- double(* eval_kf)(int i, const void *user_data)

  Function pointer for evaluating film mass transfer (cm/hr)

- const void * user_data

  Data structure for users info to calculate parameters.

- MIXED_GAS * gas_dat

  Pointer to the MIXED_GAS data structure (may or may not be used)

- MAGPIE_DATA magpie_dat

  Data structure for a magpie problem (to be used if not using skua)

- std::vector< FINCH_DATA > finch_dat

  Data structure for pore adsorption kinetics for all species (u in mol/L)
- std::vector< SCOPSOWL_PARAM_DATA > param_dat

  Data structure for parameter info for all species.
- std::vector< SKUA_DATA > skua_dat

  Data structure holding a skua object for all nodes (each skua has an object for each species)

4.37.1 Detailed Description

Primary data structure for SCOPSOWL simulations.

C-style object holding necessary information to run a SCOPSOWL simulation. SCOPSOWL is a multi-scale problem involving PDE solution for the macro-scale adsorbent pellet and the micro-scale adsorbent crystals. As such, each SCOPSOWL simulation involves multiple SKUA simulations at the nodes in the macro-scale domain. Alternatively, if the user wishes to specify that the adsorbent is homogeneous, then you can run SCOPSOWL as a single-scale problem. Additionally, you can simplfy the model by assuming that the micro-scale diffusion is very fast, and therefore replace each SKUA simulation with a simpler MAGPIE evaluation. Details on running SCOPSOWL with the various options will be discussed in the SCOPSOWL_SCENARIOS function.

4.37.2 Member Data Documentation

4.37.2.1 unsigned long int SCOPSOWL_DATA::total_steps

Running total of all calculation steps.

4.37.2.2 int SCOPSOWL_DATA::coord_macro

Coordinate system for large pellet.

4.37.2.3 int SCOPSOWL_DATA::coord_micro

Coordinate system for small crystal (if any)

4.37.2.4 int SCOPSOWL_DATA::level = 2

Level of coupling between the different scales (default = 2)

4.37.2.5 double SCOPSOWL_DATA::sim_time

Stopping time for the simulation (hrs)

4.37.2.6 double SCOPSOWL_DATA::t_old

Old time of the simulations (hrs)

4.37.2.7 double SCOPSOWL_DATA::t

Current time of the simulations (hrs)

4.37.2.8 double SCOPSOWL_DATA::t_counter = 0.0

Counter for the time output.

4.37.2.9 double SCOPSOWL_DATA::t_print

Print output at every t_print time (hrs)

4.37.2.10 bool SCOPSOWL_DATA::Print2File = true

True = results to .txt; False = no printing.

4.37.2.11 bool SCOPSOWL_DATA::Print2Console = true

True = results to console; False = no printing.

4.37.2.12 bool SCOPSOWL_DATA::SurfDiff = true

True = includes SKUA simulation if Heterogeneous; False = only uses MAGPIE.

4.37.2.13 bool SCOPSOWL_DATA::Heterogeneous = true

True = pellet is made of binder and crystals, False = all one phase.

4.37.2.14 double SCOPSOWL_DATA::gas_velocity

Superficial Gas Velocity arount pellet (cm/s)

4.37.2.15 double SCOPSOWL_DATA::total_pressure

Gas phase total pressure (kPa)

4.37.2.16 double SCOPSOWL_DATA::gas_temperature

Gas phase temperature (K)

4.37.2.17 double SCOPSOWL_DATA::pellet_radius

Nominal radius of the pellet - macroscale domain (cm)

4.37.2.18 double SCOPSOWL_DATA::crystal_radius

Nominal radius of the crystal - microscale domain (um)

4.37.2.19 double SCOPSOWL_DATA::char_macro

Characteristic size for macro scale (cm or cm^2) - only if pellet is not spherical.

4.37.2.20 double SCOPSOWL_DATA::char_micro

Characteristic size for micro scale (um or um^2) - only if crystal is not spherical.

4.37.2.21 double SCOPSOWL_DATA::binder_fraction

Volume of binder per total volume of pellet (-)

4.37.2.22 double SCOPSOWL_DATA::binder_porosity

Volume of pores per volume of binder (-)

4.37.2.23 double SCOPSOWL_DATA::binder_poresize

Nominal radius of the binder pores (cm)

4.37.2.24 double SCOPSOWL_DATA::pellet_density

Mass of the pellet per volume of pellet (kg/L)

4.37.2.25 bool SCOPSOWL_DATA::DirichletBC = false

True = Dirichlet BC; False = Neumann BC.

4.37.2.26 bool SCOPSOWL_DATA::NonLinear = true

True = Non-linear solver; False = Linear solver.

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

Outside mole fractions of each component (-)

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

Temporary place holder for gas mole fractions in other locations (-)

4.37.2.29 FILE* SCOPSOWL_DATA::OutputFile

Output file pointer to the output file for postprocesses.

4.37.2.30 double(* SCOPSOWL_DATA::eval_ads)(int i, int l, const void *user_data)

Function pointer for evaluating adsorption (mol/kg)

4.37.2.31 double(* SCOPSOWL_DATA::eval_retard)(int i, int l, const void *user_data)

Function pointer for evaluating retardation (-)

4.37.2.32 double(* SCOPSOWL_DATA::eval_diff)(int i, int l, const void *user_data)

Function pointer for evaluating pore diffusion (cm^2/hr)

4.37.2.33 double(* SCOPSOWL_DATA::eval_surfDiff)(int i, int l, const void *user_data)

Function pointer for evaluating surface diffusion (um^2/hr)

4.37.2.34 double(* SCOPSOWL_DATA::eval_kf)(int i, const void *user_data)

Function pointer for evaluating film mass transfer (cm/hr)

4.37.2.35 const void* SCOPSOWL_DATA::user_data

Data structure for users info to calculate parameters.

4.37.2.36 MIXED_GAS* SCOPSOWL_DATA::gas_dat

Pointer to the MIXED_GAS data structure (may or may not be used)

4.37.2.37 MAGPIE_DATA SCOPSOWL_DATA::magpie_dat

Data structure for a magpie problem (to be used if not using skua)

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

Data structure for pore adsorption kinetics for all species (u in mol/L)

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

Data structure for parameter info for all species.

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

Data structure holding a skua object for all nodes (each skua has an object for each species)

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

- scopsowl.h

4.38 SCOPSOWL_OPT_DATA Struct Reference

Data structure for the SCOPSOWL optmization routine.

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

Public Attributes

- int num_curves

  Number of adsorption curves to analyze.

- int evaluation

  Number of times the eval function has been called for a single curve.
- unsigned long int total_eval

  Total number of evaluations needed for completion.
- int current_points

  Number of points in the current curve.
- int num_params = 1

  Number of adjustable parameters for the current curve (currently only supports 1)
- int diffusion_type

  Flag to identify type of diffusion function to use.
- int adsorb_index

  Component index for adsorbable species.
- int max_guess_iter = 20

  Maximum allowed guess iterations (default = 20)
- bool Optimize

  True = run optimization, False = run a comparison.
- bool Rough

  True = use only a rough estimate, False = run full optimization.
- double current_temp

  Temperature for current curve.
- double current_press

  Partial pressure for current curve.
- double current_equil

  Equilibrium data point for the current curve.
- double simulation_equil

  Equilibrium simulation point for the current curve.
- double max_bias

  Positive maximum bias plausible for fitting.
- double min_bias

  Negative minimum bias plausible for fitting.
- double e_norm

  Euclidean norm of current fit.
- double f_bias

  Function bias of current fit.
- double e_norm_old

  Euclidean norm of the previous fit.
- double f_bias_old

  Function bias of the previous fit.
- double param_guess

  Parameter guess for the surface/crystal diffusivity.
- double param_guess_old

  Parameter guess for the previous curve.
- double rel_tol_norm = 0.01

  Tolerance for convergence of the guess norm.
- double abs_tol_bias = 1.0

  Tolerance for convergence of the guess bias.
- std::vector< double > y_base

  Gas phase mole fractions in absense of adsorbing species.
- std::vector< double > q_data

  Amount adsorbed at a particular point in current curve.
- std::vector< double > q_sim

Amount adsorbed based on the simulation.

- std::vector< double > t

  Time points in the current curve.

- FILE ∗ ParamFile

  Output file for parameter results.

- FILE ∗ CompareFile

  Output file for comparison of results.

- SCOPSOWL_DATA owl_dat

  Data structure for the SCOPSOWL simulation.

4.38.1 Detailed Description

Data structure for the SCOPSOWL optmization routine.

C-style object holding information about the optimization routine as well as the standard SCOPSOwl_DATA structure for SCOPSOWL simulations.

4.38.2 Member Data Documentation

4.38.2.1 int SCOPSOWL_OPT_DATA::num_curves

Number of adsorption curves to analyze.

4.38.2.2 int SCOPSOWL_OPT_DATA::evaluation

Number of times the eval function has been called for a single curve.

4.38.2.3 unsigned long int SCOPSOWL_OPT_DATA::total_eval

Total number of evaluations needed for completion.

4.38.2.4 int SCOPSOWL_OPT_DATA::current_points

Number of points in the current curve.

4.38.2.5 int SCOPSOWL_OPT_DATA::num_params = 1

Number of adjustable parameters for the current curve (currently only supports 1)

4.38.2.6 int SCOPSOWL_OPT_DATA::diffusion_type

Flag to identify type of diffusion function to use.

4.38.2.7 int SCOPSOWL_OPT_DATA::adsorb_index

Component index for adsorbable species.

4.38.2.8 int SCOPSOWL_OPT_DATA::max_guess_iter = 20

Maximum allowed guess iterations (default = 20)

4.38.2.9 bool SCOPSOWL_OPT_DATA::Optimize

True = run optimization, False = run a comparison.

4.38.2.10 bool SCOPSOWL_OPT_DATA::Rough

True = use only a rough estimate, False = run full optimization.

4.38.2.11 double SCOPSOWL_OPT_DATA::current_temp

Temperature for current curve.

4.38.2.12 double SCOPSOWL_OPT_DATA::current_press

Partial pressure for current curve.

4.38.2.13 double SCOPSOWL_OPT_DATA::current_equil

Equilibrium data point for the current curve.

4.38.2.14 double SCOPSOWL_OPT_DATA::simulation_equil

Equilibrium simulation point for the current curve.

4.38.2.15 double SCOPSOWL_OPT_DATA::max_bias

Positive maximum bias plausible for fitting.

4.38.2.16 double SCOPSOWL_OPT_DATA::min_bias

Negative minimum bias plausible for fitting.

4.38.2.17 double SCOPSOWL_OPT_DATA::e_norm

Euclidean norm of current fit.

4.38.2.18 double SCOPSOWL_OPT_DATA::f_bias

Function bias of current fit.

4.38.2.19 double SCOPSOWL_OPT_DATA::e_norm_old

Euclidean norm of the previous fit.

4.38.2.20 double SCOPSOWL_OPT_DATA::f_bias_old

Function bias of the previous fit.

4.38.2.21 double SCOPSOWL_OPT_DATA::param_guess

Parameter guess for the surface/crystal diffusivity.

4.38.2.22 double SCOPSOWL_OPT_DATA::param_guess_old

Parameter guess for the previous curve.

4.38.2.23 double SCOPSOWL_OPT_DATA::rel_tol_norm = 0.01

Tolerance for convergence of the guess norm.

4.38.2.24 double SCOPSOWL_OPT_DATA::abs_tol_bias = 1.0

Tolerance for convergence of the guess bias.

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

Gas phase mole fractions in absense of adsorbing species.

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

Amount adsorbed at a particular point in current curve.

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

Amount adsorbed based on the simulation.

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

Time points in the current curve.

4.38.2.29 FILE∗ SCOPSOWL_OPT_DATA::ParamFile

Output file for parameter results.

4.38.2.30 FILE∗ SCOPSOWL_OPT_DATA::CompareFile

Output file for comparison of results.

4.38.2.31 SCOPSOWL_DATA SCOPSOWL_OPT_DATA::owl_dat

Data structure for the SCOPSOWL simulation.

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

- scopsowl_opt.h

4.39 SCOPSOWL_PARAM_DATA Struct Reference

Data structure for the species' parameters in SCOPSOWL.

`#include <scopsowl.h>`

Public Attributes

- Matrix< double > qAvg

  Average adsorbed amount for a species at each node (mol/kg)
- Matrix< double > qAvg_old

  Old Average adsorbed amount for a species at each node (mol/kg)
- Matrix< double > Qst

  Heat of adsorption for all nodes (J/mol)
- Matrix< double > Qst_old

  Old Heat of adsorption for all nodes (J/mol)
- Matrix< double > dq_dc

  Storage vector for current adsorption slope/strength (dq/dc) (L/kg)
- double xIC

  Initial conditions for adsorbed molefractions.
- double qIntegralAvg

  Integral average of adsorption over the entire pellet (mol/kg)
- double qIntegralAvg_old

  Old Integral average of adsorption over the entire pellet (mol/kg)
- double QstAvg

  Integral average heat of adsorption (J/mol)
- double QstAvg_old

  Old integral average heat of adsorption (J/mol)
- double qo

  Boundary value of adsorption if using Dirichlet BCs (mol/kg)
- double Qsto

  Boundary value of adsorption heat if using Dirichlet BCs (J/mol)
- double dq_dco

  Boundary value of adsorption slope for Dirichelt BCs (L/kg)
- double pore_diffusion

  Value for constant pore diffusion (cm^2/hr)
- double film_transfer

  Value for constant film mass transfer (cm/hr)
- double activation_energy

  Activation energy for surface diffusion (J/mol)
- double ref_diffusion

  Reference state surface diffusivity (um^2/hr)
- double ref_temperature

  Reference temperature for empirical adjustments (K)
- double affinity

  Affinity parameter used in empirical adjustments (-)
- double ref_pressure
- bool Adsorbable

  True = species can adsorb; False = species cannot adsorb.
- std::string speciesName

  String to hold the name of each species.

4.39.1 Detailed Description

Data structure for the species' parameters in SCOPSOWL.

C-style object that holds information on all species for a particular SCOPSOWL simulation. Initial conditions, kinetic parameters, and interim matrix objects are stored here for use in various SCOSPSOWL functions.

4.39.2 Member Data Documentation

4.39.2.1 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg

Average adsorbed amount for a species at each node (mol/kg)

4.39.2.2 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg_old

Old Average adsorbed amount for a species at each node (mol/kg)

4.39.2.3 Matrix<double> SCOPSOWL_PARAM_DATA::Qst

Heat of adsorption for all nodes (J/mol)

4.39.2.4 Matrix<double> SCOPSOWL_PARAM_DATA::Qst_old

Old Heat of adsorption for all nodes (J/mol)

4.39.2.5 Matrix<double> SCOPSOWL_PARAM_DATA::dq_dc

Storage vector for current adsorption slope/strength (dq/dc) (L/kg)

4.39.2.6 double SCOPSOWL_PARAM_DATA::xIC

Initial conditions for adsorbed molefractions.

4.39.2.7 double SCOPSOWL_PARAM_DATA::qIntegralAvg

Integral average of adsorption over the entire pellet (mol/kg)

4.39.2.8 double SCOPSOWL_PARAM_DATA::qIntegralAvg_old

Old Integral average of adsorption over the entire pellet (mol/kg)

4.39.2.9 double SCOPSOWL_PARAM_DATA::QstAvg

Integral average heat of adsorption (J/mol)

4.39.2.10 double SCOPSOWL_PARAM_DATA::QstAvg_old

Old integral average heat of adsorption (J/mol)

4.39.2.11 double SCOPSOWL_PARAM_DATA::qo

Boundary value of adsorption if using Dirichlet BCs (mol/kg)

4.39.2.12 double SCOPSOWL_PARAM_DATA::Qsto

Boundary value of adsorption heat if using Dirichlet BCs (J/mol)

4.39.2.13 double SCOPSOWL_PARAM_DATA::dq_dco

Boundary value of adsorption slope for Dirichelt BCs (L/kg)

4.39.2.14 double SCOPSOWL_PARAM_DATA::pore_diffusion

Value for constant pore diffusion (cm^2/hr)

4.39.2.15 double SCOPSOWL_PARAM_DATA::film_transfer

Value for constant film mass transfer (cm/hr)

4.39.2.16 double SCOPSOWL_PARAM_DATA::activation_energy

Activation energy for surface diffusion (J/mol)

4.39.2.17 double SCOPSOWL_PARAM_DATA::ref_diffusion

Reference state surface diffusivity (um^2/hr)

4.39.2.18 double SCOPSOWL_PARAM_DATA::ref_temperature

Reference temperature for empirical adjustments (K)

4.39.2.19 double SCOPSOWL_PARAM_DATA::affinity

Affinity parameter used in empirical adjustments (-)

4.39.2.20 double SCOPSOWL_PARAM_DATA::ref_pressure

4.39.2.21 bool SCOPSOWL_PARAM_DATA::Adsorbable

True = species can adsorb; False = species cannot adsorb.

4.39.2.22 std::string SCOPSOWL_PARAM_DATA::speciesName

String to hold the name of each species.

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

- scopsowl.h

4.40 SHARK_DATA Struct Reference

Data structure for SHARK simulations.

`#include <shark.h>`

Public Attributes

- MasterSpeciesList MasterList

    Master List of species object.
- std::vector< Reaction > ReactionList

    Equilibrium reaction objects.
- std::vector< MassBalance > MassBalanceList

    Mass balance objects.
- std::vector< UnsteadyReaction > UnsteadyList

    Unsteady Reaction objects.
- std::vector< double(*)(const Matrix< double > &x, SHARK_DATA *shark_dat, const void *data) > OtherList

    Array of Other Residual functions to be defined by user.
- int numvar

    Total number of functions and species.
- int num_ssr

    Number of steady-state reactions.
- int num_mbe

    Number of mass balance equations.
- int num_usr

    Number of unsteady-state reactions.
- int num_other = 0

    Number of other functions to be used (default is always 0)
- int act_fun = IDEAL

    Flag denoting the activity function to use (default is IDEAL)
- int totalsteps = 0

    Number of iterations and function calls.
- int timesteps = 0

    Number of time steps taken to complete simulation.
- int pH_index = -1

    Contains the index of the pH variable (set internally)
- int pOH_index = -1

    Contains the index of the pOH variable (set internally)
- double simulationtime = 0.0

    Time to simulate unsteady reactions for (default = 0.0 hrs)
- double dt = 0.1

    Time step size (hrs)
- double dt_min = sqrt(DBL_EPSILON)

    Minimum allowable step size.
- double t_out = 0.0

    Time increment by which file output is made (default = print all time steps)
- double t_count = 0.0

    Running count of time increments.

- double time = 0.0

    Current value of time (starts from t = 0.0 hrs)
- double time_old = 0.0

    Previous value of time (start from t = 0.0 hrs)
- double pH = 7.0

    Value of pH if needed (default = 7)
- double Norm = 0.0

    Current value of euclidean norm in solution.
- double dielectric_const = 78.325

    Dielectric constant used in many activity models (default: water = 78.325 (1/K))
- double temperature = 298.15

    Solution temperature (default = 25 oC or 298.15 K)
- bool steadystate = true

    True = solve steady problem; False = solve transient problem.
- bool TimeAdaptivity = false

    True = solve using variable time step.
- bool const_pH = false

    True = set pH to a constant; False = solve for pH.
- bool SpeciationCurve = false

    True = runs a series of constant pH steady-state problems to produce curves.
- bool Console_Output = true

    True = display output to console.
- bool File_Output = false

    True = write output to a file.
- bool Contains_pH = false

    True = system contains pH as a variable (set internally)
- bool Contains_pOH = false

    True = system contains pOH as a variable (set internally)
- bool Converged = false

    True = system converged within tolerance.
- Matrix< double > X_old

    Solution vector for old time step - log(C)
- Matrix< double > X_new

    Solution vector for current time step - log(C)
- Matrix< double > Conc_old

    Concentration vector for old time step - 10^x.
- Matrix< double > Conc_new

    Concentration vector for current time step - 10^x.
- Matrix< double > activity_new

    Activity matrix for current time step.
- Matrix< double > activity_old

    Activity matrix from prior time step.
- int(∗ EvalActivity)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)

    Function pointer to evaluate activity coefficients.
- int(∗ Residual)(const Matrix< double > &x, Matrix< double > &F, const void ∗data)

    Function pointer to evaluate all residuals in the system.
- int(∗ lin_precon)(const Matrix< double > &r, Matrix< double > &p, const void ∗data)

    Function pointer to form a linear preconditioning operation for the Jacobian.
- PJFNK_DATA Newton_data

    Data structure for the Newton-Krylov solver (see lark.h)
- const void ∗ activity_data

User defined data structure for an activity model.
- const void * residual_data

  User defined data structure for the residual function.
- const void * precon_data

  User defined data structure for preconditioning.
- const void * other_data

  User define data structure used for user defined residuals.
- FILE * OutputFile

  Output File pointer.
- yaml_cpp_class yaml_object

  yaml object to read and access digitized yaml documents (see yaml_wrapper.h)

4.40.1 Detailed Description

Data structure for SHARK simulations.

C-style object holding data and function pointers associated with solving aqueous speciation and reaction kinetics. This object couples all other objects available in shark.h in order to provide residual calculations for each individual function that makes up the overall system model. Those residuals are brought together inside the residual function and fed into the lark.h PJFNK solver routine. That solver then attempts to find a solution to all non-linear variables simultaneously. Any function or data pointers in this structure can be overriden to change how you interface with and solve the problem. Users may also provide a set of custom residual functions through the "OtherList" vector object. Those residual function must all have the same format.

4.40.2 Member Data Documentation

4.40.2.1 MasterSpeciesList SHARK_DATA::MasterList

Master List of species object.

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

Equilibrium reaction objects.

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

Mass balance objects.

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

Unsteady Reaction objects.

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

Array of Other Residual functions to be defined by user.

This list of function pointers can be declared and set up by the user in order to add to or change the behavior of the SHARK system. Each one must be declared setup individually by the user. They will be called by the shark-_residual function when needed. Alternatively, the user is free to provide their own shark_residual function for the overall system.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
shark_dat	pointer to the SHARK_DATA data structure
data	pointer to a user defined data structure that is used to evaluate this residual

4.40.2.6 int SHARK_DATA::numvar

Total number of functions and species.

4.40.2.7 int SHARK_DATA::num_ssr

Number of steady-state reactions.

4.40.2.8 int SHARK_DATA::num_mbe

Number of mass balance equations.

4.40.2.9 int SHARK_DATA::num_usr

Number of unsteady-state reactions.

4.40.2.10 int SHARK_DATA::num_other = 0

Number of other functions to be used (default is always 0)

4.40.2.11 int SHARK_DATA::act_fun = IDEAL

Flag denoting the activity function to use (default is IDEAL)

4.40.2.12 int SHARK_DATA::totalsteps = 0

Number of iterations and function calls.

4.40.2.13 int SHARK_DATA::timesteps = 0

Number of time steps taken to complete simulation.

4.40.2.14 int SHARK_DATA::pH_index = -1

Contains the index of the pH variable (set internally)

4.40.2.15 int SHARK_DATA::pOH_index = -1

Contains the index of the pOH variable (set internally)

4.40.2.16 double SHARK_DATA::simulationtime = 0.0

Time to simulate unsteady reactions for (default = 0.0 hrs)

4.40.2.17 double SHARK_DATA::dt = 0.1

Time step size (hrs)

4.40.2.18 double SHARK_DATA::dt_min = sqrt(DBL_EPSILON)

Minimum allowable step size.

4.40.2.19 double SHARK_DATA::t_out = 0.0

Time increment by which file output is made (default = print all time steps)

4.40.2.20 double SHARK_DATA::t_count = 0.0

Running count of time increments.

4.40.2.21 double SHARK_DATA::time = 0.0

Current value of time (starts from t = 0.0 hrs)

4.40.2.22 double SHARK_DATA::time_old = 0.0

Previous value of time (start from t = 0.0 hrs)

4.40.2.23 double SHARK_DATA::pH = 7.0

Value of pH if needed (default = 7)

4.40.2.24 double SHARK_DATA::Norm = 0.0

Current value of euclidean norm in solution.

4.40.2.25 double SHARK_DATA::dielectric_const = 78.325

Dielectric constant used in many activity models (default: water = 78.325 (1/K))

4.40.2.26 double SHARK_DATA::temperature = 298.15

Solution temperature (default = 25 oC or 298.15 K)

4.40.2.27 bool SHARK_DATA::steadystate = true

True = solve steady problem; False = solve transient problem.

4.40.2.28 bool SHARK_DATA::TimeAdaptivity = false

True = solve using variable time step.

4.40.2.29 bool SHARK_DATA::const_pH = false

True = set pH to a constant; False = solve for pH.

4.40.2.30 bool SHARK_DATA::SpeciationCurve = false

True = runs a series of constant pH steady-state problems to produce curves.

4.40.2.31 bool SHARK_DATA::Console_Output = true

True = display output to console.

4.40.2.32 bool SHARK_DATA::File_Output = false

True = write output to a file.

4.40.2.33 bool SHARK_DATA::Contains_pH = false

True = system contains pH as a variable (set internally)

4.40.2.34 bool SHARK_DATA::Contains_pOH = false

True = system contains pOH as a variable (set internally)

4.40.2.35 bool SHARK_DATA::Converged = false

True = system converged within tolerance.

4.40.2.36 Matrix<double> SHARK_DATA::X_old

Solution vector for old time step - log(C)

4.40.2.37 Matrix<double> SHARK_DATA::X_new

Solution vector for current time step - log(C)

4.40.2.38 Matrix<double> SHARK_DATA::Conc_old

Concentration vector for old time step - 10^x.

4.40.2.39 Matrix<double> SHARK_DATA::Conc_new

Concentration vector for current time step - 10^x.

4.40.2.40 Matrix<double> SHARK_DATA::activity_new

Activity matrix for current time step.

4.40.2.41 Matrix< double > SHARK_DATA::activity_old

Activity matrix from prior time step.

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

Function pointer to evaluate activity coefficients.

This function pointer is called within the shark_residual function to calculate and modify the activity_new matrix entries. When using the SHARK default options, this function pointer will be automatically set to a cooresponding activity function for the list of valid functions from the valid_act enum. User may override this function pointer if they desire. Must be overriden after calling the setup function.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
F	matrix of activity coefficients that are to be altered by this function
data	pointer to a data structure needed to evaluate the activity model

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

Function pointer to evaluate all residuals in the system.

This function will be fed into the PJFNK solver (see lark.h) to solve the non-linear system of equations. By default, this pointer will be the shark_residual function (see below). However, the user may override the function and provide their own residuals for the PJFNK solver to operate on.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
F	matrix of residuals that are to be altered from the functions in the system
data	pointer to a data structure needed to evaluate the activity model

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

Function pointer to form a linear preconditioning operation for the Jacobian.

This function will be fed into the linear solver used for each non-linear step in PJFNK (see lark.h). By default, we cannot provide any linear preconditioner, because we do not know the form or sparcity of the Jacobian before hand. It will be the user's responsibility to form their own preconditioner until we can figure out a generic way to precondition the system.

4.40.2.45 PJFNK_DATA SHARK_DATA::Newton_data

Data structure for the Newton-Krylov solver (see lark.h)

4.40.2.46 const void* SHARK_DATA::activity_data

User defined data structure for an activity model.

4.40.2.47 const void* SHARK_DATA::residual_data

User defined data structure for the residual function.

4.40.2.48 const void* SHARK_DATA::precon_data

User defined data structure for preconditioning.

4.40.2.49 const void* SHARK_DATA::other_data

User define data structure used for user defined residuals.

4.40.2.50 FILE* SHARK_DATA::OutputFile

Output File pointer.

