

DGOSPREY

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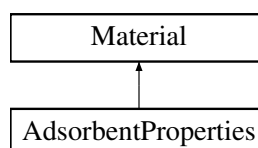
4 Class Documentation

4.1 AdsorbentProperties Class Reference

[AdsorbentProperties](#) class object inherits from Material object.

```
#include <AdsorbentProperties.h>
```

Inheritance diagram for AdsorbentProperties:



Public Member Functions

- [AdsorbentProperties](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual void [computeQpProperties](#) ()
Required function override for Material objects in MOOSE.

Private Attributes

- Real [_binder_fraction](#)
Binder fraction in the biporous adsorbent pellet (0 means no binder material)
- Real [_binder_porosity](#)
Macro-porosity of the binder material in the adsorbent pellet.
- Real [_crystal_radius](#)
Nominal radius of the adsorbent crystals suspended in the binder (um)
- Real [_pellet_diameter](#)
Nominal diameter of the adsorbent pellets in the system (cm)
- Real [_macropore_radius](#)
Nominal size of the macro-pores in the pellet (cm)
- Real [_rhos](#)
Density of the adsorbent pellet (g/cm³)
- Real [_hs](#)
Heat capacity of the adsorbent pellet (J/g/K)
- MaterialProperty< Real > & [_pellet_density](#)
MaterialProperty for the pellet density (g/cm³)
- MaterialProperty< Real > & [_pellet_heat_capacity](#)
MaterialProperty for the pellet heat capacity (J/g/K)
- VariableValue & [_temperature](#)
Reference to the coupled column temperature.
- std::vector< unsigned int > [_index](#)
List of indices for the coupled gases.
- std::vector< VariableValue * > [_gas_conc](#)
Pointer list for the coupled gases.

4.1.1 Detailed Description

[AdsorbentProperties](#) class object inherits from Material object.

This class object inherits from the Material object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will set up the structural information about adsorbent in the system that will be used when determining flow properties, as well as some kinetic properties for adsorption dynamics.

Definition at line 57 of file AdsorbentProperties.h.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 AdsorbentProperties::AdsorbentProperties (const InputParameters & parameters)

Required constructor for objects in MOOSE.

4.1.3 Member Function Documentation

4.1.3.1 virtual void AdsorbentProperties::computeQpProperties () [protected], [virtual]

Required function override for Material objects in MOOSE.

This function computes the material properties when they are needed by other MOOSE objects.

4.1.4 Member Data Documentation

4.1.4.1 Real AdsorbentProperties::_binder_fraction [private]

Binder fraction in the biporous adsorbent pellet (0 means no binder material)

Definition at line 69 of file AdsorbentProperties.h.

4.1.4.2 Real AdsorbentProperties::_binder_porosity [private]

Macro-porosity of the binder material in the adsorbent pellet.

Definition at line 70 of file AdsorbentProperties.h.

4.1.4.3 Real AdsorbentProperties::_crystal_radius [private]

Nominal radius of the adsorbent crystals suspended in the binder (um)

Definition at line 71 of file AdsorbentProperties.h.

4.1.4.4 std::vector<VariableValue*> AdsorbentProperties::_gas_conc [private]

Pointer list for the coupled gases.

Definition at line 82 of file AdsorbentProperties.h.

4.1.4.5 Real AdsorbentProperties::_hs [private]

Heat capacity of the adsorbent pellet (J/g/K)

Definition at line 75 of file AdsorbentProperties.h.

4.1.4.6 std::vector<unsigned int> AdsorbentProperties::_index [private]

List of indices for the coupled gases.

Definition at line 81 of file AdsorbentProperties.h.

4.1.4.7 Real AdsorbentProperties::_macropore_radius [private]

Nominal size of the macro-pores in the pellet (cm)

Definition at line 73 of file AdsorbentProperties.h.

4.1.4.8 MaterialProperty<Real>& AdsorbentProperties::_pellet_density [private]

MaterialProperty for the pellet density (g/cm³)

Definition at line 77 of file AdsorbentProperties.h.

4.1.4.9 Real AdsorbentProperties::_pellet_diameter [private]

Nominal diameter of the adsorbent pellets in the system (cm)

Definition at line 72 of file AdsorbentProperties.h.

4.1.4.10 MaterialProperty<Real>& AdsorbentProperties::_pellet_heat_capacity [private]

MaterialProperty for the pellet heat capacity (J/g/K)

Definition at line 78 of file AdsorbentProperties.h.

4.1.4.11 Real AdsorbentProperties::_rhos [private]

Density of the adsorbent pellet (g/cm³)

Definition at line 74 of file AdsorbentProperties.h.

4.1.4.12 VariableValue& AdsorbentProperties::_temperature [private]

Reference to the coupled column temperature.

Definition at line 80 of file AdsorbentProperties.h.

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

- [AdsorbentProperties.h](#)

4.2 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

4.2.1 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.

Definition at line 120 of file lark.h.

4.2.2 Member Data Documentation

4.2.2.1 double ARNOLDI_DATA::beta

Normalization parameter.

Definition at line 125 of file lark.h.

4.2.2.2 Matrix<double> ARNOLDI_DATA::e1

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

Definition at line 133 of file lark.h.

4.2.2.3 Matrix<double> ARNOLDI_DATA::Hkp1

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

Definition at line 131 of file lark.h.

4.2.2.4 double ARNOLDI_DATA::hp1

Additional row element of H (separate storage for holding)

Definition at line 126 of file lark.h.

4.2.2.5 int ARNOLDI_DATA::iter

Actual size of the Krylov subspace.

Definition at line 123 of file lark.h.

4.2.2.6 int ARNOLDI_DATA::k

Desired size of the Krylov subspace.

Definition at line 122 of file lark.h.

4.2.2.7 bool ARNOLDI_DATA::Output = true

True = print messages to console.

Definition at line 128 of file lark.h.

4.2.2.8 Matrix<double> ARNOLDI_DATA::sum

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

Definition at line 136 of file lark.h.

4.2.2.9 Matrix<double> ARNOLDI_DATA::v

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

Definition at line 135 of file lark.h.

4.2.2.10 `std::vector< Matrix<double> > ARNOLDI_DATA::Vk`

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

Definition at line 130 of file lark.h.

4.2.2.11 `Matrix<double> ARNOLDI_DATA::w`

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

Definition at line 134 of file lark.h.

4.2.2.12 `Matrix<double> ARNOLDI_DATA::yk`

(k) x (1) vector search direction

Definition at line 132 of file lark.h.

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

- [lark.h](#)

4.3 BACKTRACK_DATA Struct Reference

Data structure for the implementation of Backtracking Linesearch.

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

Public Attributes

- int `fun_call` = 0
Number of function calls made during line search.
- 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 Newton 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.

Definition at line 474 of file lark.h.

4.3.2 Member Data Documentation

4.3.2.1 double BACKTRACK_DATA::alpha = 1e-4

Scaling parameter for determination of search step size.

Definition at line 477 of file lark.h.

4.3.2.2 bool BACKTRACK_DATA::constRho = false

True = use a constant value for rho.

Definition at line 482 of file lark.h.

4.3.2.3 Matrix<double> BACKTRACK_DATA::Fk

Old residual vector of the Newton step.

Definition at line 484 of file lark.h.

4.3.2.4 int BACKTRACK_DATA::fun_call = 0

Number of function calls made during line search.

Definition at line 476 of file lark.h.

4.3.2.5 double BACKTRACK_DATA::lambdaMin = DBL_EPSILON

Smallest allowable step length.

Definition at line 479 of file lark.h.

4.3.2.6 double BACKTRACK_DATA::normFkp1

New residual norm of the Newton step.

Definition at line 480 of file lark.h.

4.3.2.7 double BACKTRACK_DATA::rho = 0.1

Scaling parameter for to change step size by.

Definition at line 478 of file lark.h.

4.3.2.8 Matrix<double> BACKTRACK_DATA::xk

Old solution vector of the Newton step.

Definition at line 485 of file lark.h.

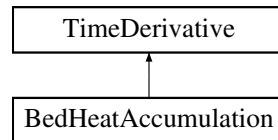
The documentation for this struct was generated from the following file:

- [lark.h](#)

4.4 BedHeatAccumulation Class Reference

```
#include <BedHeatAccumulation.h>
```

Inheritance diagram for BedHeatAccumulation:



Public Member Functions

- [BedHeatAccumulation](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_heat_retardation](#)

4.4.1 Detailed Description

Definition at line 12 of file BedHeatAccumulation.h.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 `BedHeatAccumulation::BedHeatAccumulation (const InputParameters & parameters)`

4.4.3 Member Function Documentation

4.4.3.1 `virtual Real BedHeatAccumulation::computeQpJacobian ()` [protected], [virtual]

4.4.3.2 `virtual Real BedHeatAccumulation::computeQpResidual ()` [protected], [virtual]

4.4.4 Member Data Documentation

4.4.4.1 `const MaterialProperty<Real>& BedHeatAccumulation::_heat_retardation` [private]

Definition at line 23 of file BedHeatAccumulation.h.

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

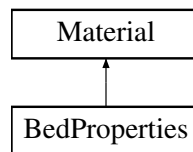
- [BedHeatAccumulation.h](#)

4.5 BedProperties Class Reference

[BedProperties](#) class object inherits from Material object.

```
#include <BedProperties.h>
```

Inheritance diagram for BedProperties:



Public Member Functions

- [BedProperties](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual void [computeQpProperties](#) ()
Required function override for Material objects in MOOSE.

Private Attributes

- Real [_length](#)
Bed length (cm)
- Real [_din](#)
Column inner diameter (cm)
- Real [_dout](#)
Column outer diameter (cm)
- Real [_eb](#)
Bulk porosity of the bed.
- Real [_Kz](#)
Axial thermal conductivity of the bed (J/hr/cm/K)
- Real [_rho_w](#)
Density of the column wall (g/cm³)
- Real [_hw](#)
Heat capacity of the column wall (J/g/K)
- Real [_Uw](#)
Bed-Wall heat transfer coefficient (J/hr/cm²/K)
- Real [_Ua](#)
External-Wall heat transfer coefficient (J/hr/cm²/K)
- MaterialProperty< Real > & [_inner_dia](#)
MaterialProperty for column inner diameter.
- MaterialProperty< Real > & [_outer_dia](#)
MaterialProperty for column outer diameter.
- MaterialProperty< Real > & [_porosity](#)
MaterialProperty for bulk porosity of the bed.
- MaterialProperty< Real > & [_conductivity](#)
MaterialProperty for thermal conductivity of the bed.
- MaterialProperty< Real > & [_wall_density](#)
MaterialProperty for column wall density.
- MaterialProperty< Real > & [_wall_heat_capacity](#)
MaterialProperty for column wall heat capacity.
- MaterialProperty< Real > & [_bed_wall_transfer_coeff](#)
MaterialProperty for bed-wall heat transfer coefficient.

- `MaterialProperty< Real > & _wall_exterior_transfer_coeff`
MaterialProperty for exterior-wall heat transfer coefficient.
- `VariableValue & _temperature`
Reference to the coupled column temperature.
- `std::vector< unsigned int > _index`
List of indices for the species in the system.
- `std::vector< VariableValue * > _gas_conc`
Pointer list of the gas species concentrations.

4.5.1 Detailed Description

`BedProperties` class object inherits from `Material` object.

This class object inherits from the `Material` object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will set up the parameters of the fixed-bed column. Those parameters include: length, diameter, thermal conductivity, heat transfer coefficients, bulk porosity, etc.

Definition at line 55 of file `BedProperties.h`.

4.5.2 Constructor & Destructor Documentation

4.5.2.1 `BedProperties::BedProperties (const InputParameters & parameters)`

Required constructor for objects in MOOSE.

4.5.3 Member Function Documentation

4.5.3.1 `virtual void BedProperties::computeQpProperties () [protected], [virtual]`

Required function override for `Material` objects in MOOSE.

This function computes the material properties when they are needed by other MOOSE objects.

4.5.4 Member Data Documentation

4.5.4.1 `MaterialProperty<Real>& BedProperties::_bed_wall_transfer_coeff [private]`

`MaterialProperty` for bed-wall heat transfer coefficient.

Definition at line 83 of file `BedProperties.h`.

4.5.4.2 `MaterialProperty<Real>& BedProperties::_conductivity [private]`

`MaterialProperty` for thermal conductivity of the bed.

Definition at line 80 of file `BedProperties.h`.

4.5.4.3 `Real BedProperties::_din [private]`

Column inner diameter (cm)

Definition at line 68 of file `BedProperties.h`.

4.5.4.4 `Real BedProperties::_dout [private]`

Column outer diameter (cm)

Definition at line 69 of file `BedProperties.h`.

4.5.4.5 Real BedProperties::_eb [private]

Bulk porosity of the bed.

Definition at line 70 of file BedProperties.h.

4.5.4.6 std::vector<VariableValue*> BedProperties::_gas_conc [private]

Pointer list of the gas species concentrations.

Definition at line 88 of file BedProperties.h.

4.5.4.7 Real BedProperties::_hw [private]

Heat capacity of the column wall (J/g/K)

Definition at line 73 of file BedProperties.h.

4.5.4.8 std::vector<unsigned int> BedProperties::_index [private]

List of indices for the species in the system.

Definition at line 87 of file BedProperties.h.

4.5.4.9 MaterialProperty<Real>& BedProperties::_inner_dia [private]

MaterialProperty for column inner diameter.

Definition at line 77 of file BedProperties.h.

4.5.4.10 Real BedProperties::_Kz [private]

Axial thermal conductivity of the bed (J/hr/cm/K)

Definition at line 71 of file BedProperties.h.

4.5.4.11 Real BedProperties::_length [private]

Bed length (cm)

Definition at line 67 of file BedProperties.h.

4.5.4.12 MaterialProperty<Real>& BedProperties::_outer_dia [private]

MaterialProperty for column outer diameter.

Definition at line 78 of file BedProperties.h.

4.5.4.13 MaterialProperty<Real>& BedProperties::_porosity [private]

MaterialProperty for bulk porosity of the bed.

Definition at line 79 of file BedProperties.h.

4.5.4.14 Real BedProperties::_rho_w [private]

Density of the column wall (g/cm³)

Definition at line 72 of file BedProperties.h.

4.5.4.15 VariableValue& BedProperties::_temperature [private]

Reference to the coupled column temperature.

Definition at line 86 of file BedProperties.h.

4.5.4.16 Real BedProperties::_Ua [private]

External-Wall heat transfer coefficient (J/hr/cm²/K)

Definition at line 75 of file BedProperties.h.

4.5.4.17 Real BedProperties::_Uw [private]

Bed-Wall heat transfer coefficient (J/hr/cm²/K)

Definition at line 74 of file BedProperties.h.

4.5.4.18 MaterialProperty<Real>& BedProperties::_wall_density [private]

MaterialProperty for column wall density.

Definition at line 81 of file BedProperties.h.

4.5.4.19 MaterialProperty<Real>& BedProperties::_wall_exterior_transfer_coeff [private]

MaterialProperty for exterior-wall heat transfer coefficient.

Definition at line 84 of file BedProperties.h.

4.5.4.20 MaterialProperty<Real>& BedProperties::_wall_heat_capacity [private]

MaterialProperty for column wall heat capacity.

Definition at line 82 of file BedProperties.h.

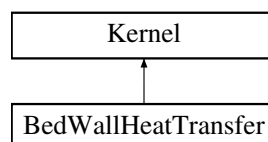
The documentation for this class was generated from the following file:

- [BedProperties.h](#)

4.6 BedWallHeatTransfer Class Reference

```
#include <BedWallHeatTransfer.h>
```

Inheritance diagram for BedWallHeatTransfer:

**Public Member Functions**

- [BedWallHeatTransfer](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_bed_wall_transfer_coeff](#)
- const MaterialProperty< Real > & [_inner_dia](#)

- `const MaterialProperty< Real > & _outer_dia`
- `VariableValue & _column_temp`

4.6.1 Detailed Description

Definition at line 11 of file `BedWallHeatTransfer.h`.

4.6.2 Constructor & Destructor Documentation

4.6.2.1 `BedWallHeatTransfer::BedWallHeatTransfer (const InputParameters & parameters)`

4.6.3 Member Function Documentation

4.6.3.1 `virtual Real BedWallHeatTransfer::computeQpJacobian ()` `[protected]`, `[virtual]`

4.6.3.2 `virtual Real BedWallHeatTransfer::computeQpResidual ()` `[protected]`, `[virtual]`

4.6.4 Member Data Documentation

4.6.4.1 `const MaterialProperty<Real>& BedWallHeatTransfer::_bed_wall_transfer_coeff` `[private]`

Definition at line 21 of file `BedWallHeatTransfer.h`.

4.6.4.2 `VariableValue& BedWallHeatTransfer::_column_temp` `[private]`

Definition at line 25 of file `BedWallHeatTransfer.h`.

4.6.4.3 `const MaterialProperty<Real>& BedWallHeatTransfer::_inner_dia` `[private]`

Definition at line 22 of file `BedWallHeatTransfer.h`.

4.6.4.4 `const MaterialProperty<Real>& BedWallHeatTransfer::_outer_dia` `[private]`

Definition at line 23 of file `BedWallHeatTransfer.h`.

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

- [BedWallHeatTransfer.h](#)

4.7 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
 - *Absolute 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 residual updates.*

4.7.1 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.

Definition at line 249 of file lark.h.

4.7.2 Member Data Documentation

4.7.2.1 double BiCGSTAB_DATA::alpha

Step size parameter for next solution.

Definition at line 255 of file lark.h.

4.7.2.2 double BiCGSTAB_DATA::bestres

Best found residual norm.

Definition at line 266 of file lark.h.

4.7.2.3 Matrix<double> BiCGSTAB_DATA::bestx

Best found solution to the linear system.

Definition at line 271 of file lark.h.

4.7.2.4 double BiCGSTAB_DATA::beta

Step size parameter for search direction.

Definition at line 256 of file lark.h.

4.7.2.5 bool BiCGSTAB_DATA::breakdown

Boolean to determine if the method broke down.

Definition at line 253 of file lark.h.

4.7.2.6 int BiCGSTAB_DATA::iter = 0

Actual number of iterations.

Definition at line 252 of file lark.h.

4.7.2.7 int BiCGSTAB_DATA::maxit = 0

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

Definition at line 251 of file lark.h.

4.7.2.8 double BiCGSTAB_DATA::omega

Scaling parameter and additional step length.

Definition at line 259 of file lark.h.

4.7.2.9 double BiCGSTAB_DATA::omega_old

Previous scaling parameter and step length.

Definition at line 260 of file lark.h.

4.7.2.10 bool BiCGSTAB_DATA::Output = true

True = print messages to console.

Definition at line 268 of file lark.h.

4.7.2.11 Matrix<double> BiCGSTAB_DATA::p

Search direction for updating.

Definition at line 275 of file lark.h.

4.7.2.12 Matrix<double> BiCGSTAB_DATA::r

Residual vector for the linear system.

Definition at line 272 of file lark.h.

4.7.2.13 Matrix<double> BiCGSTAB_DATA::r0

Initial residual vector.

Definition at line 273 of file lark.h.

4.7.2.14 double BiCGSTAB_DATA::relres

Relative residual norm.

Definition at line 264 of file lark.h.

4.7.2.15 double BiCGSTAB_DATA::relres_base

Initial residual norm.

Definition at line 265 of file lark.h.

4.7.2.16 double BiCGSTAB_DATA::res

Absolute residual norm.

Definition at line 263 of file lark.h.

4.7.2.17 double BiCGSTAB_DATA::rho

Scaling parameter for alpha and beta.

Definition at line 257 of file lark.h.