4.40.2.51 yaml_cpp_class SHARK_DATA::yaml_object

yaml object to read and access digitized yaml documents (see yaml_wrapper.h)

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

- shark.h

4.41 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

4.41.1 Member Data Documentation

4.41.1.1 unsigned long int SKUA_DATA::total_steps

4.41.1.2 int SKUA_DATA::coord

4.41.1.3 double SKUA_DATA::sim_time

4.41.1.4 double SKUA_DATA::t_old

4.41.1.5 double SKUA_DATA::t

4.41.1.6 double SKUA_DATA::t_counter = 0.0

4.41.1.7 double SKUA_DATA::t_print

4.41.1.8 double SKUA_DATA::qTn

4.41.1.9 double SKUA_DATA::qTnp1

4.41.1.10 bool SKUA_DATA::Print2File = true

4.41.1.11 bool SKUA_DATA::Print2Console = true

4.41.1.12 double SKUA_DATA::gas_velocity

4.41.1.13 double SKUA_DATA::pellet_radius

4.41.1.14 double SKUA_DATA::char_measure

4.41.1.15 bool SKUA_DATA::DirichletBC = true

4.41.1.16 bool SKUA_DATA::NonLinear = true

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

4.41.1.18 FILE* SKUA_DATA::OutputFile

4.41.1.19 double(* SKUA_DATA::eval_diff)(int i, int l, const void *user_data)

4.41.1.20 double(* SKUA_DATA::eval_kf)(int i, const void *user_data)

4.41.1.21 const void* SKUA_DATA::user_data

4.41.1.22 MAGPIE_DATA SKUA_DATA::magpie_dat

4.41.1.23 MIXED_GAS* SKUA_DATA::gas_dat

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

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

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

- skua.h

4.42 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

4.42.1 Member Data Documentation

4.42.1.1 int SKUA_OPT_DATA::num_curves

4.42.1.2 int SKUA_OPT_DATA::evaluation

4.42.1.3 unsigned long int SKUA_OPT_DATA::total_eval

4.42.1.4 int SKUA_OPT_DATA::current_points

4.42.1.5 int SKUA_OPT_DATA::num_params = 1

4.42.1.6 int SKUA_OPT_DATA::diffusion_type

4.42.1.7 int SKUA_OPT_DATA::adsorb_index

4.42.1.8 int SKUA_OPT_DATA::max_guess_iter = 20

4.42.1.9 bool SKUA_OPT_DATA::Optimize

4.42.1.10 bool SKUA_OPT_DATA::Rough

4.42.1.11 double SKUA_OPT_DATA::current_temp

4.42.1.12 double SKUA_OPT_DATA::current_press

4.42.1.13 double SKUA_OPT_DATA::current_equil

4.42.1.14 double SKUA_OPT_DATA::simulation_equil

4.42.1.15 double SKUA_OPT_DATA::max_bias

4.42.1.16 double SKUA_OPT_DATA::min_bias

4.42.1.17 double SKUA_OPT_DATA::e_norm

4.42.1.18 double SKUA_OPT_DATA::f_bias

4.42.1.19 double SKUA_OPT_DATA::e_norm_old

4.42.1.20 double SKUA_OPT_DATA::f_bias_old

4.42.1.21 double SKUA_OPT_DATA::param_guess

4.42.1.22 double SKUA_OPT_DATA::param_guess_old

4.42.1.23 double SKUA_OPT_DATA::rel_tol_norm = 0.1

4.42.1.24 double SKUA_OPT_DATA::abs_tol_bias = 0.1

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

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

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

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

4.42.1.29 FILE* SKUA_OPT_DATA::ParamFile

4.42.1.30 FILE* SKUA_OPT_DATA::CompareFile

4.42.1.31 SKUA_DATA SKUA_OPT_DATA::skua_dat

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

- skua_opt.h

4.43 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

4.43.1 Member Data Documentation

4.43.1.1 double SKUA_PARAM::activation_energy

4.43.1.2 double SKUA_PARAM::ref_diffusion

4.43.1.3 double SKUA_PARAM::ref_temperature

4.43.1.4 double SKUA_PARAM::affinity

4.43.1.5 double SKUA_PARAM::ref_pressure

4.43.1.6 double SKUA_PARAM::film_transfer

4.43.1.7 double SKUA_PARAM::xIC

4.43.1.8 double SKUA_PARAM::y_eff

4.43.1.9 double SKUA_PARAM::Qstn

4.43.1.10 double SKUA_PARAM::Qstnp1

4.43.1.11 double SKUA_PARAM::xn

4.43.1.12 double SKUA_PARAM::xnp1

4.43.1.13 bool SKUA_PARAM::Adsorbable

4.43.1.14 std::string SKUA_PARAM::speciesName

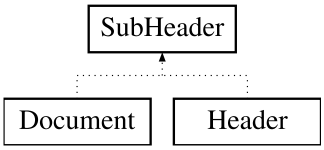
The documentation for this struct was generated from the following file:

- skua.h

4.44 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

4.44.1 Constructor & Destructor Documentation

4.44.1.1 SubHeader::SubHeader ( )

4.44.1.2 SubHeader::~SubHeader ( )

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

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

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

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

4.44.2 Member Function Documentation

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

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

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

4.44.2.4 KeyValueMap& SubHeader::getMap ( )

4.44.2.5 void SubHeader::clear ( )

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

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

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

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

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

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

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

4.44.2.13 void SubHeader::DisplayContents ( )

4.44.2.14 std::string SubHeader::getName ( )

4.44.2.15 std::string SubHeader::getAlias ( )

4.44.2.16 bool SubHeader::isAlias ( )

4.44.2.17 bool SubHeader::isAnchor ( )

4.44.2.18 int SubHeader::getState ( )

4.44.3 Member Data Documentation

4.44.3.1 KeyValueMap SubHeader::Data_Map [protected]

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

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

4.44.3.4 int SubHeader::state [protected]

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

- yaml_wrapper.h

4.45 SYSTEM_DATA Struct Reference

System Data Structure.

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

Public Attributes

- double T

    System Temperature (K)
- double PT

    Total Pressure (kPa)
- double qT

    Total Amount adsorbed (mol/kg)
- double PI

    Total Lumped Spreading Pressure (mol/kg)
- double pi

    Actual Spreading pressure (J/m^2)
- double As

    Specific surface area of adsorbent (m^2/kg)
- int N

    Total Number of Components.
- int I
- int J
- int K

    Special indices used to keep track of sub-systems.
- unsigned long int total_eval

    Counter to keep track of total number of non-linear steps.
- double avg_norm

    Used to store all norms from evaluations then average at end of run.
- double max_norm

    Used to store the maximum e.norm calculated from non-linear iterations.
- int Sys

    Number of sub-systems to solve.
- int Par

    Number of binary parameters to solve for.
- bool Recover

    If Recover == false, standard GPAST using y's as knowns.
- bool Carrier

    If there is an inert carrier gas, Carrier == true.
- bool Ideal

    If the behavior of the system is determined to be ideal, then Ideal == true.
- bool Output

    Boolean to suppress output if desired (true = display, false = no display.

4.45.1 Detailed Description

System Data Structure.

C-style object holding all the data associated with the overall system to be modeled.

4.45.2 Member Data Documentation

4.45.2.1 double SYSTEM_DATA::T

System Temperature (K)

4.45.2.2 double SYSTEM_DATA::PT

Total Pressure (kPa)

4.45.2.3 double SYSTEM_DATA::qT

Total Amount adsorbed (mol/kg)

4.45.2.4 double SYSTEM_DATA::PI

Total Lumped Spreading Pressure (mol/kg)

4.45.2.5 double SYSTEM_DATA::pi

Actual Spreading pressure (J/m^2)

4.45.2.6 double SYSTEM_DATA::As

Specific surface area of adsorbent (m^2/kg)

4.45.2.7 int SYSTEM_DATA::N

Total Number of Components.

4.45.2.8 int SYSTEM_DATA::I

4.45.2.9 int SYSTEM_DATA::J

4.45.2.10 int SYSTEM_DATA::K

Special indices used to keep track of sub-systems.

4.45.2.11 unsigned long int SYSTEM_DATA::total_eval

Counter to keep track of total number of non-linear steps.

4.45.2.12 double SYSTEM_DATA::avg_norm

Used to store all norms from evaluations then average at end of run.

4.45.2.13 double SYSTEM_DATA::max_norm

Used to store the maximum e.norm calculated from non-linear iterations.

4.45.2.14 int SYSTEM_DATA::Sys

Number of sub-systems to solve.

4.45.2.15 int SYSTEM_DATA::Par

Number of binary parameters to solve for.

4.45.2.16 bool SYSTEM_DATA::Recover

If Recover == false, standard GPAST using y's as knowns.

4.45.2.17 bool SYSTEM_DATA::Carrier

If there is an inert carrier gas, Carrier == true.

4.45.2.18 bool SYSTEM_DATA::Ideal

If the behavior of the system is determined to be ideal, then Ideal == true.

4.45.2.19 bool SYSTEM_DATA::Output

Boolean to suppress output if desired (true = display, false = no display.

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

- magpie.h

4.46 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

4.46.1 Member Data Documentation

4.46.1.1 double TRAJECTORY_DATA::mu_0 = 12.57e-7

4.46.1.2 double TRAJECTORY_DATA::rho_f = 1000.0

4.46.1.3 double TRAJECTORY_DATA::eta = 0.001

4.46.1.4 double TRAJECTORY_DATA::Hamaker = 1.3e-21

4.46.1.5 double TRAJECTORY_DATA::Temp = 298

4.46.1.6 double TRAJECTORY_DATA::k = 1.38e-23

4.46.1.7 double TRAJECTORY_DATA::Rs = 0.0026925

4.46.1.8 double TRAJECTORY_DATA::L = 0.0611

4.46.1.9 double TRAJECTORY_DATA::porosity = 0.8979

4.46.1.10 double TRAJECTORY_DATA::V_separator

4.46.1.11 double TRAJECTORY_DATA::a = 33.0e-6

4.46.1.12 double TRAJECTORY_DATA::V_wire

4.46.1.13 double TRAJECTORY_DATA::L_wire

4.46.1.14 double TRAJECTORY_DATA::A_separator

4.46.1.15 double TRAJECTORY_DATA::A_wire

4.46.1.16 double TRAJECTORY_DATA::B0 = 1.0

4.46.1.17 double TRAJECTORY_DATA::H0

4.46.1.18 double TRAJECTORY_DATA::Ms = 0.6

4.46.1.19 double TRAJECTORY_DATA::b = 0.25e-6

4.46.1.20 double TRAJECTORY_DATA::chi_p = 3.87e-6

4.46.1.21 double TRAJECTORY_DATA::rho_p = 8700.0

4.46.1.22 double TRAJECTORY_DATA::Q_in

4.46.1.23 double TRAJECTORY_DATA::V0

4.46.1.24 double TRAJECTORY_DATA::Y_initial = 20.0

4.46.1.25 double TRAJECTORY_DATA::dt

4.46.1.26 double TRAJECTORY_DATA::M

4.46.1.27 double TRAJECTORY_DATA::mp

4.46.1.28 double TRAJECTORY_DATA::beta

4.46.1.29 double TRAJECTORY_DATA::q_bar

4.46.1.30 double TRAJECTORY_DATA::sigma_v

4.46.1.31 double TRAJECTORY_DATA::sigma_vz

4.46.1.32 double TRAJECTORY_DATA::sigma_z

4.46.1.33 double TRAJECTORY_DATA::sigma_n

4.46.1.34 double TRAJECTORY_DATA::sigma_m

4.46.1.35 double TRAJECTORY_DATA::n_rand

4.46.1.36 double TRAJECTORY_DATA::m_rand

4.46.1.37 double TRAJECTORY_DATA::s_rand

4.46.1.38 double TRAJECTORY_DATA::t_rand

4.46.1.39 Matrix<double> TRAJECTORY_DATA::POL

4.46.1.40 Matrix<double> TRAJECTORY_DATA::H

4.46.1.41 Matrix<double> TRAJECTORY_DATA::dX

4.46.1.42 Matrix<double> TRAJECTORY_DATA::dY

4.46.1.43 Matrix<double> TRAJECTORY_DATA::X

4.46.1.44 Matrix<double> TRAJECTORY_DATA::Y

4.46.1.45 Matrix<int> TRAJECTORY_DATA::Cap

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

- Trajectory.h

4.47 UI_DATA Struct Reference

Data structure holding the UI arguments.

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

Public Attributes

- ValueTypePair value_type

    Data pair for input, tells what the input is and it's type.
- std::vector< std::string > user_input

    What is read in from the console at any point.
- std::vector< std::string > input_files

    A vector of input file names and directories given by user.
- std::string path

    Path to where input files are located.
- int count = 0

    Number of times a questing has been asked.
- int max = 3

    Maximum allowable recursions of a question.
- int option

    Current option choosen by the user.
- bool Path = false

    True if user gives path as an option.
- bool Files = false

    True if user gives input files as an option.
- bool MissingArg = true

    True if an input argument is missing; False if everything is ok.
- bool BasicUI = true

    True if using Basic UI; False if using Advanced UI.
- int argc

    Number of console arguments given on input.
- const char * argv []

    Actual console arguments given at execution.

4.47.1 Detailed Description

Data structure holding the UI arguments.

C-Style object for interfacing with users request upon execution of the program. User input is stored in objects below and a series of booleans is used to determine how and what to execute.

4.47.2 Member Data Documentation

4.47.2.1 ValueTypePair UI_DATA::value_type

Data pair for input, tells what the input is and it's type.

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

What is read in from the console at any point.

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

A vector of input file names and directories given by user.

4.47.2.4 std::string UI_DATA::path

Path to where input files are located.

4.47.2.5 int UI_DATA::count = 0

Number of times a questing has been asked.

4.47.2.6 int UI_DATA::max = 3

Maximum allowable recursions of a question.

4.47.2.7 int UI_DATA::option

Current option choosen by the user.

4.47.2.8 bool UI_DATA::Path = false

True if user gives path as an option.

4.47.2.9 bool UI_DATA::Files = false

True if user gives input files as an option.

4.47.2.10 bool UI_DATA::MissingArg = true

True if an input argument is missing; False if everything is ok.

4.47.2.11 bool UI_DATA::BasicUI = true

True if using Basic UI; False if using Advanced UI.

4.47.2.12 int UI_DATA::argc

Number of console arguments given on input.

4.47.2.13 const char* UI_DATA::argv[ ]

Actual console arguments given at execution.

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

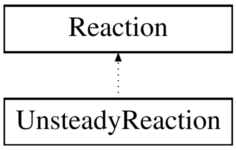
- ui.h

4.48 UnsteadyReaction Class Reference

Unsteady Reaction Object (inherits from Reaction)

`#include <shark.h>`

Inheritance diagram for UnsteadyReaction:



Public Member Functions

- UnsteadyReaction ()

  Default Constructor.
- ∼UnsteadyReaction ()

  Default Destructor.
- void Initialize_List (MasterSpeciesList &List)

  Function to initialize the UnsteadyReaction object from the MasterSpeciesList.
- void Display_Info ()

  Display the unsteady reaction information.
- void Set_Species_Index (int i)

  Set the Unsteady species index by number.
- void Set_Species_Index (std::string formula)

  Set the Unsteady species index by formula.
- void Set_Stoichiometric (int i, double v)

  Set the ith stoichiometric value (see Reaction object)
- void Set_Equilibrium (double v)

  Set the equilibrium constant (logK) (see Reaction object)
- void Set_Enthalpy (double H)

  Set the enthalpy of the reaction (J/mol) (see Reaction object)
- void Set_Entropy (double S)

  Set the entropy of the reaction (J/K/mol) (see Reaction object)

- void Set_EnthalpyANDEntropy (double H, double S)

    Set both the enthalpy and entropy (J/mol) & (J/K/mol) (see Reaction object)
- void Set_Energy (double G)

    Set the Gibb's free energy of reaction (J/mol) (see Reaction object)
- void Set_InitialValue (double ic)

    Set the initial value of the unsteady variable.
- void Set_MaximumValue (double max)

    Set the maximum value of the unsteady variable to a given value max (mol/L)
- void Set_Forward (double forward)

    Set the forward rate for the reaction (mol/L/hr)
- void Set_Reverse (double reverse)

    Set the reverse rate for the reaction (mol/L/hr)
- void Set_ForwardRef (double Fref)

    Set the forward reference rate (mol/L/hr)
- void Set_ReverseRef (double Rref)

    Set the reverse reference rate (mol/L/hr)
- void Set_ActivationEnergy (double E)

    Set the activation energy for the reaction (J/mol)
- void Set_Affinity (double b)

    Set the temperature affinity parameter for the reaction.
- void Set_TimeStep (double dt)

    Set the time step for the current simulation.
- void checkSpeciesEnergies ()

    Function to check MasterSpeciesList for species energy info (see Reaction object)
- void calculateEnergies ()

    Function to calculate the energy of the reaction (see Reaction object)
- void calculateEquilibrium (double T)

    Function to calculate the equilibrium constant (see Reaction object)
- void calculateRate (double T)

    Function to calculate the rate constant based on given temperature.
- bool haveEquilibrium ()

    True if equilibrium constant is given or can be calculated (see Reaction object)
- bool haveRate ()

    Function to return true if you have the forward or reverse rate calculated.
- int Get_Species_Index ()

    Fetch the index of the Unsteady species.
- double Get_Stoichiometric (int i)

    Fetch the ith stoichiometric value.
- double Get_Equilibrium ()

    Fetch the equilibrium constant (logK)
- double Get_Enthalpy ()

    Fetch the enthalpy of the reaction.
- double Get_Entropy ()

    Fetch the entropy of the reaction.
- double Get_Energy ()

    Fetch the energy of the reaction.
- double Get_InitialValue ()

    Fetch the initial value of the variable.
- double Get_MaximumValue ()

    Fetch the maximum value of the variable.
- double Get_Forward ()

Fetch the forward rate.

- double Get_Reverse ()

  Fetch the reverse rate.
- double Get_ForwardRef ()

  Fetch the forward reference rate.
- double Get_ReverseRef ()

  Fetch the reverse reference rate.
- double Get_ActivationEnergy ()

  Fetch the activation energy for the reaction.
- double Get_Affinity ()

  Fetch the temperature affinity for the reaction.
- double Get_TimeStep ()

  Fetch the time step.
- double Eval_ReactionRate (const Matrix< double > &x, const Matrix< double > &gama)

  Calculate reation rate (dC/dt) from concentrations and activities.
- double Eval_Residual (const Matrix< double > &x_new, const Matrix< double > &x_old, const Matrix< double > &gama_new, const Matrix< double > &gama_old)

  Calculate the unsteady residual for the reaction using and implicit time discretization.
- double Eval_Residual (const Matrix< double > &x, const Matrix< double > &gama)

  Calculate the steady-state residual for this reaction (see Reaction object)
- double Eval_IC_Residual (const Matrix< double > &x)

  Calculate the unsteady residual for initial conditions.
- double Explicit_Eval (const Matrix< double > &x, const Matrix< double > &gama)

  Return an approximate explicit solution to our unsteady variable (mol/L)

Protected Attributes

- double initial_value

  Initial value given at t=0 (in mol/L)
- double max_value

  Maximum value plausible (in mol/L)
- double forward_rate

  Forward reaction rate constant (in (mol/L)^n/hr)
- double reverse_rate

  Reverse reaction rate constant (in (mol/L)^n/hr)
- double forward_ref_rate

  Forward reference rate constant (in (mol/L)^n/hr)
- double reverse_ref_rate

  Reverse reference rate constant (in (mol/L)^n/hr)
- double activation_energy

  Activation or barrier energy for the reaction (J/mol)
- double temperature_affinity

  Temperature affinity parameter (dimensionless)
- double time_step

  Time step size for current step.
- bool HaveForward

  True if can calculate, or was given the forward rate.
- bool HaveReverse

  True if can calculate, or was given the reverse rate.
- bool HaveForRef

True if given the forward reference rate.

- bool HaveRevRef

  True if given the reverse reference rate.

- int species_index

  Index in MasterList of Unsteady Species.

Additional Inherited Members

4.48.1 Detailed Description

Unsteady Reaction Object (inherits from Reaction)

C++ style object that holds data and functions associated with unsteady chemical reactions...

i.e., aA + bB <– reverse : forward –> cC + dD

This is essentially the same as the steady reaction, but we now have a forward and reverse reaction rate to deal with. It should be noted that this is a very simple kinetic reaction model based on splitting an overall equilibrium reaction into an overall forward and reverse reaction model. Therefore, it is not expected that this representation of the reaction will provide high accuracy results for reaction kinetics, but should at least provide an overall idea of the process occuring.

4.48.2 Constructor & Destructor Documentation

4.48.2.1 UnsteadyReaction::UnsteadyReaction ( )

Default Constructor.

4.48.2.2 UnsteadyReaction::∼UnsteadyReaction ( )

Default Destructor.

4.48.3 Member Function Documentation

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

Function to initialize the UnsteadyReaction object from the MasterSpeciesList.

4.48.3.2 void UnsteadyReaction::Display_Info ( )

Display the unsteady reaction information.

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

Set the Unsteady species index by number.

This function will set the unsteady species index by the index i given. That given index must correspond to the index of the species in the MasterSpeciesList that is being considered as the unsteady species.

Parameters

i	index of the unsteady species in the MasterSpeciesList

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

Set the Unsteady species index by formula.

This function will check the MasterSpeciesList for the molecule object that has the given formula, then set the unsteady species index based on the index of that species in the master list.

Parameters

formula	molecular formula of the unsteady species (see mola.h for standard formatting)

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

Set the ith stoichiometric value (see Reaction object)

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

Set the equilibrium constant (logK) (see Reaction object)

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

Set the enthalpy of the reaction (J/mol) (see Reaction object)

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

Set the entropy of the reaction (J/K/mol) (see Reaction object)

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

Set both the enthalpy and entropy (J/mol) & (J/K/mol) (see Reaction object)

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

Set the Gibb's free energy of reaction (J/mol) (see Reaction object)

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

Set the initial value of the unsteady variable.

This function sets the initial concentration value for the unsteady species to the given value ic (mol/L). Only unsteady species need to be given an initial value. All other species initial values for the overall system is setup based on a speciation calculation performed while holding the unsteady variables constant at their respective initial values.

Parameters

ic	initial concentration value for the unsteady object (mol/L)

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

Set the maximum value of the unsteady variable to a given value max (mol/L)

This function will be called internally to help bound the unsteady variable to reasonable maximum values. That maximum is usually based on the mass balances for the current non-linear iteration.

Parameters

max	maximum allowable value for the unsteady variable (mol/L)

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

Set the forward rate for the reaction (mol/L/hr)

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

Set the reverse rate for the reaction (mol/L/hr)

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

Set the forward reference rate (mol/L/hr)

Unlike just setting the forward rate, this function sets a reference forward rate of the reaction that can be used to correct the overall forward rate based on system temperature and Arrhenius Rate Equation constants.

Parameters

Fref	forward reference rate constant (mol/L/hr)

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

Set the reverse reference rate (mol/L/hr)

Unlike just setting the reverse rate, this function sets a reference reverse rate of the reaction that can be used to correct the overall reverse rate based on system temperature and Arrhenius Rate Equation constants.

Parameters

Rref	reverse reference rate constant (mol/L/hr)

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

Set the activation energy for the reaction (J/mol)

This function will set the activation energy for the reaction to the given value of E. Note that we will only set one value for activation energy, even though there are rates for forward and reverse reactions. This is because we use the ratio of the rates and the equilibrium constant to establish the other rate. Therefore, we only need either the forward or reverse rate and the equilibrium constant to set all the rates.

Parameters

E	activation energy for the forward or reverse rate, depending on which was given

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

Set the temperature affinity parameter for the reaction.

This function will set the temperature affinity for the reaction to the given value of b. Note that we will only set one value for temperature affinity, even though there are rates for forward and reverse reactions. This is because we use the ratio of the rates and the equilibrium constant to establish the other rate. Therefore, we only need either the forward or reverse rate and the equilibrium constant to set all the rates.

Parameters

b	temperature affinity for the forward or reverse rate, depending on which was given

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

Set the time step for the current simulation.

4.48.3.20 void UnsteadyReaction::checkSpeciesEnergies ( )

Function to check MasterSpeciesList for species energy info (see Reaction object)

4.48.3.21 void UnsteadyReaction::calculateEnergies ( )

Function to calculate the energy of the reaction (see Reaction object)

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

Function to calculate the equilibrium constant (see Reaction object)

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

Function to calculate the rate constant based on given temperature.

This function will calculate and set either the forward or reverse rate for the unsteady reaction based on what information was given. If the forward rate information was given, then it sets the reverse rate and visa versa. If nothing was set correctly, an error will occur.

Parameters

T	temperature of the system in Kelvin

4.48.3.24 bool UnsteadyReaction::haveEquilibrium ( )

True if equilibrium constant is given or can be calculated (see Reaction object)

4.48.3.25 bool UnsteadyReaction::haveRate ( )

Function to return true if you have the forward or reverse rate calculated.

4.48.3.26 int UnsteadyReaction::Get_Species_Index ( )

Fetch the index of the Unsteady species.

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

Fetch the ith stoichiometric value.

4.48.3.28 double UnsteadyReaction::Get_Equilibrium ( )

Fetch the equilibrium constant (logK)

4.48.3.29 double UnsteadyReaction::Get_Enthalpy ( )

Fetch the enthalpy of the reaction.

4.48.3.30 double UnsteadyReaction::Get_Entropy ( )

Fetch the entropy of the reaction.

4.48.3.31 double UnsteadyReaction::Get_Energy ( )

Fetch the energy of the reaction.

4.48.3.32 double UnsteadyReaction::Get_InitialValue ( )

Fetch the initial value of the variable.

4.48.3.33 double UnsteadyReaction::Get_MaximumValue ( )

Fetch the maximum value of the variable.

4.48.3.34 double UnsteadyReaction::Get_Forward ( )

Fetch the forward rate.

4.48.3.35 double UnsteadyReaction::Get_Reverse ( )

Fetch the reverse rate.

4.48.3.36 double UnsteadyReaction::Get_ForwardRef ( )

Fetch the forward reference rate.

4.48.3.37 double UnsteadyReaction::Get_ReverseRef ( )

Fetch the reverse reference rate.

4.48.3.38 double UnsteadyReaction::Get_ActivationEnergy ( )

Fetch the activation energy for the reaction.

4.48.3.39 double UnsteadyReaction::Get_Affinity ( )

Fetch the temperature affinity for the reaction.

4.48.3.40 double UnsteadyReaction::Get_TimeStep ( )

Fetch the time step.

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

Calculate reation rate (dC/dt) from concentrations and activities.

This function calculates the right hand side of the unsteady reaction equation based on the available rates, the current values of the non-linear variables (x=log(C)), and the activity coefficients (gama).

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
gama	matrix of activity coefficients for each species at the current non-linear step

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

Calculate the unsteady residual for the reaction using and implicit time discretization.

This function uses the current time step and states of the non-linear variables and activities to form the residual contribution of the unsteady reaction. The time dependent functions are discretized using an implicit finite difference for best stability.

Parameters

x_new	matrix of the log(C) concentration values at the current non-linear step
gama_new	matrix of activity coefficients for each species at the current non-linear step
x_old	matrix of the log(C) concentration values at the previous non-linear step
gama_old	matrix of activity coefficients for each species at the previous non-linear step

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

Calculate the steady-state residual for this reaction (see Reaction object)

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

Calculate the unsteady residual for initial conditions.

Setting the intial conditions for all variables in the system requires a speciation calculation. However, we want the unsteady variables to be set to their respective initial conditions. Using this residual function imposes an equality constraint on those non-linear, unsteady variables allowing the rest of the speciation problem to be solved via PJFNK iterations.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step

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

Return an approximate explicit solution to our unsteady variable (mol/L)

This function will approximate the concentration of the unsteady variables based on an explicit time discretization. The purpose of this function is to try to provide the PJFNK method with a good initial guess for the values of the non-linear, unsteady variables. If we do not provide a good initial guess to these variables, then the PJFNK method may not converge to the correct solution, because the unsteady problem is the most difficult to solve.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
gama	matrix of activity coefficients for each species at the current non-linear step

4.48.4 Member Data Documentation

4.48.4.1 double UnsteadyReaction::initial_value [protected]

Initial value given at t=0 (in mol/L)

4.48.4.2 double UnsteadyReaction::max_value [protected]

Maximum value plausible (in mol/L)

4.48.4.3 double UnsteadyReaction::forward_rate [protected]

Forward reaction rate constant (in (mol/L)^n/hr)

4.48.4.4 double UnsteadyReaction::reverse_rate [protected]

Reverse reaction rate constant (in (mol/L)^n/hr)

4.48.4.5 double UnsteadyReaction::forward_ref_rate [protected]

Forward reference rate constant (in (mol/L)^n/hr)

4.48.4.6 double UnsteadyReaction::reverse_ref_rate [protected]

Reverse reference rate constant (in (mol/L)^n/hr)

4.48.4.7 double UnsteadyReaction::activation_energy [protected]

Activation or barrier energy for the reaction (J/mol)

4.48.4.8 double UnsteadyReaction::temperature_affinity [protected]

Temperature affinity parameter (dimensionless)

4.48.4.9 double UnsteadyReaction::time_step [protected]

Time step size for current step.

4.48.4.10 bool UnsteadyReaction::HaveForward [protected]

True if can calculate, or was given the forward rate.

4.48.4.11 bool UnsteadyReaction::HaveReverse [protected]

True if can calculate, or was given the reverse rate.

4.48.4.12 bool UnsteadyReaction::HaveForRef [protected]

True if given the forward reference rate.

4.48.4.13 bool UnsteadyReaction::HaveRevRef [protected]

True if given the reverse reference rate.

4.48.4.14 int UnsteadyReaction::species_index [protected]

Index in MasterList of Unsteady Species.

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

- shark.h

4.49 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

4.49.1 Constructor & Destructor Documentation

4.49.1.1 ValueTypePair::ValueTypePair ( )

4.49.1.2 ValueTypePair::~ValueTypePair ( )

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

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

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

4.49.2 Member Function Documentation

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

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

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

4.49.2.4 void ValueTypePair::findType ( )

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

4.49.2.6 void ValueTypePair::DisplayPair ( )

4.49.2.7 std::string ValueTypePair::getString ( )

4.49.2.8 bool ValueTypePair::getBool ( )

4.49.2.9 double ValueTypePair::getDouble ( )

4.49.2.10 int ValueTypePair::getInt ( )

4.49.2.11 std::string ValueTypePair::getValue ( )

4.49.2.12 int ValueTypePair::getType ( )

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

4.49.3 Member Data Documentation

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

4.49.3.2 int ValueTypePair::type [private]

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

- yaml_wrapper.h

4.50 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

4.50.1 Constructor & Destructor Documentation

4.50.1.1 yaml_cpp_class::yaml_cpp_class ( )

4.50.1.2 yaml_cpp_class::∼yaml_cpp_class ( )

4.50.2 Member Function Documentation

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

4.50.2.2 int yaml_cpp_class::readInputFile ( )

4.50.2.3 int yaml_cpp_class::cleanup ( )

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

4.50.2.5 YamlWrapper& yaml_cpp_class::getYamlWrapper ( )

4.50.2.6 void yaml_cpp_class::DisplayContents ( )

4.50.3 Member Data Documentation

4.50.3.1 YamlWrapper yaml_cpp_class::yaml_wrapper [private]

4.50.3.2 FILE∗ yaml_cpp_class::input_file [private]

4.50.3.3 const char∗ yaml_cpp_class::file_name [private]

4.50.3.4 yaml_parser_t yaml_cpp_class::token_parser [private]

4.50.3.5 yaml_token_t yaml_cpp_class::current_token [private]

4.50.3.6 yaml_token_t yaml_cpp_class::previous_token [private]

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

- yaml_wrapper.h

4.51 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

4.51.1 Constructor & Destructor Documentation

4.51.1.1 YamlWrapper::YamlWrapper ( )

4.51.1.2 YamlWrapper::∼YamlWrapper ( )

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

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

4.51.2 Member Function Documentation

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

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

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

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

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

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

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

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

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

4.51.2.10 void YamlWrapper::clear ( )

4.51.2.11 void YamlWrapper::resetKeys ( )

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

4.51.2.13 void YamlWrapper::revalidateAllKeys ( )

4.51.2.14 void YamlWrapper::DisplayContents ( )

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

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

4.51.2.17 int YamlWrapper::size ( )

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

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

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

4.51.3 Member Data Documentation

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

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

- yaml_wrapper.h

Chapter 5

File Documentation

5.1 dogfish.h File Reference

Diffusion Object Governing Fiber Interior Sorption History.

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

Classes

- struct DOGFISH_PARAM

  Data structure for species-specific parameters.
- struct DOGFISH_DATA

  Primary data structure for running the DOGFISH application.

Functions

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

  Function to print a species based header for the output file.
- void print2file_DOGFISH_header (DOGFISH_DATA ∗dog_dat)

  Function to print a time and space header for the output file.
- void print2file_DOGFISH_result_old (DOGFISH_DATA ∗dog_dat)

  Function to print out the old time results for the output file.
- void print2file_DOGFISH_result_new (DOGFISH_DATA ∗dog_dat)

  Function to print out the new time results for the output file.
- double default_Retardation (int i, int l, const void ∗data)

  Default function for the retardation coefficient.
- double default_IntraDiffusion (int i, int l, const void ∗data)

  Default function for the intraparticle diffusion coefficient.
- double default_FilmMTCoeff (int i, const void ∗data)

  Default function for the film mass transfer coefficient.
- double default_SurfaceConcentration (int i, const void ∗data)

  Default function for the fiber surface concentration.
- 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)

  Function will set up the memory and pointers for use in the DOGFISH simulations.

- int DOGFISH_Executioner (DOGFISH_DATA *dog_dat)

  Function to serially call all other functions need to solve the system at one time step.
- int set_DOGFISH_ICs (DOGFISH_DATA *dog_dat)

  Function called to evaluate the initial conditions for the time dependent problem.
- int set_DOGFISH_timestep (DOGFISH_DATA *dog_dat)

  Function sets the time step size for the next step forward in the simulation.
- int DOGFISH_preprocesses (DOGFISH_DATA *dog_dat)

  Function to perform preprocess actions to be used before calling any solver.
- int set_DOGFISH_params (const void *user_data)

  Function to calculate the values of all parameters for all species at all nodes.
- int DOGFISH_postprocesses (DOGFISH_DATA *dog_dat)

  Function to perform post-solve actions such as printing out results.
- int DOGFISH_reset (DOGFISH_DATA *dog_dat)

  Function to reset the matrices and vectors and prepare for next time step.
- int DOGFISH (DOGFISH_DATA *dog_dat)

  Function performs all necessary steps to step the diffusion simulation through time.
- int DOGFISH_TESTS ()

  Running DOGFISH tests.

5.1.1 Detailed Description

Diffusion Object Governing Fiber Interior Sorption History. dogfish.cpp

This set of objects and functions is used to numerically solve linear or non-linear diffusion physics of aqueous ions into cylindrical adsorbent fibers. Boundary conditions for this problem could be a film mass transfer, reaction, or dirichlet condition depending on the type of problem being solve.

Warning

Functions and methods in this file are still under construction.

Author

Austin Ladshaw

Date

04/09/2015

Copyright

5.1.2 Function Documentation

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

Function to print a species based header for the output file.

5.1.2.2 void print2file_DOGFISH_header (DOGFISH_DATA * *dog_dat*)

Function to print a time and space header for the output file.

5.1.2.3 void print2file_DOGFISH_result_old (DOGFISH_DATA * *dog_dat*)

Function to print out the old time results for the output file.

5.1.2.4 void print2file_DOGFISH_result_new (DOGFISH_DATA * *dog_dat*)

Function to print out the new time results for the output file.

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

Default function for the retardation coefficient.

The default retardation coefficient for this problem is 1.0 for all time and space. Therefore, this function will only ever return a 1.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
data	pointer to the DOGFISH_DATA structure

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

Default function for the intraparticle diffusion coefficient.

The default intraparticle diffusivity is to assume that each species i has a constant diffusivity. Therefore, this function returns the value of the parameter intraparticle_diffusion from the DOGFISH_PARAM structure for each adsorbing species i. Each species may have a different diffusivity.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
data	pointer to the DOGFISH_DATA structure

5.1.2.7 double default_FilmMTCoeff (int *i*, const void * *data*)

Default function for the film mass transfer coefficient.

The default film mass transfer coefficient will be to assume that this value is a constant for each species i. Therefore, this function returns the parameter value of film_transfer_coeff from the DOGFISH_PARAM structure for each adsorbing species i.

Parameters

i	index for the ith adsorbing species
data	pointer to the DOGFISH_DATA structure

5.1.2.8 double default_SurfaceConcentration (int *i*, const void * *data*)

Default function for the fiber surface concentration.

The default fiber surface concentration will be to assume that this value is a constant for each species i. Therefore, this function returns the parameter value of surface_concentration from the DOGFISH_PARAM structure for each adsorbing species i.

Parameters

i	index for the ith adsorbing species
data	pointer to the DOGFISH_DATA structure

5.1.2.9 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*)

Function will set up the memory and pointers for use in the DOGFISH simulations.

The pointers to the output file, parameter functions, and data structures are passed into this function to setup the problem in memory. This function must always be called prior to calling any other DOGFISH routine and after the DOGFISH_DATA structure has been initialized.

Parameters

file	pointer to the output file to print out results
eval_R	function pointer for the retardation coefficient function
eval_DI	function pointer for the intraparticle diffusion function
eval_kf	function pointer for the film mass transfer function
eval_qs	function pointer for the surface concentration function
user_data	pointer for the user's own data structure (only if using custom functions)
dog_dat	pointer for the DOGFISH_DATA structure

5.1.2.10 int DOGFISH_Executioner (DOGFISH_DATA * *dog_dat*)

Function to serially call all other functions need to solve the system at one time step.

This function will call the DOGFISH_preprocesses function, followed by the FINCH solver functions for each species i, then call the DOGFISH_postprocesses function. After completion, this would have solved the diffusion physics for a single time step.

5.1.2.11 int set_DOGFISH_ICs (DOGFISH_DATA * *dog_dat*)

Function called to evaluate the initial conditions for the time dependent problem.

This function will use information in DOGFISH_DATA to setup the initial conditions, initial parameter values, and initial sorption averages for each species. This function always assumes a constant initial condition for the sorption of each species.

5.1.2.12 int set_DOGFISH_timestep (DOGFISH_DATA * *dog_dat*)

Function sets the time step size for the next step forward in the simulation.

This function will set the next time step size based on the spatial discretization of the fiber. Maximum time step size is locked at 0.5 hours.

5.1.2.13 int DOGFISH_preprocesses (DOGFISH_DATA * *dog_dat*)

Function to perform preprocess actions to be used before calling any solver.

This function will call all of the parameter functions in order to establish boundary condition parameter values prior to calling the FINCH solvers.

5.1.2.14 int set_DOGFISH_params (const void * *user_data*)

Function to calculate the values of all parameters for all species at all nodes.

This function is passed to the FINCH_DATA data structure and set as the setparams function pointer. FINCH calls this function during it's solver routine to setup the non-linear form of the problem and solve the non-linear system.

Parameters

user_data	this is actually the DOGFISH_DATA structure, but is passed anonymously to FINCH

5.1.2.15 int DOGFISH_postprocesses (DOGFISH_DATA * *dog_dat*)

Function to perform post-solve actions such as printing out results.

This function increments the total_steps counter in DOGFISH_DATA to keep a running total of all solver steps taken. Additionally, it prints out the results of the current time simulation to the output file.

5.1.2.16 int DOGFISH_reset (DOGFISH_DATA * *dog_dat*)

Function to reset the matrices and vectors and prepare for next time step.

This function will reset the matrix and vector information of DOGFISH_DATA and FINCH_DATA to prepare for the next simulation step in time.

5.1.2.17 int DOGFISH (DOGFISH_DATA * *dog_dat*)

Function performs all necessary steps to step the diffusion simulation through time.

This function calls the initial conditions, set time step, executioner, and reset functions to step the simulation through time. It will only exit when the simulation time is reached or if an error occurs.

5.1.2.18 int DOGFISH_TESTS ( )

Running DOGFISH tests.

This function is called from the UI to run a test simulation of DOGFISH. Ouput is stored in a DOGFISH_TestOutput.-txt file in a sub-directory "output" from the directory in which the executable was called.

5.2 eel.h File Reference

Easy-access Element Library.

```
#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

  Atom object to hold information about specific atoms in the periodic table (click Atom to go to function definitions)
- class PeriodicTable

  Class object that store a digitial copy of all Atom objects.

Functions

- int EEL_TESTS ()

  Test function to exercise the class objects and check for errors.

5.2.1 Detailed Description

Easy-access Element Library. eel.cpp

This file contains two C++ objects: (i) Atom and (ii) PeriodicTable.

```
The Atom class defines all relavent information necessary for dealing with actual
atoms. However, this is not necessarily all the information that one may need for
any simulation dealing with atoms. Instead, it is really just a place holder used
to construct Molecules and hold oxidation state and molecular/atomic wieght information.

The PeriodicTable class creates a digital version of a complete periodic table. Further
development of this object can make it possible to query this structure for a particular
atom upon user request.
```

Warning

The Atom class is mostly complete, but the PeriodicTable object is just a place holder.

Author

Austin Ladshaw

Date

02/23/2015

Copyright

5.2.2 Function Documentation

5.2.2.1 int EEL_TESTS ( )

Test function to exercise the class objects and check for errors.

5.3 egret.h File Reference

Estimation of Gas-phase pRopErTies.

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

Classes

- struct PURE_GAS

  Data structure holding all the parameters for each pure gas spieces.
- struct MIXED_GAS

  Data structure holding information necessary for computing mixed gas properties.

Macros

- #define Rstd 8.3144621

  Gas Constant in J/K/mol (or) L∗kPa/K/mol (Standard Units)
- #define RE3 8.3144621E+3

  Gas Constant in cm^3∗kPa/K/mol (Convenient for density calculations)
- #define Po 100.0

  Standard state pressure (kPa)
- #define Cstd(p, T) ((p)/(Rstd∗T))

  Calculation of concentration/density from partial pressure (Cstd = mol/L)
- #define CE3(p, T) ((p)/(RE3∗T))

  Calculation of concentration/density from partial pressure (CE3 = mol/cm^3)
- #define Pstd(c, T) ((c)∗Rstd∗T)

  Calculation of partial pressure from concentration/density (c = mol/L)
- #define PE3(c, T) ((c)∗RE3∗T)

  Calculation of partial pressure from concentration/density (c = mol/cm^3)
- #define Nu(mu, rho) ((mu)/(rho))

  Calculation of kinematic viscosity from dynamic viscosity and density (cm^2/s)
- #define PSI(T) (0.873143 + (0.000072375∗T))

  Calculation of temperature correction factor for dynamic viscosity.
- #define Dp_ij(Dij, PT) ((PT∗Dij)/Po)

  Calculation of the corrected binary diffusivity (cm^2/s)
- #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)

  Calculation of binary diffusion based on MW, density, and viscosity info (cm^2/s)
- #define Mu(muo, To, C, T) (muo ∗ ((To + C)/(T + C)) ∗ pow((T/To),1.5))

  Calculation of single species viscosity from Sutherland's Equ. (g/cm/s)
- #define D_ii(rhoi, mui) (1.385∗mui/rhoi)

  Calculation of self-diffusivity (cm^2/s)
- #define ReNum(u, L, nu) (u∗L/nu)

  Calculation of the Reynold's Number (-)
- #define ScNum(nu, D) (nu/D)

  Calculation of the Schmidt Number (-)
- #define FilmMTCoeff(D, L, Re, Sc) ((D/L)∗(2.0 + (1.1∗pow(Re,0.6)∗pow(Sc,0.3))))

  Calculation of film mass transfer coefficient (cm/s)

Functions

- int initialize_data (int N, MIXED_GAS ∗gas_dat)

  Function to initialize the MIXED_GAS structure based on number of gas species.
- int set_variables (double PT, double T, double us, double L, std::vector< double > &y, MIXED_GAS ∗gas_-dat)

  Function to set the values of the parameters in the gas phase.
- int calculate_properties (MIXED_GAS ∗gas_dat)

Function to calculate the gas properties based on information in MIXED_GAS.

- int EGRET_TESTS ()

  Function runs a series of tests for the EGRET file.

5.3.1 Detailed Description

Estimation of Gas-phase pRopErTies. egret.cpp

This file is responsible for estimating various temperature, pressure, and concentration dependent parameters to be used in other models for gas phase adsorption, mass transfer, and or mass transport. The goal of this file is to eliminate redundancies in code such that the higher level programs operate more efficiently and cleanly. Calculations made here are based on kinetic theory of gases, ideal gas law, and some emperical models that were developed to account for changes in density and viscosity with changes in temperature between standard temperatures and up to 1000 K.

Author

Austin Ladshaw

Date

01/29/2015

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5.3.2 Macro Definition Documentation

5.3.2.1 #define Rstd 8.3144621

Gas Constant in J/K/mol (or) L∗kPa/K/mol (Standard Units)

5.3.2.2 #define RE3 8.3144621E+3

Gas Constant in cm^3∗kPa/K/mol (Convenient for density calculations)

5.3.2.3 #define Po 100.0

Standard state pressure (kPa)

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

Calculation of concentration/density from partial pressure (Cstd = mol/L)

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

Calculation of concentration/density from partial pressure (CE3 = mol/cm^3)

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

Calculation of partial pressure from concentration/density (c = mol/L)

5.3.2.7 #define PE3(c, T) ((c)∗RE3∗T)

Calculation of partial pressure from concentration/density (c = mol/cm^3)

5.3.2.8 #define Nu(mu, rho) ((mu)/(rho))

Calculation of kinematic viscosity from dynamic viscosity and density (cm^2/s)

5.3.2.9 #define PSI(T) (0.873143 + (0.000072375∗T))

Calculation of temperature correction factor for dynamic viscosity.

5.3.2.10 #define Dp_ij(Dij, PT) ((PT∗Dij)/Po)

Calculation of the corrected binary diffusivity (cm^2/s)

5.3.2.11 #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)

Calculation of binary diffusion based on MW, density, and viscosity info (cm^2/s)

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

Calculation of single species viscosity from Sutherland's Equ. (g/cm/s)

5.3.2.13 #define D_ii(rhoi, mui) (1.385∗mui/rhoi)

Calculation of self-diffusivity (cm^2/s)

5.3.2.14 #define ReNum(u, L, nu) (u∗L/nu)

Calculation of the Reynold's Number (-)

5.3.2.15 #define ScNum(nu, D) (nu/D)

Calculation of the Schmidt Number (-)

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

Calculation of film mass transfer coefficient (cm/s)

5.3.3 Function Documentation

5.3.3.1 int initialize_data (int N, MIXED_GAS ∗ gas_dat)

Function to initialize the MIXED_GAS structure based on number of gas species.

This function will initialize the sizes of all vector objects in the MIXED_GAS structure based on the number of gas species indicated by N.

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

Function to set the values of the parameters in the gas phase.

The gas phase properties are a function of total pressure, gas temperature, gas velocity, characteristic length, and the mole fractions of each species in the gas phase. Prior to calculating the gas phase properties, these parameters must be set and updated as they change.

Parameters

PT	total gas pressure in kPa
T	gas temperature in K
us	gas velocity in cm/s
L	characteristic length in cm (this depends on the particular system)
y	vector of gas mole fractions of each species in the mixture
gas_dat	pointer to the MIXED_GAS data structure

5.3.3.3 int calculate_properties (MIXED_GAS * *gas_dat*)

Function to calculate the gas properties based on information in MIXED_GAS.

This function uses the kinetic theory of gases, combined with other semi-empirical models, to predict and approximate several properties of the mixed gas phase that might be necessary when running any gas dynamical simulation. This includes mass and energy transfer equations, as well as adsorption kinetics in porous adsorbents.

5.3.3.4 int EGRET_TESTS ( )

Function runs a series of tests for the EGRET file.

The test looks at a standard air with 5 primary species of interest and calculates the gas properties from 273 K to 373 K. This function can be called from the UI.

5.4 error.h File Reference

All error types are defined here.

```
#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 }

  List of names for error type.

Functions

- void error (int flag)

  Error function customizes output message based on flag.

5.4.1 Detailed Description

All error types are defined here. error.cpp

This file defines all the different errors that may occur in any simulation in any file. Those errors are recognized by an enum with is then passed through to the error.cpp file that customizes the error message to the console. A macro will also print out the file name and line number where the error occured.

Author

Austin Ladshaw

Date

04/28/2014

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5.4.2 Macro Definition Documentation

5.4.2.1 #define mError(*i*)

Value:

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

5.4.3 Enumeration Type Documentation

5.4.3.1 enum error_type

List of names for 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

5.4.4 Function Documentation

5.4.4.1 void error (int *flag*)

Error function customizes output message based on flag.

This error function is reference in the error.cpp file, but is not called by any other file. Instead, all other files call the mError(i) macro that expands into this error function call plus prints out the file name and line number where the error occured.

5.5 finch.h File Reference

Flux-limiting Implicit Non-oscillatory Conservative High-resolution scheme.

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

Classes

- struct FINCH_DATA

  Data structure for the FINCH object.

Enumerations

- enum finch_solve_type { FINCH_Picard, LARK_Picard, LARK_PJFNK }

  List of enum options to define the solver type in FINCH.
- enum finch_coord_type { Cartesian, Cylindrical, Spherical }

  List of enum options to define the coordinate system in FINCH.

Functions

- double max (std::vector< double > &values)

  Function returns the maximum in a list of values.
- double min (std::vector< double > &values)

Function returns the minimum in a list of values.
- double minmod (std::vector< double > &values)

  Function returns the result of the minmod function acting on a list of values.
- int uTotal (FINCH_DATA *dat)

  Function integrates the conserved quantity to return it's total in the domain.
- int uAverage (FINCH_DATA *dat)

  Function integrates the conserved quantity to reture it's average in the domain.
- int check_Mass (FINCH_DATA *dat)

  Function checks the unp1 vector for negative values and will adjust if needed.
- int l_direct (FINCH_DATA *dat)

  Function solves the discretized FINCH problem directly by assuming it is linear.
- int lark_picard_step (const Matrix< double > &x, Matrix< double > &G, const void *data)

  Function to perform the necessary LARK Picard iterative method (not typically used)
- int nl_picard (FINCH_DATA *dat)

  Function to solve the discretized FINCH problem iteratively by assuming it is non-linear.
- 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)

  Function to setup memory and set user defined functions into the FINCH object.
- void print2file_dim_header (FILE *Output, FINCH_DATA *dat)

  Function will print out a dimension header for FINCH output.
- void print2file_time_header (FILE *Output, FINCH_DATA *dat)

  Function will print out a time header for FINCH output.
- void print2file_result_old (FILE *Output, FINCH_DATA *dat)

  Function will print out the old results to the variable u.
- void print2file_result_new (FILE *Output, FINCH_DATA *dat)

  Function will print out the new results to the variable u.
- void print2file_newline (FILE *Output, FINCH_DATA *dat)

  Function will force print out a blank line.
- void print2file_tab (FILE *Output, FINCH_DATA *dat)

  Function will force print out a tab.
- int default_execution (const void *user_data)

  Default executioner function for FINCH.
- int default_ic (const void *user_data)

  Default initial conditions function for FINCH.
- int default_timestep (const void *user_data)

  Default time step function for FINCH.
- int default_preprocess (const void *user_data)

  Default preprocesses function for FINCH.
- int default_solve (const void *user_data)

  Default solve function for FINCH.
- int default_params (const void *user_data)

  Default params function for FINCH.
- int minmod_discretization (const void *user_data)

  Minmod Discretization function for FINCH.
- int vanAlbada_discretization (const void *user_data)

  Van Albada Discretization function for FINCH.

- int ospre_discretization (const void ∗user_data)

  Ospre Discretization function for FINCH.
- int default_bcs (const void ∗user_data)

  Default boundary conditions function for FINCH.
- int default_res (const Matrix< double > &x, Matrix< double > &res, const void ∗user_data)

  Default residual function for FINCH.
- int default_precon (const Matrix< double > &b, Matrix< double > &p, const void ∗user_data)

  Default preconditioning function for FINCH.
- int default_postprocess (const void ∗user_data)
- int default_reset (const void ∗user_data)

  Default reset function for FINCH.
- int FINCH_TESTS ()

  Function runs a particular FINCH test.

5.5.1 Detailed Description

Flux-limiting Implicit Non-oscillatory Conservative High-resolution scheme. finch.cpp

This is a conservative finite differences scheme based on the Kurganov and Tadmoor (2000) MUSCL scheme for non-linear conservation laws. It can solve 1-D conservation law problems in three different coordinate systems: (i) Cartesian - axial, (ii) Cylindrical - radial, and (iii) Spherical - radial. It is the backbone algorithm behind all 1-D PDE problems in the ecosystem software.

The form of the general conservation law problem that FINCH solves is...

z^d∗R∗du/dt = d/dz(z^d∗D∗du/dz) - d/dz(z^d∗v∗u) - z^d∗k∗u + z^d∗S

where R, D, v, k, and S are the parameters of the problem and d, z, and u are the coordinates, spatial dimension, and conserved quantities, respectively. The parameter R is a retardation coefficient, D is a diffusion coefficient, v is a velocity, k is a reaction coefficient, and S is a forcing function or source/sink term.

FINCH supports the use of both Dirichlet and Neuman boundary conditions as the input/inlet condition and uses the No Flux (or Natural) boundary condition for the output/outlet of the domain. For radial problems, the outlet is always taken to the the center of the cylindrical or spherical particle. This enforces the symmetry of the problem. For axial problems, the outlet is determined by the sign of the velocity term and is therefore choosen by the routine based on the actual flow direction in the domain.

Parameters of the problem can be coupled to the variable u and also be functions of space and time. The coupling of the parameters with the variable forces the problem to become non-linear, which requires iteration to solve. The default iterative method is a built-in Picard's method. This method is equivalent to an inexact Newton method, because we use the Linear Solve of this system as a weak approximation to the non-linear solve. Generally, this method is sufficient and is the most efficient. However, if a problem is particularly difficult to solve, then we can call some of the non-linear solvers developed in LARK. If PJFNK is used, then the Linear Solve for the FINCH problem is used as the Preconditioner for the Linear Solve in PJFNK.

This algorithm comes packaged with three different slope limiter functions to stabilize the velocity term for highly advectively dominate problems. The available slope limiters are: (i) minmod, (ii) van Albada, and (iii) ospre. By default, the FINCH setup function will set the slope limiter to ospre, because this method provides a reasonable compromise between accuracy and efficiency.

Slope Limiter Stats:

minmod -> Highest Accuracy, Lowest Efficiency

van Albada -> Lowest Accuracy, Highest Efficiency

ospre -> Average Accuracy, Average Efficiency

Author

Austin Ladshaw

Date

01/29/2015

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5.5.2 Enumeration Type Documentation

5.5.2.1 enum finch_solve_type

List of enum options to define the solver type in FINCH.

Enumerator

FINCH_Picard

LARK_Picard

LARK_PJFNK

5.5.2.2 enum finch_coord_type

List of enum options to define the coordinate system in FINCH.

Enumerator

Cartesian

Cylindrical

Spherical

5.5.3 Function Documentation

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

Function returns the maximum in a list of values.

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

Function returns the minimum in a list of values.

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

Function returns the result of the minmod function acting on a list of values.

5.5.3.4 int uTotal (FINCH_DATA * *dat*)

Function integrates the conserved quantity to return it's total in the domain.

5.5.3.5 int uAverage (FINCH_DATA * *dat*)

Function integrates the conserved quantity to reture it's average in the domain.

5.5.3.6 int check_Mass (FINCH_DATA * *dat*)

Function checks the unp1 vector for negative values and will adjust if needed.

This function can be turned off or on in the FINCH_DATA structure. Typically, you will want to leave this on so that the routine does not return negative values for u. However, if you want to get negative values of u, then turn this option off.

5.5.3.7 int l_direct (FINCH_DATA * *dat*)

Function solves the discretized FINCH problem directly by assuming it is linear.

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

Function to perform the necessary LARK Picard iterative method (not typically used)

5.5.3.9 int nl_picard (FINCH_DATA * *dat*)

Function to solve the discretized FINCH problem iteratively by assuming it is non-linear.

Note

> If the problem is actually linear, then this will solve it in one iteration. So it may be best to always assume the problem is non-linear.

5.5.3.10 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*)

Function to setup memory and set user defined functions into the FINCH object.

This function MUST be called prior to running any FINCH based simulation. However, you are only every required to provide this function with the FINCH_DATA pointer. It is recommended, however, that you do provide the user_-setparams and param_data pointers, as these will likely vary significantly from problem to problem.

After the problem is setup in memory, you do not technically have to have FINCH call all of it's own functions. You can write your own executioner, initial conditions, and other functions and decided how and when everything is called. Then just call the solve function in FINCH_DATA when you want to use the FINCH solver. This is how FINCH is used in SKUA, SCOPSOWL, DOGFISH, and MONKFISH.