4.7.2.18 double BiCGSTAB_DATA::rho_old

Previous scaling parameter for alpha and beta.

Definition at line 258 of file lark.h.

4.7.2.19 Matrix<double> BiCGSTAB_DATA::s

Residual updating vector.

Definition at line 277 of file lark.h.

4.7.2.20 Matrix<double> BiCGSTAB_DATA::t

Search direction for residual updates.

Definition at line 279 of file lark.h.

4.7.2.21 double BiCGSTAB_DATA::tol_abs = 1e-6

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

Definition at line 262 of file lark.h.

4.7.2.22 double BiCGSTAB_DATA::tol_rel = 1e-6

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

Definition at line 261 of file lark.h.

4.7.2.23 Matrix<double> BiCGSTAB_DATA::v

Search direction for p.

Definition at line 274 of file lark.h.

4.7.2.24 Matrix<double> BiCGSTAB_DATA::x

Current solution to the linear system.

Definition at line 270 of file lark.h.

4.7.2.25 Matrix<double> BiCGSTAB_DATA::y

Preconditioned search direction.

Definition at line 276 of file lark.h.

4.7.2.26 Matrix<double> BiCGSTAB_DATA::z

Preconditioned residual updating vector.

Definition at line 278 of file lark.h.

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

- [lark.h](#)

4.8 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.*

4.8.1 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.

Definition at line 288 of file lark.h.

4.8.2 Member Data Documentation

4.8.2.1 double CGS_DATA::alpha

Step size parameter for next solution.

Definition at line 294 of file lark.h.

4.8.2.2 double CGS_DATA::bestres

Best found residual norm.

Definition at line 303 of file lark.h.

4.8.2.3 Matrix<double> CGS_DATA::bestx

Best found solution to the linear system.

Definition at line 308 of file lark.h.

4.8.2.4 double CGS_DATA::beta

Step size parameter for search direction.

Definition at line 295 of file lark.h.

4.8.2.5 bool CGS_DATA::breakdown

Boolean to determine if the method broke down.

Definition at line 292 of file lark.h.

4.8.2.6 Matrix<double> CGS_DATA::c

Holds the matvec result between A and p.

Definition at line 315 of file lark.h.

4.8.2.7 int CGS_DATA::iter = 0

Actual number of iterations.

Definition at line 291 of file lark.h.

4.8.2.8 int CGS_DATA::maxit = 0

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

Definition at line 290 of file lark.h.

4.8.2.9 bool CGS_DATA::Output = true

True = print messages to console.

Definition at line 305 of file lark.h.

4.8.2.10 Matrix<double> CGS_DATA::p

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

Definition at line 314 of file lark.h.

4.8.2.11 Matrix<double> CGS_DATA::r

Residual vector for the linear system.

Definition at line 309 of file lark.h.

4.8.2.12 Matrix<double> CGS_DATA::r0

Initial residual vector.

Definition at line 310 of file lark.h.

4.8.2.13 double CGS_DATA::relres

Relative residual norm.

Definition at line 301 of file lark.h.

4.8.2.14 double CGS_DATA::relres_base

Initial residual norm.

Definition at line 302 of file lark.h.

4.8.2.15 double CGS_DATA::res

Absolute residual norm.

Definition at line 300 of file lark.h.

4.8.2.16 double CGS_DATA::rho

Scaling parameter for alpha and beta.

Definition at line 296 of file lark.h.

4.8.2.17 double CGS_DATA::sigma

Scaling parameter and additional step length.

Definition at line 297 of file lark.h.

4.8.2.18 double CGS_DATA::tol_abs = 1e-6

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

Definition at line 299 of file lark.h.

4.8.2.19 double CGS_DATA::tol_rel = 1e-6

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

Definition at line 298 of file lark.h.

4.8.2.20 Matrix<double> CGS_DATA::u

Search direction for v.

Definition at line 311 of file lark.h.

4.8.2.21 Matrix<double> CGS_DATA::v

Search direction for x.

Definition at line 313 of file lark.h.

4.8.2.22 Matrix<double> CGS_DATA::w

Updates sigma and u.

Definition at line 312 of file lark.h.

4.8.2.23 Matrix<double> CGS_DATA::x

Current solution to the linear system.

Definition at line 307 of file lark.h.

4.8.2.24 Matrix<double> CGS_DATA::z

Full search direction for x.

Definition at line 316 of file lark.h.

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

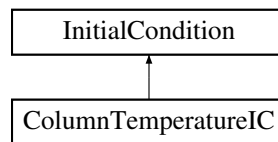
- [lark.h](#)

4.9 ColumnTemperatureIC Class Reference

[ColumnTemperatureIC](#) class object inherits from [InitialCondition](#) object.

```
#include <ColumnTemperatureIC.h>
```

Inheritance diagram for [ColumnTemperatureIC](#):



Public Member Functions

- [ColumnTemperatureIC](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.
- virtual Real [value](#) (const Point &p)
Required function override for setting the value of the non-linear variable at a given point.

Private Attributes

- Real [_TC_IC](#)
Initial condition value for the column temperature (K)

4.9.1 Detailed Description

[ColumnTemperatureIC](#) class object inherits from [InitialCondition](#) object.

This class object inherits from the [InitialCondition](#) object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will establish the initial conditions for column temperature as constant throughout the domain.

Note

You can have the non-linear variable vary spatially in the domain by inheriting from and or modifying this file to do so.

Definition at line 58 of file [ColumnTemperatureIC.h](#).

4.9.2 Constructor & Destructor Documentation

4.9.2.1 [ColumnTemperatureIC::ColumnTemperatureIC](#) (const InputParameters & *parameters*)

Required constructor for objects in MOOSE.

4.9.3 Member Function Documentation

4.9.3.1 virtual Real [ColumnTemperatureIC::value](#) (const Point & *p*) [virtual]

Required function override for setting the value of the non-linear variable at a given point.

This function passes a point *p* as an argument. The return value will be the value of the non-linear variable at that point. That information is used to establish the spatially varying initial condition for the given non-linear variable.

4.9.4 Member Data Documentation

4.9.4.1 Real `ColumnTemperatureIC::TC_IC` [private]

Initial condition value for the column temperature (K)

Definition at line 70 of file `ColumnTemperatureIC.h`.

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

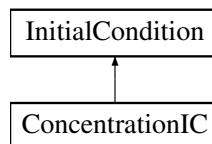
- [ColumnTemperatureIC.h](#)

4.10 ConcentrationIC Class Reference

`ConcentrationIC` class object inherits from `InitialCondition` object.

```
#include <ConcentrationIC.h>
```

Inheritance diagram for `ConcentrationIC`:



Public Member Functions

- `ConcentrationIC` (const `InputParameters` ¶meters)
Required constructor for objects in MOOSE.
- virtual Real `value` (const `Point` &p)
Required function override for setting the value of the non-linear variable at a given point.

Private Attributes

- Real `_y_IC`
Initial molefraction of the species in the gas phase.
- Real `_PT_IC`
Initial total pressure in the column (kPa)
- Real `_T_IC`
Initial temperature in the column (K)

4.10.1 Detailed Description

`ConcentrationIC` class object inherits from `InitialCondition` object.

This class object inherits from the `InitialCondition` object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will establish the initial conditions for a species' concentration as constant throughout the domain.

Note

You can have the non-linear variable vary spatially in the domain by inheriting from and or modifying this file to do so.

Definition at line 58 of file `ConcentrationIC.h`.

4.10.2 Constructor & Destructor Documentation

4.10.2.1 ConcentrationIC::ConcentrationIC (const InputParameters & *parameters*)

Required constructor for objects in MOOSE.

4.10.3 Member Function Documentation

4.10.3.1 virtual Real ConcentrationIC::value (const Point & *p*) [virtual]

Required function override for setting the value of the non-linear variable at a given point.

This function passes a point *p* as an argument. The return value will be the value of the non-linear variable at that point. That information is used to establish the spatially varying initial condition for the given non-linear variable.

4.10.4 Member Data Documentation

4.10.4.1 Real ConcentrationIC::_PT_IC [private]

Initial total pressure in the column (kPa)

Definition at line 71 of file ConcentrationIC.h.

4.10.4.2 Real ConcentrationIC::_T_IC [private]

Initial temperature in the column (K)

Definition at line 72 of file ConcentrationIC.h.

4.10.4.3 Real ConcentrationIC::_y_IC [private]

Initial molefraction of the species in the gas phase.

Definition at line 70 of file ConcentrationIC.h.

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

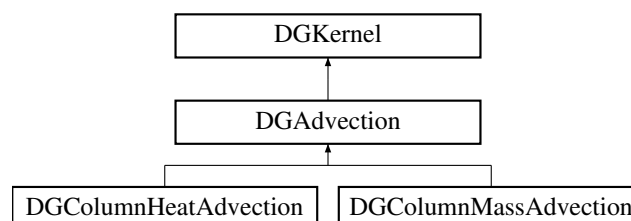
- [ConcentrationIC.h](#)

4.11 DGAdvection Class Reference

[DGAdvection](#) class object inherits from DGKernel object.

```
#include <DGAdvection.h>
```

Inheritance diagram for DGAdvection:



Public Member Functions

- [DGAdvection](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Vector of velocity.
- Real [_vx](#)
x-component of velocity (optional - set in input file)
- Real [_vy](#)
y-component of velocity (optional - set in input file)
- Real [_vz](#)
z-component of velocity (optional - set in input file)

4.11.1 Detailed Description

[DGAdvection](#) class object inherits from DGKernel object.

This class object inherits from the DGKernel object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of advection physics in the MOOSE framework. The only parameter for this kernel is a generic velocity vector, whose components can be set piecewise in the input file or by inheriting from this base class and manually altering the velocity vector.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 66 of file DGAdvection.h.

4.11.2 Constructor & Destructor Documentation

4.11.2.1 DGAdvection::DGAdvection (const InputParameters & parameters)

Required constructor for objects in MOOSE.

4.11.3 Member Function Documentation

4.11.3.1 virtual Real DGAdvection::computeQpJacobian (Moose::DGJacobianType type) [protected], [virtual]

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented in [DGColumnHeatAdvection](#), and [DGColumnMassAdvection](#).

4.11.3.2 virtual Real DGAdvection::computeQpResidual (Moose::DGResidualType type) [protected], [virtual]

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented in [DGColumnHeatAdvection](#), and [DGColumnMassAdvection](#).

4.11.4 Member Data Documentation

4.11.4.1 RealVectorValue DGAdvection::_velocity [protected]

Vector of velocity.

Definition at line 82 of file DGAdvection.h.

4.11.4.2 Real DGAdvection::_vx [protected]

x-component of velocity (optional - set in input file)

Definition at line 83 of file DGAdvection.h.

4.11.4.3 Real DGAdvection::_vy [protected]

y-component of velocity (optional - set in input file)

Definition at line 84 of file DGAdvection.h.

4.11.4.4 Real DGAdvection::_vz [protected]

z-component of velocity (optional - set in input file)

Definition at line 85 of file DGAdvection.h.

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

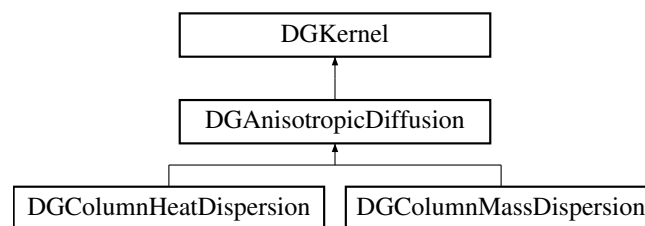
- [DGAdvection.h](#)

4.12 DGAnisotropicDiffusion Class Reference

[DGAnisotropicDiffusion](#) class object inherits from DGKernel object.

```
#include <DGAnisotropicDiffusion.h>
```

Inheritance diagram for DGAnisotropicDiffusion:



Public Member Functions

- [DGAnisotropicDiffusion](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- Real [_epsilon](#)
Penalty term for gradient jumps between the solution and test functions.
- Real [_sigma](#)
Penalty term applied to element size.
- RealTensorValue [_Diffusion](#)
Diffusion tensor matrix parameter.
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

4.12.1 Detailed Description

[DGAnisotropicDiffusion](#) class object inherits from DGKernel object.

This class object inherits from the DGKernel object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of advection physics in the MOOSE framework. The only parameter for this kernel is a diffusion tensor, whose components can be set piecewise in the input file or by inheriting from this base class and manually altering the tensor matrix.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 66 of file DGAnisotropicDiffusion.h.

4.12.2 Constructor & Destructor Documentation

4.12.2.1 DGAnisotropicDiffusion::DGAnisotropicDiffusion (const InputParameters & *parameters*)

Required constructor for objects in MOOSE.

4.12.3 Member Function Documentation

4.12.3.1 virtual Real DGAnisotropicDiffusion::computeQpJacobian (Moose::DGJacobianType *type*) [protected], [virtual]

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented in [DGColumnMassDispersion](#), and [DGColumnHeatDispersion](#).

4.12.3.2 `virtual Real DGAnisotropicDiffusion::computeQpResidual (Moose::DGResidualType type)` `[protected]`,
`[virtual]`

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented in [DGColumMassDispersion](#), and [DGColumHeatDispersion](#).

4.12.4 Member Data Documentation

4.12.4.1 `RealTensorValue DGAnisotropicDiffusion::_Diffusion` `[protected]`

Diffusion tensor matrix parameter.

Definition at line 84 of file `DGAnisotropicDiffusion.h`.

4.12.4.2 `Real DGAnisotropicDiffusion::_Dxx` `[protected]`

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.12.4.3 `Real DGAnisotropicDiffusion::_Dxy` `[protected]`

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.12.4.4 `Real DGAnisotropicDiffusion::_Dxz` `[protected]`

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.12.4.5 `Real DGAnisotropicDiffusion::_Dyx` `[protected]`

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.12.4.6 `Real DGAnisotropicDiffusion::_Dyy` `[protected]`

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.12.4.7 `Real DGAnisotropicDiffusion::_Dyz` `[protected]`

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.12.4.8 `Real DGAnisotropicDiffusion::_Dzx` `[protected]`

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.12.4.9 `Real DGAnisotropicDiffusion::_Dzy` `[protected]`

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.12.4.10 `Real DGAnisotropicDiffusion::_Dzz` `[protected]`

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.12.4.11 `Real DGAnisotropicDiffusion::_epsilon` `[protected]`

Penalty term for gradient jumps between the solution and test functions.

Definition at line 82 of file `DGAnisotropicDiffusion.h`.

4.12.4.12 `Real DGAnisotropicDiffusion::_sigma` `[protected]`

Penalty term applied to element size.

Definition at line 83 of file DGAnisotropicDiffusion.h.

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

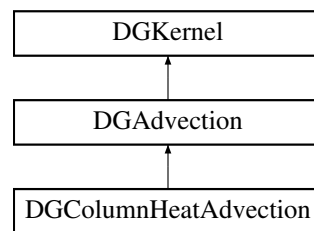
- [DGAnisotropicDiffusion.h](#)

4.13 DGColumnHeatAdvection Class Reference

[DGColumnHeatAdvection](#) class object inherits from [DGAdvection](#) object.

```
#include <DGColumnHeatAdvection.h>
```

Inheritance diagram for DGColumnHeatAdvection:



Public Member Functions

- [DGColumnHeatAdvection](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Vector of velocity.
- Real [_vx](#)
x-component of velocity (optional - set in input file)
- Real [_vy](#)
y-component of velocity (optional - set in input file)
- Real [_vz](#)
z-component of velocity (optional - set in input file)

Private Attributes

- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.
- const MaterialProperty< Real > & [_gas_density](#)
Reference to the gas density material property.
- const MaterialProperty< Real > & [_gas_heat_capacity](#)
Reference to the gas heat capacity material property.

4.13.1 Detailed Description

[DGColumnHeatAdvection](#) class object inherits from [DGAdvection](#) object.

This class object inherits from the [DGAdvection](#) object in DGOSPREY. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of the heat advection physics in a fixed-bed column. Parameters for this kernel are given as material properties and will be used to override the inherited classes velocity vector.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 64 of file [DGColumnHeatAdvection.h](#).

4.13.2 Constructor & Destructor Documentation

4.13.2.1 [DGColumnHeatAdvection::DGColumnHeatAdvection \(const InputParameters & parameters \)](#)

Required constructor for objects in MOOSE.

4.13.3 Member Function Documentation

4.13.3.1 [virtual Real DGColumnHeatAdvection::computeQpJacobian \(Moose::DGJacobianType type \)](#) [protected], [virtual]

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGAdvection](#).

4.13.3.2 [virtual Real DGColumnHeatAdvection::computeQpResidual \(Moose::DGResidualType type \)](#) [protected], [virtual]

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGAdvection](#).

4.13.4 Member Data Documentation

4.13.4.1 [const MaterialProperty<Real>& DGColumnHeatAdvection::_gas_density](#) [private]

Reference to the gas density material property.

Definition at line 82 of file [DGColumnHeatAdvection.h](#).

4.13.4.2 [const MaterialProperty<Real>& DGColumnHeatAdvection::_gas_heat_capacity](#) [private]

Reference to the gas heat capacity material property.

Definition at line 83 of file [DGColumnHeatAdvection.h](#).

4.13.4.3 [const MaterialProperty<Real>& DGColumnHeatAdvection::_vel](#) [private]

Reference to the velocity material property.

Definition at line 81 of file [DGColumnHeatAdvection.h](#).

4.13.4.4 RealVectorValue DGAdvection::_velocity [protected],[inherited]

Vector of velocity.

Definition at line 82 of file DGAdvection.h.

4.13.4.5 Real DGAdvection::_vx [protected],[inherited]

x-component of velocity (optional - set in input file)

Definition at line 83 of file DGAdvection.h.

4.13.4.6 Real DGAdvection::_vy [protected],[inherited]

y-component of velocity (optional - set in input file)

Definition at line 84 of file DGAdvection.h.

4.13.4.7 Real DGAdvection::_vz [protected],[inherited]

z-component of velocity (optional - set in input file)

Definition at line 85 of file DGAdvection.h.

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

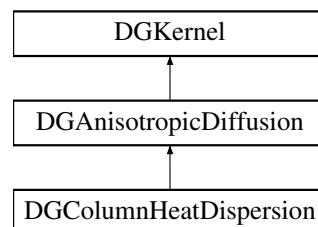
- [DGColumnHeatAdvection.h](#)

4.14 DGColumnHeatDispersion Class Reference

[DGColumnHeatDispersion](#) class object inherits from [DGAnisotropicDiffusion](#) object.

```
#include <DGColumnHeatDispersion.h>
```

Inheritance diagram for DGColumnHeatDispersion:



Public Member Functions

- [DGColumnHeatDispersion](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- Real [_epsilon](#)

Penalty term for gradient jumps between the solution and test functions.

- Real [_sigma](#)

Penalty term applied to element size.

- RealTensorValue [_Diffusion](#)

Diffusion tensor matrix parameter.

- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

Private Attributes

- const MaterialProperty< Real > & [_conductivity](#)

Reference to the thermal conductivity material property.

4.14.1 Detailed Description

[DGColumnHeatDispersion](#) class object inherits from [DGAnisotropicDiffusion](#) object.

This class object inherits from the [DGAnisotropicDiffusion](#) object in OSPREY. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of the heat dispersion physics in a fixed-bed column. Parameters for this kernel are given as material properties and will be used to override the inherited classes diffusion tensor.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 64 of file [DGColumnHeatDispersion.h](#).

4.14.2 Constructor & Destructor Documentation

4.14.2.1 [DGColumnHeatDispersion::DGColumnHeatDispersion \(const InputParameters & parameters \)](#)

Required constructor for objects in MOOSE.