Parameters

user_callroutine	function pointer the the call routine function
user_setic	function pointer to set initial conditions for problem
user_timestep	function pointer to set the next time step
user_preprocess	function pointer to setup a preprocess operation
user_solve	function pointer to solve the system of equations
user_setparams	function pointer to set the parameters in the problem (always override this)

user_discretize	function pointer to select discretization scheme for the problem
user_bcs	function pointer to evaluate boundary conditions for the problem
user_res	function pointer to evaluate non-linear residuals for the problem
user_precon	function pointer to perform a linear preconditioning operation
user_-postprocess	function pointer to setup a postprocess operation
user_reset	function pointer to reset stateful data for next simulation
dat	pointer to the FINCH_DATA structure
param_data	user supplied pointer to a data structure needed in user_setparams

5.5.3.11 void print2file_dim_header (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will print out a dimension header for FINCH output.

5.5.3.12 void print2file_time_header (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will print out a time header for FINCH output.

5.5.3.13 void print2file_result_old (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will print out the old results to the variable u.

5.5.3.14 void print2file_result_new (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will print out the new results to the variable u.

5.5.3.15 void print2file_newline (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will force print out a blank line.

5.5.3.16 void print2file_tab (FILE ∗ *Output*, FINCH_DATA ∗ *dat*)

Function will force print out a tab.

5.5.3.17 int default_execution (const void ∗ *user_data*)

Default executioner function for FINCH.

The default executioner function for FINCH assumes the user_data parameter is the FINCH_DATA structure and calls the preprocesses, solve, postprocesses, checkMass, uTotal, and uAverage functions in that order.

5.5.3.18 int default_ic (const void ∗ *user_data*)

Default initial conditions function for FINCH.

The default initial condition function for FINCH assumes the user_data parameter is the FINCH_DATA structure and sets the initial values of all system parameters according to the given constants in that structure.

5.5.3.19 int default_timestep (const void * *user_data*)

Default time step function for FINCH.

The default time step function for FINCH assumes the user_data parameter is the FINCH_DATA structure and sets the time step to 1/2 the mesh size or bases the time step off of the CFL condition if the problem is not being solved iteratively and involves an advective portion.

5.5.3.20 int default_preprocess (const void * *user_data*)

Default preprocesses function for FINCH.

The default preprocesses function for FINCH assumes the user_data parameter is the FINCH_DATA structure and does nothing.

5.5.3.21 int default_solve (const void * *user_data*)

Default solve function for FINCH.

The default solve function for FINCH assumes the user_data parameter is the FINCH_DATA structure and calls the corresponding solution method depending on the users conditions.

5.5.3.22 int default_params (const void * *user_data*)

Default params function for FINCH.

The default params function for FINCH assumes the user_data parameter is the FINCH_DATA structure and sets the values of all parameters at all nodes equal to the values of those parameters at the boundaries.

5.5.3.23 int minmod_discretization (const void * *user_data*)

Minmod Discretization function for FINCH.

The minmod discretization function for FINCH assumes the user_data parameter is the FINCH_DATA structure and discretizes the time and space portion of the problem with 2nd order finite differences and uses the minmod slope limiter function to stabilize the advective physics.

5.5.3.24 int vanAlbada_discretization (const void * *user_data*)

Van Albada Discretization function for FINCH.

The van Albada discretization function for FINCH assumes the user_data parameter is the FINCH_DATA structure and discretizes the time and space portion of the problem with 2nd order finite differences and uses the van Albada slope limiter function to stabilize the advective physics.

5.5.3.25 int ospre_discretization (const void * *user_data*)

Ospre Discretization function for FINCH.

The ospre discretization function for FINCH assumes the user_data parameter is the FINCH_DATA structure and discretizes the time and space portion of the problem with 2nd order finite differences and uses the ospre slope limiter function to stabilize the advective physics. This is the default discretization function.

5.5.3.26 int default_bcs (const void * *user_data*)

Default boundary conditions function for FINCH.

The default boundary conditions function for FINCH assumes the user_data parameter is the FINCH_DATA structure and sets the boundary conditions according to the type of problem requested. The input BCs will always be either Neumann or Dirichlet and the output BC will always be a zero flux Neumann BC.

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

Default residual function for FINCH.

The default residual function for FINCH assumes the user_data parameter is the FINCH_DATA structure and calls the setparams function (passing the param_data structure), the discretization function, and the set BCs functions, in that order. It then forms the implicit and explicit side residuals that go into the iterative solver.

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

Default preconditioning function for FINCH.

The default preconditioning function for FINCH assumes the user_data parameter is the FINCH_DATA structure and performs a tridiagonal linear solve using a Modified Thomas Algorithm. This preconditioner will solve the linear problem exactly if there is no advective portion of the physics. Additionally, this preconditioner is also used as the basis for forming the default FINCH non-linear iterations and is sufficient for solving most problems.

5.5.3.29 int default_postprocess (const void * *user_data*)

The default postprocesses function for FINCH assumes the user_data parameter is the FINCH_DATA structure and does nothing.

5.5.3.30 int default_reset (const void * *user_data*)

Default reset function for FINCH.

The default reset function for FINCH assumes the user_data parameter is the FINCH_DATA structure and sets all old state parameters and variables to the new state.

5.5.3.31 int FINCH_TESTS ( )

Function runs a particular FINCH test.

The FINCH_TESTS function is used to exercise and test out the FINCH algorithms for correctness, efficiency, and accuracy. This test should never report a failure.

5.6 flock.h File Reference

FundamentaL Off-gas Collection of Kernels.

```
#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"
```

5.6.1 Detailed Description

FundamentaL Off-gas Collection of Kernels. This is just a .h file that holds all the includes necessary to develop and run simulations for adsorption and/or mass/energy transfer problems for gaseous systems. Include this file into any other project or source code that needs the methods below.

Files Included in FLOCK

macaw.h egret.h finch.h lark.h skua.h scopsowl.h gsta_opt.h magpie.h skua_opt.h scopsowl_opt.h yaml_wrapper.h

Author

Austin Ladshaw

Date

04/28/2014

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5.7 gsta_opt.h File Reference

Generalized Statistical Thermodynamic Adsorption (GSTA) Optimization Routine.

```
#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

    Data structure used in the GSTA optimization routines.

Macros

- #define Po 100.0

    Standard State Pressure - Units: kPa.
- #define R 8.3144621

    Gas Constant - Units: J/(K∗mol) = kB ∗ Na.
- #define Na 6.0221413E+23

    Avagadro's Number - Units: molecules/mol.

Functions

- int roundIt (double d)

    Function rounds a double to an integer.
- int twoFifths (int m)

    Function returns the rounded two-fifths result of int m.
- int orderMag (double x)

    Function returns the order of magnitude for the parameter x.
- int minValue (std::vector< int > &array)

    Function returns the minimum integer in an array of integers.
- int minIndex (std::vector< double > &array)

    Function returns the index of the minimum integer in an array of integers.
- int avgPar (std::vector< int > &array)

    Function returns the average integer value in an array of integers.
- double avgValue (std::vector< double > &array)

    Function returns an average in an array of doubles.
- double weightedAvg (double *enorm, double *x, int n)

    Function returns a weighted average in an array.
- double rSq (double *x, double *y, double slope, double vint, int m_dat)

    Function calculates the Coefficient of Determination (R Squared) for the temperature regression.
- bool isSmooth (double *par, void *data)

    Function looks at the list of parameters to check if they are smoothly changing.
- void orthoLinReg (double *x, double *y, double *par, int m_dat, int n_par)

    Function performs an Orthogonal Linear Regression on a set of data.
- void eduGuess (double *P, double *q, double *par, int k, int m_dat, void *data)

    Function will formed an educated guess for the next set of parameters in the GSTA analysis.
- double gstaFunc (double p, const double *K, double qmax, int n_par)

    Function evaluates the result of the GSTA isotherm model.
- double gstaObjFunc (double *t, double *y, double *par, int m_dat, void *data)

    Function to evaulate the GSTA objective function value.
- void eval_GSTA (const double *par, int m_dat, const void *data, double *fvec, int *info)

    Function to evaluate the GSTA model and feed into the lmfit routine.
- int gsta_optimize (const char *fileName)

    Function to perform the GSTA optimization routine.

5.7.1 Detailed Description

Generalized Statistical Thermodynamic Adsorption (GSTA) Optimization Routine. gsta_opt.cpp

Optimization routine developed for the GSTA isotherm and data analysis. This algorithm was the primary subject of a publication made in Fluid Phase Equilibria. Please refer to the below paper for technical information about the algorithms.

Reference: Ladshaw, Yiacoumi, Tsouris, and DePaoli, Fluid Phase Equilibria, 388, 169-181, 2015.

The GSTA model was first introduced by Llano-Restrepo and Mosquera (2009). Please refer to the below reference for theoretical information about the model.

Reference: Llano-Restrepo and Mosquera, Fluid Phase Equilibria, 283, 73-88, 2009.

Author

Austin Ladshaw

Date

12/17/2013

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5.7.2 Macro Definition Documentation

5.7.2.1 #define Po 100.0

Standard State Pressure - Units: kPa.

5.7.2.2 #define R 8.3144621

Gas Constant - Units: J/(K∗mol) = kB ∗ Na.

5.7.2.3 #define Na 6.0221413E+23

Avagadro's Number - Units: molecules/mol.

5.7.3 Function Documentation

5.7.3.1 int roundIt (double *d*)

Function rounds a double to an integer.

This function returns a rounded value of d. Rounding up for any decimal larger than 0.5 and down for all else.

5.7.3.2 int twoFifths (int *m*)

Function returns the rounded two-fifths result of int m.

This function is used to determine what the maximum number of parameters should be based on the number of data points m. It is designed to prevent the algorithms from "over fitting" the data.

5.7.3.3 int orderMag (double *x*)

Function returns the order of magnitude for the parameter x.

This function is used to help create initial guesses for the new GSTA parameters that are being optimized for. In order to make sure that those parameters are considered relavent in the optimization routine, we need to make the initial guesses to be around the same order of magnitude of the other GSTA parameters.

5.7.3.4 int minValue (std::vector< int > & *array*)

Function returns the minimum integer in an array of integers.

This function is used to determine the minimum number of GSTA parameters that were required to adequately fit the isotherm data.

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

Function returns the index of the minimum integer in an array of integers.

This function identifies the index of the minimum number of parameters needed for the GSTA model to fit the data. This index is common for all vectors in the GSTA_OPT_DATA structure and is used to identify the most suitable solution.

5.7.3.6 int avgPar (std::vector< int > & *array*)

Function returns the average integer value in an array of integers.

This function is used to identify the average number of parameters that all the data fitting needed for each GSTA analysis.

5.7.3.7 double avgValue (std::vector< double > & *array*)

Function returns an average in an array of doubles.

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

Function returns a weighted average in an array.

This averaging scheme is used to approximate the qmax parameter for the GSTA isotherm model, if that value is unknown. The weighting is based on the euclidean norms of all the fits of the data. Smaller norms are more heavily weighted since they represent a better fit of the data. Once averaging is complete and we have an estimate for qmax, the entire algorithm is re-run holding that qmax constant.

Parameters

enorm	array of euclidean norms from the fitting of the data
x	array of optimum qmax values to be averaged
n	the number of enorm and x values in the array

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

Function calculates the Coefficient of Determination (R Squared) for the temperature regression.

This function is used to determine the "fittness" of the linear regression performed on the temperature independent parameters of the GSTA isotherm. A good linear regression should return a value between 1.0 and 0.9.

Parameters

x	observations in the x-axis
y	observations in the y-axis
slope	slope of the linear regression
vint	intercept of the linear regression
m_dat	number of data points used in the linear regression

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

Function looks at the list of parameters to check if they are smoothly changing.

This function takes the parameter array par and GSTA_OPT_DATA structure and checks to see if those parameters are changing smoothly. If they are erratic or non-smooth, then it could be an indication of "over fitting" of the data.

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

Function performs an Orthogonal Linear Regression on a set of data.

This function takes an array of x and y observations and performs an orthogonal linear regression on that information to find optimum parameters for slope and intercept.

Parameters

x	array of x-axis observations
y	array of y-axis observations
par	array of parameter results after regression
m_dat	number of data points or observations
n_par	number of parameters to seek (if n_par != 1 or 2, then par[0] = intercept and par[1] = slope)

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

Function will formed an educated guess for the next set of parameters in the GSTA analysis.

This function takes partial pressure and adsorption observations, P and q, and tries to give a decent initial guess to what the GSTA parameters, par, will be for the next iteration.

Parameters

P	partial pressure observations in the data (kPa)
q	adsorption observations in the data (any units)
par	parameter array for the GSTA isotherm
k	index of the current number of parameters being considered
m_dat	number of pressure-adsorption observations in the isotherm
data	pointer to the GSTA_OPT_DATA data structure

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

Function evaluates the result of the GSTA isotherm model.

This function will evaluate the GSTA model and return the adsorbed amount given the current partial pressure p and the equilibrium parameters K.

Parameters

p	current partial pressure (kPa)
K	array of equilibrium parameters (1/kPa^n)
qmax	the theorectical maximum capacity for the isotherm
n_par	the number of equilibrium parameters

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

Function to evaulate the GSTA objective function value.

The objective function seeks to penalize the relative fittness of the model based on the number of parameters it took to minimize the euclidean norms. By penalizing the fittness of the model in this fashion, we can find the best solution to the system that required the least number of equilibrium parameters.

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

Function to evaluate the GSTA model and feed into the lmfit routine.

This function will formulate the residuals that go into the Levenberg-Marquardt's Algorithm for non-linear least squares regression. The form of this function is specific to how we interface with the lmfit routines.

5.7.3.16 int gsta_optimize (const char * *fileName*)

Function to perform the GSTA optimization routine.

This function is callable from the UI and is used to find the optimum parameters of the GSTA isotherm model given a particular set of isotherm data for single-component adsorption equilibria.

Parameters

fileName	name of the input file that holds the isotherm data

Note

The input file for the GSTA optimization routine is a text file holding the necessary information and data needed to run the routine. That input file has a very specific format that is detailed below.

Number of Isotherm Curves

Theoretical Maximum Adsorption Capacity (if unknown, provide 0)

Temperature of the ith Isotherm (K)

Number of Data points for the ith Isotherm

Partial Pressure (kPa) [tab] Corresponding Adsorbed Amount (any units)

(2nd Line down is repeated for all isotherms you are optimizing on...)

Example:

2

21.0

298.15

4

0.000165483 2.77

0.000306379 2.75

0.00044922 5.00

0.000939259 10.40

313.15

4

0.000589636 2.75

0.001063584 3.70

0.001351836 4.2

0.001543464 4.6

The above example would be for 2 sets of isotherms at 298.15 and 313.15 K, respectively. Maximum adsorption capacity is given as 21 (which in this has units of wt%). Each isotherm has 4 data points, which are given in a list as p (kPa) and q (wt%) pairs. Units of adsorption don't matter as long as they are consistent. If you give maximum capacity in mol/kg, then the q's in the lists must also be in mol/kg.

5.8 lark.h File Reference

Linear Algebra Residual Kernels.

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

Classes

- struct ARNOLDI_DATA

    Data structure for the construction of the Krylov subspaces for a linear system.
- struct GMRESLP_DATA

    Data structure for implementation of the Restarted GMRES algorithm with Left Preconditioning.
- struct GMRESRP_DATA

    Data structure for the Restarted GMRES algorithm with Right Preconditioning.
- struct PCG_DATA

    Data structure for implementation of the PCG algorithms for symmetric linear systems.
- struct BiCGSTAB_DATA

    Data structure for the implementation of the BiCGSTAB algorithm for non-symmetric linear systems.
- struct CGS_DATA

    Data structure for the implementation of the CGS algorithm for non-symmetric linear systems.
- struct OPTRANS_DATA

    Data structure for implementation of linear operator transposition.
- struct GCR_DATA

    Data structure for the implementation of the GCR algorithm for non-symmetric linear systems.
- struct GMRESR_DATA

    Data structure for the implementation of GCR with Nested GMRES preconditioning (i.e., GMRESR)
- struct KMS_DATA

    Data structure for the implemenation of the Krylov Multi-Space (KMS) Method.
- struct PICARD_DATA

    Data structure for the implementation of a Picard or Fixed-Point iteration for non-linear systems.
- struct BACKTRACK_DATA

    Data structure for the implementation of Backtracking Linesearch.
- struct PJFNK_DATA

    Data structure for the implementation of the PJFNK algorithm for non-linear systems.
- struct NUM_JAC_DATA

    Data structure to form a numerical jacobian matrix with finite differences.

Macros

- #define MIN_TOL 1e-15

    Minimum Allowable Tolerance for linear and non-linear problems.

Enumerations

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

    Enum of definitions for linear solver types in PJFNK.

Functions

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

  Function to update the linear vector x based on the Arnoldi Krylov subspace.
- 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)

  Function to factor a linear operator into an orthonormal basis and upper Hessenberg matrix.
- 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)

  Function to iteratively solve a non-symmetric, indefinite linear system with GMRESLP.
- 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)

  Function to directly solve a non-symmetric, indefinite linear system with FOM.
- 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)

  Function to iteratively solve a non-symmetric, indefinite linear system with GMRESRP.
- 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)

  Function to iteratively solve a symmetric, definite linear system with PCG.
- 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)

  Function to iteratively solve a non-symmetric, definite linear system with BiCGSTAB.
- 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)

  Function to iteratively solve a non-symmetric, definite linear system with CGS.
- 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)

  *Function that is used to perform transposition of a linear operator and results in a new vector A^T*r=u.*
- 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)

  Function to iteratively solve a non-symmetric, definite linear system with GCR.
- int gmresrPreconditioner (const Matrix< double > &r, Matrix< double > &Mr, const void *data)

  Function used in conjunction with GMRESR to apply GMRESRP iterations as a preconditioner.
- 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)

  Function to iteratively solve a non-symmetric, indefinite linear system with GMRESR.
- int kmsPreconditioner (const Matrix< double > &r, Matrix< double > &Mr, const void *data)

  Preconditioner function for the Krylov Multi-Space.
- int krylovMultiSpace (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, KMS_DATA *kms_dat, const void *matvec_data, const void *term_precon_data)

  Function to iteratively solve a non-symmetric, indefinite linear system with KMS.
- 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)

Function to iteratively solve a non-linear system using the Picard or Fixed-Point method.

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

  Function to form a linear operator of a Jacobian matrix used along with the PJFNK method.
- 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)

  Function to perform a Backtracking Line Search operation to smooth out convergence of PJFNK.
- 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)

  Function to perform the PJFNK algorithm to solve a non-linear system of equations.
- 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)

  Function to form a full numerical Jacobian matrix from a given non-linear function.
- int LARK_TESTS ()

  Function that runs a variety of tests on all the functions in LARK.

5.8.1 Detailed Description

Linear Algebra Residual Kernels. lark.cpp

The functions contained within are designed to solve generic linear and non-linear square systems of equations given a function argument and data from the user. Optionally, the user can also provide a function to return a preconditioning result that will be applied to the system.

Having the user define how the preconditioning is carried out provides two major advantages: (1) we do not need to store and large, sparse preconditioning matrices and instead only store the preconditioned vector result and (2) this allows the user to use any kind of preconditioner they see fit for their problem.

The Arnoldi function is typically not called by the user, but can be if desired. It accepts the function arguments and a residual vector to form an orthonormal basis of the Krylov subspace using the Modified Gram-Schmidt process (aka Arnoldi Iteration). This function is called by GMRES to iteratively solve a linear system of equations. Note that you can use this function to directly solve the linear system as long as that system is not too large. Construction of the basis is expensive, which is why this is used as a sub-function of an iterative method.

The Restarted GMRES function will accept function arguments for a linear system and attempt to solve said system iteratively by constructing an orthonormal basis from the Krylov function. Note that this GMRES function does support restarting and will use restarting by default if the linear system is too large.

Also included is a GMRES algorithm without restarting. This will directly solve the linear system within residual tolerance using a Full Orthogonal basis set of that system. It is equivalent to calling the Krylov method with the k parameter equal to N (i.e. the number of equations). This method is nick-named the Full Othogonalization Method (FOM), although the true FOM algorithm in literature is slightly different.

The PJFNK function will accept function arguments for a square, non-linear system of equations and attempt to solve it iteratively using both the GMRES and Krylov functions with Newton's method to convert the non-linear system into a linear system.

Also built here is a PCG implementation for solving symmetric linear systems. Can also be called by PJFNK if we know that the linear system (i.e. the Jacobian) is symmetric. This algorithm is significantly more efficient than GMRES, but is only valid if the system of equations is symmetric.

Other linear solvers implemented in this work are the BiCGSTAB and CGS algorithms for non-symmetric, positive definite matrices. These algorithms are significantly more computationally efficient than GMRES or FOM. However, they can both break down if the linear system is poorly conditioned. In general, you only want to use these methods if you have preconditioning available and your linear system is very, very large. Otherwise, you will be better suited to using GMRES or FOM.

There is also an implementation of the Generalized Conjugate Residual (GCR) method with and without restarting. This is a GMRES-like method that should give the exact solution within N iterations, where N is the original size of the matrix. Built ontop of the GCR method is a GMRESR (or GMRES Recursive) algorithm that uses GCR as the base method and performs GMRESRP iterations as a preconditioner at each iteration of GCR. This is the only linear solver that has built-in preconditioning. As a result, it may be slower than other algorithms for simple problems, but generally will have much better convergence behavior and will almost always give better residual reduction, even for hard to solve problems.

We have also developed a novel/experimental iterative method based on the idea of recursively preconditioning a Krylov Subspace with more Krylov Subspaces. We have called with algorithm the Krylov Multi-Space (KMS) method. This algorithm is based on publications from Vorst and Vuik (1991) and Saad (1993). The idea is too use the FGMRES algorithm developed by Saad (1993) and precondition it with more FGMRES steps, i.e., nesting the iterations as Vorst and Vuik (1991) had proposed. In this way, we have created a generalized Krylov Subspace method that has it's own variable preconditioner that can be adjusted depending on the user's desired complexity and convergence rate. If the levels of recursion requested is zero, then this algorithm is exactly equal to GMRES with right preconditioning. If the level is one, then it is FGMRES with a GMRES preconditioner. However, we allow the levels of recursion to reach up to 5, thus allowing us to precondition the preconitioners with more GMRES steps. This can result is significantly faster convergence rates, but is typically only necessary for very large or difficult to solve problems.

NOTE: There are three GMRES implementations: (i) gmresLP, (ii) fom, and (iii) gmresRP. GMRESLP is a restarted GMRES implementation that is left preconditioned and only checks the residual on the outer loops. This may be less efficient than GMRESRP, which can check both outer and inner loop residuals. However, GMRESRP has to use right preconditioning, which also slightly changes the convergence behavior of the linear system. GMRES with left preconditioning and without restarting will just build the full subspace by default, thus solving the system exactly, but may require too much memory. You can do a GMRESRP unrestarted by specifying that the restart parameter be equal to the size of the problem.

Basic Implementation Details:

Linear Solvers -> Solve Ax=b for x

Non-Linear Solvers -> Solve F(x)=0 for x

All implementations require system size to be 2 or greater

Author

Austin Ladshaw

Date

10/14/2014

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5.8.2 Macro Definition Documentation

5.8.2.1 #define MIN_TOL 1e-15

Minimum Allowable Tolerance for linear and non-linear problems.

5.8.3 Enumeration Type Documentation

5.8.3.1 enum krylov_method

Enum of definitions for linear solver types in PJFNK.

Enum delineates the available Krylov Subspace methods that can be used to solve the linear sub-problem at each non-linear iteration in a Newton method.

Enumerator

GMRESLP

PCG

BiCGSTAB

CGS

FOM

GMRESRP

GCR

GMRESR

5.8.4 Function Documentation

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

Function to update the linear vector x based on the Arnoldi Krylov subspace.

This function will update a solution vector x based on the previous solution x0 given the orthonormal basis and upper Hessenberg matrix formed in the Arnoldi algorithm. Updating is automatically called by the GMRESLP function. It is expected that the Arnoldi algorithm has already been called prior to calling this function.

Parameters

x	matrix that will hold the new updated solution to the linear system
x0	matrix that holds the previous solution to the linear system
arnoldi_dat	pointer to the ARNOLDI_DATA data structure

5.8.4.2 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*)

Function to factor a linear operator into an orthonormal basis and upper Hessenberg matrix.

This function performs the Arnoldi algorithm to factor a linear operator into an orthonormal basis and upper Hessenberg matrix. Each orthonormal vector is formed using a Modified Gram-Schmidt procedure. When used in conjunction with GMRESLP, user may supply a preconditioning operator to improve convergence of the linear system. However, this function can be used by itself to factor the user's linear operator.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
r0	user supplied vector to serve as the first basis vector in the orthonormal basis
arnoldi_dat	pointer to the ARNOLDI_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (*matvec) (const Matrix<double>& v, Matrix<double> &Av, const void *data)

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

--—

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

--—

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

--—

5.8.4.3 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*)

Function to iteratively solve a non-symmetric, indefinite linear system with GMRESLP.

This function iteratively solves a non-symmetric, indefinite linear system using the Generalized Minimum RESidual method with Left Preconditioning (GMRESLP). It calls the Arnoldi algorithm to factor a linear operator into an orthonormal basis and upper Hessenberg matrix, then uses that factorization to form an approximation to the linear system. Because this algorithm uses left-side preconditioning, it can only check the linear residuals at the outer iterations.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
gmreslp_dat	pointer to the GMRESLP_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

--—

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

--—

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

--—

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

--—

5.8.4.4 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*)

Function to directly solve a non-symmetric, indefinite linear system with FOM.

This function directly solves a non-symmetric, indefinite linear system using the Full Orthogonalization Method (F-OM). This algorithm is exactly equivalent to GMRESLP without restarting. Therefore, it uses the GMRESLP_DATA structure and calls the GMRESLP algorithm without using restarts. As a result, it never checks linear residuals. However, this should give the exact solution upon completion, assuming the linear operator is not singular.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
gmreslp_dat	pointer to the GMRESLP_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

----

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

5.8.4.5 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*)

Function to iteratively solve a non-symmetric, indefinite linear system with GMRESRP.

This function iteratively solves a non-symmetric, indefinite linear system using the Generalized Minimum RESidual method with Right Preconditioning (GMRESRP). Because this algorithm uses right preconditioning, it is able to check the linear residuals at both the outer and inner iterations. This may be much for efficient compared to G-MRESLP. In order to check inner residuals, this algorithm has to perform it's own internal Modified Gram-Schmidt procedure and will not call the Arnoldi algorithm.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
gmresrp_dat	pointer to the GMRESRP_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

---

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

5.8.4.6 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*)

Function to iteratively solve a symmetric, definite linear system with PCG.

This function iteratively solves a symmetric, definite linear system using the Preconditioned Conjugate Gradient (PCG) method. The PCG algorithm is optimal in terms of efficiency and residual reduction, but only if the linear system is symmetric. PCG will fail if the linear operator is non-symmetric!

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
pcg_dat	pointer to the PCG_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

---

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

5.8.4.7 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*)

Function to iteratively solve a non-symmetric, definite linear system with BiCGSTAB.

This function iteratively solves a non-symmetric, definite linear system using the Bi-Conjugate Gradient STABilized (BiCGSTAB) method. This is a highly efficient algorithm for solving non-symmetric problems, but will occassionally breakdown and fail. Most common failures are caused by poor preconditioning. Works very well for grid-based linear systems.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
bicg_dat	pointer to the BiCGSTAB_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

--——

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

--——

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

--——

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

--——

5.8.4.8 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*)

Function to iteratively solve a non-symmetric, definite linear system with CGS.

This function iteratively solves a non-symmetric, definite linear system using the Conjugate Gradient Squared (CGS) method. This is an extremely efficient algorithm for solving non-symmetric problems, but will often breakdown and fail. Most common failures are caused by poor or no preconditioning. Works very will for grid-based linear systems.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
cgs_dat	pointer to the CGS_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

---—

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

---—

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

---—

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

---—

5.8.4.9 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*)

Function that is used to perform transposition of a linear operator and results in a new vector A^T∗r=u.

This function takes a user supplied linear operator and forms the result of that operator transposed and multiplied by a given vector r (A^T∗r=u). Transposition is accomplised by reordering the transpose operator and multiplying the non-transposed operator by a complete set of orthonormal vectors. The end result gives the ith component of the vector u for each operation (u_i = r^T∗A∗i). Here, i is a vector made from the ith column of the identity matrix. If the linear system if sufficiently large, then this operation may take some time.

Parameters

matvec	user supplied linear operator given as an int function
r	vector to be multiplied by the transpose of the operator
u	vector to store the result of the operator transposition (u=A^T∗r)
transpose_dat	pointer to the OPTRANS_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

---—

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

---—

5.8.4.10 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*)

Function to iteratively solve a non-symmetric, definite linear system with GCR.

This function iteratively solves a non-symmetric, definite linear system using the Generalized Conjugate Residual (GCR) method. Similar to GMRESRP, this algorithm will construct a growing orthonormal basis set that will eventually form the exact solution to the linear system. However, this algorithm is less efficient than GMRESRP and can suffer breakdowns if the linear system is indefinite.

Parameters

matvec	user supplied linear operator given as an int function
precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
gcr_dat	pointer to the GCR_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
precon_data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

--——

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

--——

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

---—

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

---—

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

Function used in conjunction with GMRESR to apply GMRESRP iterations as a preconditioner.

This function is required to take the form of the user supplied preconditioning functions for other iterative methods. However, it cannot be used in conjunction with any other Krylov method. It is only called by the GMRESR function when the preconditioner needs to be applied.

Parameters

r	vector supplied to the preconditioner to operate on
Mr	vector to hold the result of the preconditioning operation
data	void pointer to the GMRESR_DATA data structure

5.8.4.12 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*)

Function to iteratively solve a non-symmetric, indefinite linear system with GMRESR.

This function iteratively solves a non-symmetric, indefinite linear system using the Generalized Minimum RESidual Recursive (GMRESR) method. This algorithm actually uses GCR at the outer iterations, but stabilizes GCR with GMRESRP inner iterations to implicitly form a variable preconditioner to the linear system. As such, this is one of only two methods that inherently includes preconditioning (the other is KMS), without any user supplied preconditioning operator. However, this algorithms is signficantly more computationally expensive than GCR or GMRESRP separately. It should only be used for solving very large or very hard to solve linear systems.

Parameters

matvec	user supplied linear operator given as an int function
terminal_precon	user supplied preconditioning operator given as an int function

b	matrix of boundary conditions in the linear system Ax=b
gmresr_dat	pointer to the GMRESR_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
term_precon_-data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

--—

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

--—

int (∗terminal_precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

--—

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

--—

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

Preconditioner function for the Krylov Multi-Space.

This function is required to take the form of the user supplied preconditioning functions for other iterative methods. However, it cannot be used in conjunction with any other Krylov method. It is only called by the KMS function when the preconditioner needs to be applied.

Parameters

r	vector supplied to the preconditioner to operate on
Mr	vector to hold the result of the preconditioning operation
data	void pointer to the KMS_DATA data structure

5.8.4.14 int krylovMultiSpace (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*, KMS_DATA ∗ *kms_dat*, const void ∗ *matvec_data*, const void ∗ *term_precon_data*)

Function to iteratively solve a non-symmetric, indefinite linear system with KMS.

This function iteratively solves a non-symmetric, indefinite linear system using the Krylov Multi-Space (KMS) method. This algorithm uses GMRESRP at both outer and inner iterations to implicitly form a variable preconditioner to the linear system. As such, this is one of only two methods that inherently includes preconditioning, without any user supplied preconditioning operator (the other being GMRESR). The advantage to this method over GMRESR is that this method is GMRES at its core, and will therefore never breakdown or need to be stabilized. Additionally, you can call this method and set it's max_level parameter (see KMS_DATA) to 0, which will make this algorithm exactly equal to GMRESRP. If the max_level is set to 1, then this algorithm is exactly FGMRES (Saad, 1993) with the GMRES algorithm as a preconditioner. However, you can set max_level higher to precondition the preconditioners with more preconditioners. Thus creating a method with any desired complexity or rate of convergence.

Parameters

matvec	user supplied linear operator given as an int function
terminal_precon	user supplied preconditioning operator given as an int function
b	matrix of boundary conditions in the linear system Ax=b
kms_dat	pointer to the KMS_DATA data structure
matvec_data	user supplied void pointer to a data structure needed for the linear operator
term_precon_-data	user supplied void pointer to a data structure needed for the precondtioning operator

Note

int (∗matvec) (const Matrix<double>& v, Matrix<double> &Av, const void ∗data)

This is a user supplied function for a linear operator. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix v that will act on the linear operator a modified the matrix entries of Av to form the result of a matrix-vector product. Void pointer data is used to pass any user data structure that the function may need in order to perform the linear operation.

----

int (∗terminal_precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

This is a user supplied function for a preconditioning operator. It has the same form as the above linear operator function and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the original linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

5.8.4.15 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*)

Function to iteratively solve a non-linear system using the Picard or Fixed-Point method.

This function iteratively solves a non-linear system using the Picard method. User supplies a residual function and a weak solution form function. The weak form function is used to approximate the next solution vector for the non-linear system and the residual function is used to determine convergence. User also supplies an initial guess to the non-linear system as a matix x, which will also be used to store the solution. This algorithm is very simple and may not be sufficient to solve complex non-linear systems.

Parameters

res	user supplied function for the non-linear residuals of the system
evalx	user supplied function for the weak form to estimate the next solution
x	user supplied matrix holding the initial guess to the non-linear system
picard_dat	pointer to the PICARD_DATA data structure
res_data	user supplied void pointer to a data structure used for residual evaluations
evalx_data	user supplied void pointer to a data structure used for evaluation of weak form

Note

int (∗res) (const Matrix<double>& x, Matrix<double> &F, const void ∗data)

This is a user supplied function for the non-linear residuals. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix x representing the current non-linear variables. Those variables are used to evaluate the users functions and return the residuals in the matrix F. The void pointer data is a data structure provided by the user to hold information the function may need in order to form the residuals.

----

int (∗evalx) (const Matrix<double>& x0, Matrix<double> &x, const void ∗data)

This is a user supplied function to approximate the next solution vector x based on the previous solution vector x0. The x0 matrix is passed to this function and must be used to edit the entries of x based on the weak form of the problem. The user is free to define any weak form approximation. Void pointer data is the users data structure that may be used to pass additional information into this function in order to evaluate the weak form.

Example Residual: F(x) = x^2 + x - 1 Goal is to make this function equal zero

Example Weak Form: x = 1 - x0^2 Rearrage residual to form a weak solution

----

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

Function to form a linear operator of a Jacobian matrix used along with the PJFNK method.

This function is used in conjunction with the PJFNK routine to form a linear operator that a Krylov method can operate on. This linear operator is formed from the current residual vector of the non-linear iteration in PJFNK using a finite difference approximation.

Jacobian Linear Operator: J∗v = (F(x_k + eps∗v) - F(x_k)) / eps

Parameters

v	vector to be multiplied by the Jacobian matrix
Jv	storage vector for the result of the Jacobi-vector product
data	void pointer to the PJFNK_DATA data structure holding solver information

5.8.4.17 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*)

Function to perform a Backtracking Line Search operation to smooth out convergence of PJFNK.

This function performs a simple backtracking line search operation on the residuals from the PJFNK method. The step size of the non-linear iteration is checked against a level of tolerance for residual reduction, then adjusted down if necessary. This method always starts out with the maximum allowable step size. If the largest step size is fine, then the algorithm does nothing. Otherwise, it iteratively adjusts the step size down, until a suitable step is found. In the case that no suitable step is found, this algorithm will report failure to the PJFNK method and PJFNK will decide whether to continue trying to find a global minimum or report that it is stuck in a local minimum.

Parameters

feval	user supplied residual function for the non-linear system
Fkp1	vector holding the residuals for the next non-linear step
xkp1	vector holding the solution for the next non-linear step
pk	vector holding the current non-linear search direction
normFk	value of the current non-linear residual
backtrack_dat	pointer to the BACKTRACK_DATA data structure
feval_data	user supplied void pointer to the data structure needed for residual evaluation

Note

int (∗feval) (const Matrix<double>& x, Matrix<double> &F, const void ∗data)

This is a user supplied function for the non-linear residuals. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix x representing the current non-linear variables. Those variables are used to evaluate the users functions and return the residuals in the matrix F. The void pointer data is a data structure provided by the user to hold information the function may need in order to form the residuals.

5.8.4.18 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*)

Function to perform the PJFNK algorithm to solve a non-linear system of equations.

This function solves a non-linear system of equations using the Preconditioned Jacobian- Free Newton-Krylov (P-JFNK) algorithm. Each non-linear step of this method results in a linear sub-problem that is solved iteratively with one of the Krylov methods in the krylov_method enum. User must supplied a residual function that computes the non-linear residuals of the system given the current state of the variables x. Additionally, the user must also supplied an initial guess to the non-linear system. Optionally, the user may supply a preconditioning function for the linear sub-problem.

Basic Steps: (i) Calc F(x_k), (ii) Solve J(x_k)∗s_k=-F(x_k) for s_k, (iii) Form x_kp1 = x_k + s_k

Parameters

res	user supplied residual function for the non-linear system
precon	user supplied preconditioning function for the linear sub-problems
x	user supplied initial guess and storage location of the solution
pjfnk_dat	pointer to the PJFNK_DATA data structure
res_data	user supplied void pointer to data structure used in residual function
precon_data	user supplied void pointer to data structure used in preconditioning function

Note

int (∗res) (const Matrix<double>& x, Matrix<double> &F, const void ∗data)

This is a user supplied function for the non-linear residuals. User's function must return an int of 0 upon success and anything else denotes a failure. The function accepts a matrix x representing the current non-linear variables. Those variables are used to evaluate the users functions and return the residuals in the matrix F. The void pointer data is a data structure provided by the user to hold information the function may need in order to form the residuals.

----

int (∗precon) (const Matrix<double>& b, Matrix<double> &Mb, const void ∗data)

This is a user supplied function for a preconditioning operator. It has the same form as the linear operators from the Krylov methods and should have all the same properties. The only difference is that this function must form an approximate matrix inversion on the jacvec linear operator and modify the entries of Mb to represent the result of that approximate matrix inversion. The matrix b is given as the vector that this operator is acting on and the void pointer data is for any user data structure that the operator may need.

5.8.4.19 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*)

Function to form a full numerical Jacobian matrix from a given non-linear function.

This function uses finite differences to form a full rank Jacobian matrix for a user supplied non-linear function. The Jacobian matrix will be formed at the current state of the non-linear variables x and stored in a full matrix J. Integers Nx and Nf are used to determine the size of the Jacobian matrix.

Parameters

Func	user supplied function for evaluation of the non-linear system
x	matrix holding the current value of the non-linear variables
J	matrix that will store the numerical Jacobian result
Nx	number of non-linear variables in the system
Nf	number of non-linear functions in the system
jac_dat	pointer to the NUM_JAC_DATA data structure
user_data	user supplied void pointer to a data structure used in the non-linear function

5.8.4.20 int LARK_TESTS ( )

Function that runs a variety of tests on all the functions in LARK.

This function runs a variety of tests on the linear and non-linear methods developed in LARK. It can be called from the UI.

5.9 macaw.h File Reference

MAtrix CAlculation Workspace.