4.14.3 Member Function Documentation

4.14.3.1 [virtual Real DGColumnHeatDispersion::computeQpJacobian \(Moose::DGJacobianType type \) \[protected\], \[virtual\]](#)

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGAnisotropicDiffusion](#).

4.14.3.2 `virtual Real DGColumnHeatDispersion::computeQpResidual (Moose::DGResidualType type)` [protected], [virtual]

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGAnisotropicDiffusion](#).

4.14.4 Member Data Documentation

4.14.4.1 `const MaterialProperty<Real>& DGColumnHeatDispersion::_conductivity` [private]

Reference to the thermal conductivity material property.

Definition at line 81 of file `DGColumnHeatDispersion.h`.

4.14.4.2 `RealTensorValue DGAnisotropicDiffusion::_Diffusion` [protected], [inherited]

Diffusion tensor matrix parameter.

Definition at line 84 of file `DGAnisotropicDiffusion.h`.

4.14.4.3 `Real DGAnisotropicDiffusion::_Dxx` [protected], [inherited]

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.14.4.4 `Real DGAnisotropicDiffusion::_Dxy` [protected], [inherited]

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.14.4.5 `Real DGAnisotropicDiffusion::_Dxz` [protected], [inherited]

Definition at line 86 of file `DGAnisotropicDiffusion.h`.

4.14.4.6 `Real DGAnisotropicDiffusion::_Dyx` [protected], [inherited]

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.14.4.7 `Real DGAnisotropicDiffusion::_Dyy` [protected], [inherited]

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.14.4.8 `Real DGAnisotropicDiffusion::_Dyz` [protected], [inherited]

Definition at line 87 of file `DGAnisotropicDiffusion.h`.

4.14.4.9 `Real DGAnisotropicDiffusion::_Dzx` [protected], [inherited]

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.14.4.10 `Real DGAnisotropicDiffusion::_Dzy` [protected], [inherited]

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.14.4.11 `Real DGAnisotropicDiffusion::_Dzz` [protected], [inherited]

Definition at line 88 of file `DGAnisotropicDiffusion.h`.

4.14.4.12 `Real DGAnisotropicDiffusion::_epsilon` [protected], [inherited]

Penalty term for gradient jumps between the solution and test functions.

Definition at line 82 of file DGAnisotropicDiffusion.h.

4.14.4.13 Real DGAnisotropicDiffusion::sigma [protected],[inherited]

Penalty term applied to element size.

Definition at line 83 of file DGAnisotropicDiffusion.h.

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

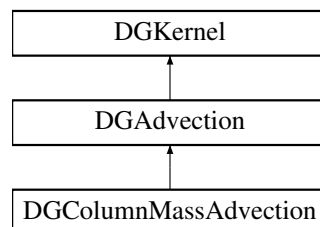
- [DGColumnHeatDispersion.h](#)

4.15 DGColumnMassAdvection Class Reference

[DGColumnMassAdvection](#) class object inherits from [DGAdvection](#) object.

```
#include <DGColumnMassAdvection.h>
```

Inheritance diagram for DGColumnMassAdvection:



Public Member Functions

- [DGColumnMassAdvection](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Vector of velocity.
- Real [_vx](#)
x-component of velocity (optional - set in input file)
- Real [_vy](#)
y-component of velocity (optional - set in input file)
- Real [_vz](#)
z-component of velocity (optional - set in input file)

Private Attributes

- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.

4.15.1 Detailed Description

[DGColumnMassAdvection](#) class object inherits from [DGAdvection](#) object.

This class object inherits from the [DGAdvection](#) object in DGOSPREY. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of the heat advection physics in a fixed-bed column. Parameters for this kernel are given as material properties and will be used to override the inherited classes velocity vector.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 63 of file [DGColumnMassAdvection.h](#).

4.15.2 Constructor & Destructor Documentation

4.15.2.1 [DGColumnMassAdvection::DGColumnMassAdvection \(const InputParameters & parameters \)](#)

Required constructor for objects in MOOSE.

4.15.3 Member Function Documentation

4.15.3.1 [virtual Real DGColumnMassAdvection::computeQpJacobian \(Moose::DGJacobianType type \)](#) [protected], [virtual]

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGAdvection](#).

4.15.3.2 [virtual Real DGColumnMassAdvection::computeQpResidual \(Moose::DGResidualType type \)](#) [protected], [virtual]

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGAdvection](#).

4.15.4 Member Data Documentation

4.15.4.1 [const MaterialProperty<Real>& DGColumnMassAdvection::_vel](#) [private]

Reference to the velocity material property.

Definition at line 80 of file [DGColumnMassAdvection.h](#).

4.15.4.2 [RealVectorValue DGAdvection::_velocity](#) [protected],[inherited]

Vector of velocity.

Definition at line 82 of file [DGAdvection.h](#).

4.15.4.3 [Real DGAdvection::_vx](#) [protected],[inherited]

x-component of velocity (optional - set in input file)

Definition at line 83 of file [DGAdvection.h](#).

4.15.4.4 Real DGAdvection::_vy [protected],[inherited]

y-component of velocity (optional - set in input file)

Definition at line 84 of file DGAdvection.h.

4.15.4.5 Real DGAdvection::_vz [protected],[inherited]

z-component of velocity (optional - set in input file)

Definition at line 85 of file DGAdvection.h.

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

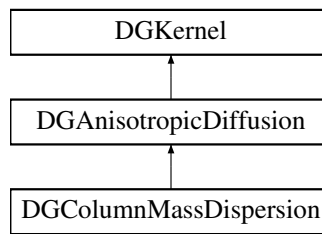
- [DGColumnMassAdvection.h](#)

4.16 DGColumnMassDispersion Class Reference

[DGColumnMassDispersion](#) class object inherits from [DGAnisotropicDiffusion](#) object.

```
#include <DGColumnMassDispersion.h>
```

Inheritance diagram for DGColumnMassDispersion:



Public Member Functions

- [DGColumnMassDispersion](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) (Moose::DGResidualType type)
Required residual function for DG kernels in MOOSE.
- virtual Real [computeQpJacobian](#) (Moose::DGJacobianType type)
Required Jacobian function for DG kernels in MOOSE.

Protected Attributes

- Real [_epsilon](#)
Penalty term for gradient jumps between the solution and test functions.
- Real [_sigma](#)
Penalty term applied to element size.
- RealTensorValue [_Diffusion](#)
Diffusion tensor matrix parameter.
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)

- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

Private Attributes

- unsigned int [_index](#)
Index of the species of interest for this kernel.
- const MaterialProperty
< std::vector< Real > > & [_dispersion](#)
Reference to the axial dispersion material property.
- const MaterialProperty
< std::vector< Real > > & [_molecular_diffusion](#)
Reference to the molecular diffusion material property.

4.16.1 Detailed Description

[DGColumnMassDispersion](#) class object inherits from [DGAnisotropicDiffusion](#) object.

This class object inherits from the [DGAnisotropicDiffusion](#) object in OSPREY. All public and protected members of this class are required function overrides. The object will provide residuals and Jacobians for the discontinuous Galerkin formulation of the mass dispersion physics in a fixed-bed column. Parameters for this kernel are given as material properties and will be used to override the inherited classes diffusion tensor.

Note

As a reminder, any DGKernel in MOOSE was be accompanied by the equivalent GKernel in order to provide the full residuals and Jacobians for the system.

Definition at line 65 of file [DGColumnMassDispersion.h](#).

4.16.2 Constructor & Destructor Documentation

4.16.2.1 [DGColumnMassDispersion::DGColumnMassDispersion \(const InputParameters & parameters \)](#)

Required constructor for objects in MOOSE.

4.16.3 Member Function Documentation

4.16.3.1 [virtual Real DGColumnMassDispersion::computeQpJacobian \(Moose::DGJacobianType type \)](#) `[protected]`, `[virtual]`

Required Jacobian function for DG kernels in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGAnisotropicDiffusion](#).

4.16.3.2 `virtual Real DGColumnMassDispersion::computeQpResidual (Moose::DGResidualType type)` `[protected]`,
`[virtual]`

Required residual function for DG kernels in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGAnisotropicDiffusion](#).

4.16.4 Member Data Documentation

4.16.4.1 `RealTensorValue DGAnisotropicDiffusion::_Diffusion` `[protected]`, `[inherited]`

Diffusion tensor matrix parameter.

Definition at line 84 of file [DGAnisotropicDiffusion.h](#).

4.16.4.2 `const MaterialProperty<std::vector<Real>>& DGColumnMassDispersion::dispersion` `[private]`

Reference to the axial dispersion material property.

Definition at line 83 of file [DGColumnMassDispersion.h](#).

4.16.4.3 `Real DGAnisotropicDiffusion::_Dxx` `[protected]`, `[inherited]`

Definition at line 86 of file [DGAnisotropicDiffusion.h](#).

4.16.4.4 `Real DGAnisotropicDiffusion::_Dxy` `[protected]`, `[inherited]`

Definition at line 86 of file [DGAnisotropicDiffusion.h](#).

4.16.4.5 `Real DGAnisotropicDiffusion::_Dxz` `[protected]`, `[inherited]`

Definition at line 86 of file [DGAnisotropicDiffusion.h](#).

4.16.4.6 `Real DGAnisotropicDiffusion::_Dyx` `[protected]`, `[inherited]`

Definition at line 87 of file [DGAnisotropicDiffusion.h](#).

4.16.4.7 `Real DGAnisotropicDiffusion::_Dyy` `[protected]`, `[inherited]`

Definition at line 87 of file [DGAnisotropicDiffusion.h](#).

4.16.4.8 `Real DGAnisotropicDiffusion::_Dyz` `[protected]`, `[inherited]`

Definition at line 87 of file [DGAnisotropicDiffusion.h](#).

4.16.4.9 `Real DGAnisotropicDiffusion::_Dzx` `[protected]`, `[inherited]`

Definition at line 88 of file [DGAnisotropicDiffusion.h](#).

4.16.4.10 `Real DGAnisotropicDiffusion::_Dzy` `[protected]`, `[inherited]`

Definition at line 88 of file [DGAnisotropicDiffusion.h](#).

4.16.4.11 `Real DGAnisotropicDiffusion::_Dzz` `[protected]`, `[inherited]`

Definition at line 88 of file [DGAnisotropicDiffusion.h](#).

4.16.4.12 `Real DGAnisotropicDiffusion::_epsilon` `[protected]`, `[inherited]`

Penalty term for gradient jumps between the solution and test functions.

Definition at line 82 of file DGAisotropicDiffusion.h.

4.16.4.13 `unsigned int DGColumnMassDispersion::_index` `[private]`

Index of the species of interest for this kernel.

Definition at line 82 of file DGColumnMassDispersion.h.

4.16.4.14 `const MaterialProperty<std::vector<Real>>& DGColumnMassDispersion::_molecular_diffusion` `[private]`

Reference to the molecular diffusion material property.

Definition at line 84 of file DGColumnMassDispersion.h.

4.16.4.15 `Real DGAisotropicDiffusion::_sigma` `[protected]`, `[inherited]`

Penalty term applied to element size.

Definition at line 83 of file DGAisotropicDiffusion.h.

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

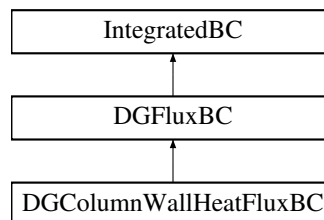
- [DGColumnMassDispersion.h](#)

4.17 DGColumnWallHeatFluxBC Class Reference

[DGColumnWallHeatFluxBC](#) class object inherits from [DGFluxBC](#) object.

```
#include <DGColumnWallHeatFluxBC.h>
```

Inheritance diagram for [DGColumnWallHeatFluxBC](#):



Public Member Functions

- [DGColumnWallHeatFluxBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)

Diffusivity tensor in the system or at the boundary.

- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)

Value of the non-linear variable at the input of the boundary.

Private Attributes

- VariableValue & [_wall_temp](#)

Reference to the coupled variable for wall temperature of the column.

- const MaterialProperty< Real > & [_bed_wall_transfer_coeff](#)

Reference to the bed-wall transfer coefficient material property.

- const MaterialProperty< Real > & [_conductivity](#)

Reference to the thermal conductivity material property.

4.17.1 Detailed Description

[DGColumnWallHeatFluxBC](#) class object inherits from [DGFluxBC](#) object.

This class object inherits from the [DGFluxBC](#) object (see [DGFluxBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxBC](#) functions.

Definition at line 62 of file [DGColumnWallHeatFluxBC.h](#).

4.17.2 Constructor & Destructor Documentation

4.17.2.1 [DGColumnWallHeatFluxBC::DGColumnWallHeatFluxBC \(const InputParameters & parameters \)](#)

Required constructor for BC objects in MOOSE.

4.17.3 Member Function Documentation

4.17.3.1 `virtual Real DGColumnWallHeatFluxBC::computeQpJacobian ()` [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxBC](#).

4.17.3.2 `virtual Real DGColumnWallHeatFluxBC::computeQpResidual ()` `[protected]`, `[virtual]`

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxBC](#).

4.17.4 Member Data Documentation

4.17.4.1 `const MaterialProperty<Real>& DGColumnWallHeatFluxBC::_bed_wall_transfer_coeff` `[private]`

Reference to the bed-wall transfer coefficient material property.

Definition at line 81 of file `DGColumnWallHeatFluxBC.h`.

4.17.4.2 `const MaterialProperty<Real>& DGColumnWallHeatFluxBC::_conductivity` `[private]`

Reference to the thermal conductivity material property.

Definition at line 82 of file `DGColumnWallHeatFluxBC.h`.

4.17.4.3 `RealTensorValue DGFluxBC::_Diffusion` `[protected]`, `[inherited]`

Diffusivity tensor in the system or at the boundary.

Definition at line 83 of file `DGFluxBC.h`.

4.17.4.4 `Real DGFluxBC::_Dxx` `[protected]`, `[inherited]`

Definition at line 89 of file `DGFluxBC.h`.

4.17.4.5 `Real DGFluxBC::_Dxy` `[protected]`, `[inherited]`

Definition at line 89 of file `DGFluxBC.h`.

4.17.4.6 `Real DGFluxBC::_Dxz` `[protected]`, `[inherited]`

Definition at line 89 of file `DGFluxBC.h`.

4.17.4.7 `Real DGFluxBC::_Dyx` `[protected]`, `[inherited]`

Definition at line 90 of file `DGFluxBC.h`.

4.17.4.8 `Real DGFluxBC::_Dyy` `[protected]`, `[inherited]`

Definition at line 90 of file `DGFluxBC.h`.

4.17.4.9 `Real DGFluxBC::_Dyz` `[protected]`, `[inherited]`

Definition at line 90 of file `DGFluxBC.h`.

4.17.4.10 `Real DGFluxBC::_Dzx` `[protected]`, `[inherited]`

Definition at line 91 of file `DGFluxBC.h`.

4.17.4.11 `Real DGFluxBC::_Dzy` `[protected]`, `[inherited]`

Definition at line 91 of file `DGFluxBC.h`.

4.17.4.12 `Real DGFluxBC::_Dzz` `[protected]`, `[inherited]`

Definition at line 91 of file `DGFluxBC.h`.

4.17.4.13 `Real DGFluxBC::_u_input` `[protected]`, `[inherited]`

Value of the non-linear variable at the input of the boundary.

Definition at line 94 of file DGFluxBC.h.

4.17.4.14 `RealVectorValue DGFluxBC::_velocity` `[protected]`, `[inherited]`

Velocity vector in the system or at the boundary.

Definition at line 80 of file DGFluxBC.h.

4.17.4.15 `Real DGFluxBC::_vx` `[protected]`, `[inherited]`

Definition at line 85 of file DGFluxBC.h.

4.17.4.16 `Real DGFluxBC::_vy` `[protected]`, `[inherited]`

Definition at line 86 of file DGFluxBC.h.

4.17.4.17 `Real DGFluxBC::_vz` `[protected]`, `[inherited]`

Definition at line 87 of file DGFluxBC.h.

4.17.4.18 `VariableValue& DGColumnWallHeatFluxBC::_wall_temp` `[private]`

Reference to the coupled variable for wall temperature of the column.

Definition at line 80 of file DGColumnWallHeatFluxBC.h.

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

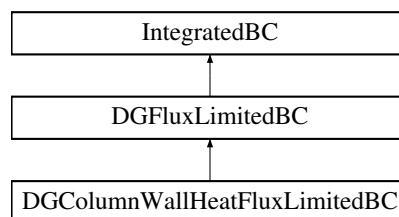
- [DGColumnWallHeatFluxBC.h](#)

4.18 DGColumnWallHeatFluxLimitedBC Class Reference

[DGColumnWallHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

```
#include <DGColumnWallHeatFluxLimitedBC.h>
```

Inheritance diagram for [DGColumnWallHeatFluxLimitedBC](#):



Public Member Functions

- [DGColumnWallHeatFluxLimitedBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.

- virtual Real [computeQpJacobian](#) ()

Required function override for BC objects in MOOSE.

Protected Attributes

- Real [_epsilon](#)
Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.
- Real [_sigma](#)
Penalty term based on the size of the element at the boundary.
- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

Private Attributes

- VariableValue & [_wall_temp](#)
Reference to the coupled variable for wall temperature of the column.
- const MaterialProperty< Real > & [_bed_wall_transfer_coeff](#)
Reference to the bed-wall transfer coefficient material property.
- const MaterialProperty< Real > & [_conductivity](#)
Reference to the thermal conductivity material property.

4.18.1 Detailed Description

[DGColumnWallHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

This class object inherits from the [DGFluxLimitedBC](#) object (see [DGFluxLimitedBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxLimitedBC](#) functions.

Definition at line 55 of file [DGColumnWallHeatFluxLimitedBC.h](#).

4.18.2 Constructor & Destructor Documentation

4.18.2.1 [DGColumnWallHeatFluxLimitedBC::DGColumnWallHeatFluxLimitedBC](#) (const InputParameters & *parameters*)

Required constructor for BC objects in MOOSE.

4.18.3 Member Function Documentation

4.18.3.1 virtual Real DGColumnWallHeatFluxLimitedBC::computeQpJacobian () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxLimitedBC](#).

4.18.3.2 virtual Real DGColumnWallHeatFluxLimitedBC::computeQpResidual () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxLimitedBC](#).

4.18.4 Member Data Documentation

4.18.4.1 const MaterialProperty<Real>& DGColumnWallHeatFluxLimitedBC::bed_wall_transfer_coeff [private]

Reference to the bed-wall transfer coefficient material property.

Definition at line 74 of file DGColumnWallHeatFluxLimitedBC.h.

4.18.4.2 const MaterialProperty<Real>& DGColumnWallHeatFluxLimitedBC::conductivity [private]

Reference to the thermal conductivity material property.

Definition at line 75 of file DGColumnWallHeatFluxLimitedBC.h.

4.18.4.3 RealTensorValue DGFluxLimitedBC::_Diffusion [protected], [inherited]

Diffusivity tensor in the system or at the boundary.

Definition at line 79 of file DGFluxLimitedBC.h.

4.18.4.4 Real DGFluxLimitedBC::_Dxx [protected], [inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.18.4.5 Real DGFluxLimitedBC::_Dxy [protected], [inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.18.4.6 Real DGFluxLimitedBC::_Dxz [protected], [inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.18.4.7 Real DGFluxLimitedBC::_Dyx [protected], [inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.18.4.8 Real DGFluxLimitedBC::_Dyy [protected], [inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.18.4.9 Real DGFluxLimitedBC::_Dyz [protected], [inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.18.4.10 `Real DGFluxLimitedBC::_Dzx` [protected],[inherited]

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.18.4.11 `Real DGFluxLimitedBC::_Dzy` [protected],[inherited]

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.18.4.12 `Real DGFluxLimitedBC::_Dzz` [protected],[inherited]

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.18.4.13 `Real DGFluxLimitedBC::_epsilon` [protected],[inherited]

Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.

Definition at line 72 of file `DGFluxLimitedBC.h`.

4.18.4.14 `Real DGFluxLimitedBC::_sigma` [protected],[inherited]

Penalty term based on the size of the element at the boundary.

Definition at line 74 of file `DGFluxLimitedBC.h`.

4.18.4.15 `Real DGFluxLimitedBC::_u_input` [protected],[inherited]

Value of the non-linear variable at the input of the boundary.

Definition at line 90 of file `DGFluxLimitedBC.h`.

4.18.4.16 `RealVectorValue DGFluxLimitedBC::_velocity` [protected],[inherited]

Velocity vector in the system or at the boundary.

Definition at line 77 of file `DGFluxLimitedBC.h`.

4.18.4.17 `Real DGFluxLimitedBC::_vx` [protected],[inherited]

Definition at line 81 of file `DGFluxLimitedBC.h`.

4.18.4.18 `Real DGFluxLimitedBC::_vy` [protected],[inherited]

Definition at line 82 of file `DGFluxLimitedBC.h`.

4.18.4.19 `Real DGFluxLimitedBC::_vz` [protected],[inherited]

Definition at line 83 of file `DGFluxLimitedBC.h`.

4.18.4.20 `VariableValue& DGColumnWallHeatFluxLimitedBC::_wall_temp` [private]

Reference to the coupled variable for wall temperature of the column.

Definition at line 73 of file `DGColumnWallHeatFluxLimitedBC.h`.

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

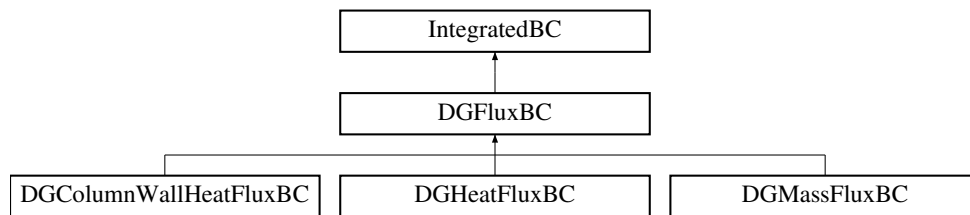
- [DGColumnWallHeatFluxLimitedBC.h](#)

4.19 DGFluxBC Class Reference

[DGFluxBC](#) class object inherits from `IntegratedBC` object.

```
#include <DGFluxBC.h>
```

Inheritance diagram for `DGFluxBC`:



Public Member Functions

- [DGFluxBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

4.19.1 Detailed Description

[DGFluxBC](#) class object inherits from IntegratedBC object.

This class object inherits from the IntegratedBC object. All public and protected members of this class are required function overrides. The flux BC uses the velocity and diffusivity in the system to apply a boundary condition based on whether or not material is leaving or entering the boundary.

Definition at line 63 of file DGFluxBC.h.

4.19.2 Constructor & Destructor Documentation

4.19.2.1 DGFluxBC::DGFluxBC (const InputParameters & *parameters*)

Required constructor for BC objects in MOOSE.

4.19.3 Member Function Documentation

4.19.3.1 virtual Real DGFluxBC::computeQpJacobian () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented in [DGColumnWallHeatFluxBC](#), [DGHeatFluxBC](#), and [DGMassFluxBC](#).

4.19.3.2 virtual Real DGFluxBC::computeQpResidual () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented in [DGColumnWallHeatFluxBC](#), [DGHeatFluxBC](#), and [DGMassFluxBC](#).

4.19.4 Member Data Documentation

4.19.4.1 RealTensorValue DGFluxBC::_Diffusion [protected]

Diffusivity tensor in the system or at the boundary.

Definition at line 83 of file DGFluxBC.h.

4.19.4.2 Real DGFluxBC::_Dxx [protected]

Definition at line 89 of file DGFluxBC.h.

4.19.4.3 Real DGFluxBC::_Dxy [protected]

Definition at line 89 of file DGFluxBC.h.

4.19.4.4 Real DGFluxBC::_Dxz [protected]

Definition at line 89 of file DGFluxBC.h.

4.19.4.5 Real DGFluxBC::_Dyx [protected]

Definition at line 90 of file DGFluxBC.h.

4.19.4.6 Real DGFluxBC::_Dyy [protected]

Definition at line 90 of file DGFluxBC.h.

4.19.4.7 Real DGFluxBC::_Dyz [protected]

Definition at line 90 of file DGFluxBC.h.

4.19.4.8 Real DGFluxBC::_Dzx [protected]

Definition at line 91 of file DGFluxBC.h.

4.19.4.9 Real DGFluxBC::_Dzy [protected]

Definition at line 91 of file DGFluxBC.h.

4.19.4.10 Real DGFluxBC::_Dzz [protected]

Definition at line 91 of file DGFluxBC.h.

4.19.4.11 Real DGFluxBC::_u.input [protected]

Value of the non-linear variable at the input of the boundary.

Definition at line 94 of file DGFluxBC.h.

4.19.4.12 RealVectorValue DGFluxBC::_velocity [protected]

Velocity vector in the system or at the boundary.

Definition at line 80 of file DGFluxBC.h.

4.19.4.13 Real DGFluxBC::_vx [protected]

Definition at line 85 of file DGFluxBC.h.

4.19.4.14 Real DGFluxBC::_vy [protected]

Definition at line 86 of file DGFluxBC.h.

4.19.4.15 Real DGFluxBC::_vz [protected]

Definition at line 87 of file DGFluxBC.h.

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

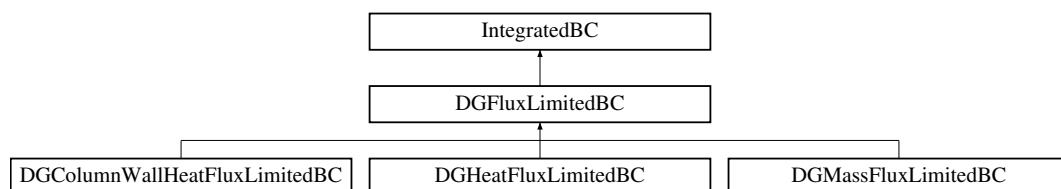
- [DGFluxBC.h](#)

4.20 DGFluxLimitedBC Class Reference

[DGFluxLimitedBC](#) class object inherits from IntegratedBC object.

```
#include <DGFluxLimitedBC.h>
```

Inheritance diagram for DGFluxLimitedBC:



Public Member Functions

- [DGFluxLimitedBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()

Required function override for BC objects in MOOSE.

- virtual Real [computeQpJacobian](#) ()

Required function override for BC objects in MOOSE.

Protected Attributes

- Real [_epsilon](#)

Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.

- Real [_sigma](#)

Penalty term based on the size of the element at the boundary.

- RealVectorValue [_velocity](#)

Velocity vector in the system or at the boundary.

- RealTensorValue [_Diffusion](#)

Diffusivity tensor in the system or at the boundary.

- Real [_vx](#)

- Real [_vy](#)

- Real [_vz](#)

- Real [_Dxx](#)

- Real [_Dxy](#)

- Real [_Dxz](#)

- Real [_Dyx](#)

- Real [_Dyy](#)

- Real [_Dyz](#)

- Real [_Dzx](#)

- Real [_Dzy](#)

- Real [_Dzz](#)

- Real [_u_input](#)

Value of the non-linear variable at the input of the boundary.

4.20.1 Detailed Description

[DGFluxLimitedBC](#) class object inherits from [IntegratedBC](#) object.

This class object inherits from the [IntegratedBC](#) object. All public and protected members of this class are required function overrides.

Definition at line 55 of file [DGFluxLimitedBC.h](#).

4.20.2 Constructor & Destructor Documentation

4.20.2.1 [DGFluxLimitedBC::DGFluxLimitedBC](#) (const [InputParameters](#) & *parameters*)

Required constructor for BC objects in MOOSE.

4.20.3 Member Function Documentation

4.20.3.1 virtual Real [DGFluxLimitedBC::computeQpJacobian](#) () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented in [DGColumnWallHeatFluxLimitedBC](#), [DGHeatFluxLimitedBC](#), and [DGMassFluxLimitedBC](#).

4.20.3.2 `virtual Real DGFluxLimitedBC::computeQpResidual () [protected], [virtual]`

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented in [DGColumnWallHeatFluxLimitedBC](#), [DGHeatFluxLimitedBC](#), and [DGMassFluxLimitedBC](#).

4.20.4 Member Data Documentation

4.20.4.1 `RealTensorValue DGFluxLimitedBC::_Diffusion [protected]`

Diffusivity tensor in the system or at the boundary.

Definition at line 79 of file `DGFluxLimitedBC.h`.

4.20.4.2 `Real DGFluxLimitedBC::_Dxx [protected]`

Definition at line 85 of file `DGFluxLimitedBC.h`.

4.20.4.3 `Real DGFluxLimitedBC::_Dxy [protected]`

Definition at line 85 of file `DGFluxLimitedBC.h`.

4.20.4.4 `Real DGFluxLimitedBC::_Dxz [protected]`

Definition at line 85 of file `DGFluxLimitedBC.h`.

4.20.4.5 `Real DGFluxLimitedBC::_Dyx [protected]`

Definition at line 86 of file `DGFluxLimitedBC.h`.

4.20.4.6 `Real DGFluxLimitedBC::_Dyy [protected]`

Definition at line 86 of file `DGFluxLimitedBC.h`.

4.20.4.7 `Real DGFluxLimitedBC::_Dyz [protected]`

Definition at line 86 of file `DGFluxLimitedBC.h`.

4.20.4.8 `Real DGFluxLimitedBC::_Dzx [protected]`

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.20.4.9 `Real DGFluxLimitedBC::_Dzy [protected]`

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.20.4.10 `Real DGFluxLimitedBC::_Dzz [protected]`

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.20.4.11 `Real DGFluxLimitedBC::_epsilon [protected]`

Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.

Definition at line 72 of file `DGFluxLimitedBC.h`.

4.20.4.12 `Real DGFluxLimitedBC::_sigma [protected]`

Penalty term based on the size of the element at the boundary.

Definition at line 74 of file `DGFluxLimitedBC.h`.

4.20.4.13 Real DGFluxLimitedBC::_u_input [protected]

Value of the non-linear variable at the input of the boundary.

Definition at line 90 of file DGFluxLimitedBC.h.

4.20.4.14 RealVectorValue DGFluxLimitedBC::_velocity [protected]

Velocity vector in the system or at the boundary.

Definition at line 77 of file DGFluxLimitedBC.h.

4.20.4.15 Real DGFluxLimitedBC::_vx [protected]

Definition at line 81 of file DGFluxLimitedBC.h.

4.20.4.16 Real DGFluxLimitedBC::_vy [protected]

Definition at line 82 of file DGFluxLimitedBC.h.

4.20.4.17 Real DGFluxLimitedBC::_vz [protected]

Definition at line 83 of file DGFluxLimitedBC.h.

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

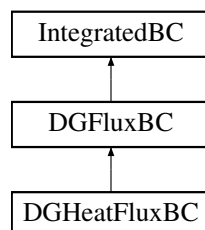
- [DGFluxLimitedBC.h](#)

4.21 DGHeatFluxBC Class Reference

DGHeatFluxBC class object inherits from DGFluxBC object.

```
#include <DGHeatFluxBC.h>
```

Inheritance diagram for DGHeatFluxBC:



Public Member Functions

- [DGHeatFluxBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

Private Attributes

- Real [_input_temperature](#)
Value of the column temperature at the inlet of the system.
- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.
- const MaterialProperty< Real > & [_gas_density](#)
Reference to the gas density material property.
- const MaterialProperty< Real > & [_gas_heat_capacity](#)
Reference to the gas heat capacity material property.
- const MaterialProperty< Real > & [_conductivity](#)
Reference to the thermal conductivity material property.

4.21.1 Detailed Description

[DGHeatFluxBC](#) class object inherits from [DGFluxBC](#) object.

This class object inherits from the [DGFluxBC](#) object (see [DGFluxBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxBC](#) functions.

Definition at line 62 of file [DGHeatFluxBC.h](#).

4.21.2 Constructor & Destructor Documentation

4.21.2.1 [DGHeatFluxBC::DGHeatFluxBC](#) (const InputParameters & *parameters*)

Required constructor for BC objects in MOOSE.

4.21.3 Member Function Documentation

4.21.3.1 virtual Real DGHeatFluxBC::computeQpJacobian () [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxBC](#).

4.21.3.2 virtual Real DGHeatFluxBC::computeQpResidual () [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxBC](#).

4.21.4 Member Data Documentation

4.21.4.1 const MaterialProperty<Real>& DGHeatFluxBC::_conductivity [private]

Reference to the thermal conductivity material property.

Definition at line 85 of file DGHeatFluxBC.h.

4.21.4.2 RealTensorValue DGFluxBC::_Diffusion [protected],[inherited]

Diffusivity tensor in the system or at the boundary.

Definition at line 83 of file DGFluxBC.h.

4.21.4.3 Real DGFluxBC::_Dxx [protected],[inherited]

Definition at line 89 of file DGFluxBC.h.

4.21.4.4 Real DGFluxBC::_Dxy [protected],[inherited]

Definition at line 89 of file DGFluxBC.h.

4.21.4.5 Real DGFluxBC::_Dxz [protected],[inherited]

Definition at line 89 of file DGFluxBC.h.

4.21.4.6 Real DGFluxBC::_Dyx [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.21.4.7 Real DGFluxBC::_Dyy [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.21.4.8 Real DGFluxBC::_Dyz [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.21.4.9 Real DGFluxBC::_Dzx [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.21.4.10 Real DGFluxBC::_Dzy [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.21.4.11 `Real DGFluxBC::_Dzz` [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.21.4.12 `const MaterialProperty<Real>& DGHeatFluxBC::_gas_density` [private]

Reference to the gas density material property.

Definition at line 83 of file DGHeatFluxBC.h.

4.21.4.13 `const MaterialProperty<Real>& DGHeatFluxBC::_gas_heat_capacity` [private]

Reference to the gas heat capacity material property.

Definition at line 84 of file DGHeatFluxBC.h.

4.21.4.14 `Real DGHeatFluxBC::_input_temperature` [private]

Value of the column temperature at the inlet of the system.

Definition at line 80 of file DGHeatFluxBC.h.

4.21.4.15 `Real DGFluxBC::_u_input` [protected],[inherited]

Value of the non-linear variable at the input of the boundary.

Definition at line 94 of file DGFluxBC.h.

4.21.4.16 `const MaterialProperty<Real>& DGHeatFluxBC::_vel` [private]

Reference to the velocity material property.

Definition at line 82 of file DGHeatFluxBC.h.

4.21.4.17 `RealVectorValue DGFluxBC::_velocity` [protected],[inherited]

Velocity vector in the system or at the boundary.

Definition at line 80 of file DGFluxBC.h.

4.21.4.18 `Real DGFluxBC::_vx` [protected],[inherited]

Definition at line 85 of file DGFluxBC.h.

4.21.4.19 `Real DGFluxBC::_vy` [protected],[inherited]

Definition at line 86 of file DGFluxBC.h.

4.21.4.20 `Real DGFluxBC::_vz` [protected],[inherited]

Definition at line 87 of file DGFluxBC.h.

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

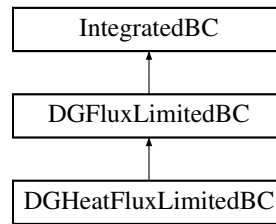
- [DGHeatFluxBC.h](#)

4.22 DGHeatFluxLimitedBC Class Reference

[DGHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

```
#include <DGHeatFluxLimitedBC.h>
```

Inheritance diagram for DGHeatFluxLimitedBC:



Public Member Functions

- [DGHeatFluxLimitedBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- Real [_epsilon](#)
Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.
- Real [_sigma](#)
Penalty term based on the size of the element at the boundary.
- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

Private Attributes

- Real [_input_temperature](#)
Value of the column temperature at the inlet of the system.
- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.
- const MaterialProperty< Real > & [_gas_density](#)
Reference to the gas density material property.
- const MaterialProperty< Real > & [_gas_heat_capacity](#)
Reference to the gas heat capacity material property.
- const MaterialProperty< Real > & [_conductivity](#)
Reference to the thermal conductivity material property.

4.22.1 Detailed Description

[DGHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

This class object inherits from the [DGFluxLimitedBC](#) object (see [DGFluxLimitedBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxLimitedBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxLimitedBC](#) functions.

Definition at line 55 of file [DGHeatFluxLimitedBC.h](#).

4.22.2 Constructor & Destructor Documentation

4.22.2.1 [DGHeatFluxLimitedBC::DGHeatFluxLimitedBC \(const InputParameters & parameters \)](#)

Required constructor for BC objects in MOOSE.

4.22.3 Member Function Documentation

4.22.3.1 [virtual Real DGHeatFluxLimitedBC::computeQpJacobian \(\)](#) [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxLimitedBC](#).

4.22.3.2 [virtual Real DGHeatFluxLimitedBC::computeQpResidual \(\)](#) [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxLimitedBC](#).

4.22.4 Member Data Documentation

4.22.4.1 [const MaterialProperty<Real>& DGHeatFluxLimitedBC::_conductivity](#) [private]

Reference to the thermal conductivity material property.

Definition at line 78 of file [DGHeatFluxLimitedBC.h](#).

4.22.4.2 RealTensorValue DGFluxLimitedBC::_Diffusion [protected],[inherited]

Diffusivity tensor in the system or at the boundary.

Definition at line 79 of file DGFluxLimitedBC.h.

4.22.4.3 Real DGFluxLimitedBC::_Dxx [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.22.4.4 Real DGFluxLimitedBC::_Dxy [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.22.4.5 Real DGFluxLimitedBC::_Dxz [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.22.4.6 Real DGFluxLimitedBC::_Dyx [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.22.4.7 Real DGFluxLimitedBC::_Dyy [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.22.4.8 Real DGFluxLimitedBC::_Dyz [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.22.4.9 Real DGFluxLimitedBC::_Dzx [protected],[inherited]

Definition at line 87 of file DGFluxLimitedBC.h.

4.22.4.10 Real DGFluxLimitedBC::_Dzy [protected],[inherited]

Definition at line 87 of file DGFluxLimitedBC.h.

4.22.4.11 Real DGFluxLimitedBC::_Dzz [protected],[inherited]

Definition at line 87 of file DGFluxLimitedBC.h.

4.22.4.12 Real DGFluxLimitedBC::_epsilon [protected],[inherited]

Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.

Definition at line 72 of file DGFluxLimitedBC.h.

4.22.4.13 const MaterialProperty<Real>& DGHeatFluxLimitedBC::_gas_density [private]

Reference to the gas density material property.

Definition at line 76 of file DGHeatFluxLimitedBC.h.

4.22.4.14 const MaterialProperty<Real>& DGHeatFluxLimitedBC::_gas_heat_capacity [private]

Reference to the gas heat capacity material property.

Definition at line 77 of file DGHeatFluxLimitedBC.h.

4.22.4.15 Real DGHeatFluxLimitedBC::_input_temperature [private]

Value of the column temperature at the inlet of the system.

Definition at line 73 of file DGHeatFluxLimitedBC.h.

4.22.4.16 `Real DGFluxLimitedBC::_sigma` `[protected]`, `[inherited]`

Penalty term based on the size of the element at the boundary.

Definition at line 74 of file DGFluxLimitedBC.h.