```
#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 >

    Templated C++ Matrix Class Object (click Matrix to go to function definitions)

Macros

- #define M_PI 3.14159265358979323846264338327950288

    Value of PI with double precision.

Functions

- int MACAW_TESTS ()

    Function to run the MACAW tests.

5.9.1 Detailed Description

MAtrix CAlculation Workspace. macaw.cpp

This is a small C++ library that faciltates the use and construction of real matrices using vector objects. The Matrix class is templated so that users are able to work with matrices of any type including, but not limited to: (i) doubles, (ii) ints, (iii) floats, and (iv) even other matrices! Routines and functions are defined for Dense matrix operations. As a result, we typically only use Column Matrices (or Vectors) when doing any actual simulations. However, the development of this class was integral to the development and testing of the Sparse matrix operators in lark.h.

While the primary goal of this object was to define how to operate on real matrices, we could extend this idea to complex matrices as well. For this, we could develop objects that represent imaginary and complex numbers and then create a Matrix of those objects. For this reason, the matrix operations here are all templated to abstract away the specificity of the type of matrix being operated on.

Author

Austin Ladshaw

Date

01/07/2014

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5.9.2 Macro Definition Documentation

5.9.2.1 #define M_PI 3.14159265358979323846264338327950288

Value of PI with double precision.

5.9.3 Function Documentation

5.9.3.1 int MACAW_TESTS ( )

Function to run the MACAW tests.

This function is callable from the UI and is used to run several algorithm tests for the Matrix objects. This test should never report any errors.

5.10 magpie.h File Reference

Multicomponent Adsorption Generalized Procedure for Isothermal Equilibria.

```
#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

  GSTA Data Structure.
- struct mSPD_DATA

  MSPD Data Structure.
- struct GPAST_DATA

  GPAST Data Structure.
- struct SYSTEM_DATA

  System Data Structure.
- struct MAGPIE_DATA

  MAGPIE Data Structure.

Macros

- #define DBL_EPSILON 2.2204460492503131e-016

  Machine precision value used for approximating gradients.
- #define Z 10.0

  Surface coordination number used in the MSPD activity model.
- #define A 3.13E+09

  Corresponding van der Waals standard area for our coordination number (cm^2/mol)
- #define V 18.92

  Corresponding van der Waals standard volume for our coordination number (cm^3/mol)
- #define Po 100.0

  Standard State Pressure - Units: kPa.
- #define R 8.3144621

  Gas Constant - Units: J/(K∗mol) = kB ∗ Na.
- #define Na 6.0221413E+23

  Avagadro's Number - Units: molecules/mol.
- #define kB 1.3806488E-23

  Boltzmann's Constant - Units: J/K.
- #define shapeFactor(v_i) (((Z - 2) ∗ v_i) / (Z ∗ V)) + (2 / Z)

  This macro replaces all instances of shapeFactor(#) with the following single line calculation.
- #define lnKo(H, S, T) -(H / (R ∗ T)) + (S / R)

  This macro calculates the natural log of the dimensionless isotherm parameter.
- #define He(qm, K1, m) (qm ∗ K1) / (m ∗ Po)

  This macro calculates the Henry's Coefficient for the ith component.

Functions

- double qo (double po, const void ∗data, int i)

  Function computes the result of the GSTA isotherm for the ith species.
- double dq_dp (double p, const void ∗data, int i)

  Function computes the derivative of the GSTA model with respect to partial pressure.
- double q_p (double p, const void ∗data, int i)

  Function computes the ratio between the adsorbed amount and partial pressure for the GSTA isotherm.
- double PI (double po, const void ∗data, int i)

  Function computes the spreading pressure integral of the ith species.
- double Qst (double po, const void ∗data, int i)

  Function computes the heat of adsorption based on the ith species GSTA parameters.

- double eMax (const void ∗data, int i)

  Function to approximate the maximum lateral energy term for the ith species.
- double lnact_mSPD (const double ∗par, const void ∗data, int i, volatile double PI)

  Function to evaluate the MSPD activity coefficient for the ith species.
- double grad_mSPD (const double ∗par, const void ∗data, int i)

  Function to approximate the derivative of the MSPD activity model with spreading pressure.
- double qT (const double ∗par, const void ∗data)

  Function to calculate the total adsorbed amount (mol/kg) for the mixed surface phase.
- void initialGuess_mSPD (double ∗par, const void ∗data)

  Function to provide an initial guess to the unknown parameters being solved for in GPAST.
- void eval_po_PI (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function used with lmfit to evaluate the reference state pressure of a species based on spreading pressure.
- void eval_po_qo (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function used with lmfit to evaluate the reference state pressure of a species based on that species isotherm.
- void eval_po (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function used with lmfit to evaluate the reference state pressure of a species based on a sub-system.
- void eval_eta (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function used with lmfit to evaluate the binary interaction parameters for each unique species pair.
- void eval_GPAST (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function used with lmfit to solve the GPAST system of equations.
- int MAGPIE (const void ∗data)

  Function to call all sub-routines to solve a MAGPIE/GPAST problem at a given temperature and pressure.
- int MAGPIE_SCENARIOS (const char ∗inputFileName, const char ∗sceneFileName)

  Function to perform a series of MAGPIE simulations based on given input files.

5.10.1 Detailed Description

Multicomponent Adsorption Generalized Procedure for Isothermal Equilibria. magpie.cpp

This file contains all functions and routines associated with predicting isothermal adsorption equilibria from only single component isotherm information. The basis of the model is the Adsorbed Solution Theory developed by Myers and Prausnitz (1965). Added to that base model is a procedure by which we can predict the non-idealities present at the surface phase by solving a closed system of equations involving the activity model.

For more details on this procedure, check out our publication in AIChE where we give a fully feature explaination of our Generalized Predictive Adsorbed Solution Theory (GPAST).

Reference: Ladshaw, A., Yiacoumi, S., and Tsouris, C., "A generalized procedure for the prediction of multicomponent adsorption equilibria", AIChE J., vol. 61, No. 8, p. 2600-2610, 2015.

MAGPIE represents a special case of the more general GPAST procedure, wherin the isotherm for each species is respresent by the GSTA isotherm (see gsta_opt.h) and the activity model for non-ideality at the adsorbent surface is a Modified Spreading Pressure Dependent (MSPD) model. See the above paper reference for more details.

Author

Austin Ladshaw

Date

12/17/2013

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5.10.2 Macro Definition Documentation

5.10.2.1 #define DBL_EPSILON 2.2204460492503131e-016

Machine precision value used for approximating gradients.

5.10.2.2 #define Z 10.0

Surface coordination number used in the MSPD activity model.

5.10.2.3 #define A 3.13E+09

Corresponding van der Waals standard area for our coordination number (cm^2/mol)

5.10.2.4 #define V 18.92

Corresponding van der Waals standard volume for our coordination number (cm^3/mol)

5.10.2.5 #define Po 100.0

Standard State Pressure - Units: kPa.

5.10.2.6 #define R 8.3144621

Gas Constant - Units: J/(K∗mol) = kB ∗ Na.

5.10.2.7 #define Na 6.0221413E+23

Avagadro's Number - Units: molecules/mol.

5.10.2.8 #define kB 1.3806488E-23

Boltzmann's Constant - Units: J/K.

5.10.2.9 #define shapeFactor(*v_i*) (((Z - 2) ∗ v_i) / (Z ∗ V)) + (2 / Z)

This macro replaces all instances of shapeFactor(#) with the following single line calculation.

5.10.2.10 #define lnKo(*H,* *S,* *T*) -(H / (R ∗ T)) + (S / R)

This macro calculates the natural log of the dimensionless isotherm parameter.

5.10.2.11 #define He(*qm,* *K1,* *m*) (qm ∗ K1) / (m ∗ Po)

This macro calculates the Henry's Coefficient for the ith component.

5.10.3 Function Documentation

5.10.3.1 double qo (double *po*, const void ∗ *data*, int *i*)

Function computes the result of the GSTA isotherm for the ith species.

This function just computes the result of the GSTA isotherm model for the ith species given the partial pressure po.

Parameters

po	partial pressure in kPa at which to evaluate the GSTA model
data	void pointer to the MAGPIE_DATA data structure
i	index of the gas species for which the GSTA model is being evaluated

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

Function computes the derivative of the GSTA model with respect to partial pressure.

This function just computes the result of the derivative of GSTA isotherm model for the ith species at the given the partial pressure p.

Parameters

p	partial pressure in kPa at which to evaluate the GSTA model
data	void pointer to the MAGPIE_DATA data structure
i	index of the gas species for which the GSTA model is being evaluated

5.10.3.3 double q_p (double *p*, const void ∗ *data*, int *i*)

Function computes the ratio between the adsorbed amount and partial pressure for the GSTA isotherm.

This function just computes the ratio between the adsorbed amount q (mol/kg) and the partial pressure p (kPa) at the given partial pressure. If p == 0, then this function returns the Henry's Law constant for the isotherm of the ith species.

Parameters

p	partial pressure in kPa at which to evaluate the GSTA model
data	void pointer to the MAGPIE_DATA data structure
i	index of the gas species for which the GSTA model is being evaluated

5.10.3.4 double PI (double *po*, const void ∗ *data*, int *i*)

Function computes the spreading pressure integral of the ith species.

This function uses an analytical solution to the spreading pressure integral with the GSTA isotherm to evaluate and return the value computed by that integral equation.

Parameters

po	partial pressure in kPa at which to evaluate the lumped spreading pressure
data	void pointer to the MAGPIE_DATA data structure
i	index of the gas species for which the GSTA model is being evaluated

5.10.3.5 double Qst (double *po*, const void ∗ *data*, int *i*)

Function computes the heat of adsorption based on the ith species GSTA parameters.

This function computes the isosteric heat of adsorption (J/mol) for the GSTA parameters of the ith species.

Parameters

po	partial pressure in kPa at which to evaluate the heat of adsorption
data	void pointer to the MAGPIE_DATA data structure
i	index of the gas species for which the GSTA model is being evaluated

5.10.3.6 double eMax (const void ∗ *data*, int *i*)

Function to approximate the maximum lateral energy term for the ith species.

The function attempts to approximate the maximum lateral energy term for the ith species. This is not a true maximum, but a cheaper estimate. Value being computed is used to shift the geometric mean and formulate the average cross-lateral energy term between species i and j.

5.10.3.7 double lnact_mSPD (const double ∗ *par*, const void ∗ *data*, int *i*, volatile double *PI*)

Function to evaluate the MSPD activity coefficient for the ith species.

This function will return the natural log of the ith species activity coefficient using the Modified Spreading Pressure Dependent (MSPD) activity model. The par argument holds the variable values being solved for by GPAST and their contents will change depending on whether we are doing a forward or reverse evaluation. This function should not be called by the user and will only be called when needed in the GPAST routine.

Parameters

par	list of parameters representing variables to be solved for in GPAST
data	void pointer for the MAGPIE_DATA data structure
i	ith species that we want to calculate the activity coefficient for
PI	lumped spreading pressure term used in gradient estimations

5.10.3.8 double grad_mSPD (const double ∗ *par*, const void ∗ *data*, int *i*)

Function to approximate the derivative of the MSPD activity model with spreading pressure.

This function returns a 2nd order, finite different approximation of the derivative of the MSPD activity model with the spreading pressure. The par argument will either hold the current iterates estimate of spreading pressure or should be passed as null. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
data	void pointer for the MAGPIE_DATA data structure
i	ith species for which we will approximate the activty model gradient

5.10.3.9 double qT (const double ∗ *par*, const void ∗ *data*)

Function to calculate the total adsorbed amount (mol/kg) for the mixed surface phase.

This function will uses the obtained system parameters from par and estimate the total amount of gases adsorbed to the surface in mol/kg. The user does not need to call this function, since this result will be stored in the SYSTE-M_DATA structure.

Parameters

par	list of parameters representing variables to be solved for in GPAST
data	void pointer for the MAGPIE_DATA data structure

5.10.3.10 void initialGuess_mSPD (double * *par*, const void * *data*)

Function to provide an initial guess to the unknown parameters being solved for in GPAST.

This function intends to provide an initial guess for the unknown values being solved for in the GPAST system. Depending on what type of solve is requested, this algorithm will provide a guess for the adsorbed or gas phase composition.

Parameters

par	list of parameters representing variables to be solved for in GPAST
data	void pointer for the MAGPIE_DATA data structure

5.10.3.11 void eval_po_PI (const double * *par*, int *m_dat*, const void * *data*, double * *fvec*, int * *info*)

Function used with lmfit to evaluate the reference state pressure of a species based on spreading pressure.

This function is used inside of the MSPD activity model to calculate the reference state pressure of a particular species at a given spreading pressure for the system. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
m_dat	number of functions/variables in the GPAST system of equations
data	void pointer for the MAGPIE_DATA data structure
fvec	list of residuals formed by the functions in GPAST
info	integer flag variable used in the lmfit routine

5.10.3.12 void eval_po_qo (const double * *par*, int *m_dat*, const void * *data*, double * *fvec*, int * *info*)

Function used with lmfit to evaluate the reference state pressure of a species based on that species isotherm.

This function is used to evaluate the partial pressure or reference state pressure for a particular species given single-component adsorbed amount. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
m_dat	number of functions/variables in the GPAST system of equations
data	void pointer for the MAGPIE_DATA data structure
fvec	list of residuals formed by the functions in GPAST
info	integer flag variable used in the lmfit routine

5.10.3.13 void eval_po (const double * *par*, int *m_dat*, const void * *data*, double * *fvec*, int * *info*)

Function used with lmfit to evaluate the reference state pressure of a species based on a sub-system.

This function is used to approximate reference state pressures based on the spreading pressure of a sub-system in GPAST. The sub-system will be one of the unique binary systems that exist in the overall mixed gas system. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
m_dat	number of functions/variables in the GPAST system of equations
data	void pointer for the MAGPIE_DATA data structure
fvec	list of residuals formed by the functions in GPAST
info	integer flag variable used in the lmfit routine

5.10.3.14 void eval_eta (const double * *par,* int *m_dat,* const void * *data,* double * *fvec,* int * *info*)

Function used with lmfit to evaluate the binary interaction parameters for each unique species pair.

This function is used to estimate the binary interaction parameters for all species pairs in a given sub-system. Those parameters are then stored for later used when evaluating the activity coefficients for the overall mixture. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
m_dat	number of functions/variables in the GPAST system of equations
data	void pointer for the MAGPIE_DATA data structure
fvec	list of residuals formed by the functions in GPAST
info	integer flag variable used in the lmfit routine

5.10.3.15 void eval_GPAST (const double * *par,* int *m_dat,* const void * *data,* double * *fvec,* int * *info*)

Function used with lmfit to solve the GPAST system of equations.

This function is used after having calculated and stored all necessary information to solve a closed form GPAST system of equations. User does not need to call this function. GPAST will call automatically when needed.

Parameters

par	list of parameters representing variables to be solved for in GPAST
m_dat	number of functions/variables in the GPAST system of equations
data	void pointer for the MAGPIE_DATA data structure
fvec	list of residuals formed by the functions in GPAST
info	integer flag variable used in the lmfit routine

5.10.3.16 int MAGPIE (const void * *data*)

Function to call all sub-routines to solve a MAGPIE/GPAST problem at a given temperature and pressure.

This is the function that a typical user will want to incorporate into their own codes when evaluating adsorption of a gas mixture. Prior to calling this function, all required structures and information in the MAGPIE_DATA structure must have been properly initialized. After this function has completed it's operations, it will return an integer used to denote a success or failure of the routine. Integers 0, 1, 2, and 3 all denote success. Anything else is considered a failure.

To setup the MAGPIE_DATA structure correctly, you must reserve space for all vector objects based on the number of gas species in the mixture. In general, you only need to reserve space for the adsorbing species. However, you can also reserve space for non-adsorbing species, but you MUST give a gas/adsorbed mole fraction of the non-adsorbing species 0.0 so that the routine knows to ignore them (very important)!

After setting up the memory for the vector objects, you can intialize information specific to the simulation you want to request. The number of species (N), total pressure (PT) and gas temperature (T) must always be given. You can neglect the non-idealities of the surface phase by setting the Ideal bool to true. This will result in faster calculations, because MAGPIE will just revert down to the Ideal Adsorbed Solution Theory (IAST).

The Recover bool will denote whether we are doing a forward or reverse GPAST evaluation. Forward evaluation is for solving for the composition of the adsorbed phase given the composition of the gas phase (Recover = false). Reverse evaluation is for solve for the composition of the gas phase given the composition of the adsorbed phase (Recover = true).

For a reverse evaluation (Recover = true) you will also need to stipulate whether or not there is a carrier gas (Carrier = true or false). A carrier gas is considered any non-adsorbing species that may be present in the gas phase and contributing to the total pressure in the system.

The parameters that must be initialized for all species include all GSTA_DATA parameters and the van der Waals volume parameter (v) in the mSPD_DATA structure. For non-adsorbing species, you can ignore these parameters, but need to set the sites (m) from GSTA_DATA to 1. GPAST cannot run any evaluations without these parameters being set properly AND set in the same order for all species (i.e., make sure that gpast_dat[i].qmax corresponds to mspd_dat[i].v and so on).

Lastly, you need to give either the gas phase or adsorbed phase mole fractions, depending on whether you are going to run a forward or reverse evaluation, respectively. For a forward evaluation, provide the gas mole fractions (y) in GPAST_DATA for each species (non-adsorbing species should have this value set to 0.0). For a reverse evaluation, provide the adsorbed mole fractions (x) in GPAST_DATA for each species, as well as the total adsorbed amount (qT) in SYSTEM_DATA. Again, non-adsorbing species should have their respective phase mole fractions set to 0.0 to exclude them from the simulation. Additionally, if there are non-adsorbing species present, then the Carrier bool in SYSTEM_DATA must be set to true.

Parameters

data	void pointer for the MAGPIE_DATA data structure holding all necessary information

5.10.3.17 int MAGPIE_SCENARIOS (const char * *inputFileName,* const char * *sceneFileName*)

Function to perform a series of MAGPIE simulations based on given input files.

This function is callable from the UI and is used to perform a series of isothermal equilibria evaluations using the MAGPIE routines. There are two input files that must be provided: (i) inputFileName - containing parameter information for the species and (ii) sceneFileName - containing information for each MAGPIE simulation. Each of these files have a specific structure (see below). NOTE: this may change in future versions.

inputFileName Text File Structure:

Integer for Number of Adsorbing Species

van der Waals Volume (cm^3/mol) of ith species

GSTA adsorption capacity (mol/kg) of ith species

Number of GSTA parameters of ith species

Enthalpy (J/mol) of nth site [tab] Entropy of nth site (J/K/mol) of ith species

(repeat above for all n sites in species i)

(repeat above for all species i)

Example Input File:

5

17.1

5.8797

1

-20351.9 -81.8369

16.2

5.14934

1

-16662.7 -74.4766

19.7

9.27339

4

-46597.5 -53.6994

-125024 -221.073

-193619 -356.728

-272228 -567.459

13.25

4.59144

1

-13418.5 -84.888

18.0

10.0348

1

-20640.4 -72.6119

(The above input file gives the parameter information for 5 adsorbing species)

sceneFileName Text File Structure:

Integer Flag to mark Forward (0) or { Reverse (1) evaluations }

Number of Simulations to Run

Total Pressure (kPa) [tab] Temperature (K) { [tab] Total Adsorption (mol/kg) [tab] Carrier Gas Flag (0=false, 1=true) }

Gas/Adsorbed Mole Fractions for each species in the order given in prior file (tab separated)

(repeat above for all simulations desired)

NOTE: only provide the Total Adsorption and Carrier Flag if doing Reverse evaluations!

Example Scenario File 1:

0

4

0.65 303.15

0.364 0.318 0.318

3.25 303.15

0.371 0.32 0.309

6.85 303.15

0.388 0.299 0.313

13.42 303.15

0.349 0.326 0.325

(The above scenario file is for 4 forward evaluations/simulations for a 3-adsorbing species system)

Example Scenario File 2:

1

4

0.65 303.15 5.4 0

0.364 0.318 0.318

3.25 303.15 7.7 0

0.371 0.32 0.309

6.85 303.15 9.8 0

0.388 0.299 0.313

13.42 303.15 10.4 0

0.349 0.326 0.325

(The above scenario file is for 4 reverse evaluations/simulations for a 3-adsorbing species system and no carrier gas)

5.11 mola.h File Reference

Molecule Object Library from Atoms.

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

Classes

- class Molecule

    C++ Molecule Object built from Atom Objects (click Molecule to go to function definitions)

Functions

- int MOLA_TESTS ()

    Function to run the MOLA tests.

5.11.1 Detailed Description

Molecule Object Library from Atoms. mola.cpp

This file contains a C++ Class for creating Molecule objects from the Atom objects that were defined in eel.h. Molecules can be created and registered from basic information or can be registered from a growing list of pre-registered molecules that are accessible by name/formula.

Registered Molecules are are known and defined prior to runtime. They have a charge, energy characteristics, phase, name, and formula that they are recongized by. The formula is used to create the atoms that they are made from. If some information is incomplete, it must be specified as to what information is missing (i.e. denote whether the formation energies are known).

Formation energies are used to determine stability/dissociation/acidity equilibrium constants during runtime. If the formation energies are unknown, then the equilibrium constants must be given to a reaction object on when it is initialized.

The molecule formula's are given as strings which are parsed in the constructor to determine what atoms from the EEL files will be registered and used. Note, you will be able to build molecules from an input file, but the library molecules here are ready to be used in applications and require no more input other that the molecule's formula.

List of Currently Registered Molecules

CO3 2- (aq)

Cl - (aq)

H2O (l)

H + (aq)

H2CO3 (aq)

HCO3 - (aq)

HNO3 (aq)

HCl (aq)

NaHCO3 (aq)

NaCO3 - (aq)

Na + (aq)

NaCl (aq)

NaOH (aq)

NO3 - (aq)

OH - (aq)

UO2 2+ (aq)

UO2NO3 + (aq)

UO2(NO3)2 (aq)

UO2OH + (aq)

UO2(OH)2 (aq)

UO2(OH)3 - (aq)

UO2(OH)4 2- (aq)

(UO2)2OH 3+ (aq)

(UO2)2(OH)2 2+ (aq)

(UO2)3(OH)4 2+ (aq)

(UO2)3(OH)5 + (aq)

(UO2)3(OH)7 - (aq)

(UO2)4(OH)7 + (aq)

UO2CO3 (aq)

UO2(CO3)2 2- (aq)

UO2(CO3)3 4- (aq)

Those registered molecules follow a strict naming convention by which they can be recognized (see below)...

Naming Convention

Plus (+) and minus (-) charges are denoted by the numeric value of the charge followed by a + or - sign, respectively (e.g. UO2(CO3)3 4- (aq))

The phase is always denoted last and will be marked as (l) for liquid, (s) for solid, (aq) for aqueous, and (g) for gas (see above).

When registering a molecule that is not in the library, you must also provide a linear formula during construction or registration. This is needed so that the string parsing is easier to handle when the molecule subsequently registers the necessary atoms. (e.g. UO2(CO3)3 = UO2C3O9 or UO11C3).

Author

Austin Ladshaw

Date

02/24/2014

Copyright

5.11.2 Function Documentation

5.11.2.1 int MOLA_TESTS ( )

Function to run the MOLA tests.

This function is callable from the UI and is used to run several algorithm tests for the Molecule objects. This test should never report any errors.

5.12 monkfish.h File Reference

Multi-fiber wOven Nest Kernel For Interparticle Sorption History.

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

Classes

- struct MONKFISH_PARAM

  Data structure for species specific information and parameters.
- struct MONKFISH_DATA

  Primary data structure for running MONKFISH.

Functions

- double default_porosity (int i, int l, const void ∗user_data)

  Default porosity function for MONKFISH.

- double default_density (int i, int l, const void ∗user_data)

  Default density function for MONKFISH.
- double default_interparticle_diffusion (int i, int l, const void ∗user_data)

  Default interparticle diffusion function.
- double default_monk_adsorption (int i, int l, const void ∗user_data)

  Default adsorption strength function.
- double default_monk_equilibrium (int i, int l, const void ∗user_data)

  Default equilibrium adsorption function in mg/g.
- double default_monkfish_retardation (int i, int l, const void ∗user_data)

  Default retardation coefficient function.
- double default_exterior_concentration (int i, const void ∗user_data)

  Default exterior concentratio function.
- double default_film_transfer (int i, const void ∗user_data)

  Default film mass transfer function.
- 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)

  Setup function to allocate memory and setup function pointers for the MONKFISH simulation.
- int MONKFISH_TESTS ()

  Function to run tests on the MONKFISH algorithms.

5.12.1 Detailed Description

Multi-fiber wOven Nest Kernel For Interparticle Sorption History. monkfish.cpp

This file contains structures and functions associated with modeling the sorption characteristics of woven fiber bundles used to recover uranium from seawater. It is coupled with the DOGFISH kernel that determines the sorption of individual fibers. This kernel will resolve the interparticle diffusion between bundles of individual fibers in a woven ball-like domain.

Warning

Functions and methods in this file are still under construction.

Author

Austin Ladshaw

Date

04/14/2015

Copyright

5.12.2 Function Documentation

5.12.2.1 double default_porosity (int *i*, int *l*, const void * *user_data*)

Default porosity function for MONKFISH.

This function assumes a linear relationship between the maximum porosity at the center of the woven fibers and the minimum porosity at the edge of the woven fiber bundle.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.2 double default_density (int *i*, int *l*, const void * *user_data*)

Default density function for MONKFISH.

This function calls the porosity function and uses the single fiber density to provide an estimate of the bulk fiber density locally in the woven fiber bundle.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.3 double default_interparticle_diffusion (int *i*, int *l*, const void * *user_data*)

Default interparticle diffusion function.

This function assumes that the interparticle diffusivity is a contant and returns that diffusivity multiplied by the domain porosity to form the effective diffusion coefficient in the domain.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.4 double default_monk_adsorption (int *i*, int *l*, const void * *user_data*)

Default adsorption strength function.

This function will either use the default equilibrium function or the DOGFISH simulation result to produce the approximate adsorption strength using perturbation theory.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.5 double default_monk_equilibrium (int *i*, int *l*, const void ∗ *user_data*)

Default equilibirium adsorption function in mg/g.

This function uses the exterior species' concentration (mol/L), the species' molecular weight (g/mol), and the bulk fiber density (g/L) to calculate the adsorption equilibrium in mg/g. It assumes that the exterior concentration represents the moles of species per liter of solution that is being sorbed.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.6 double default_monkfish_retardation (int *i*, int *l*, const void ∗ *user_data*)

Default retardation coefficient function.

This function calls the porosity, density, and adsorption functions to evaluate the retardation coefficient of the diffusing material.

Parameters

i	index for the ith adsorbing species
l	index for the lth node in the domain
user_data	pointer to the MONKFISH_DATA structure

5.12.2.7 double default_exterior_concentration (int *i*, const void ∗ *user_data*)

Default exterior concentratio function.

This function assumes that the exterior concentration for sorption is just equal to the value of exterior_concentration given in MONKFISH_PARAM.

Parameters

i	index for the ith adsorbing species
user_data	pointer to the MONKFISH_DATA structure

5.12.2.8 double default_film_transfer (int *i*, const void ∗ *user_data*)

Default film mass transfer function.

This function assumes that the film mass transfer coefficient is just equal to the value of the film_transfer_coeff in MONKFISH_PARAM.

Parameters

i	index for the ith adsorbing species
user_data	pointer to the MONKFISH_DATA structure

5.12.2.9 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*)

Setup function to allocate memory and setup function pointers for the MONKFISH simulation.

This function will allocate memory and setup the MONKFISH problem. To specify use of the default functions in MONKFISH, pass NULL args for all function pointers and the user_data data structure. Otherwise, pass in your own custom arguments. The MONKFISH_DATA pointer must always be passed to this function.

Parameters

file	pointer to the output file to print out results
eval_porosity	function pointer for the bulk domain porosity function
eval_density	function pointer for the bulk domain density function
eval_ext_diff	function pointer for the interparticle diffusion function
eval_adsorb	function pointer for the adsorption strength function
eval_retard	function pointer for the retardation coefficient function
eval_ext_conc	function pointer for the external concentration function
eval_ext_film	function pointer for the external film mass transfer function
dog_diffusion	function pointer for the DOGFISH diffusion function (see dogfish.h)
dog_ext_film	function pointer for the DOGFISH film mass transfer (see dogfish.h)
dog_surf_conc	function pointer for the DOGFISH surface concentration (see dogfish.h)
user_data	pointer for the user's own data structure (only if using custom functions)
monk_dat	pointer for the MONKFISH_DATA structure

5.12.2.10 int MONKFISH_TESTS ( )

Function to run tests on the MONKFISH algorithms.

This function currently does nothing and is not callable from the UI.

5.13 sandbox.h File Reference

Coding Test Area.