4.22.4.17 `Real DGFluxLimitedBC::_u_input` `[protected]`, `[inherited]`

Value of the non-linear variable at the input of the boundary.

Definition at line 90 of file DGFluxLimitedBC.h.

4.22.4.18 `const MaterialProperty<Real>& DGHeatFluxLimitedBC::_vel` `[private]`

Reference to the velocity material property.

Definition at line 75 of file DGHeatFluxLimitedBC.h.

4.22.4.19 `RealVectorValue DGFluxLimitedBC::_velocity` `[protected]`, `[inherited]`

Velocity vector in the system or at the boundary.

Definition at line 77 of file DGFluxLimitedBC.h.

4.22.4.20 `Real DGFluxLimitedBC::_vx` `[protected]`, `[inherited]`

Definition at line 81 of file DGFluxLimitedBC.h.

4.22.4.21 `Real DGFluxLimitedBC::_vy` `[protected]`, `[inherited]`

Definition at line 82 of file DGFluxLimitedBC.h.

4.22.4.22 `Real DGFluxLimitedBC::_vz` `[protected]`, `[inherited]`

Definition at line 83 of file DGFluxLimitedBC.h.

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

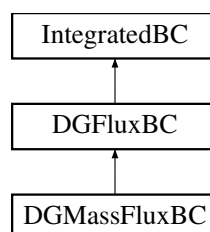
- [DGHeatFluxLimitedBC.h](#)

4.23 DGMassFluxBC Class Reference

[DGMassFluxBC](#) class object inherits from [DGFluxBC](#) object.

```
#include <DGMassFluxBC.h>
```

Inheritance diagram for DGMassFluxBC:



Public Member Functions

- [DGMassFluxBC](#) (const InputParameters ¶meters)

Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

Private Attributes

- Real [_input_temperature](#)
Value of the column temperature at the inlet of the system.
- Real [_input_pressure](#)
Value of the column total pressure at the inlet of the system.
- Real [_input_molefraction](#)
Value of the molefraction of the specific species at the inlet of the system.
- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.
- unsigned int [_index](#)
Index of the species of interest at the boundary.
- const MaterialProperty
< std::vector< Real > > & [_dispersion](#)
Reference to the dispersion coefficient material property.
- const MaterialProperty
< std::vector< Real > > & [_molecular_diffusion](#)
Reference to the molecular diffusion material property.

4.23.1 Detailed Description

[DGMassFluxBC](#) class object inherits from [DGFluxBC](#) object.

This class object inherits from the [DGFluxBC](#) object (see [DGFluxBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxBC](#) functions.

Definition at line 62 of file [DGMassFluxBC.h](#).

4.23.2 Constructor & Destructor Documentation

4.23.2.1 [DGMassFluxBC::DGMassFluxBC](#) (const [InputParameters](#) & *parameters*)

Required constructor for BC objects in MOOSE.

4.23.3 Member Function Documentation

4.23.3.1 virtual Real [DGMassFluxBC::computeQpJacobian](#) () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxBC](#).

4.23.3.2 virtual Real [DGMassFluxBC::computeQpResidual](#) () [protected], [virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxBC](#).

4.23.4 Member Data Documentation

4.23.4.1 RealTensorValue [DGFluxBC::Diffusion](#) [protected], [inherited]

Diffusivity tensor in the system or at the boundary.

Definition at line 83 of file [DGFluxBC.h](#).

4.23.4.2 const MaterialProperty<std::vector<Real>> & [DGMassFluxBC::dispersion](#) [private]

Reference to the dispersion coefficient material property.

Definition at line 88 of file [DGMassFluxBC.h](#).

4.23.4.3 Real [DGFluxBC::Dxx](#) [protected], [inherited]

Definition at line 89 of file [DGFluxBC.h](#).

4.23.4.4 Real [DGFluxBC::Dxy](#) [protected], [inherited]

Definition at line 89 of file [DGFluxBC.h](#).

4.23.4.5 Real [DGFluxBC::Dxz](#) [protected], [inherited]

Definition at line 89 of file [DGFluxBC.h](#).

4.23.4.6 **Real DGFluxBC::_Dyx** [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.23.4.7 **Real DGFluxBC::_Dyy** [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.23.4.8 **Real DGFluxBC::_Dyz** [protected],[inherited]

Definition at line 90 of file DGFluxBC.h.

4.23.4.9 **Real DGFluxBC::_Dzx** [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.23.4.10 **Real DGFluxBC::_Dzy** [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.23.4.11 **Real DGFluxBC::_Dzz** [protected],[inherited]

Definition at line 91 of file DGFluxBC.h.

4.23.4.12 **unsigned int DGMassFluxBC::_index** [private]

Index of the species of interest at the boundary.

Definition at line 87 of file DGMassFluxBC.h.

4.23.4.13 **Real DGMassFluxBC::_input_molefraction** [private]

Value of the molefraction of the specific species at the inlet of the system.

Definition at line 84 of file DGMassFluxBC.h.

4.23.4.14 **Real DGMassFluxBC::_input_pressure** [private]

Value of the column total pressure at the inlet of the system.

Definition at line 82 of file DGMassFluxBC.h.

4.23.4.15 **Real DGMassFluxBC::_input_temperature** [private]

Value of the column temperature at the inlet of the system.

Definition at line 80 of file DGMassFluxBC.h.

4.23.4.16 **const MaterialProperty<std::vector<Real>>& DGMassFluxBC::_molecular_diffusion** [private]

Reference to the molecular diffusion material property.

Definition at line 89 of file DGMassFluxBC.h.

4.23.4.17 **Real DGFluxBC::_u_input** [protected],[inherited]

Value of the non-linear variable at the input of the boundary.

Definition at line 94 of file DGFluxBC.h.

4.23.4.18 **const MaterialProperty<Real>& DGMassFluxBC::_vel** [private]

Reference to the velocity material property.

Definition at line 86 of file DGMassFluxBC.h.

4.23.4.19 RealVectorValue DGFluxBC::_velocity [protected], [inherited]

Velocity vector in the system or at the boundary.

Definition at line 80 of file DGFluxBC.h.

4.23.4.20 Real DGFluxBC::_vx [protected], [inherited]

Definition at line 85 of file DGFluxBC.h.

4.23.4.21 Real DGFluxBC::_vy [protected], [inherited]

Definition at line 86 of file DGFluxBC.h.

4.23.4.22 Real DGFluxBC::_vz [protected], [inherited]

Definition at line 87 of file DGFluxBC.h.

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

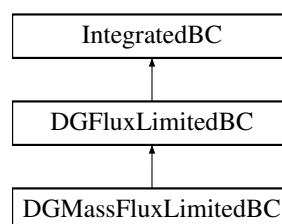
- [DGMassFluxBC.h](#)

4.24 DGMassFluxLimitedBC Class Reference

[DGMassFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

```
#include <DGMassFluxLimitedBC.h>
```

Inheritance diagram for DGMassFluxLimitedBC:



Public Member Functions

- [DGMassFluxLimitedBC](#) (const InputParameters ¶meters)
Required constructor for BC objects in MOOSE.

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
Required function override for BC objects in MOOSE.
- virtual Real [computeQpJacobian](#) ()
Required function override for BC objects in MOOSE.

Protected Attributes

- Real [_epsilon](#)
Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.
- Real [_sigma](#)
Penalty term based on the size of the element at the boundary.

- RealVectorValue [_velocity](#)
Velocity vector in the system or at the boundary.
- RealTensorValue [_Diffusion](#)
Diffusivity tensor in the system or at the boundary.
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)
- Real [_u_input](#)
Value of the non-linear variable at the input of the boundary.

Private Attributes

- Real [_input_temperature](#)
Value of the column temperature at the inlet of the system.
- Real [_input_pressure](#)
Value of the column total pressure at the inlet of the system.
- Real [_input_molefraction](#)
Value of the molefraction of the specific species at the inlet of the system.
- const MaterialProperty< Real > & [_vel](#)
Reference to the velocity material property.
- unsigned int [_index](#)
Index of the species of interest at the boundary.
- const MaterialProperty
< std::vector< Real > > & [_dispersion](#)
Reference to the dispersion coefficient material property.
- const MaterialProperty
< std::vector< Real > > & [_molecular_diffusion](#)
Reference to the molecular diffusion material property.

4.24.1 Detailed Description

[DGMassFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

This class object inherits from the [DGFluxLimitedBC](#) object (see [DGFluxLimitedBC.h](#) for more details). All public and protected members of this class are required function overrides. The object will take in the given variable and material properties to override some objects declared for the generic [DGFluxLimitedBC](#) to fit this particular boundary condition. Then, it just calls the appropriate [DGFluxLimitedBC](#) functions.

Definition at line 55 of file [DGMassFluxLimitedBC.h](#).

4.24.2 Constructor & Destructor Documentation

4.24.2.1 [DGMassFluxLimitedBC::DGMassFluxLimitedBC](#) (const InputParameters & *parameters*)

Required constructor for BC objects in MOOSE.

4.24.3 Member Function Documentation

4.24.3.1 virtual Real DGMassFluxLimitedBC::computeQpJacobian () [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a Jacobian contribution for this object. The Jacobian being computed is the associated diagonal element in the overall Jacobian matrix for the system and is used in preconditioning of the linear sub-problem.

Reimplemented from [DGFluxLimitedBC](#).

4.24.3.2 virtual Real DGMassFluxLimitedBC::computeQpResidual () [protected],[virtual]

Required function override for BC objects in MOOSE.

This function returns a residual contribution for this object.

Reimplemented from [DGFluxLimitedBC](#).

4.24.4 Member Data Documentation

4.24.4.1 RealTensorValue DGFluxLimitedBC::_Diffusion [protected],[inherited]

Diffusivity tensor in the system or at the boundary.

Definition at line 79 of file DGFluxLimitedBC.h.

4.24.4.2 const MaterialProperty<std::vector<Real> >& DGMassFluxLimitedBC::_dispersion [private]

Reference to the dispersion coefficient material property.

Definition at line 81 of file DGMassFluxLimitedBC.h.

4.24.4.3 Real DGFluxLimitedBC::_Dxx [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.24.4.4 Real DGFluxLimitedBC::_Dxy [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.24.4.5 Real DGFluxLimitedBC::_Dxz [protected],[inherited]

Definition at line 85 of file DGFluxLimitedBC.h.

4.24.4.6 Real DGFluxLimitedBC::_Dyx [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.24.4.7 Real DGFluxLimitedBC::_Dyy [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.24.4.8 Real DGFluxLimitedBC::_Dyz [protected],[inherited]

Definition at line 86 of file DGFluxLimitedBC.h.

4.24.4.9 Real DGFluxLimitedBC::_Dzx [protected],[inherited]

Definition at line 87 of file DGFluxLimitedBC.h.

4.24.4.10 Real DGFluxLimitedBC::_Dzy [protected],[inherited]

Definition at line 87 of file DGFluxLimitedBC.h.

4.24.4.11 `Real DGFluxLimitedBC::_Dzz` `[protected]`, `[inherited]`

Definition at line 87 of file `DGFluxLimitedBC.h`.

4.24.4.12 `Real DGFluxLimitedBC::_epsilon` `[protected]`, `[inherited]`

Penalty term applied to the difference between the solution at the inlet and the value it is supposed to be.

Definition at line 72 of file `DGFluxLimitedBC.h`.

4.24.4.13 `unsigned int DGMassFluxLimitedBC::_index` `[private]`

Index of the species of interest at the boundary.

Definition at line 80 of file `DGMassFluxLimitedBC.h`.

4.24.4.14 `Real DGMassFluxLimitedBC::_input_molefraction` `[private]`

Value of the molefraction of the specific species at the inlet of the system.

Definition at line 77 of file `DGMassFluxLimitedBC.h`.

4.24.4.15 `Real DGMassFluxLimitedBC::_input_pressure` `[private]`

Value of the column total pressure at the inlet of the system.

Definition at line 75 of file `DGMassFluxLimitedBC.h`.

4.24.4.16 `Real DGMassFluxLimitedBC::_input_temperature` `[private]`

Value of the column temperature at the inlet of the system.

Definition at line 73 of file `DGMassFluxLimitedBC.h`.

4.24.4.17 `const MaterialProperty<std::vector<Real>>& DGMassFluxLimitedBC::_molecular_diffusion` `[private]`

Reference to the molecular diffusion material property.

Definition at line 82 of file `DGMassFluxLimitedBC.h`.

4.24.4.18 `Real DGFluxLimitedBC::_sigma` `[protected]`, `[inherited]`

Penalty term based on the size of the element at the boundary.

Definition at line 74 of file `DGFluxLimitedBC.h`.

4.24.4.19 `Real DGFluxLimitedBC::_u_input` `[protected]`, `[inherited]`

Value of the non-linear variable at the input of the boundary.

Definition at line 90 of file `DGFluxLimitedBC.h`.

4.24.4.20 `const MaterialProperty<Real>& DGMassFluxLimitedBC::_vel` `[private]`

Reference to the velocity material property.

Definition at line 79 of file `DGMassFluxLimitedBC.h`.

4.24.4.21 `RealVectorValue DGFluxLimitedBC::_velocity` `[protected]`, `[inherited]`

Velocity vector in the system or at the boundary.

Definition at line 77 of file `DGFluxLimitedBC.h`.

4.24.4.22 `Real DGFluxLimitedBC::_vx` `[protected]`, `[inherited]`

Definition at line 81 of file `DGFluxLimitedBC.h`.

4.24.4.23 Real DGFluxLimitedBC::vy [protected], [inherited]

Definition at line 82 of file DGFluxLimitedBC.h.

4.24.4.24 Real DGFluxLimitedBC::vz [protected], [inherited]

Definition at line 83 of file DGFluxLimitedBC.h.

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

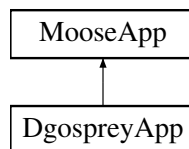
- [DGMassFluxLimitedBC.h](#)

4.25 DgospreyApp Class Reference

[DgospreyApp](#) inherits from the MooseApp object.

```
#include <DgospreyApp.h>
```

Inheritance diagram for DgospreyApp:



Public Member Functions

- [DgospreyApp](#) (InputParameters parameters)
DgospreyApp constructor (required)
- virtual [~DgospreyApp](#) ()
DgospreyApp destructor (required)

Static Public Member Functions

- static void [registerApps](#) ()
Function to the DgospreyApp into MOOSE (required)
- static void [registerObjects](#) (Factory &factory)
Function to register kernels/objects created in DGOSPNEY into the application (required)
- static void [associateSyntax](#) (Syntax &syntax, ActionFactory &action_factory)
Function to associate syntax with the DgospreyApp (required?)

4.25.1 Detailed Description

[DgospreyApp](#) inherits from the MooseApp object.

This object defines the required constructors, destructors, and functions that must be a part of every MooseApp based object. All MooseApp objects must be created in this way and override these functions.

Definition at line 54 of file DgospreyApp.h.

4.25.2 Constructor & Destructor Documentation

4.25.2.1 DgospreyApp::DgospreyApp (InputParameters parameters)

[DgospreyApp](#) constructor (required)

4.25.2.2 `virtual DgospreyApp::~DgospreyApp () [virtual]`

[DgospreyApp](#) destructor (required)

4.25.3 Member Function Documentation

4.25.3.1 `static void DgospreyApp::associateSyntax (Syntax & syntax, ActionFactory & action_factory) [static]`

Function to associate syntax with the [DgospreyApp](#) (required?)

I don't know what this is or does or what is actually being registered.

4.25.3.2 `static void DgospreyApp::registerApps () [static]`

Function to the [DgospreyApp](#) into MOOSE (required)

4.25.3.3 `static void DgospreyApp::registerObjects (Factory & factory) [static]`

Function to register kernels/objects created in DGOSPNEY into the application (required)

This is the function where the user must register all the kernels and other modules that are to be used in DGOSPNEY. Each time a new kernel or other object is created in DGOSPNEY, it must be registered here prior to building and running the application. Otherwise, the new functionality added will not show up or be utilized.

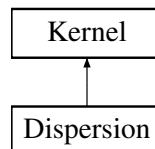
The documentation for this class was generated from the following file:

- [DgospreyApp.h](#)

4.26 Dispersion Class Reference

```
#include <Dispersion.h>
```

Inheritance diagram for Dispersion:



Public Member Functions

- [Dispersion](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- int [_index](#)
- const MaterialProperty
< std::vector< Real > > & [_dispersion](#)

4.26.1 Detailed Description

Definition at line 12 of file Dispersion.h.

4.26.2 Constructor & Destructor Documentation

4.26.2.1 Dispersion::Dispersion (const InputParameters & *parameters*)

4.26.3 Member Function Documentation

4.26.3.1 virtual Real Dispersion::computeQpJacobian () [protected], [virtual]

4.26.3.2 virtual Real Dispersion::computeQpResidual () [protected], [virtual]

4.26.4 Member Data Documentation

4.26.4.1 const MaterialProperty<std::vector<Real> >& Dispersion::_dispersion [private]

Definition at line 24 of file Dispersion.h.

4.26.4.2 int Dispersion::_index [private]

Definition at line 23 of file Dispersion.h.

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

- [Dispersion.h](#)

4.27 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_I_I`

- `std::vector< double > uz_lm1_l`
- `std::vector< double > uz_lp1_l`
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 > gl`
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 overridden)

4.27.1 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 overridden 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.

Definition at line 81 of file finch.h.

4.27.2 Member Data Documentation

4.27.2.1 double FINCH_DATA::beta = 0.5

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

Definition at line 123 of file finch.h.

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

Function pointer to executioner (DEFAULT = default_execution)

Definition at line 186 of file finch.h.

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

Centered, explicit coefficients (Calculated at Runtime)

Definition at line 134 of file finch.h.

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

Centered, implicit coefficients (Calculated at Runtime)

Definition at line 133 of file finch.h.

4.27.2.5 bool FINCH_DATA::CheckMass = false

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

Definition at line 117 of file finch.h.

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

Left side, explicit coefficients (Calculated at Runtime)

Definition at line 132 of file finch.h.

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

Left side, implicit coefficients (Calculated at Runtime)

Definition at line 131 of file finch.h.

4.27.2.8 bool FINCH_DATA::CN = true

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

Definition at line 114 of file finch.h.

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

Right side, explicit coefficients (Calculated at Runtime)

Definition at line 136 of file finch.h.

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

Right side, implicit coefficients (Calculated at Runtime)

Definition at line 135 of file finch.h.

4.27.2.11 int FINCH_DATA::d = 0

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

Definition at line 84 of file finch.h.

4.27.2.12 double FINCH_DATA::DIC = 1.0

Initial condition of [Dispersion](#) (if constant)

Definition at line 100 of file finch.h.

4.27.2.13 `bool FINCH_DATA::Dirichlet = false`

Flag to indicate use of Dirichlet or Neumann starting boundary.

Definition at line 116 of file finch.h.

4.27.2.14 `int(* FINCH_DATA::discretize)(const void *user_data)`

Function pointer to discretization (DEFAULT = `ospre_discretization`)

Definition at line 192 of file finch.h.

4.27.2.15 `Matrix<double> FINCH_DATA::Dn`

[Dispersion](#) Old.

Definition at line 166 of file finch.h.

4.27.2.16 `Matrix<double> FINCH_DATA::Dnp1`

[Dispersion](#) New.

Definition at line 167 of file finch.h.

4.27.2.17 `double FINCH_DATA::Do = 1.0`

Boundary Value of [Dispersion](#).

Definition at line 105 of file finch.h.

4.27.2.18 `double FINCH_DATA::dt = 0.0125`

Time step.

Definition at line 85 of file finch.h.

4.27.2.19 `double FINCH_DATA::dt_old = 0.0125`

Previous time step.

Definition at line 86 of file finch.h.

4.27.2.20 `double FINCH_DATA::dz = 0.1`

Space step.

Definition at line 88 of file finch.h.

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

Function pointer to the preconditioning function (DEFAULT = `default_precon`)

Definition at line 197 of file finch.h.

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

Function pointer to the residual function (DEFAULT = `default_res`)

Definition at line 195 of file finch.h.

4.27.2.23 `bool FINCH_DATA::ExplicitFlux = false`

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

Definition at line 118 of file finch.h.

4.27.2.24 `std::vector<double> FINCH_DATA::fC_E`

Centered, explicit fluxes (Calculated at Runtime)

Definition at line 141 of file finch.h.

4.27.2.25 `std::vector<double> FINCH_DATA::fC_I`

Centered, implicit fluxes (Calculated at Runtime)

Definition at line 140 of file finch.h.

4.27.2.26 `std::vector<double> FINCH_DATA::fL_E`

Left side, explicit fluxes (Calculated at Runtime)

Definition at line 139 of file finch.h.

4.27.2.27 `std::vector<double> FINCH_DATA::fL_I`

Left side, implicit fluxes (Calculated at Runtime)

Definition at line 138 of file finch.h.

4.27.2.28 `Matrix<double> FINCH_DATA::Fn`

Flux Limiter Old.

Definition at line 175 of file finch.h.

4.27.2.29 `Matrix<double> FINCH_DATA::Fnp1`

Flux Limiter New.

Definition at line 176 of file finch.h.

4.27.2.30 `std::vector<double> FINCH_DATA::fR_E`

Right side, explicit fluxes (Calculated at Runtime)

Definition at line 143 of file finch.h.

4.27.2.31 `std::vector<double> FINCH_DATA::fR_I`

Right side, implicit fluxes (Calculated at Runtime)

Definition at line 142 of file finch.h.

4.27.2.32 `Matrix<double> FINCH_DATA::gE`

Explicit Side Boundary Conditions.

Definition at line 178 of file finch.h.

4.27.2.33 `Matrix<double> FINCH_DATA::gl`

Implicit Side Boundary Conditions.

Definition at line 177 of file finch.h.

4.27.2.34 `bool FINCH_DATA::iterative = true`

Flag to indicate whether to solve directly, or iteratively.

Definition at line 119 of file finch.h.

4.27.2.35 double FINCH_DATA::kfn = 1.0

Film mass transfer coefficient Old.

Definition at line 108 of file finch.h.

4.27.2.36 double FINCH_DATA::kfnp1 = 1.0

Film mass transfer coefficient New.

Definition at line 109 of file finch.h.

4.27.2.37 double FINCH_DATA::klC = 1.0

Initial condition of Reaction (if constant)

Definition at line 101 of file finch.h.

4.27.2.38 Matrix<double> FINCH_DATA::kn

Reaction Old.

Definition at line 168 of file finch.h.

4.27.2.39 Matrix<double> FINCH_DATA::knp1

Reaction New.

Definition at line 169 of file finch.h.

4.27.2.40 double FINCH_DATA::ko = 1.0

Boundary Value of Reaction.

Definition at line 106 of file finch.h.

4.27.2.41 double FINCH_DATA::L = 1.0

Total space.

Definition at line 89 of file finch.h.

4.27.2.42 double FINCH_DATA::lambda_E

Boundary Coefficient for Explicit Neumann (Calculated at Runtime)

Definition at line 111 of file finch.h.

4.27.2.43 double FINCH_DATA::lambda_I

Boundary Coefficient for Implicit Neumann (Calculated at Runtime)

Definition at line 110 of file finch.h.

4.27.2.44 int FINCH_DATA::LN = 10

Number of nodes.

Definition at line 113 of file finch.h.

4.27.2.45 int FINCH_DATA::max_iter = 20

Maximum number of iterations allowed.

Definition at line 126 of file finch.h.

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

Explicit lower diagonal matrix elements (Calculated at Runtime)

Definition at line 151 of file finch.h.

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

Implicit lower diagonal matrix elements (Calculated at Runtime)

Definition at line 150 of file finch.h.

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

Explicit diagonal matrix elements (Calculated at Runtime)

Definition at line 149 of file finch.h.

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

Implicit diagonal matrix elements (Calculated at Runtime)

Definition at line 148 of file finch.h.

4.27.2.50 int FINCH_DATA::nl_method = FINCH_Picard

Non-linear solution method - default = FINCH_Picard.

Definition at line 128 of file finch.h.

4.27.2.51 bool FINCH_DATA::NormTrack = true

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

Definition at line 121 of file finch.h.

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

Explicit upper diagonal matrix elements (Calculated at Runtime)

Definition at line 147 of file finch.h.

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

Implicit upper diagonal matrix elements (Calculated at Runtime)

Definition at line 146 of file finch.h.

4.27.2.54 const void* FINCH_DATA::param_data

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

Definition at line 204 of file finch.h.

4.27.2.55 PICARD_DATA FINCH_DATA::picard_dat

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

Definition at line 202 of file finch.h.

4.27.2.56 PJFNK_DATA FINCH_DATA::pjfnk_dat

Data structure for PJFNK method (more rigours method)

Definition at line 203 of file finch.h.

4.27.2.57 Matrix<double> FINCH_DATA::pres

Current search direction.

Definition at line 181 of file finch.h.

4.27.2.58 Matrix<double> FINCH_DATA::res

Current residual.

Definition at line 180 of file finch.h.

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

Function pointer to reset time (DEFAULT = default_reset)

Definition at line 199 of file finch.h.

4.27.2.60 double FINCH_DATA::RIC = 1.0

Initial condition of the Time Coefficient (if constant)

Definition at line 102 of file finch.h.

4.27.2.61 Matrix<double> FINCH_DATA::Rn

Time Coeff Old.

Definition at line 172 of file finch.h.

4.27.2.62 Matrix<double> FINCH_DATA::Rnp1

Time Coeff New.

Definition at line 173 of file finch.h.

4.27.2.63 double FINCH_DATA::Ro = 1.0

Boundary Value of Time Coefficient.

Definition at line 107 of file finch.h.

4.27.2.64 double FINCH_DATA::s = 1.0

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

Definition at line 90 of file finch.h.

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

Function pointer to set boundary conditions (DEFAULT = default_bcs)

Definition at line 193 of file finch.h.

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

Function pointer to initial conditions (DEFAULT = default_ic)

Definition at line 187 of file finch.h.

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

Function pointer to set parameters (DEFAULT = default_params)

Definition at line 191 of file finch.h.

4.27.2.68 `int(* FINCH_DATA::setpostprocess)(const void *user_data)`

Function pointer to the postprocesses (DEFAULT = default_postprocess)

Definition at line 198 of file finch.h.

4.27.2.69 `int(* FINCH_DATA::setpreprocess)(const void *user_data)`

Function pointer to preprocesses (DEFAULT = default_preprocess)

Definition at line 189 of file finch.h.

4.27.2.70 `int(* FINCH_DATA::settime)(const void *user_data)`

Function pointer to set time step (DEFAULT = default_timestep)

Definition at line 188 of file finch.h.

4.27.2.71 `Matrix<double> FINCH_DATA::Sn`

Forcing Function Old.

Definition at line 170 of file finch.h.

4.27.2.72 `Matrix<double> FINCH_DATA::SnP1`

Forcing Function New.

Definition at line 171 of file finch.h.

4.27.2.73 `int(* FINCH_DATA::solve)(const void *user_data)`

Function pointer to the solver (DEFAULT = default_solve)

Definition at line 190 of file finch.h.

4.27.2.74 `bool FINCH_DATA::SteadyState = false`

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

Definition at line 120 of file finch.h.

4.27.2.75 `double FINCH_DATA::T = 1.0`

Total time.

Definition at line 87 of file finch.h.

4.27.2.76 `double FINCH_DATA::t = 0.0`

Current Time.

Definition at line 91 of file finch.h.

4.27.2.77 `double FINCH_DATA::t_old = 0.0`

Previous Time.

Definition at line 92 of file finch.h.

4.27.2.78 `double FINCH_DATA::tol_abs = 1e-6`

Absolute Tolerance for Convergence.

Definition at line 125 of file finch.h.

4.27.2.79 double FINCH_DATA::tol_rel = 1e-6

Relative Tolerance for Convergence.

Definition at line 124 of file finch.h.

4.27.2.80 int FINCH_DATA::total_iter = 0

Total number of iterations made.

Definition at line 127 of file finch.h.

4.27.2.81 Matrix<double> FINCH_DATA::u_star

Conserved Quantity Projected New.

Definition at line 161 of file finch.h.

4.27.2.82 double FINCH_DATA::uAvg = 0.0

Average amount of conserved quantity in domain.

Definition at line 96 of file finch.h.

4.27.2.83 double FINCH_DATA::uAvg_old = 0.0

Old Average amount of conserved quantity.

Definition at line 97 of file finch.h.

4.27.2.84 Matrix<double> FINCH_DATA::ubest

Best found solution if solving iteratively.

Definition at line 162 of file finch.h.

4.27.2.85 double FINCH_DATA::uIC = 0.0

Initial condition of Conserved Quantity (if constant)

Definition at line 98 of file finch.h.

4.27.2.86 Matrix<double> FINCH_DATA::un

Conserved Quantity Old.

Definition at line 159 of file finch.h.

4.27.2.87 Matrix<double> FINCH_DATA::unm1

Conserved Quantity Older.

Definition at line 158 of file finch.h.

4.27.2.88 Matrix<double> FINCH_DATA::unp1

Conserved Quantity New.

Definition at line 160 of file finch.h.

4.27.2.89 double FINCH_DATA::uo = 1.0

Boundary Value of Conserved Quantity.

Definition at line 103 of file finch.h.

4.27.2.90 `bool FINCH_DATA::Update = false`

Flag to check if the system needs updating.

Definition at line 115 of file finch.h.

4.27.2.91 `double FINCH_DATA::uT = 0.0`

Total amount of conserved quantity in domain.

Definition at line 94 of file finch.h.

4.27.2.92 `double FINCH_DATA::uT_old = 0.0`

Old Total amount of conserved quantity.

Definition at line 95 of file finch.h.

4.27.2.93 `std::vector<double> FINCH_DATA::uz_I_E`

Definition at line 155 of file finch.h.

4.27.2.94 `std::vector<double> FINCH_DATA::uz_I_I`

Definition at line 154 of file finch.h.

4.27.2.95 `std::vector<double> FINCH_DATA::uz_lm1_E`

Definition at line 155 of file finch.h.

4.27.2.96 `std::vector<double> FINCH_DATA::uz_lm1_I`

Definition at line 154 of file finch.h.

4.27.2.97 `std::vector<double> FINCH_DATA::uz_lp1_E`

Explicit local slopes (Calculated at Runtime)

Definition at line 155 of file finch.h.

4.27.2.98 `std::vector<double> FINCH_DATA::uz_lp1_I`

Implicit local slopes (Calculated at Runtime)

Definition at line 154 of file finch.h.

4.27.2.99 `double FINCH_DATA::vIC = 1.0`

Initial condition of Velocity (if constant)

Definition at line 99 of file finch.h.

4.27.2.100 `Matrix<double> FINCH_DATA::vn`

Velocity Old.

Definition at line 164 of file finch.h.

4.27.2.101 `Matrix<double> FINCH_DATA::vnp1`

Velocity New.

Definition at line 165 of file finch.h.

4.27.2.102 double FINCH_DATA::vo = 1.0

Boundary Value of Velocity.

Definition at line 104 of file finch.h.

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

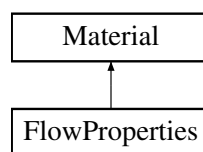
- [finch.h](#)

4.28 FlowProperties Class Reference

[FlowProperties](#) class object inherits from Material object.

```
#include <FlowProperties.h>
```

Inheritance diagram for FlowProperties:



Public Member Functions

- [FlowProperties](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual void [computeQpProperties](#) ()
Required function override for Material objects in MOOSE.

Private Attributes

- std::vector< Real > [_molecular_wieght](#)
Molecular wieghts for each gas species (g/mol)
- std::vector< Real > [_comp_heat_capacity](#)
Heat capacities for each gas species (J/g/K)
- std::vector< Real > [_comp_ref_viscosity](#)
Sutherland's reference viscosity for each gas species (g/cm/s)
- std::vector< Real > [_comp_ref_temp](#)
Sutherland's reference temperature for each species (K)
- std::vector< Real > [_comp_Sutherland_const](#)
Sutherland's constant for each gas species (K)
- Real [_flow_rate](#)
Inlet flow rate for the fixed-bed column (cm³/hr)
- Real [_column_length](#)
Length of the fixed-bed column (cm)
- MaterialProperty< Real > & [_velocity](#)
MaterialProperty for the linear velocity in the bed (cm/hr)
- MaterialProperty< Real > & [_gas_density](#)
MaterialProperty for the gas density (g/cm³)

- MaterialProperty< Real > & [_gas_viscosity](#)
MaterialProperty for the gas viscosity (g/cm/s)
- MaterialProperty< Real > & [_gas_heat_capacity](#)
MaterialProperty for the gas heat capacity (J/g/K)
- MaterialProperty< Real > & [_gas_molecular_wieght](#)
MaterialProperty for the gas total molecular wieght (g/mol)
- const MaterialProperty< Real > & [_inner_dia](#)
Coupled material property for bed inner diameter.
- const MaterialProperty< Real > & [_porosity](#)
Coupled material property for bed bulk porosity.
- const MaterialProperty< Real > & [_pellet_density](#)
Coupled material property for adsorbent pellet density.
- const MaterialProperty< Real > & [_pellet_heat_capacity](#)
Coupled material property for adsorbent heat capacity.
- MaterialProperty< Real > & [_heat_retardation](#)
MaterialProperty for energy balance retardation coefficient.
- MaterialProperty< std::vector
< Real > > & [_molecular_diffusion](#)
MaterialProperty for each species' molecular diffusion (cm²/s)
- MaterialProperty< std::vector
< Real > > & [_dispersion](#)
MaterialProperty for each species' dispersion coefficient (cm²/hr)
- MaterialProperty< std::vector
< Real > > & [_retardation](#)
MaterialProperty for each species' retardation coefficient.
- VariableValue & [_temperature](#)
Reference to the coupled column temperature.
- VariableValue & [_total_pressure](#)
Reference to the coupled column pressure.
- std::vector< unsigned int > [_index](#)
Indices for the gas species in the system.
- std::vector< VariableValue * > [_gas_conc](#)
Pointer list to the coupled gases.
- std::vector< VariableValue * > [_solid_conc](#)
Pointer list to the coupled adsorption concentrations.
- std::vector< VariableValue * > [_solid_perturb](#)
Pointer list to the coupled adsorption perturbations.

4.28.1 Detailed Description

[FlowProperties](#) class object inherits from Material object.

This class object inherits from the Material object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will set up and calculate various flow properties including linear velocities, molecular diffusion, mechanical dispersion, gas density, gas viscosity, gas heat capacity, etc. This object also approximates the effective retardation coefficient for each species in the mass balance. The evaluation of that parameter is dependent on the solid phase concentration variable, which will either be calculated by MAGPIE (see [magpie.h](#)) or SCOPSOWL (see [scopsowl.h](#)) depending on whether or not we will consider adsorption kinetics in the simulation.

Definition at line 63 of file FlowProperties.h.

4.28.2 Constructor & Destructor Documentation

4.28.2.1 FlowProperties::FlowProperties (const InputParameters & *parameters*)

Required constructor for objects in MOOSE.

4.28.3 Member Function Documentation

4.28.3.1 virtual void FlowProperties::computeQpProperties () [protected], [virtual]

Required function override for Material objects in MOOSE.

This function computes the material properties when they are needed by other MOOSE objects.

4.28.4 Member Data Documentation

4.28.4.1 Real FlowProperties::_column_length [private]

Length of the fixed-bed column (cm)

Definition at line 81 of file FlowProperties.h.

4.28.4.2 std::vector<Real> FlowProperties::_comp_heat_capacity [private]

Heat capacities for each gas species (J/g/K)

Definition at line 76 of file FlowProperties.h.

4.28.4.3 std::vector<Real> FlowProperties::_comp_ref_temp [private]

Sutherland's reference temperature for each species (K)

Definition at line 78 of file FlowProperties.h.

4.28.4.4 std::vector<Real> FlowProperties::_comp_ref_viscosity [private]

Sutherland's reference viscosity for each gas species (g/cm/s)

Definition at line 77 of file FlowProperties.h.

4.28.4.5 std::vector<Real> FlowProperties::_comp_Sutherland_const [private]

Sutherland's constant for each gas species (K)

Definition at line 79 of file FlowProperties.h.

4.28.4.6 MaterialProperty<std::vector<Real> >& FlowProperties::_dispersion [private]

MaterialProperty for each species' dispersion coefficient (cm²/hr)

Definition at line 96 of file FlowProperties.h.

4.28.4.7 Real FlowProperties::_flow_rate [private]

Inlet flow rate for the fixed-bed column (cm³/hr)

Definition at line 80 of file FlowProperties.h.

4.28.4.8 std::vector<VariableValue *> FlowProperties::_gas_conc [private]

Pointer list to the coupled gases.

Definition at line 102 of file FlowProperties.h.

4.28.4.9 MaterialProperty<Real>& FlowProperties::_gas_density [private]

MaterialProperty for the gas density (g/cm³)

Definition at line 84 of file FlowProperties.h.

4.28.4.10 MaterialProperty<Real>& FlowProperties::_gas_heat_capacity [private]

MaterialProperty for the gas heat capacity (J/g/K)

Definition at line 86 of file FlowProperties.h.

4.28.4.11 MaterialProperty<Real>& FlowProperties::_gas_molecular_wieght [private]

MaterialProperty for the gas total molecular wieght (g/mol)

Definition at line 87 of file FlowProperties.h.

4.28.4.12 MaterialProperty<Real>& FlowProperties::_gas_viscosity [private]

MaterialProperty for the gas viscosity (g/cm/s)

Definition at line 85 of file FlowProperties.h.

4.28.4.13 MaterialProperty<Real>& FlowProperties::_heat_retardation [private]

MaterialProperty for energy balance retardation coefficient.

Definition at line 94 of file FlowProperties.h.

4.28.4.14 std::vector<unsigned int> FlowProperties::_index [private]

Indices for the gas species in the system.

Definition at line 101 of file FlowProperties.h.

4.28.4.15 const MaterialProperty<Real>& FlowProperties::_inner_dia [private]

Coupled material property for bed inner diameter.

Definition at line 89 of file FlowProperties.h.

4.28.4.16 MaterialProperty<std::vector<Real> >& FlowProperties::_molecular_diffusion [private]

MaterialProperty for each species' molecular diffusion (cm²/s)

Definition at line 95 of file FlowProperties.h.

4.28.4.17 std::vector<Real> FlowProperties::_molecular_wieght [private]

Molecular wieghts for each gas species (g/mol)

Definition at line 75 of file FlowProperties.h.

4.28.4.18 const MaterialProperty<Real>& FlowProperties::_pellet_density [private]

Coupled material property for adsorbent pellet density.

Definition at line 91 of file FlowProperties.h.

4.28.4.19 const MaterialProperty<Real>& FlowProperties::_pellet_heat_capacity [private]

Coupled material property for adsorbent heat capacity.

Definition at line 92 of file FlowProperties.h.

4.28.4.20 `const MaterialProperty<Real>& FlowProperties::_porosity` [private]

Coupled material property for bed bulk porosity.

Definition at line 90 of file FlowProperties.h.