```
#include "flock.h"
#include "school.h"
```

Functions

- int RUN_SANDBOX ()

    Function to run the methods implemented in the Sandbox.

5.13.1 Detailed Description

Coding Test Area. sandbox.cpp

This file contains a series of simple tests for routines used in other files and algorithms. Before any code or methods are used, they are tested here to make sure that they are useful. The tests in the sandbox are callable from the UI to make it easier to alter existing sandbox code and run tests on new proposed methods or algorithms.

Warning

Functions and methods in this file are not meant to be used anywhere else.

Author

Austin Ladshaw

Date

04/11/2015

Copyright

5.13.2 Function Documentation

5.13.2.1 int RUN_SANDBOX ( )

Function to run the methods implemented in the Sandbox.

This function is callable from the UI and is used to observe results from the tests of newly developed algorithms. Edit header and source files here to test out your own routines or functions. Then you can run those functions by rebuilding the Ecosystem executable and running the sandbox tests.

5.14 school.h File Reference

Seawater Codes from a Highly Object-Oriented Library.

```
#include "eel.h"
#include "mola.h"
#include "shark.h"
#include "dogfish.h"
#include "monkfish.h"
#include "yaml_wrapper.h"
```

5.14.1 Detailed Description

Seawater Codes from a Highly Object-Oriented Library. This file contains include statements for all files used in the aqueous adsorption problems, primarily targeted at Seawater simulations. Include this file into any other project or source code that needs the methods below.

Files Included in SCHOOL

eel.h mola.h shark.h dogfish.h monkfish.h yaml_wrapper.h

Note

(1) shark.h also includes methods from macaw.h and lark.h
(2) dogfish.h also includes methods from finch.h

Author

Austin Ladshaw

Date

02/23/2015

Copyright

5.15 scopsowl.h File Reference

Simultaneously Coupled Objects for Pore and Surface diffusion Operations With Linear systems.

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

Classes

- struct SCOPSOWL_PARAM_DATA

  Data structure for the species' parameters in SCOPSOWL.
- struct SCOPSOWL_DATA

  Primary data structure for SCOPSOWL simulations.

Macros

- #define SCOPSOWL_HPP_
- #define Dp(Dm, ep) (ep∗ep∗Dm)

  Estimate of Pore Diffusivity (cm^2/s)
- #define Dk(rp, T, MW) (9700.0∗rp∗pow((T/MW),0.5))

  Estimate of Knudsen Diffusivity (cm^2/s)
- #define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)),-1.0))

  Estimate of Average Pore Diffusion (cm^2/s)

Functions

- void print2file_species_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)

  Function to print out the main header for the output file.
- void print2file_SCOPSOWL_time_header (FILE ∗Output, SCOPSOWL_DATA ∗owl_dat, int i)

  Function to print out the time and space header for the output file.
- void print2file_SCOPSOWL_header (SCOPSOWL_DATA ∗owl_dat)

  Function to call the species and time header functions.
- void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA ∗owl_dat)

  Function to print out the old time results to the output file.
- void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA ∗owl_dat)

  Function to print out the new time results to the output file.
- double default_adsorption (int i, int l, const void ∗user_data)

  Default function for evaluating adsorption and adsorption strength.

- double default_retardation (int i, int l, const void *user_data)

  Default function for evaluating retardation coefficient.
- double default_pore_diffusion (int i, int l, const void *user_data)

  Default function for evaluating pore diffusivity.
- double default_surf_diffusion (int i, int l, const void *user_data)

  Default function for evaluating surface diffusion for HOMOGENEOUS pellets.
- double default_effective_diffusion (int i, int l, const void *user_data)

  Default function for evaluating effective diffusivity for HOMOGENEOUS pellets.
- double const_pore_diffusion (int i, int l, const void *user_data)

  Constant pore diffusion function for homogeneous or heterogeneous pellets.
- double default_filmMassTransfer (int i, const void *user_data)

  Default function for evaluating the film mass transfer coefficient.
- double const_filmMassTransfer (int i, const void *user_data)

  Constant film mass transfer coefficient function.
- 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)

  Setup function to allocate memory and setup function pointers for the SCOPSOWL simulation.
- int SCOPSOWL_Executioner (SCOPSOWL_DATA *owl_dat)

  SCOPSOWL executioner function to solve a time step.
- int set_SCOPSOWL_ICs (SCOPSOWL_DATA *owl_dat)

  Function to set the initial conditions for a SCOPSOWL simulation.
- int set_SCOPSOWL_timestep (SCOPSOWL_DATA *owl_dat)

  Function to set the timestep of the SCOPSOWL simulation.
- int SCOPSOWL_preprocesses (SCOPSOWL_DATA *owl_dat)

  Function to perform all preprocess SCOPSOWL operations.
- int set_SCOPSOWL_params (const void *user_data)

  Function to set the values of all non-linear system parameters during simulation.
- int SCOPSOWL_postprocesses (SCOPSOWL_DATA *owl_dat)

  Function to perform all postprocess SCOPSOWL operations.
- int SCOPSOWL_reset (SCOPSOWL_DATA *owl_dat)

  Function to reset all stateful information to prepare for next simulation.
- int SCOPSOWL (SCOPSOWL_DATA *owl_dat)

  Function to progress the SCOPSOWL simulation through time till complete.
- int SCOPSOWL_SCENARIOS (const char *scene, const char *sorbent, const char *comp, const char *sorbate)

  Function to perform a SCOPSOWL simulation based on a set of parameters given in input files.
- int SCOPSOWL_TESTS ()

  Function to run a SCOPSOWL test simulation.

5.15.1 Detailed Description

Simultaneously Coupled Objects for Pore and Surface diffusion Operations With Linear systems. scopsowl.cpp

This file contains structures and functions associated with modeling adsorption in commercial, bi-porous adsorbents such as zeolites and mordenites. The pore diffusion and mass transfer equations are coupled with adsorption and surface diffusion through smaller crystals embedded in a binder matrix. However, you can also direct this simulation to treat the adsorbent as homogeneous (instead of heterogeneous) in order to model an even greater variety of gaseous adsorption kinetic problems. This object is coupled with either MAGPIE, SKUA, or BOTH depending on the type of simulation requested.

Author

Austin Ladshaw

Date

01/29/2015

Copyright

5.15.2 Macro Definition Documentation

5.15.2.1 #define SCOPSOWL_HPP_

5.15.2.2 #define Dp(*Dm*, *ep*) (ep*ep*Dm)

Estimate of Pore Diffusivity (cm^2/s)

5.15.2.3 #define Dk(*rp*, *T*, *MW*) (9700.0*rp*pow((T/MW),0.5))

Estimate of Knudsen Diffusivity (cm^2/s)

5.15.2.4 #define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)),-1.0))

Estimate of Average Pore Diffusion (cm^2/s)

5.15.3 Function Documentation

5.15.3.1 void print2file_species_header (FILE * *Output*, SCOPSOWL_DATA * *owl_dat*, int *i*)

Function to print out the main header for the output file.

5.15.3.2 void print2file_SCOPSOWL_time_header (FILE * *Output*, SCOPSOWL_DATA * *owl_dat*, int *i*)

Function to print out the time and space header for the output file.

5.15.3.3 void print2file_SCOPSOWL_header (SCOPSOWL_DATA * *owl_dat*)

Function to call the species and time header functions.

5.15.3.4 void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA * *owl_dat*)

Function to print out the old time results to the output file.

5.15.3.5 void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA * *owl_dat*)

Function to print out the new time results to the output file.

5.15.3.6 double default_adsorption (int *i*, int *l*, const void ∗ *user_data*)

Default function for evaluating adsorption and adsorption strength.

This function is called in the preprocesses and postprocesses to estimate the strength of adsorption in the macro-scale problem from perturbations. It will use perturbations in either the MAGPIE simulation or SKUA simulation, depending on the type of problem the user is solving.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.7 double default_retardation (int *i*, int *l*, const void ∗ *user_data*)

Default function for evaluating retardation coefficient.

This function is called in the preprocesses and postprocesses to estimate the retardation coefficient for the simulation. It is recalculated at every time step to keep track of all changing conditions in the simulation.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.8 double default_pore_diffusion (int *i*, int *l*, const void ∗ *user_data*)

Default function for evaluating pore diffusivity.

This function is called during the evaluation of non-linear residuals to more accurately represent non-linearities in the pore diffusion behavior. The pore diffusion is calculated based on kinetic theory of gases (see egret.h) and is adjusted according to the Knudsen Diffusion model and the porosity of the binder material.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.9 double default_surf_diffusion (int *i*, int *l*, const void ∗ *user_data*)

Default function for evaluating surface diffusion for HOMOGENEOUS pellets.

This function is ONLY used if the pellet is determined to be homogeneous. Otherwise, this is replaced by the surface diffusion function for the SKUA simulation. The diffusivity is calculated based on the Arrhenius rate expression and then adjusted by the outside partial pressure of the adsorbing species.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.10 double default_effective_diffusion (int *i*, int *l*, const void ∗ *user_data*)

Default function for evaluating effective diffusivity for HOMOGENEOUS pellets.

This function is ONLY used if the pellet is determined to be homogeneous. Otherwise, this is replaced by the pore diffusion function. The effective diffusivity is determined by the combination of pore diffusivity and surface diffusivity with adsorption strength in an homogeneous pellet.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.11 double const_pore_diffusion (int *i*, int *l*, const void ∗ *user_data*)

Constant pore diffusion function for homogeneous or heterogeneous pellets.

This function should be used if the user wants to specify a constant pore diffusivity. The value of pore diffusion is then set equal to the value of pore_diffusion in the SCOPSOWL_PARAM_DATA structure.

Parameters

i	index for the ith species in the system
l	index for the lth node in the macro-scale domain
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.12 double default_filmMassTransfer (int *i*, const void ∗ *user_data*)

Default function for evaluating the film mass transfer coefficient.

This function is called during the setup of the boundary conditions and is used to estimate the film mass transfer coefficient for the macro-scale problem. The coefficient is calculated according to the kinetic theory of gases (see egret.h).

Parameters

i	index for the ith species in the system
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.13 double const_filmMassTransfer (int *i*, const void ∗ *user_data*)

Constant film mass transfer coefficient function.

This function is used when the user wants to specify a constant value for film mass transfer. The value of that coefficient is then set equal to the value of film_transfer in the SCOPSOWL_PARAM_DATA structure.

Parameters

i	index for the ith species in the system
user_data	pointer for the SCOSPOWL_DATA structure

5.15.3.14 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*)

Setup function to allocate memory and setup function pointers for the SCOPSOWL simulation.

This function sets up the memory and function pointers used in SCOPSOWL simulations. User can provide NULL in place of functions for the function pointers and the setup will automatically use just the default settings. However, the user is required to pass the necessary data structure pointers for MIXED_GAS and SCOPSOWL_DATA.

Parameters

file	pointer to the output file to print out results
eval_sorption	pointer to the adsorption evaluation function
eval_retardation	pointer to the retardation evaluation function
eval_pore_diff	pointer to the pore diffusion function
eval_filmMT	pointer to the film mass transfer function
eval_surface_diff	pointer to the surface diffusion function (required)
user_data	pointer to the user's data structure used for the parameter functions
gas_data	pointer to the MIXED_GAS structure used to evaluate kinetic gas theory
owl_data	pointer to the SCOPSOWL_DATA structure

5.15.3.15 int SCOPSOWL_Executioner (SCOPSOWL_DATA * *owl_dat*)

SCOPSOWL executioner function to solve a time step.

This function will call the preprocess, solver, and postprocess functions to evaluate a single time step in a simulation. All simulation conditions must be set prior to calling this function. This function will typically be the one called from other simulations that will involve a SCOPSOWL evaluation to resolve kinetic coupling.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.16 int set_SCOPSOWL_ICs (SCOPSOWL_DATA * *owl_dat*)

Function to set the initial conditions for a SCOPSOWL simulation.

This function will setup the initial conditions of the simulation based on the initial temperature, pressure, and adsorbed molefractions. It assumes that the initial conditions are constant throughout the domain of the problem. This function should only be called once during a simulation.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.17 int set_SCOPSOWL_timestep (SCOPSOWL_DATA * *owl_dat*)

Function to set the timestep of the SCOPSOWL simulation.

This function is used to set the next time step to be used in the SCOPSOWL simulation. A constant time step based on the size of the pellet discretization will be used. Users may want to use a custom time step to ensure that coupled-multi-scale systems are all in sync.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.18 int SCOPSOWL_preprocesses (SCOPSOWL_DATA * *owl_dat*)

Function to perform all preprocess SCOPSOWL operations.

This function will update the boundary conditions and simulation conditions based on the current temperature, pressure, and gas phase composition, which may all vary in time. Since this function is called by the SCOPSOWL-_Executioner, it does not need to be called explicitly by the user.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.19 int set_SCOPSOWL_params (const void * *user_data*)

Function to set the values of all non-linear system parameters during simulation.

This is the function override for the FINCH setparams function (see finch.h). It will update the values of non-linear parameters in the residuals so that all variables in a species' system are fully coupled.

Parameters

user_data	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.20 int SCOPSOWL_postprocesses (SCOPSOWL_DATA * *owl_dat*)

Function to perform all postprocess SCOPSOWL operations.

This function will update the retardation coefficients based on newly obtained simulation results for the current time step and calculate the average and total amount of adsorption of each species in the domain. Additionally, this function will call the print functions to store simulation results in the output file.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.21 int SCOPSOWL_reset (SCOPSOWL_DATA * *owl_dat*)

Function to reset all stateful information to prepare for next simulation.

This function will update the stateful information used in SCOPSOWL to prepare the system for the next time step in the simulation. However, because updating the states erases the old state, the user must be absolutely sure that the simulation is ready to be updated. For just running standard simulations, this is not an issue, but in coupling with other simulations it is very important.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.22 int SCOPSOWL (SCOPSOWL_DATA * *owl_dat*)

Function to progress the SCOPSOWL simulation through time till complete.

This function will call the initial conditions, then progressively call the executioner, time step, and reset functions to propagate the simulation in time. As such, this function is primarily used when running a SCOPSOWL simulation by itself and not when coupling it to an other problem.

Parameters

owl_dat	pointer to the SCOPSOWL_DATA structure (must be initialized)

5.15.3.23 int SCOPSOWL_SCENARIOS (const char $*$ *scene*, const char $*$ *sorbent*, const char $*$ *comp*, const char $*$ *sorbate*)

Function to perform a SCOPSOWL simulation based on a set of parameters given in input files.

This is the primary function to be called when running a stand-alone SCOPSOWL simulation. Parameters and system information for the simulation are given in a series of input files that come in as character arrays. These inputs are all required to call this function.

Parameters

scene	Sceneario Input File
sorbent	Adsorbent Input File
comp	Component Input File
sorbate	Adsorbate Input File

Note

Each input file has a particular format that must be strictly adhered to in order for the simulation to be carried out correctly. The format for each input file, and an example, is provided below...

Scenario Input Format

System Temperature (K) [tab] Total Pressure (kPa) [tab] Gas Velocity (cm/s)

Simulation Time (hrs) [tab] Print Out Time (hrs)

BC Type (0 = Neumann, 1 = Dirichlet)

Number of Gas Species

Initial Total Adsorption (mol/kg)

Name of ith Species [tab] Adsorbable? (0 = false, 1 = true) [tab] Gas Phase Molefraction [tab] Initial Sorbed Molefraction

(repeat above for all species)

Example Scenario Input

353.15 101.35 0.36

4.0 0.05

0

5

0.0

N2 0 0.7634 0.0

O2 0 0.2081 0.0

Ar 0 0.009 0.0

CO2 0 0.0004 0.0

H2O 1 0.0191 0.0

Above example is for a 5-component mixture of N2, O2, Ar, CO2, and H2O, but we are only considering the H2O as adsorbable.

Adsorbent Input File

Heterogeneous Pellet? (0 = false, 1 = true) [tab] Surface Diffusion Included? (0 = false, 1 = true)

Macro Coord. (2 = spherical, 1 = cylindrical) { [tab] Char. Length (cm) (i.e., cylinder length) }

(NOTE: Char. Length is only needed if problem is not spherical)

Pellet Radius (cm) [tab] Pellet Density (kg/L) [tab] Porosity (vol. void / vol. binder) [tab] Pore Radius (cm)

(Below is only needed if pellet is Heterogeneous)

Micro Coord. (2 = spherical, 1 = cylindrical) { [tab] Char. Length (cm) (i.e., cylinder length) }

Crystal Radius (um) [tab] Binder Fraction (vol. binder / vol. pellet)

Example Adsorbent Input

1 1

2

0.118 1.69 0.272 3.5E-6

2

2.0 0.175

Above example is for a heterogeneous adsorbent with surface diffusion. The pellet and crystals are both considered spherical. Pellet radius is 0.118 cm, density is 1.69 kg/L, porosity is 0.272, and pore size is 3.5e-6 cm. The pellet is made up of 17.5 % binder material and contains crystals roughly 2.0 um in radius.

Component Input File

Molar Weight of ith species (g/mol) [tab] Specific Heat of ith species (J/g/K)

Sutherland Viscosity (g/cm/s) [tab] Sutherland Temperature (K) [tab] Sutherland Constant (K) of ith species

(repeat above for all species in same order they appeared in the Scenario Input File)

Example Component Input

28.016 1.04

0.0001781 300.55 111.0

32.0 0.919

0.0002018 292.25 127.0

39.948 0.522

0.0002125 273.11 144.4

44.009 0.846

0.000148 293.15 240.0

18.0 1.97

0.0001043 298.16 784.72

Above example is a continuation of the Scenario Input example wherein each grouping represents parameters that are associated with N2, O2, Ar, CO2, and H2O, respectively. The order is VERY important!

Adsorbate Input File

{ Type of Surface Diffusion Function (0 = constant, 1 = simple Darken, 2 = theoretical Darken) }

(NOTE: The above option is only given IF the pellet was specified as Heterogeneous!)

Reference Diffusivity (um^2/hr) [tab] Activation Energy (J/mol) of ith adsorbable species

Reference Temperature (K) [tab] Affinity Constant (-) of ith adsorbable species

van der Waals Volume (cm^3/mol) of ith species

GSTA adsorption capacity (mol/kg) of ith species

Number of GSTA parameters of ith species

Enthalpy (J/mol) of nth site [tab] Entropy of nth site (J/K/mol) of ith species

(repeat enthalpy and entropy for all n sites in species i)

(repeat above for all species i)

Example Adsorbate Input

0

0.8814 0.0

267.999 0.0

13.91

11.67

4

-46597.5 -53.6994

-125024 -221.073

-193619 -356.728

-272228 -567.459

1.28 540.1

374.99 0.01

3.01

1.27

2

-46597.5 -53.6994

-125024 -221.073

Above example would be for a simulation involving two adsorbable species using a constant surface diffusion function. Each adsorbable species has it's own set of kinetic and equilibrium parameters that must be given in the same order as the species appeared in the Scenario Input. Note: we do not need to supply this information for non-adsorbable species.

5.15.3.24 int SCOPSOWL_TESTS ( )

Function to run a SCOPSOWL test simulation.

This function runs a test of the SCOPSOWL physics and prints out results to a text file. It is callable from the UI.

5.16 scopsowl_opt.h File Reference

Optimization Routine for Surface Diffusivities in SCOPSOWL.