4.28.4.21 `MaterialProperty<std::vector<Real>>& FlowProperties::_retardation` [private]

MaterialProperty for each species' retardation coefficient.

Definition at line 97 of file FlowProperties.h.

4.28.4.22 `std::vector<VariableValue*> FlowProperties::_solid_conc` [private]

Pointer list to the coupled adsorption concentrations.

Definition at line 103 of file FlowProperties.h.

4.28.4.23 `std::vector<VariableValue*> FlowProperties::_solid_perturb` [private]

Pointer list to the coupled adsorption perturbations.

Definition at line 104 of file FlowProperties.h.

4.28.4.24 `VariableValue& FlowProperties::_temperature` [private]

Reference to the coupled column temperature.

Definition at line 99 of file FlowProperties.h.

4.28.4.25 `VariableValue& FlowProperties::_total_pressure` [private]

Reference to the coupled column pressure.

Definition at line 100 of file FlowProperties.h.

4.28.4.26 `MaterialProperty<Real>& FlowProperties::_velocity` [private]

MaterialProperty for the linear velocity in the bed (cm/hr)

Definition at line 83 of file FlowProperties.h.

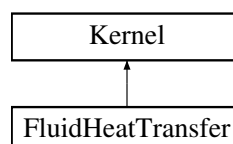
The documentation for this class was generated from the following file:

- [FlowProperties.h](#)

4.29 FluidHeatTransfer Class Reference

```
#include <FluidHeatTransfer.h>
```

Inheritance diagram for FluidHeatTransfer:



Public Member Functions

- [FluidHeatTransfer](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_bed_wall_transfer_coeff](#)
- const MaterialProperty< Real > & [_inner_dia](#)
- const MaterialProperty< Real > & [_porosity](#)
- VariableValue & [_wall_temp](#)

4.29.1 Detailed Description

Definition at line 11 of file FluidHeatTransfer.h.

4.29.2 Constructor & Destructor Documentation

4.29.2.1 [FluidHeatTransfer::FluidHeatTransfer \(const InputParameters & *parameters* \)](#)

4.29.3 Member Function Documentation

4.29.3.1 [virtual Real FluidHeatTransfer::computeQpJacobian \(\)](#) [protected],[virtual]

4.29.3.2 [virtual Real FluidHeatTransfer::computeQpResidual \(\)](#) [protected],[virtual]

4.29.4 Member Data Documentation

4.29.4.1 [const MaterialProperty<Real>& FluidHeatTransfer::_bed_wall_transfer_coeff](#) [private]

Definition at line 21 of file FluidHeatTransfer.h.

4.29.4.2 [const MaterialProperty<Real>& FluidHeatTransfer::_inner_dia](#) [private]

Definition at line 22 of file FluidHeatTransfer.h.

4.29.4.3 [const MaterialProperty<Real>& FluidHeatTransfer::_porosity](#) [private]

Definition at line 23 of file FluidHeatTransfer.h.

4.29.4.4 [VariableValue& FluidHeatTransfer::_wall_temp](#) [private]

Definition at line 25 of file FluidHeatTransfer.h.

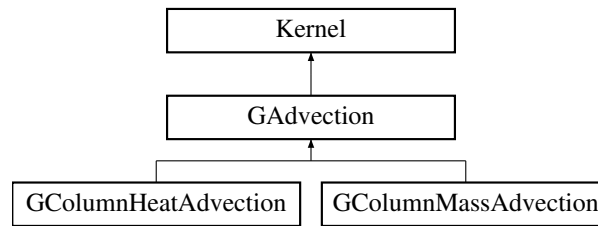
The documentation for this class was generated from the following file:

- [FluidHeatTransfer.h](#)

4.30 GAdvection Class Reference

```
#include <GAdvection.h>
```

Inheritance diagram for GAdvection:



Public Member Functions

- [GAdvection](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealVectorValue [_velocity](#)
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)

4.30.1 Detailed Description

Definition at line 13 of file GAdvection.h.

4.30.2 Constructor & Destructor Documentation

4.30.2.1 GAdvection::GAdvection (const InputParameters & parameters)

4.30.3 Member Function Documentation

4.30.3.1 virtual Real GAdvection::computeQpJacobian () [protected], [virtual]

Reimplemented in [GColumnHeatAdvection](#), and [GColumnMassAdvection](#).

4.30.3.2 virtual Real GAdvection::computeQpResidual () [protected], [virtual]

Reimplemented in [GColumnHeatAdvection](#), and [GColumnMassAdvection](#).

4.30.4 Member Data Documentation

4.30.4.1 RealVectorValue GAdvection::_velocity [protected]

Definition at line 23 of file GAdvection.h.

4.30.4.2 Real GAdvection::_vx [protected]

Definition at line 25 of file GAdvection.h.

4.30.4.3 Real GAdvection::_vy [protected]

Definition at line 26 of file GAdvection.h.

4.30.4.4 Real GAdvection::_vz [protected]

Definition at line 27 of file GAdvection.h.

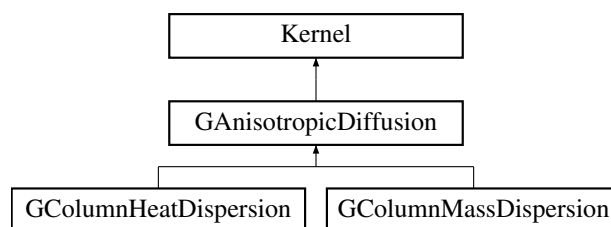
The documentation for this class was generated from the following file:

- [GAdvection.h](#)

4.31 GAnisotropicDiffusion Class Reference

```
#include <GAnisotropicDiffusion.h>
```

Inheritance diagram for GAnisotropicDiffusion:



Public Member Functions

- [GAnisotropicDiffusion](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealTensorValue [_Diffusion](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

4.31.1 Detailed Description

Definition at line 12 of file GAnisotropicDiffusion.h.

4.31.2 Constructor & Destructor Documentation

4.31.2.1 GAnisotropicDiffusion::GAnisotropicDiffusion (const InputParameters & *parameters*)

4.31.3 Member Function Documentation

4.31.3.1 virtual Real GAnisotropicDiffusion::computeQpJacobian () [protected], [virtual]

Reimplemented in [GColumnHeatDispersion](#), and [GColumnMassDispersion](#).

4.31.3.2 virtual Real GAnisotropicDiffusion::computeQpResidual () [protected], [virtual]

Reimplemented in [GColumnHeatDispersion](#), and [GColumnMassDispersion](#).

4.31.4 Member Data Documentation

4.31.4.1 RealTensorValue GAnisotropicDiffusion::_Diffusion [protected]

Definition at line 22 of file GAnisotropicDiffusion.h.

4.31.4.2 Real GAnisotropicDiffusion::_Dxx [protected]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.31.4.3 Real GAnisotropicDiffusion::_Dxy [protected]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.31.4.4 Real GAnisotropicDiffusion::_Dxz [protected]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.31.4.5 Real GAnisotropicDiffusion::_Dyx [protected]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.31.4.6 Real GAnisotropicDiffusion::_Dyy [protected]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.31.4.7 Real GAnisotropicDiffusion::_Dyz [protected]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.31.4.8 Real GAnisotropicDiffusion::_Dzx [protected]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.31.4.9 Real GAnisotropicDiffusion::_Dzy [protected]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.31.4.10 Real GAnisotropicDiffusion::_Dzz [protected]

Definition at line 26 of file GAnisotropicDiffusion.h.

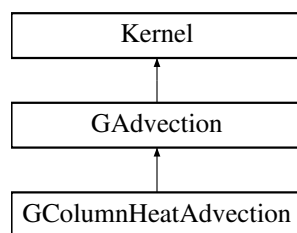
The documentation for this class was generated from the following file:

- [GAnisotropicDiffusion.h](#)

4.32 GColumnHeatAdvection Class Reference

```
#include <GColumnHeatAdvection.h>
```

Inheritance diagram for GColumnHeatAdvection:



Public Member Functions

- [GColumnHeatAdvection](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealVectorValue [_velocity](#)
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)

Private Attributes

- const MaterialProperty< Real > & [_vel](#)
- const MaterialProperty< Real > & [_gas_density](#)
- const MaterialProperty< Real > & [_gas_heat_capacity](#)

4.32.1 Detailed Description

Definition at line 21 of file GColumnHeatAdvection.h.

4.32.2 Constructor & Destructor Documentation

4.32.2.1 [GColumnHeatAdvection::GColumnHeatAdvection](#) (const InputParameters & *parameters*)

4.32.3 Member Function Documentation

4.32.3.1 virtual Real [GColumnHeatAdvection::computeQpJacobian](#) () [protected], [virtual]

Reimplemented from [GAdvection](#).

4.32.3.2 virtual Real [GColumnHeatAdvection::computeQpResidual](#) () [protected], [virtual]

Reimplemented from [GAdvection](#).

4.32.4 Member Data Documentation

4.32.4.1 `const MaterialProperty<Real>& GColumnHeatAdvection::_gas_density` `[private]`

Definition at line 33 of file GColumnHeatAdvection.h.

4.32.4.2 `const MaterialProperty<Real>& GColumnHeatAdvection::_gas_heat_capacity` `[private]`

Definition at line 34 of file GColumnHeatAdvection.h.

4.32.4.3 `const MaterialProperty<Real>& GColumnHeatAdvection::_vel` `[private]`

Definition at line 32 of file GColumnHeatAdvection.h.

4.32.4.4 `RealVectorValue GAdvection::_velocity` `[protected], [inherited]`

Definition at line 23 of file GAdvection.h.

4.32.4.5 `Real GAdvection::_vx` `[protected], [inherited]`

Definition at line 25 of file GAdvection.h.

4.32.4.6 `Real GAdvection::_vy` `[protected], [inherited]`

Definition at line 26 of file GAdvection.h.

4.32.4.7 `Real GAdvection::_vz` `[protected], [inherited]`

Definition at line 27 of file GAdvection.h.

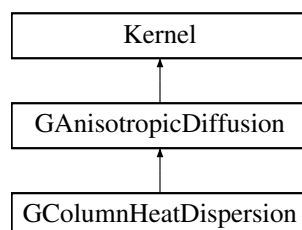
The documentation for this class was generated from the following file:

- [GColumnHeatAdvection.h](#)

4.33 GColumnHeatDispersion Class Reference

```
#include <GColumnHeatDispersion.h>
```

Inheritance diagram for GColumnHeatDispersion:



Public Member Functions

- [GColumnHeatDispersion](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealTensorValue [_Diffusion](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

Private Attributes

- const MaterialProperty< Real > & [_conductivity](#)

4.33.1 Detailed Description

Definition at line 20 of file GColumnHeatDispersion.h.

4.33.2 Constructor & Destructor Documentation

4.33.2.1 GColumnHeatDispersion::GColumnHeatDispersion (const InputParameters & *parameters*)

4.33.3 Member Function Documentation

4.33.3.1 virtual Real GColumnHeatDispersion::computeQpJacobian () [protected], [virtual]

Reimplemented from [GAnisotropicDiffusion](#).

4.33.3.2 virtual Real GColumnHeatDispersion::computeQpResidual () [protected], [virtual]

Reimplemented from [GAnisotropicDiffusion](#).

4.33.4 Member Data Documentation

4.33.4.1 const MaterialProperty<Real>& GColumnHeatDispersion::_conductivity [private]

Definition at line 31 of file GColumnHeatDispersion.h.

4.33.4.2 RealTensorValue GAnisotropicDiffusion::_Diffusion [protected], [inherited]

Definition at line 22 of file GAnisotropicDiffusion.h.

4.33.4.3 Real GAnisotropicDiffusion::_Dxx [protected], [inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.33.4.4 Real GAnisotropicDiffusion::_Dxy [protected], [inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.33.4.5 Real GAnisotropicDiffusion::_Dxz [protected], [inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.33.4.6 Real GAnisotropicDiffusion::Dyx [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.33.4.7 Real GAnisotropicDiffusion::Dyy [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.33.4.8 Real GAnisotropicDiffusion::Dyz [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.33.4.9 Real GAnisotropicDiffusion::Dzx [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.33.4.10 Real GAnisotropicDiffusion::Dzy [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.33.4.11 Real GAnisotropicDiffusion::Dzz [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

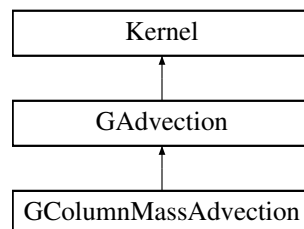
The documentation for this class was generated from the following file:

- [GColumnHeatDispersion.h](#)

4.34 GColumnMassAdvection Class Reference

```
#include <GColumnMassAdvection.h>
```

Inheritance diagram for GColumnMassAdvection:



Public Member Functions

- [GColumnMassAdvection](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealVectorValue [_velocity](#)
- Real [_vx](#)
- Real [_vy](#)
- Real [_vz](#)

Private Attributes

- `const MaterialProperty< Real > & _vel`

4.34.1 Detailed Description

Definition at line 21 of file GColumnMassAdvection.h.

4.34.2 Constructor & Destructor Documentation

4.34.2.1 GColumnMassAdvection::GColumnMassAdvection (const InputParameters & *parameters*)

4.34.3 Member Function Documentation

4.34.3.1 virtual Real GColumnMassAdvection::computeQpJacobian () [protected], [virtual]

Reimplemented from [GAdvection](#).

4.34.3.2 virtual Real GColumnMassAdvection::computeQpResidual () [protected], [virtual]

Reimplemented from [GAdvection](#).

4.34.4 Member Data Documentation

4.34.4.1 const MaterialProperty<Real>& GColumnMassAdvection::_vel [private]

Definition at line 32 of file GColumnMassAdvection.h.

4.34.4.2 RealVectorValue GAdvection::_velocity [protected], [inherited]

Definition at line 23 of file GAdvection.h.

4.34.4.3 Real GAdvection::_vx [protected], [inherited]

Definition at line 25 of file GAdvection.h.

4.34.4.4 Real GAdvection::_vy [protected], [inherited]

Definition at line 26 of file GAdvection.h.

4.34.4.5 Real GAdvection::_vz [protected], [inherited]

Definition at line 27 of file GAdvection.h.

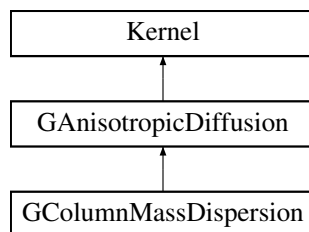
The documentation for this class was generated from the following file:

- [GColumnMassAdvection.h](#)

4.35 GColumnMassDispersion Class Reference

```
#include <GColumnMassDispersion.h>
```

Inheritance diagram for GColumnMassDispersion:



Public Member Functions

- [GColumnMassDispersion](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Protected Attributes

- RealTensorValue [_Diffusion](#)
- Real [_Dxx](#)
- Real [_Dxy](#)
- Real [_Dxz](#)
- Real [_Dyx](#)
- Real [_Dyy](#)
- Real [_Dyz](#)
- Real [_Dzx](#)
- Real [_Dzy](#)
- Real [_Dzz](#)

Private Attributes

- unsigned int [_index](#)
- const MaterialProperty
< std::vector< Real > > & [_dispersion](#)
- const MaterialProperty
< std::vector< Real > > & [_molecular_diffusion](#)

4.35.1 Detailed Description

Definition at line 20 of file GColumnMassDispersion.h.

4.35.2 Constructor & Destructor Documentation

4.35.2.1 [GColumnMassDispersion::GColumnMassDispersion](#) (const InputParameters & *parameters*)

4.35.3 Member Function Documentation

4.35.3.1 virtual Real [GColumnMassDispersion::computeQpJacobian](#) () [protected],[virtual]

Reimplemented from [GAnisotropicDiffusion](#).

4.35.3.2 virtual Real GColumnMassDispersion::computeQpResidual () [protected],[virtual]

Reimplemented from [GAnisotropicDiffusion](#).

4.35.4 Member Data Documentation

4.35.4.1 RealTensorValue GAnisotropicDiffusion::_Diffusion [protected],[inherited]

Definition at line 22 of file GAnisotropicDiffusion.h.

4.35.4.2 const MaterialProperty<std::vector<Real>>& GColumnMassDispersion::_dispersion [private]

Definition at line 32 of file GColumnMassDispersion.h.

4.35.4.3 Real GAnisotropicDiffusion::_Dxx [protected],[inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.35.4.4 Real GAnisotropicDiffusion::_Dxy [protected],[inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.35.4.5 Real GAnisotropicDiffusion::_Dxz [protected],[inherited]

Definition at line 24 of file GAnisotropicDiffusion.h.

4.35.4.6 Real GAnisotropicDiffusion::_Dyx [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.35.4.7 Real GAnisotropicDiffusion::_Dyy [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.35.4.8 Real GAnisotropicDiffusion::_Dyz [protected],[inherited]

Definition at line 25 of file GAnisotropicDiffusion.h.

4.35.4.9 Real GAnisotropicDiffusion::_Dzx [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.35.4.10 Real GAnisotropicDiffusion::_Dzy [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.35.4.11 Real GAnisotropicDiffusion::_Dzz [protected],[inherited]

Definition at line 26 of file GAnisotropicDiffusion.h.

4.35.4.12 unsigned int GColumnMassDispersion::_index [private]

Definition at line 31 of file GColumnMassDispersion.h.

4.35.4.13 const MaterialProperty<std::vector<Real>>& GColumnMassDispersion::_molecular_diffusion [private]

Definition at line 33 of file GColumnMassDispersion.h.

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

- [GColumnMassDispersion.h](#)

4.36 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.

4.36.1 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.

Definition at line 336 of file lark.h.

4.36.2 Member Data Documentation

4.36.2.1 double GCR_DATA::alpha

Inner iteration step size.

Definition at line 345 of file lark.h.

4.36.2.2 double GCR_DATA::bestres

Best found residual norm of the linear system.

Definition at line 352 of file lark.h.

4.36.2.3 Matrix<double> GCR_DATA::bestx

Best found solution to the linear system.

Definition at line 357 of file lark.h.

4.36.2.4 double GCR_DATA::beta

Outer iteration step size.

Definition at line 346 of file lark.h.

4.36.2.5 bool GCR_DATA::breakdown = false

Boolean to determine if a step has failed.

Definition at line 343 of file lark.h.

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

Vector span for updating r.

Definition at line 362 of file lark.h.

4.36.2.7 Matrix<double> GCR_DATA::c_temp

Temporary c vector to be updated.

Definition at line 359 of file lark.h.

4.36.2.8 int GCR_DATA::iter_inner = 0

Number of inner iterations taken.

Definition at line 341 of file lark.h.

4.36.2.9 int GCR_DATA::iter_outer = 0

Number of outer iterations taken.

Definition at line 340 of file lark.h.

4.36.2.10 `int GCR_DATA::maxit = 0`

Maximum allowable outer iterations.

Definition at line 339 of file lark.h.

4.36.2.11 `bool GCR_DATA::Output = true`

True = print messages to the console.

Definition at line 354 of file lark.h.

4.36.2.12 `Matrix<double> GCR_DATA::r`

Residual Vector.

Definition at line 358 of file lark.h.

4.36.2.13 `double GCR_DATA::relres`

Relative residual norm for linear system.

Definition at line 350 of file lark.h.

4.36.2.14 `double GCR_DATA::relres_base`

Initial residual norm of the linear system.

Definition at line 351 of file lark.h.

4.36.2.15 `double GCR_DATA::res`

Absolute residual norm for linear system.

Definition at line 349 of file lark.h.

4.36.2.16 `int GCR_DATA::restart = -1`

Restart parameter for outer iterations - default = 20.

Definition at line 338 of file lark.h.