```
#include "scopsowl.h"
```

Classes

- struct SCOPSOWL_OPT_DATA

  Data structure for the SCOPSOWL optmization routine.

Functions

- int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA ∗owl_opt)

  Function to set the rest of the gas phase mole fractions based on current mole fraction of adsorbing gas.
- int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA ∗owl_opt)

  Function to set up an initial guess for the surface diffusivity parameter in SCOPSOWL.
- void eval_SCOPSOWL_Uptake (const double ∗par, int m_dat, const void ∗data, double ∗fvec, int ∗info)

  Function that works in conjunction with the lmfit routine to minimize the euclidean norm between function and data.
- int SCOPSOWL_OPTIMIZE (const char ∗scene, const char ∗sorbent, const char ∗comp, const char ∗sorbate, const char ∗data)

  Function called to perform the optimization routine given a specific set of information and data.

5.16.1 Detailed Description

Optimization Routine for Surface Diffusivities in SCOPSOWL. scopsowl_opt.cpp

This file contains structures and functions associated with performing non-linear least-squares optimization of the SCOPSOWL simulation results against actual kinetic adsorption data. The optimization routine here allows you to run data comparisons and optimizations in three forms: (i) Rough optimizations - cheaper operations, but less accurate, (ii) Exact optmizations - much more expensive, but greater accuracy, and (iii) data/model comparisons - no optimization, just using system parameters to compare simulation results agains a set of data.

Depending on the level of optimization desired, this routine could take several minutes or several hours. The optimization/comparisons are printed out in two files: (i) a parameter file, which contains the simulation partial pressures and temperatures and the optimized diffusivities with the euclidean norm of the fitting and (ii) a comparison file that shows the model value and data value at each time step for each kinetic curve.

The optimized diffusion parameters are given for each individual kinetic data curve. Each data curve will have a different pairing of partial pressure and temperature. Because of this, you will get a list of different diffusivities for each data curve. To get the optimum kinetic parameters from this list of diffusivities, you must fit the diffusion parameter values to the following diffusion function model...

D_opt = D_ref ∗ exp(-E / (R∗T)) ∗ pow(p , (T_ref/T) - B)

where D_ref is the Reference Diffusivity (um^2/hr), E is the activation energy for adsorption (J/mol), R is the gas law constant (J/K/mol), T is the system temperature (K), p is the partial pressure of the adsorbing species (kPa), T_ref is the Reference Temperature (K), and B is the Affinity constant. This algorithm does not automatically produce these parameters for you, but gives you everything you need to produce them yourself.

This routine allows you to optimize multiple kinetic curves at one time. However, all data must be for the same adsorbent-adsorbate system. In other words, the adsorbent and adsorbate pair must be the same for each kinetic curve analyzed. Also, each experiment must have been done in a thin bed or continuous flow system where the adsorbents were exposed to a nearly constant outside partial pressure for all time steps and the gas velocity of that system is assumed constant for all experiments. This experimental setup is very typical for studying adsorption kinetics for gas-solid systems.

Author

Austin Ladshaw

Date

05/14/2015

Copyright

5.16.2 Function Documentation

5.16.2.1 int SCOPSOWL_OPT_set_y (SCOPSOWL_OPT_DATA * *owl_opt*)

Function to set the rest of the gas phase mole fractions based on current mole fraction of adsorbing gas.

This function takes the current mole fraction of the adsorbing gas and calculates the gas mole fractions of the other gases in the sytem based on the standard inlet gas composition given in the scenario file.

5.16.2.2 int initial_guess_SCOPSOWL (SCOPSOWL_OPT_DATA * *owl_opt*)

Function to set up an initial guess for the surface diffusivity parameter in SCOPSOWL.

This function performs the Rough optimization on the surface diffusivity based on the idea of reducing or eliminating function bias between data and simulation. A positive function bias means that the simulation curve is "higher" than the data curve and a negative function bias means that the simulation curve is "lower" than the data curve. We use this information to incrementally adjust the rate of surface diffusion until this bias is near zero. When bias is near zero, the simulation is nearly optimized, but further refinement may be necessary to find the true minimum solution.

5.16.2.3 void eval_SCOPSOWL_Uptake (const double * *par,* int *m_dat,* const void * *data,* double * *fvec,* int * *info*)

Function that works in conjunction with the lmfit routine to minimize the euclidean norm between function and data.

This function will run the SCOPSOWL simulation at a given value of surface diffusivity and produce residuals that feed into the Levenberg-Marquardt's algorithm for non-linear least-squares regression. The form of this function is specific to the format required by the lmfit routine.

Parameters

par	array of parameters that are to be optimized
m_dat	number of data points or functions to evaluate
data	user supplied data structure holding information necessary to form the residuals
fvec	array of residuals computed at the current parameter values
info	integer pointer denoting whether or not the user requests to end a particular simulation

5.16.2.4 int SCOPSOWL_OPTIMIZE (const char * *scene,* const char * *sorbent,* const char * *comp,* const char * *sorbate,* const char * *data*)

Function called to perform the optimization routine given a specific set of information and data.

This is the function that is callable by the UI. The user must provide 5 input files to the routine in order to establish simulation conditions, adsborbent properties, component properties, adsorbate equilibrium parameters, and the set of data that we are comparing the simulations to. Each input file has a very specific structure and order to the information that it contains. The structure here is DIFFERENT than the structure for just running standard SCOPS-OWL simulations (see scopsowl.h).

Parameters

scene	Sceneario Input File
sorbent	Adsorbent Input File
comp	Component Input File
sorbate	Adsorbate Input File
data	Kinetic Adsorption Data File

Note

Much of the structure of these input files are "similar" to that of the input files used in SCOPSOWL_SCENA-RIOS (see scopsowl.h), but with some notable differences. Below gives the format for each input file with an example. Make sure your input files follow this format before calling this routine from the UI.

Scenario Input File

Optimization? (0 = false, 1 = true) [tab] Rough Optimization? (0 = false, 1 = true)

Surf. Diff. (0 = constant, 1 = simple Darken, 2 = theoretical Darken) [tab] BC Type (0 = Neumann, 1 = Dirichlet)

Total Pressure (kPa) [tab] Gas Velocity (cm/s)

Number of Gaseous Species

Initial Adsorption Total (mol/kg)

Name [tab] Adsorbable? (0 = false, 1 = true) [tab] Inlet Gas Mole Fraction [tab] Initial Adsorbed Mole Fraction

(NOTE: The above line is repeated for all species in gas phase. Also, this algorithm only allows you to consider one adsorbable gas component. Inlet gas mole fractions must be non-zero for all non-adsorbing gases and must sum to 1.)

Example Scenario Input

1 0

0 0

101.35 0.36

5

0.0

N2 0 0.7825 0.0

O2 0 0.2081 0.0

Ar 0 0.009 0.0

CO2 0 0.0004 0.0

H2O 1 0.0 0.0

Above example is for running optimizations on data collected with a gas stream at 0.36 cm/s with 5 gas species in the mixture, only H_2O of which is adsorbing. The "base line" or "inlet gas" without H_2O has a composition of N_2 at 0.7825, O_2 at 0.2081, Ar at 0.009, and CO_2 at 0.0004.

Adsorbent Input File

Heterogeneous Pellet? (0 = false, 1 = true)

Macro Coord. (2 = spherical, 1 = cylindrical) { [tab] Char. Length (cm) (i.e., cylinder length) }

(NOTE: Char. Length is only needed if problem is not spherical)

Pellet Radius (cm) [tab] Pellet Density (kg/L) [tab] Porosity (vol. void / vol. binder) [tab] Pore Radius (cm)

(Below is only needed if pellet is Heterogeneous)

Micro Coord. (2 = spherical, 1 = cylindrical) { [tab] Char. Length (cm) (i.e., cylinder length) }

Crystal Radius (um) [tab] Binder Fraction (vol. binder / vol. pellet)

Example Adsorbent Input

1

2

0.118 1.69 0.272 3.5E-6

2

2.0 0.175

Above example is nearly identical to the file given in the SCOPSOWL_SCENARIO example (see scopsowl.h). However, here we do not give an integer flag denoting whether or not we are considering surface diffusion as a mechanism. This is because we automatically assume that surface diffusion is a mechanism in the system, since that is the unknown parameter that we are performing the optimizations for.

Component Input File

Molar Weight of ith species (g/mol) [tab] Specific Heat of ith species (J/g/K)

Sutherland Viscosity (g/cm/s) [tab] Sutherland Temperature (K) [tab] Sutherland Constant (K) of ith species

(repeat above for all species in same order they appeared in the Scenario Input File)

Example Component Input

28.016 1.04

0.0001781 300.55 111.0

32.0 0.919

0.0002018 292.25 127.0

39.948 0.522

0.0002125 273.11 144.4

44.009 0.846

0.000148 293.15 240.0

18.0 1.97

0.0001043 298.16 784.72

Above example is exactly the same as in the SCOPSOWL_SCENARIO example (see scopsowl.h). There is no difference in the input file formats for this input. Keep in mind that the order is VERY important! All species information must be in the same order that the species appeared in the Scenario input file.

Adsorbate Input File

Reference Diffusivity (um^2/hr) [tab] Activation Energy (J/mol) of ith adsorbable species

Reference Temperature (K) [tab] Affinity Constant (-) of ith adsorbable species

van der Waals Volume (cm^3/mol) of ith species

GSTA adsorption capacity (mol/kg) of ith species

Number of GSTA parameters of ith species

Enthalpy (J/mol) of nth site [tab] Entropy of nth site (J/K/mol) of ith species

(repeat enthalpy and entropy for all n sites in species i)

(repeat above for all species i)

Example Adsorbate Input

0 0

0 0

13.91

11.67

4

-46597.5 -53.6994

-125024 -221.073

-193619 -356.728

-272228 -567.459

Above example gives the equilibrium parameters associated with the H2O-MS3A single component adsorption system. Note that the kinetic parameters (Ref. Diff., Act. Energy, Ref. Temp., and Affinity) were all given a value of zero. These values are irrelavent if we are running an optimization because they will be replaced with a single estimate for the diffusivity that is being optimization for. However, if we wanted to run this routine with comparisons and not do any optmization, then you would need to provide non-zero values for these parameters (at least for Ref. Diff.).

Data Input File

Number of Kinetic Data Curves

Number of data points in the ith curve

Temperature (K) [tab] Partial Pressure (kPa) [tab] Equilibrium Adsorption (mol/kg) all of ith curve

Time point 1 (hrs) [tab] Adsorption 1 (mol/kg) of ith curve

Time point 1 (hrs) [tab] Adsorption 2 (mol/kg) of ith curve

... (Repeat for all time-adsorption data points)

(Repeat above for all curves i)

Example Data Input

40

2990

298.15 0.000310922 2.9

0 0

0.166666667 0.001834419

0.333611111 0.004880247

0.5 0.008306803

...

2789

298.15 0.00055189 5

0 0

0.166944444 0.003350185

0.333611111 0.007418267

0.5 0.009930906

0.666666667 0.014597236

0.833611111 0.021377373

....

Above is a partial example for a data set of 40 kinetic curves. The first curve contains 2990 data points and has temperature of 298.15 K, partial pressure of 0.000310922 kPa, and an equilibrium adsorption of 2.9. Each first time point should start from 0 hours and each initial adsorption should correspond to the value of initial adsorption indicated in the Scenario input file. Then, this structure is repeated for all adsorptio curves.

5.17 shark.h File Reference

Speciation-object Hierarchy for Aqueous Reaction Kinetics.

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

Classes

- class MasterSpeciesList

  Master Species List Object.
- class Reaction

  Reaction Object.
- class MassBalance

  Mass Balance Object.
- class UnsteadyReaction

  Unsteady Reaction Object (inherits from Reaction)
- struct SHARK_DATA

  Data structure for SHARK simulations.

Macros

- #define Rstd 8.3144621

    Gas Law Constant in J/K/mol (or) L∗kPa/K/mol (Standard Units)

Typedefs

- typedef struct SHARK_DATA SHARK_DATA

    Data structure for SHARK simulations.

Enumerations

- enum valid_act {
  IDEAL, DAVIES, DEBYE_HUCKEL, SIT,
  PITZER }

    Enumeration for the list of valid activity models for non-ideal solutions.

Functions

- void print2file_shark_info (SHARK_DATA ∗shark_dat)

    Function to print out simulation conditions and options to the output file.
- void print2file_shark_header (SHARK_DATA ∗shark_dat)

    Function to print out the head of species and time stamps to the output file.
- void print2file_shark_results_new (SHARK_DATA ∗shark_dat)

    Function to print out the simulation results for the current time step.
- void print2file_shark_results_old (SHARK_DATA ∗shark_dat)

    Function to print out the simulation results for the previous time step.
- int ideal_solution (const Matrix< double > &x, Matrix< double > &F, const void ∗data)

    Activity function for Ideal Solution.
- int Davies_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)

    Activity function for Davies Equation.
- int DebyeHuckel_equation (const Matrix< double > &x, Matrix< double > &F, const void ∗data)

    Activity function for Debye-Huckel Equation.
- int act_choice (const std::string &input)

    Function takes a given string and returns a flag denoting which activity model was choosen.
- bool linesearch_choice (const std::string &input)

    Function returns a bool to determine the form of line search requested.
- int linearsolve_choice (const std::string &input)

    Function returns the linear solver flag for the PJFNK method.
- int Convert2LogConcentration (const Matrix< double > &x, Matrix< double > &logx)

    Function to convert the given values of variables (x) to the log of those variables (logx)
- int Convert2Concentration (const Matrix< double > &logx, Matrix< double > &x)

    Function to convert the given log values of variables (logx) to the values of those variables (x)
- int read_scenario (SHARK_DATA ∗shark_dat)

    Function to go through the yaml object for the scenario document.
- int read_options (SHARK_DATA ∗shark_dat)

    Function to go through the yaml object for the solver options document.
- int read_species (SHARK_DATA ∗shark_dat)

    Function to go through the yaml object for the master species document.
- int read_massbalance (SHARK_DATA ∗shark_dat)

Function to go through the yaml object for the mass balance document.

- int read_equilrxn (SHARK_DATA ∗shark_dat)

  Function to go through the yaml object for the equilibrium reaction document.

- int read_unsteadyrxn (SHARK_DATA ∗shark_dat)

  Function to go through the yaml object for the unsteady reaction document.

- 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)

  Function to setup the memory and pointers for the SHARK_DATA structure for the current simulation.

- 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)

  Function to add user defined custom residual functions to the OtherList vector object in SHARK_DATA.

- int shark_parameter_check (SHARK_DATA ∗shark_dat)

  Function to check the Reaction and UnsteadyReaction objects for missing info.

- int shark_energy_calculations (SHARK_DATA ∗shark_dat)

  Function to calculate all Reaction and UnsteadyReaction energies.

- int shark_temperature_calculations (SHARK_DATA ∗shark_dat)

  Function to calculate all Reaction and UnsteadyReaction parameters as a function of temperature.

- int shark_pH_finder (SHARK_DATA ∗shark_dat)

  Function will search MasterSpeciesList for existance of H + (aq) and OH - (aq) molecules.

- int shark_guess (SHARK_DATA ∗shark_dat)

  Function provides a rough initial guess for the values of all non-linear variables.

- int shark_initial_conditions (SHARK_DATA ∗shark_dat)

  Function to establish the initial conditions of the shark simulation.

- int shark_executioner (SHARK_DATA ∗shark_dat)

  Function to execute a shark simulation at a single time step or pH value.

- int shark_timestep_const (SHARK_DATA ∗shark_dat)

  Function to set up all time steps in the simulation to a specified constant.

- int shark_timestep_adapt (SHARK_DATA ∗shark_dat)

  Function to set up all time steps in the simulation based on success or failure to converge.

- int shark_preprocesses (SHARK_DATA ∗shark_dat)

  Function to call other functions for calculation of parameters and setting of time steps.

- int shark_solver (SHARK_DATA ∗shark_dat)

  Function to call the PJFNK solver routine given the current SHARK_DATA information.

- int shark_postprocesses (SHARK_DATA ∗shark_dat)

  Function to convert PJFNK solutions to concentration values and print to the output file.

- int shark_reset (SHARK_DATA ∗shark_dat)

  Function to reset the values of all stateful information in SHARK_DATA.

- int shark_residual (const Matrix< double > &x, Matrix< double > &F, const void ∗data)

  Default residual function for shark evaluations.

- int SHARK (SHARK_DATA ∗shark_dat)

  Function to call all above functions to perform a shark simulation.

- int SHARK_SCENARIO (const char ∗yaml_input)

  Function to perform a shark simulation based on the conditions in a yaml formatted input file.

- int SHARK_TESTS ()

  Function to perform a series of shark calculation tests.

5.17.1 Detailed Description

Speciation-object Hierarchy for Aqueous Reaction Kinetics. shark.cpp

This file contains structures and functions associated with solving speciation and kinetic problems in aqueous systems. The primary aim for the development of these algorithms was to solve speciation and adsorption problems for the recovery of uranium resources from seawater. Seawater is an extradorinarily complex medium in which to work, which is why these algorithms are being constructed in a piece-wise, object-oriented fashion. This allows us to displace much of the complexity of the problem by breaking it down into smaller, more managable pieces.

Each piece of SHARK contributes to a residual function when solving the overall speciation, reaction, kinetic chemical problem. These residuals are then fed into the PJFNK solver function in lark.h. The variables of the system are the log(C) concentration values of each species in the system. We solve for log(C) concentrations, rather than just C, because the PJFNK method is an unbounded solution algorithm. So to prevent the algorithm from producing negative values for concentration, we reformulate all residuals in terms of the log(C) values. In this way, regardless of the value found for log(C), the concentration C will always be greater than 0.

Currenty, SHARK supports standard aqueous speciation problems with simple kinetic models based on an unsteady form of the standard reaction stoichiometry. As more methods and algorithms are completed, the SHARK simulations will be capable of doing much, much more.

Warning

Much of this is still underconstruction and many methods or interfaces may change. Use with caution.

Author

Austin Ladshaw

Date

05/27/2015

Copyright

5.17.2 Macro Definition Documentation

5.17.2.1 #define Rstd 8.3144621

Gas Law Constant in J/K/mol (or) L∗kPa/K/mol (Standard Units)

5.17.3 Typedef Documentation

5.17.3.1 typedef struct SHARK_DATA SHARK_DATA

Data structure for SHARK simulations.

C-style object holding data and function pointers associated with solving aqueous speciation and reaction kinetics. This object couples all other objects available in shark.h in order to provide residual calculations for each individual function that makes up the overall system model. Those residuals are brought together inside the residual function and fed into the lark.h PJFNK solver routine. That solver then attempts to find a solution to all non-linear variables simultaneously. Any function or data pointers in this structure can be overriden to change how you interface with and solve the problem. Users may also provide a set of custom residual functions through the "OtherList" vector object. Those residual function must all have the same format.

5.17.4 Enumeration Type Documentation

5.17.4.1 enum valid_act

Enumeration for the list of valid activity models for non-ideal solutions.

Note

The SIT and PITZER models are not currently supported.

Enumerator

IDEAL

DAVIES

DEBYE_HUCKEL

SIT

PITZER

5.17.5 Function Documentation

5.17.5.1 void print2file_shark_info (SHARK_DATA ∗ *shark_dat*)

Function to print out simulation conditions and options to the output file.

5.17.5.2 void print2file_shark_header (SHARK_DATA ∗ *shark_dat*)

Function to print out the head of species and time stamps to the output file.

5.17.5.3 void print2file_shark_results_new (SHARK_DATA ∗ *shark_dat*)

Function to print out the simulation results for the current time step.

5.17.5.4 void print2file_shark_results_old (SHARK_DATA ∗ *shark_dat*)

Function to print out the simulation results for the previous time step.

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

Activity function for Ideal Solution.

This is one of the default activity models available. It assumes the system behaves ideally and sets the activity coefficients to 1 for all species.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
F	matrix of activity coefficients that are to be altered by this function
data	pointer to a data structure needed to evaluate the activity model

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

Activity function for Davies Equation.

This is one of the default activity models available. It uses the Davies semi-empirical model to calculate average activities of each species in solution. This model is typically valid for systems involving high ionic strengths upto 0.5 M (mol/L).

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
F	matrix of activity coefficients that are to be altered by this function
data	pointer to a data structure needed to evaluate the activity model

5.17.5.7 int DebyeHuckel_equation (const Matrix< double > & *x*, Matrix< double > & *F*, const void * *data*)

Activity function for Debye-Huckel Equation.

This is one of the default activity models available. It uses the Debye-Huckel limiting model to calculate average activities of each species in solution. This model is typically valid for systems involving low ionic strengths and is only good for solutions between 0 and 0.01 M.

Parameters

x	matrix of the log(C) concentration values at the current non-linear step
F	matrix of activity coefficients that are to be altered by this function
data	pointer to a data structure needed to evaluate the activity model

5.17.5.8 int act_choice (const std::string & *input*)

Function takes a given string and returns a flag denoting which activity model was choosen.

This function returns an integer flag that will be one of the valid activity model flags from the valid_act enum. If the input string was not recognized, then it defaults to returning the IDEAL flag.

Parameters

input	string for the name of the activity model

5.17.5.9 bool linesearch_choice (const std::string & *input*)

Function returns a bool to determine the form of line search requested.

This function returns true if the user requests a bouncing line search algorithm and false if the user wants a standard line search. If the input string is unrecognized, then it returns false.

Parameters

input	string for the line search method option

5.17.5.10 int linearsolve_choice (const std::string & *input*)

Function returns the linear solver flag for the PJFNK method.

This function takes in a string argument and returns the integer flag for the appropriate linear solver in PJFNK. If the input string was unrecognized, then it returns the GMRESRP flag.

Parameters

input	string for the linear solver method option

5.17.5.11 int Convert2LogConcentration (const Matrix< double > & *x*, Matrix< double > & *logx*)

Function to convert the given values of variables (x) to the log of those variables (logx)

This function returns an integer flag to denote success of failure. It takes a constant matrix argument x and replaces the elements of the matrix logx with the base 10 log of those x values. This is used mainly to convert a set of concentrations (x) to their respective log(C) values (logx).

Parameters

x	matrix of values to take the base 10 log of
logx	matrix whose entries are to be changed to base 10 log(x)

5.17.5.12 int Convert2Concentration (const Matrix< double > & *logx*, Matrix< double > & *x*)

Function to convert the given log values of variables (logx) to the values of those variables (x)

This function returns an integer flag to denote success of failure. It takes a constant matrix argument logx and replaces the elements of the matrix x with 10^logx. This is used mainly to convert a set of log(C) values (logx) to their respective concentration values (x).

Parameters

logx	matrix of values to apply as the power of 10 (i.e., 10^logx)
x	matrix whose entries are to be changed to the result of 10^logx

5.17.5.13 int read_scenario (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the scenario document.

This function checks the yaml object for the expected keys and values of the scenario document to setup the shark simulation for the input given in the input file.

5.17.5.14 int read_options (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the solver options document.

This function checks the yaml object for the expected keys and values of the solver options document to setup the shark simulation for the input given in the input file.

5.17.5.15 int read_species (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the master species document.

This function checks the yaml object for the expected keys and values of the master species document to setup the shark simulation for the input given in the input file.

5.17.5.16 int read_massbalance (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the mass balance document.

This function checks the yaml object for the expected keys and values of the mass balance document to setup the shark simulation for the input given in the input file.

5.17.5.17 int read_equilrxn (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the equilibrium reaction document.

This function checks the yaml object for the expected keys and values of the equilibrium reaction document to setup the shark simulation for the input given in the input file.

5.17.5.18 int read_unsteadyrxn (SHARK_DATA * *shark_dat*)

Function to go through the yaml object for the unsteady reaction document.

This function checks the yaml object for the expected keys and values of the unsteady reaction document to setup the shark simulation for the input given in the input file.

5.17.5.19 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*)

Function to setup the memory and pointers for the SHARK_DATA structure for the current simulation.

This function will be called after reading the scenario file and is used to setup the memory and other pointers for the user requested simulation. This function must be called before running a simulation or trying to read in the remander of the yaml formatted input file. Options may be overriden manually after calling this function.

Parameters

file	pointer for the output file where shark results will be stored
residual	pointer to the residual function that will be fed into the PJFNK solver
activity	pointer to the activity function that will determine the activity coefficients
precond	pointer to the linear preconditioning operation to be applied to the Jacobian
dat	pointer to the SHARK_DATA data structure
activity_data	optional pointer for data needed in activity functions
residual_data	optional pointer for data needed in residual functions
precon_data	optional pointer for data needed in preconditioning functions
other_data	optional pointer for data needed in the evaluation of user defined residual functions

5.17.5.20 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*)

Function to add user defined custom residual functions to the OtherList vector object in SHARK_DATA.

This function will need to be used if the user wants to include custom residuals into the system via the OtherList object in SHARK_DATA. For each i residual you want to add, you must call this function passing your residual function and the SHARK_DATA structure pointer. The order that those functions are executed in are determined by the integer i.

Parameters

i	index that the other_res function will appear at in the OtherList object
other_res	function pointer for the user's custom residual function
shark_dat	pointer to the SHARK_DATA data structure

5.17.5.21 int shark_parameter_check (SHARK_DATA * *shark_dat*)

Function to check the Reaction and UnsteadyReaction objects for missing info.

This function checks the Reaction and UnsteadyReaction objects for missing information. If information is missing, this function will return an error that will cause the program to force quit.

5.17.5.22 int shark_energy_calculations (SHARK_DATA * *shark_dat*)

Function to calculate all Reaction and UnsteadyReaction energies.

This function will call the calculate energy functions for Reaction and UnsteadyReaction objects.

5.17.5.23 int shark_temperature_calculations (SHARK_DATA * *shark_dat*)

Function to calculate all Reaction and UnsteadyReaction parameters as a function of temperature.

This function will call all temperature dependent functions in Reaction and UnsteadyReaction to calculate equilibirium and reaction rate parameters as a function of system temperature.

5.17.5.24 int shark_pH_finder (SHARK_DATA * *shark_dat*)

Function will search MasterSpeciesList for existance of H + (aq) and OH - (aq) molecules.

This function searches all molecules in the MasterSpeciesList object for the H + (aq) and OH - (aq) molecules. If they are found, then it sets the pH_index and pOH_index of the SHARK_DATA structure and indicates that the system contains these variables.

5.17.5.25 int shark_guess (SHARK_DATA * *shark_dat*)

Function provides a rough initial guess for the values of all non-linear variables.

This function constructs an rough initial guess for the values of all non-linear variables in the system. The guess is based primarily off of trying to statisfy all mass balance constraints, initial conditions, and pH constraints if any apply.

5.17.5.26 int shark_initial_conditions (SHARK_DATA * *shark_dat*)

Function to establish the initial conditions of the shark simulation.

This function will establish the initial conditions for a transient problem by solving the speciation of the system while holding the transient/unsteady variables constant at their respective initial values. However, if the system we are trying to solve is steady, then this function just calls the shark_guess function.

5.17.5.27 int shark_executioner (SHARK_DATA * *shark_dat*)

Function to execute a shark simulation at a single time step or pH value.

This function calls the preprocess, solver, and postprocess functions in order. If a particular solve did not converge, then it will retry the solver routine until it runs out of tries or attains convergence.

5.17.5.28 int shark_timestep_const (SHARK_DATA * *shark_dat*)

Function to set up all time steps in the simulation to a specified constant.

This function will set all time steps for the current simulation to a constant that is specified in the input file. The time step will not be changed unless the simulation fails, then it will be reduced in order to try to get the system to converge.

5.17.5.29 int shark_timestep_adapt (SHARK_DATA * *shark_dat*)

Function to set up all time steps in the simulation based on success or failure to converge.

This function will set all time steps for the current simulation based on some factor multiple of the prior time step used and whether or not the previous solution step was successful. If the previous step converged, then the new time step will be 1.5x the old time step. If it failed, then the simulation will be retried with a new time step of 0.5x the old time step.

5.17.5.30 int shark_preprocesses (SHARK_DATA * *shark_dat*)

Function to call other functions for calculation of parameters and setting of time steps.

This function will call the shark_temperature_calculations function and the appropriate time step function. If the user requests a constant time step, it will call the shark_timestep_const function. Otherwise, it calls the shark_timestep-_adapt function.

5.17.5.31 int shark_solver (SHARK_DATA * *shark_dat*)

Function to call the PJFNK solver routine given the current SHARK_DATA information.

This function will perform the necessary steps before and after calling the PJFNK solver routine. Based on the simulation flags, the solver function will perform an intial guess for unsteady variables, call the PJFNK method, and the printout a console message about the performance. If a terminal failure occurs during the solver, it will print out the current state of residuals, variables, and the Jacobian matrix to the console. Analyzing this information could provide clues as to why failure occured.

5.17.5.32 int shark_postprocesses (SHARK_DATA * *shark_dat*)

Function to convert PJFNK solutions to concentration values and print to the output file.

This function will convert the non-linear variables to their respective concentration values, then print the solve information out to the output file.

5.17.5.33 int shark_reset (SHARK_DATA * *shark_dat*)

Function to reset the values of all stateful information in SHARK_DATA.

This function will reset all stateful matrix data in the SHARK_DATA structure in preparation of the next time step simulation.

5.17.5.34 int shark_residual (const Matrix< double > & *x*, Matrix< double > & *F*, const void * *data*)

Default residual function for shark evaluations.

This function calls each individual object's residual function to formulate the overall residual function used in the PJ-FNK solver routine. It will also call the activity function. The order in which these function calls occurs is as follows: (i) activities, (ii) Reaction, (iii) UnsteadyReaction, (iv) MassBalance, (v) OtherList, and (vi) MasterSpeciesList. If a constant pH is specified, then the MasterSpeciesList residual call is replaced with a constraint on the H + (aq) variable (if one exists).

5.17.5.35 int SHARK (SHARK_DATA * *shark_dat*)

Function to call all above functions to perform a shark simulation.

This function is called after reading in all inputs, setting all constants, and calling the setup function. It will call all the necessary functions and subroutines iteratively until the desired simulation is complete.

5.17.5.36 int SHARK_SCENARIO (const char * *yaml_input*)

Function to perform a shark simulation based on the conditions in a yaml formatted input file.

This is the primary function used to run shark simulations from the UI. It requires that ths user provide one input file that is formatted with yaml keys, symbols, and spacing so that it can be recognized by the parser. This style of input file is much easier to use and understand than the input files used for SCOPSOWL or SKUA. Below shows an example of a typical input file. Note that the # symbol is used in the input file to comment out lines of text that the parser does not need to read.

Example Yaml Input for SHARK

#This will serve as a test input file for shark to demo how to structure the document

#In practice, this section should be listed first, but it doesn't really matter

#DO NOT USE TABS IN THESE INPUT FILES

#— Starts a document ... Ends a document

#All keys must be proceeded by a :

#All lists/header must be preceeded by a -

#Spacing of the keys will indicate which list/header they belong to

Scenario:

—

- vars_fun:

  numvar: 25

  num_ssr: 15

  num_mbe: 7

  num_usr: 2

  num_other: 0 #Not required or used in current version

- sys_data:

  act_fun: davies

  const_pH: false

  pH: 7 #Only required if we are specifying a const_pH

  temp: 298.15 #Units must be in Kelvin

  dielec: 78.325 #Units must be in (1/Kelvin)

  res_alk: 0 #Units must be in mol/L (Residual Alkalinity)

- run_time:

  steady: false #NOTE: All time must be represented in hours

  specs_curve: false #Only needed if steady = true, and will default to false

  dt: 0.001 #Only required if steady = false

  time_adapt: true #Only needed if steady = false, and will default to false

  sim_time: 96.0 #Only required if steady = false

  t_out: 0.01 #Only required if steady = false

  ...

#The following header is entirely optional, but is used to set solver options

SolverOptions:

—

line_search: true #Default = true, and is recommended to be true

search_type: standard

linear_solve: gmresrp #Note: FOM will be fastest for small problems

restart: 25 #Note: restart only used if using GMRES or GCR type solvers

nl_maxit: 50

nl_abstol: 1e-5

nl_reltol: 1e-8

lin_reltol: 1e-10 #Min Tol = 1e-15

lin_abstol: 1e-10 #Min Tol = 1e-15

nl_print: true

l_print: true

...

#After the Scenario read, shark will call the setup_function, then read info below

MasterSpecies:

—

#Header names are specific

#Keys are chosen by user, but must span numbers 0 through numvar-1

#Keys will denote the ordering of the variables

#Note: Currently, the number of reg molecules is very limited

- reg:

  0: Cl - (aq)

  1: NaHCO3 (aq)

  2: NaCO3 - (aq)

  3: Na + (aq)

  4: HNO3 (aq)

  5: NO3 - (aq)

  6: H2CO3 (aq)

  7: HCO3 - (aq)

  8: CO3 2- (aq)

  9: UO2 2+ (aq)

  10: UO2NO3 + (aq)

  11: UO2(NO3)2 (aq)

  12: UO2OH + (aq)

  13: UO2(OH)3 - (aq)

  14: (UO2)2(OH)2 2+ (aq)

  15: (UO2)3(OH)5 + (aq)

  16: UO2CO3 (aq)

  17: UO2(CO3)2 2- (aq)

18: UO2(CO3)3 4- (aq)

19: H2O (l)

20: OH - (aq)

21: H + (aq)

#Keys for the sub-headers must follow same rules as keys from above

- unreg:
  - 22:
    formula: A(OH)2 (aq)
    charge: 0
    enthalpy: 0
    entropy: 0
    have_HS: false
    energy: 0
    have_G: false
    phase: Aqueous
    name: Amidoxime
    lin_form: none
  - 23:
    formula: UO2AO2 (aq)
    charge: 0
    enthalpy: 0
    entropy: 0
    have_HS: false
    energy: 0
    have_G: false
    phase: Aqueous
    name: Uranyl-amidoximate
    lin_form: none
  - 24:
    formula: UO2CO3AO2 2- (aq)
    charge: -2
    enthalpy: 0
    entropy: 0
    have_HS: false
    energy: 0
    have_G: false
    phase: Aqueous
    name: Uranyl-carbonate-amidoximate
    lin_form: none
    ...

#NOTE: Total concentrations must be given in mol/L

MassBalance:

—

#Header names under MassBalance are choosen by the user

#All other keys will be checked

- water:

  total_conc: 1

  - delta:
    "H2O (l)": 1

- carbonate:

  total_conc: 0.0004175

  - delta:
    "NaHCO3 (aq)": 1
    "NaCO3 - (aq)": 1
    "H2CO3 (aq)": 1
    "HCO3 - (aq)": 1
    "CO3 2- (aq)": 1
    "UO2CO3 (aq)": 1
    "UO2(CO3)2 2- (aq)": 2
    "UO2(CO3)3 4- (aq)": 3
    "UO2CO3AO2 2- (aq)": 1

#Other mass balances skipped for demo purposes...

...

#Document for equilibrium or steady reactions

EquilRxn:

—

#Headers under EquilRxn separate out each reaction object

#Keys for these headers only factor into the order of the equations

#Stoichiometry follows the convention that products are pos(+) and reactants are neg(-)

#Note: logK is only required if any species in stoichiometry is unregistered

#Example: below represents - {H2O (l)} –> {H + (aq)} + {OH - (aq)}

#Note: a valid reaction statement requires at least 1 stoichiometry args

#Note: You can also provide reaction energies: enthalpy, entropy, and energy

- rxn00:

  logK: -14

  - stoichiometry:
    "H2O (l)": -1
    "OH - (aq)": 1
    "H + (aq)": 1

- rxn01:

  logK: -6.35

  - stoichiometry:
    "H2CO3 (aq)": -1
    "HCO3 - (aq)": 1
    "H + (aq)": 1

#Other reactions skipped for demo purposes...

...

#Document for unsteady reactions

UnsteadyRxn:

—

#Same basic standards for this doc as the EquilRxn

#Main difference is the inclusion of rate information

#You are required to give at least 1 rate

#You are also required to denote which variable is unsteady

#You must give the initial concentration for the variable in mol/L

#Rate units are in (L/mol)^n/hr

#Note: we also have keys for forward_ref, reverse_ref,

#activation_energy, and temp_affinity.

#These are optional if forward and/or reverse are given

#Note: You can also provide reaction energies: enthalpy, entropy, and energy

- rxn00:
  unsteady_var: UO2AO2 (aq)
  initial_condition: 0
  logK: -1.35
  forward: 4.5e+6
  reverse: 1.00742e+8
  - stoichiometry:
    "UO2 2+ (aq)": -1
    "A(OH)2 (aq)": -1
    "UO2AO2 (aq)": 1
    "H + (aq)": 2
- rxn01:
  unsteady_var: UO2CO3AO2 2- (aq)
  initial_condition: 0
  logK: 3.45
  forward: 2.55e+15
  reverse: 9.04774e+11
  - stoichiometry:
    "UO2 2+ (aq)": -1
    "CO3 2- (aq)": -1
    "A(OH)2 (aq)": -1
    "UO2CO3AO2 2- (aq)": 1
    "H + (aq)": 2

...

Note

It may be advantageous to look at some other shark input file examples. More input files are provided in the input_files/SHARK directory of the ecosystem project folder. Please refer to your own source file location for more input file examples for SHARK.

5.17.5.37 int SHARK_TESTS ( )

Function to perform a series of shark calculation tests.

This function sets up and solves a test problem for shark. It is callable from the UI.

5.18 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 ()

5.18.1 Macro Definition Documentation

5.18.1.1 #define SKUA_HPP_

5.18.1.2 #define D_inf(*Dref,* *Tref,* *B,* *p,* *T*) (Dref * pow(p+sqrt(DBL_EPSILON),(Tref/T)-B))

5.18.1.3 #define D_o(*Diff,* *E,* *T*) (Diff * exp(-E/(Rstd*T)))

5.18.1.4 #define D_c(*Diff,* *phi*) (Diff * (1.0/((1.0+1.1E-6)-phi)))

5.18.2 Function Documentation

5.18.2.1 void print2file_species_header (FILE * *Output,* SKUA_DATA * *skua_dat,* int *i*)

5.18.2.2 void print2file_SKUA_time_header (FILE * *Output,* SKUA_DATA * *skua_dat,* int *i*)

5.18.2.3 void print2file_SKUA_header (SKUA_DATA * *skua_dat*)

5.18.2.4 void print2file_SKUA_results_old (SKUA_DATA * *skua_dat*)

5.18.2.5 void print2file_SKUA_results_new (SKUA_DATA * *skua_dat*)

5.18.2.6 double default_Dc (int *i,* int *l,* const void * *data*)

5.18.2.7 double default_kf (int *i,* const void * *data*)

5.18.2.8 double const_Dc (int *i,* int *l,* const void * *data*)

5.18.2.9 double simple_darken_Dc (int *i,* int *l,* const void * *data*)

5.18.2.10 double theoretical_darken_Dc (int *i,* int *l,* const void * *data*)

5.18.2.11 double empirical_kf (int *i,* const void * *data*)

5.18.2.12 double const_kf (int *i,* const void * *data*)

5.18.2.13 int molefractionCheck (SKUA_DATA * *skua_dat*)

5.18.2.14 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*)

5.18.2.15 int SKUA_Executioner (SKUA_DATA * *skua_dat*)

5.18.2.16 int set_SKUA_ICs (SKUA_DATA * *skua_dat*)

5.18.2.17 int set_SKUA_timestep (SKUA_DATA * *skua_dat*)

5.18.2.18 int SKUA_preprocesses (SKUA_DATA * *skua_dat*)

5.18.2.19 int set_SKUA_params (const void * *user_data*)

5.18.2.20 int SKUA_postprocesses (SKUA_DATA ∗ *skua_dat*)

5.18.2.21 int SKUA_reset (SKUA_DATA ∗ *skua_dat*)

5.18.2.22 int SKUA (SKUA_DATA ∗ *skua_dat*)

5.18.2.23 int SKUA_CYCLE_TEST01 (SKUA_DATA ∗ *skua_dat*)

5.18.2.24 int SKUA_CYCLE_TEST02 (SKUA_DATA ∗ *skua_dat*)

5.18.2.25 int SKUA_LOW_TEST03 (SKUA_DATA ∗ *skua_dat*)

5.18.2.26 int SKUA_MID_TEST04 (SKUA_DATA ∗ *skua_dat*)

5.18.2.27 int SKUA_SCENARIOS (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate*)

5.18.2.28 int SKUA_TESTS ( )

5.19 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)

5.19.1 Function Documentation

5.19.1.1 int SKUA_OPT_set_y (SKUA_OPT_DATA ∗ *skua_opt*)

5.19.1.2 int initial_guess_SKUA (SKUA_OPT_DATA ∗ *skua_opt*)

5.19.1.3 void eval_SKUA_Uptake (const double ∗ *par,* int *m_dat,* const void ∗ *data,* double ∗ *fvec,* int ∗ *info*)

5.19.1.4 int SKUA_OPTIMIZE (const char ∗ *scene,* const char ∗ *sorbent,* const char ∗ *comp,* const char ∗ *sorbate,* const char ∗ *data*)

5.20 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 ()

5.20.1 Function Documentation

5.20.1.1 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*)

5.20.1.2 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*)

5.20.1.3 double Grav_R (const Matrix< double > & *dX*, int *i*, double *b*, double *rho_p*, double *rho_f*)

5.20.1.4 double Grav_T (const Matrix< double > & *dX*, int *i*, double *b*, double *rho_p*, double *rho_f*)

5.20.1.5 double Van_R (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *Hamaker*, double *b*, double *a*)

5.20.1.6 double V_RAD (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *V0*, double *rho_f*, double *a*, double *eta*)

5.20.1.7 double V_THETA (const Matrix< double > & *dX*, const Matrix< double > & *dY*, int *i*, double *V0*, double *rho_f*, double *a*, double *eta*)

5.20.1.8 double Brown_RAD (double *n_rand*, double *m_rand*, double *sigma_n*, double *sigma_m*)

5.20.1.9 double Brown_THETA (double *s_rand*, double *t_rand*, double *sigma_n*, double *sigma_m*)

5.20.1.10 int POLAR (Matrix< double > & *POL*, const Matrix< double > & *dX*, const Matrix< double > & *dY*, const void * *data*, int *i*)

5.20.1.11 double RADIAL_FORCE (const Matrix< double > & *POL*, double *eta*, double *b*, double *mp*, double *t*, double *a*)

5.20.1.12 double TANGENTIAL_FORCE (const Matrix< double > & *POL*, const Matrix< double > & *dY*, double *eta*, double *b*, double *mp*, double *t*, double *a*, int *i*)

5.20.1.13 int CARTESIAN (const Matrix< double > & *POL*, Matrix< double > & *H*, const Matrix< double > & *dY*, double *i*, const void * *data*)

5.20.1.14 int DISPLACEMENT (Matrix< double > & *dX*, Matrix< double > & *dY*, const Matrix< double > & *H*, int *i*)

5.20.1.15 int LOCATION (const Matrix< double > & *dY*, const Matrix< double > & *dX*, Matrix< double > & *X*, Matrix< double > & *Y*, int *i*)

5.20.1.16 double Removal_Efficiency (double *Sum_Cap*, const void * *data*)

5.20.1.17 int Trajectory_SetupConstants (TRAJECTORY_DATA * *dat*)

5.20.1.18 int Number_Generator (TRAJECTORY_DATA * *dat*)

5.20.1.19 int Run_Trajectory ( )

5.21 ui.h File Reference

User Interface for Ecosystem.

```
#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

  Data structure holding the UI arguments.

Macros

- #define UI_HPP_
- #define ECO_VERSION "0.0 alpha"

Macro expansion for executable current version number.

- #define ECO_EXECUTABLE "eco0"

  Macro expansion for executable current name.

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 }

  Valid options available upon execution of the code.

Functions

- void aui_help ()

  Function to display help for Advanced User Interface.
- void bui_help ()

  Function to display help for Basic User Interface.
- std::string allLower (const std::string &input)

  Function to return an all lower case string based on the passed argument.
- bool exit (const std::string &input)

  Function returns true if user requests exit.
- bool help (const std::string &input)

  Function returns trun if the user requests help.
- bool version (const std::string &input)

  Function returns true if user requests to know the executable version.
- bool test (const std::string &input)

  Function returns true if user requests to run a test.
- bool exec (const std::string &input)

  Function returns true if the user requests to run a simulation/executable.
- bool path (const std::string &input)

  Function returns true if the user indicates that input files share a common path.
- bool input (const std::string &input)

  Function returns true if the user indicates that the next arguments are input files.
- bool valid_test_string (const std::string &input, UI_DATA ∗ui_dat)

  Function returns true if the user gave a valid test option.
- bool valid_exec_string (const std::string &input, UI_DATA ∗ui_dat)

  Function returns true if the user gave a valid execution option.
- int number_files (UI_DATA ∗ui_dat)

  Function returns the number of expected input files for the user's run option.
- bool valid_addon_options (UI_DATA ∗ui_dat)

  Function returns true if the user has choosen a valid additional runtime option.
- void display_help (UI_DATA ∗ui_dat)

  Function to call the appropriate help menu based on type of interface.
- void display_version (UI_DATA ∗ui_dat)

  Function to display ecosystem version information to the console.
- int invalid_input (int count, int max)

  Function returns a CONTINUE or EXIT when invalid input is given.

- bool valid_input_main (UI_DATA *ui_dat)

  Function returns true if user gave valid input in Basic UI.
- bool valid_input_tests (UI_DATA *ui_dat)

  Function returns true if user gave a valid test function to run.
- bool valid_input_execute (UI_DATA *ui_dat)

  Function returns true if user gave a valid executable function to run.
- int test_loop (UI_DATA *ui_dat)

  Function that loops the Basic UI until a valid test option was selected.
- int exec_loop (UI_DATA *ui_dat)

  Function that loops the Basic UI until a valid executable option was selected.
- int run_test (UI_DATA *ui_dat)

  Function will call the user requested test function.
- int run_exec (UI_DATA *ui_dat)

  Function will call the user requested executable function.
- int run_executable (int argc, const char *argv[])

  Function called by the main and runs both user interfaces for the program.

5.21.1 Detailed Description

User Interface for Ecosystem. ui.cpp

These routines define how the user will interface with the software

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Date

08/25/2015

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This software was designed and built at the Georgia Institute of Technology by Austin Ladshaw for PhD research in the area of adsorption and surface science. Copyright (c) 2015, all rights reserved.

5.21.2 Macro Definition Documentation

5.21.2.1 #define UI_HPP_

5.21.2.2 #define ECO_VERSION "0.0 alpha"

Macro expansion for executable current version number.

5.21.2.3 #define ECO_EXECUTABLE "eco0"

Macro expansion for executable current name.

5.21.3 Enumeration Type Documentation

5.21.3.1 enum valid_options

Valid options available upon execution of the code.

Enumeration of valid options for executing the ecosystem code. More options become available as the code updates. Some options that appear here may not be viewable in the "help" screen of the executable. Those options are hidden, but are still valid entries.

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***

5.21.4 Function Documentation

5.21.4.1 void aui_help ( )

Function to display help for Advanced User Interface.

The Advanved User Interface help screen is accessed by including run option -h or –help when executing the program from command line.

5.21.4.2 void bui_help ( )

Function to display help for Basic User Interface.

The Basic User Interface help screen is accessed by running the executable, then typing "help" at any point during the console prompts. Exception to this occurs when the console prompts you to provide input files for your choosen routine. In this circumstance, the executable always assumes that what the user types in will be an input file.

5.21.4.3 std::string allLower (const std::string & *input*)

Function to return an all lower case string based on the passed argument.

This function will copy the input paramter and convert that copy to all lower case. The copy is then returned and can be checked against valid or allowed strings.

Parameters

input	string to copy and convert to lower case

5.21.4.4 bool exit (const std::string & *input*)

Function returns true if user requests exit.

This function will check the input string for "exit" or "quit" and terminate the executable. Only checked if using the Basic User Interface.

Parameters

input	input string user gives to the console

5.21.4.5 bool help (const std::string & *input*)

Function returns trun if the user requests help.

This function will check the input string for "help", "-h", or "–help" and will tell the executable to display the help menu. The help menu that gets displayed depends on how the executable was run to begin with.

Parameters

input	input string user gives to the console

5.21.4.6 bool version (const std::string & *input*)

Function returns true if user requests to know the executable version.

This function will check the input string for "version", "-v", or "–version" and will tell the executable to display version information about the executable.

Parameters

input	input string user gives to the console

5.21.4.7 bool test (const std::string & *input*)

Function returns true if user requests to run a test.

This function will check the input string for "-t" or "–test" and determine whether or not the user requests to run an ecosystem test function.

Parameters

input	input string user gives to the console

5.21.4.8 bool exec (const std::string & *input*)

Function returns true if the user requests to run a simulation/executable.

This function will check the input string for "-e" or "–execute" and determine whether or not the user requests to run an ecosystem executable function.

Parameters

input	input string the user gives to the console

5.21.4.9 bool path (const std::string & *input*)

Function returns true if the user indicates that input files share a common path.

This function will check the input string for "-p" or "–path" and determine whether or not the user will give a common path to all input files needed for the specified simulation. Only used in Advanced User Interface.

Parameters

input	input string the user gives to the console

5.21.4.10 bool input (const std::string & *input*)

Function returns true if the user indicates that the next arguments are input files.

This function will check the input string for "-i" or "–input" and determine whether or not the user's next arguments are input files for a specific simulation. Only used in Advanced User Interface.

Parameters

input	input string the user gives to the console

5.21.4.11 bool valid_test_string (const std::string & *input*, UI_DATA * *ui_dat*)

Function returns true if the user gave a valid test option.

This function will check the input string given by the user and determine whether that string denotes a valid test. Then, it will mark the option variable in ui_dat with the appropriate option from the valid_options enum.

Parameters

input	input string the user gives to the console
ui_dat	pointer to the data structure for the ui object

5.21.4.12 bool valid_exec_string (const std::string & *input*, UI_DATA * *ui_dat*)

Function returns true if the user gave a valid execution option.

This function will check the input string given by the user and determine whether that string denotes a valid execution option. Then, it will mark the option variable in ui_dat with the appropriate option from the valid_options enum.

Parameters

input	input string the user gives to the console
ui_dat	pointer to the data structure for the ui object

5.21.4.13 int number_files (UI_DATA * *ui_dat*)

Function returns the number of expected input files for the user's run option.

This function will check the option variable in the ui_dat structure to determine the number of input files that is expected to be given. Running different executable functions in ecosystem may require various number of input files.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.14 bool valid_addon_options (UI_DATA * *ui_dat*)

Function returns true if the user has choosen a valid additional runtime option.

This function will check all additional input options in the user_input variable of ui_dat to determine if the user requests any additional options during runtime. Valid additional options are -p or –path and -i or –input.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.15 void display_help (UI_DATA * *ui_dat*)

Function to call the appropriate help menu based on type of interface.

This function looks at the ui_dat structure and the user's OS files to determine what help menu to display and how to display it. There are two different types of help menus that can be displayed: (i) Advanced Help and (ii) Basic Help. Additionally, this function checks the OS file system for the existence of installed help files. If it finds those files, then it instructs the command terminal to read the contents of those files with the "less" command. Otherwise, it will just print the appropriate help menu to the console window.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.16 void display_version (UI_DATA * *ui_dat*)

Function to display ecosystem version information to the console.

This function will check the ui_dat structure to see which type of interface the user is using, then print out the version information for the executable being run.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.17 int invalid_input (int *count,* int *max*)

Function returns a CONTINUE or EXIT when invalid input is given.

This function looks at the current count and the max iterations and determines whether or not to force the executable to terminate. If the user provides too many incorrect options during the Basic User Interface, then the executable will force quit.

Parameters

count	number of times the user has provided a bad option
max	maximum allowable bad options before force quit

5.21.4.18 bool valid_input_main (UI_DATA * *ui_dat*)

Function returns true if user gave valid input in Basic UI.

This function is only called if the user is running the Basic UI. It checks the given console argument stored in user_input of ui_dat for a valid option. If no valid option is given, then this function returns false.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.19 bool valid_input_tests (UI_DATA * *ui_dat*)

Function returns true if user gave a valid test function to run.

This function checks the user_input argument of ui_dat for a valid test option. If no valid test was given, then this function returns false.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.20 bool valid_input_execute (UI_DATA * *ui_dat*)

Function returns true if user gave a valid executable function to run.

This function checks the user_input argument of ui_dat for a valid executable option. If no valid executable was given, then this function returns false.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.21 int test_loop (UI_DATA * *ui_dat*)

Function that loops the Basic UI until a valid test option was selected.

This function loops the Basic UI menu for running a test until a valid test is selected by the user. If a valid test is not selected, and the maximum number of loops has been reached, then this function will cause the program to force quit.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.22 int exec_loop (UI_DATA * *ui_dat*)

Function that loops the Basic UI until a valid executable option was selected.

This function loops the Basic UI menu for running an executable until a valid executable is selected by the user. If a valid executable is not selected, and the maximum number of loops has been reached, then this function will cause the program to force quit.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.23 int run_test (UI_DATA * *ui_dat*)

Function will call the user requested test function.

This function checks the option variable of the ui_dat structure and runs the corresponding test function.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.24 int run_exec (UI_DATA * *ui_dat*)

Function will call the user requested executable function.

This function checks the option variable of the ui_dat structure and runs the corresponding executable function.

Parameters

ui_dat	pointer to the data structure for the ui object

5.21.4.25 int run_executable (int *argc*, const char * *argv[]*)

Function called by the main and runs both user interfaces for the program.

This function is called in the main.cpp file and passes the console arguments given at run time.

Parameters

argc	number of arguments provided by the user at the time of execution
argv	list of C-strings that was provided by the user at the time of execution

5.22 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)

5.22.1 Typedef Documentation

5.22.1.1 typedef enum **data_type data_type**

5.22.1.2 typedef enum **header_state header_state**

5.22.2 Enumeration Type Documentation

5.22.2.1 enum **data_type**

Enumerator

STRING

BOOLEAN

DOUBLE

INT

UNKNOWN

5.22.2.2 enum **header_state**

Enumerator

ANCHOR

ALIAS

NONE

5.22.3 Function Documentation

5.22.3.1 int YAML_WRAPPER_TESTS ( )

5.22.3.2 int YAML_CPP_TEST (const char * *file*)

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