4.36.2.17 `double GCR_DATA::tol_abs = 1e-6`

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

Definition at line 348 of file lark.h.

4.36.2.18 `double GCR_DATA::tol_rel = 1e-6`

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

Definition at line 347 of file lark.h.

4.36.2.19 `int GCR_DATA::total_iter = 0`

Total number of iterations taken.

Definition at line 342 of file lark.h.

4.36.2.20 `OPTRANS_DATA GCR_DATA::transpose_dat`

Data structure for Operator Transposition.

Definition at line 364 of file lark.h.

4.36.2.21 `std::vector<Matrix<double> > GCR_DATA::u`

Vector span for updating x.

Definition at line 361 of file lark.h.

4.36.2.22 `Matrix<double> GCR_DATA::u_temp`

Temporary u vector to be updated.

Definition at line 360 of file lark.h.

4.36.2.23 `Matrix<double> GCR_DATA::x`

Current solution to the linear system.

Definition at line 356 of file lark.h.

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

- [lark.h](#)

4.37 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
Absolute tolerance for convergence - default = 1e-6.
- double `res`
Absolute residual 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.

4.37.1 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-Preconditioned (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.

Definition at line 147 of file lark.h.

4.37.2 Member Data Documentation

4.37.2.1 **ARNOLDI_DATA** GMRESLP_DATA::arnoldi_dat

Data structure for the kyrlov subspace.

Definition at line 167 of file lark.h.

4.37.2.2 **double** GMRESLP_DATA::bestres

Best found residual norm of the linear system.

Definition at line 159 of file lark.h.

4.37.2.3 **Matrix**<double> GMRESLP_DATA::bestx

Best found solution to the linear system.

Definition at line 164 of file lark.h.

4.37.2.4 **int** GMRESLP_DATA::iter = 0

Number of iterations needed for convergence.

Definition at line 151 of file lark.h.

4.37.2.5 **int** GMRESLP_DATA::maxit = 0

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

Definition at line 150 of file lark.h.

4.37.2.6 **bool** GMRESLP_DATA::Output = true

True = print messages to console.

Definition at line 161 of file lark.h.

4.37.2.7 **Matrix**<double> GMRESLP_DATA::r

Residual vector for the linear system.

Definition at line 165 of file lark.h.

4.37.2.8 double GMRESLP_DATA::relres

Relative residual norm of the linear system.

Definition at line 157 of file lark.h.

4.37.2.9 double GMRESLP_DATA::relres_base

Initial residual norm of the linear system.

Definition at line 158 of file lark.h.

4.37.2.10 double GMRESLP_DATA::res

Absolution redisual norm of the linear system.

Definition at line 156 of file lark.h.

4.37.2.11 int GMRESLP_DATA::restart = -1

Restart parameter - default = min(vector_size,20)

Definition at line 149 of file lark.h.

4.37.2.12 int GMRESLP_DATA::steps = 0

Total number of gmres iterations and krylov iterations.

Definition at line 152 of file lark.h.

4.37.2.13 double GMRESLP_DATA::tol_abs = 1e-6

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

Definition at line 155 of file lark.h.

4.37.2.14 double GMRESLP_DATA::tol_rel = 1e-6

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

Definition at line 154 of file lark.h.

4.37.2.15 Matrix<double> GMRESLP_DATA::x

Current solution to the linear system.

Definition at line 163 of file lark.h.

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

- [lark.h](#)

4.38 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.

4.38.1 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).

Definition at line 373 of file lark.h.

4.38.2 Member Data Documentation

4.38.2.1 `Matrix<double> GMRESR_DATA::arg`

Argument matrix passed between preconditioner and iterator.

Definition at line 391 of file lark.h.

4.38.2.2 double GMRESR_DATA::gcr_abs_tol = 1e-6

Absolute outer residual tolerance.

Definition at line 389 of file lark.h.

4.38.2.3 GCR_DATA GMRESR_DATA::gcr_dat

Data structure for the outer GCR steps.

Definition at line 393 of file lark.h.

4.38.2.4 int GMRESR_DATA::gcr_maxit = 0

Number of GCR iterations.

Definition at line 376 of file lark.h.

4.38.2.5 bool GMRESR_DATA::GCR_Output = true

True = print GCR messages.

Definition at line 384 of file lark.h.

4.38.2.6 double GMRESR_DATA::gcr_rel_tol = 1e-6

Relative outer residual tolerance.

Definition at line 388 of file lark.h.

4.38.2.7 int GMRESR_DATA::gcr_restart = -1

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

Definition at line 375 of file lark.h.

4.38.2.8 GMRESRP_DATA GMRESR_DATA::gmres_dat

Data structure for the inner GMRES steps.

Definition at line 394 of file lark.h.

4.38.2.9 int GMRESR_DATA::gmres_maxit = 1

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

Definition at line 378 of file lark.h.

4.38.2.10 bool GMRESR_DATA::GMRES_Output = false

True = print GMRES messages.

Definition at line 385 of file lark.h.

4.38.2.11 int GMRESR_DATA::gmres_restart = -1

Number of GMRES restarts (max = 20)

Definition at line 377 of file lark.h.

4.38.2.12 double GMRESR_DATA::gmres_tol = 0.1

Tolerance relative to GCR iterations.

Definition at line 387 of file lark.h.

4.38.2.13 int GMRESR_DATA::iter_inner

Total GMRES iterations.

Definition at line 382 of file lark.h.

4.38.2.14 int GMRESR_DATA::iter_outer

Total GCR iterations.

Definition at line 381 of file lark.h.

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

User supplied matrix-vector product function.

Definition at line 397 of file lark.h.

4.38.2.16 const void* GMRESR_DATA::matvec_data

Data structure for the user's matvec function.

Definition at line 401 of file lark.h.

4.38.2.17 int GMRESR_DATA::N

Dimension of the linear system.

Definition at line 379 of file lark.h.

4.38.2.18 const void* GMRESR_DATA::term_precon

Data structure for the user's terminal preconditioner.

Definition at line 402 of file lark.h.

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

Optional user supplied terminal preconditioner.

Definition at line 399 of file lark.h.

4.38.2.20 int GMRESR_DATA::total_iter

Total GMRES and GCR iterations.

Definition at line 380 of file lark.h.

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

- [lark.h](#)

4.39 GMRESR_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*

4.39.1 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.

Definition at line 177 of file lark.h.

4.39.2 Member Data Documentation

4.39.2.1 `double GMRESRP_DATA::bestres`

Best found residual norm of the linear system.

Definition at line 190 of file lark.h.

4.39.2.2 `Matrix<double> GMRESRP_DATA::bestx`

Best found solution to the linear system.

Definition at line 195 of file lark.h.

4.39.2.3 `std::vector< double > GMRESRP_DATA::e0`

($k+1 \times 1$) Normalized vector with residual info

Definition at line 203 of file lark.h.

4.39.2.4 `std::vector< double > GMRESRP_DATA::e0_bar`

($k+1 \times 1$) Factorized normal vector

Definition at line 204 of file lark.h.

4.39.2.5 `std::vector< std::vector< double > > GMRESRP_DATA::H`

($k+1 \times k$) upper Hessenberg storage matrix

Definition at line 200 of file lark.h.

4.39.2.6 `std::vector< std::vector< double > > GMRESRP_DATA::H_bar`

($k+1 \times k$) Factorized matrix

Definition at line 201 of file lark.h.

4.39.2.7 `int GMRESRP_DATA::iter_inner = 0`

Total number of inner iterations.

Definition at line 182 of file lark.h.

4.39.2.8 `int GMRESRP_DATA::iter_outer = 0`

Total number of outer iterations.

Definition at line 181 of file lark.h.

4.39.2.9 `int GMRESRP_DATA::iter_total = 0`

Total number of overall iterations.

Definition at line 183 of file lark.h.

4.39.2.10 `int GMRESRP_DATA::maxit = 0`

Maximum allowable outer iterations.

Definition at line 180 of file lark.h.

4.39.2.11 `bool GMRESRP_DATA::Output = true`

True = print messages to console.

Definition at line 192 of file lark.h.

4.39.2.12 `Matrix<double> GMRESRP_DATA::r`

Residual vector for the linear system.

Definition at line 196 of file lark.h.

4.39.2.13 `double GMRESRP_DATA::relres`

Relative residual norm for linear system.

Definition at line 188 of file lark.h.

4.39.2.14 `double GMRESRP_DATA::relres_base`

Initial residual norm of the linear system.

Definition at line 189 of file lark.h.

4.39.2.15 `double GMRESRP_DATA::res`

Absolute residual norm for linear system.

Definition at line 187 of file lark.h.

4.39.2.16 `int GMRESRP_DATA::restart = -1`

Restart parameter - default = min(20,vector_size)

Definition at line 179 of file lark.h.

4.39.2.17 `Matrix<double> GMRESRP_DATA::sum`

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

Definition at line 208 of file lark.h.

4.39.2.18 `double GMRESRP_DATA::tol_abs = 1e-6`

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

Definition at line 186 of file lark.h.

4.39.2.19 `double GMRESRP_DATA::tol_rel = 1e-6`

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

Definition at line 185 of file lark.h.

4.39.2.20 `Matrix<double> GMRESRP_DATA::v`

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

Definition at line 207 of file lark.h.

4.39.2.21 `std::vector< Matrix<double> > GMRESRP_DATA::Vk`

(N x k) orthonormal vector basis

Definition at line 198 of file lark.h.

4.39.2.22 `Matrix<double> GMRESRP_DATA::w`

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

Definition at line 206 of file lark.h.

4.39.2.23 `Matrix<double> GMRESRP_DATA::x`

Current solution to the linear system.

Definition at line 194 of file lark.h.

4.39.2.24 `std::vector< double > GMRESRP_DATA::y`

(k x 1) Vector search direction

Definition at line 202 of file lark.h.

4.39.2.25 `std::vector< Matrix<double> > GMRESRP_DATA::Zk`

(N x k) preconditioned vector set

Definition at line 199 of file lark.h.

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

- [lark.h](#)

4.40 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 [Plo](#)
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.

4.40.1 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.

Definition at line 123 of file `magpie.h`.

4.40.2 Member Data Documentation

4.40.2.1 `std::vector<double> GPAST_DATA::gama_inf`

Infinite dilution activities.

Definition at line 129 of file `magpie.h`.

4.40.2.2 `double GPAST_DATA::He`

Henry's Coefficient (mol/kg/kPa)

Definition at line 127 of file `magpie.h`.

4.40.2.3 `double GPAST_DATA::Plo`

Pure component spreading pressures (mol/kg)

Definition at line 131 of file `magpie.h`.

4.40.2.4 `std::vector<double> GPAST_DATA::po`

Pure component reference state pressures (kPa)

Definition at line 132 of file `magpie.h`.

4.40.2.5 `double GPAST_DATA::poi`

Reference state pressures solved for using Recover eval GPAST.

Definition at line 133 of file `magpie.h`.

4.40.2.6 `bool GPAST_DATA::present`

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

Definition at line 134 of file `magpie.h`.

4.40.2.7 `double GPAST_DATA::q`

Amount adsorbed for each component (mol/kg)

Definition at line 128 of file `magpie.h`.

4.40.2.8 `double GPAST_DATA::qo`

Pure component capacities (mol/kg)

Definition at line 130 of file `magpie.h`.

4.40.2.9 double GPAST_DATA::x

Adsorbed mole fraction.

Definition at line 125 of file magpie.h.

4.40.2.10 double GPAST_DATA::y

Gas phase mole fraction.

Definition at line 126 of file magpie.h.

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

- [magpie.h](#)

4.41 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))*

4.41.1 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.

Definition at line 98 of file magpie.h.

4.41.2 Member Data Documentation

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

Enthalpies for each site (J/mol)

Definition at line 102 of file magpie.h.

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

Entropies for each site (J/(K*mol))

Definition at line 103 of file magpie.h.

4.41.2.3 int GSTA_DATA::m

Number of parameters in the GSTA isotherm.

Definition at line 101 of file magpie.h.

4.41.2.4 double GSTA_DATA::qmax

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

Definition at line 100 of file magpie.h.

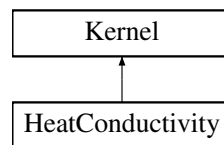
The documentation for this struct was generated from the following file:

- [magpie.h](#)

4.42 HeatConductivity Class Reference

```
#include <HeatConductivity.h>
```

Inheritance diagram for HeatConductivity:



Public Member Functions

- [HeatConductivity](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_conductivity](#)
- const MaterialProperty< Real > & [_porosity](#)

4.42.1 Detailed Description

Definition at line 12 of file HeatConductivity.h.

4.42.2 Constructor & Destructor Documentation

4.42.2.1 [HeatConductivity::HeatConductivity](#) (const InputParameters & *parameters*)

4.42.3 Member Function Documentation

4.42.3.1 virtual Real [HeatConductivity::computeQpJacobian](#) () [protected], [virtual]

4.42.3.2 virtual Real [HeatConductivity::computeQpResidual](#) () [protected], [virtual]

4.42.4 Member Data Documentation

4.42.4.1 const MaterialProperty<Real>& [HeatConductivity::_conductivity](#) [private]

Definition at line 23 of file HeatConductivity.h.

4.42.4.2 `const MaterialProperty<Real>& HeatConductivity::porosity` `[private]`

Definition at line 24 of file HeatConductivity.h.

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

- [HeatConductivity.h](#)

4.43 KMS_DATA Struct Reference

Data structure for the implementation 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.

4.43.1 Detailed Description

Data structure for the implementation 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 progressively 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.

Definition at line 413 of file lark.h.

4.43.2 Member Data Documentation

4.43.2.1 `std::vector<GMRESRP_DATA> KMS_DATA::gmres_in`

Data structures for each recursion level.

Definition at line 431 of file lark.h.

4.43.2.2 `GMRESRP_DATA KMS_DATA::gmres_out`

Data structure for the outer steps.

Definition at line 430 of file lark.h.

4.43.2.3 `int KMS_DATA::inner_iter = 0`

Number of inner steps taken.

Definition at line 419 of file lark.h.

4.43.2.4 `double KMS_DATA::inner_reltol = 0.1`

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

Definition at line 425 of file lark.h.

4.43.2.5 `int KMS_DATA::level = 0`

Current level in the recursion.

Definition at line 415 of file lark.h.

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

User supplied matrix-vector product function.

Definition at line 434 of file lark.h.

4.43.2.7 `const void* KMS_DATA::matvec_data`

Data structure for the user's matvec function.

Definition at line 438 of file lark.h.

4.43.2.8 `int KMS_DATA::max_level = 0`

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

Definition at line 416 of file lark.h.

4.43.2.9 `int KMS_DATA::maxit = 0`

Maximum allowable iterations for the outer steps.

Definition at line 418 of file lark.h.

4.43.2.10 `double KMS_DATA::outer_abstol = 1e-6`

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

Definition at line 424 of file lark.h.

4.43.2.11 `int KMS_DATA::outer_iter = 0`

Number of outer steps taken.

Definition at line 420 of file lark.h.

4.43.2.12 `double KMS_DATA::outer_reltol = 1e-6`

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

Definition at line 423 of file lark.h.

4.43.2.13 `bool KMS_DATA::Output_in = false`

True = Print the inner steps residuals.

Definition at line 428 of file lark.h.

4.43.2.14 `bool KMS_DATA::Output_out = true`

True = Print the outer steps residuals.

Definition at line 427 of file lark.h.

4.43.2.15 `int KMS_DATA::restart = -1`

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

Definition at line 417 of file lark.h.

4.43.2.16 `const void* KMS_DATA::term_precon`

Data structure for the user's terminal preconditioner.

Definition at line 439 of file lark.h.

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

Optional user supplied terminal preconditioner.

Definition at line 436 of file lark.h.

4.43.2.18 `int KMS_DATA::total_iter = 0`

Total number of iterations in all steps.

Definition at line 421 of file lark.h.

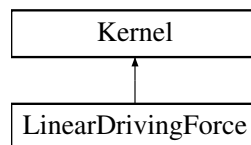
The documentation for this struct was generated from the following file:

- [lark.h](#)

4.44 LinearDrivingForce Class Reference

```
#include <LinearDrivingForce.h>
```

Inheritance diagram for LinearDrivingForce:



Public Member Functions

- [LinearDrivingForce](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- bool [_gaining](#)
- Real [_coef](#)
- Real [_driving_value](#)
- VariableValue & [_var](#)

4.44.1 Detailed Description

Definition at line 11 of file LinearDrivingForce.h.

4.44.2 Constructor & Destructor Documentation

4.44.2.1 [LinearDrivingForce::LinearDrivingForce](#) (const InputParameters & *parameters*)

4.44.3 Member Function Documentation

4.44.3.1 virtual Real [LinearDrivingForce::computeQpJacobian](#) () [protected],[virtual]

4.44.3.2 virtual Real [LinearDrivingForce::computeQpResidual](#) () [protected],[virtual]

4.44.4 Member Data Documentation

4.44.4.1 Real [LinearDrivingForce::_coef](#) [private]

Definition at line 22 of file LinearDrivingForce.h.

4.44.4.2 Real [LinearDrivingForce::_driving_value](#) [private]

Definition at line 23 of file LinearDrivingForce.h.

4.44.4.3 bool [LinearDrivingForce::_gaining](#) [private]

Definition at line 21 of file LinearDrivingForce.h.

4.44.4.4 VariableValue& LinearDrivingForce::var [private]

Definition at line 24 of file LinearDrivingForce.h.

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

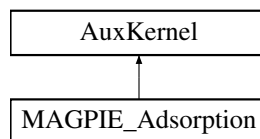
- [LinearDrivingForce.h](#)

4.45 MAGPIE_Adsorption Class Reference

Magpie Adsorption class inherits from AuxKernel.

```
#include <MAGPIE_Adsorption.h>
```

Inheritance diagram for MAGPIE_Adsorption:



Public Member Functions

- [MAGPIE_Adsorption](#) (const InputParameters ¶meters)
Standard MOOSE public constructor.

Protected Member Functions

- virtual Real [computeValue](#) ()
Required MOOSE function override.

Private Attributes

- unsigned int [_index](#)
Index of the gaseous species to calculate equilibria for.
- const MaterialProperty
< [MAGPIE_DATA](#) > & [_magpie_dat](#)
Material Property holding the MAGPIE data structure.

4.45.1 Detailed Description

Magpie Adsorption class inherits from AuxKernel.

This class object creates an AuxKernel for use in the MOOSE framework. The AuxKernel will calculate the adsorption equilibria for a given species in the gas phase based on parameters, variables, and constants set in the MAGPIE object. Those values include temperature, pressure, concentration, and associated equilibrium energy constants. The return value is the adsorption equilibrium value in mol/kg.

Definition at line 63 of file MAGPIE_Adsorption.h.

4.45.2 Constructor & Destructor Documentation

4.45.2.1 MAGPIE_Adsorption::MAGPIE_Adsorption (const InputParameters & parameters)

Standard MOOSE public constructor.

4.45.3 Member Function Documentation

4.45.3.1 virtual Real MAGPIE_Adsorption::computeValue () [protected],[virtual]

Required MOOSE function override.

This is the function that is called by the MOOSE framework when a calculation of the AuxVariable is needed. You are required to override this function for any inherited AuxKernel.

4.45.4 Member Data Documentation

4.45.4.1 unsigned int MAGPIE_Adsorption::_index [private]

Index of the gaseous species to calculate equilibria for.

Definition at line 76 of file MAGPIE_Adsorption.h.

4.45.4.2 const MaterialProperty< MAGPIE_DATA >& MAGPIE_Adsorption::_magpie_dat [private]

Material Property holding the MAGPIE data structure.

Definition at line 77 of file MAGPIE_Adsorption.h.

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

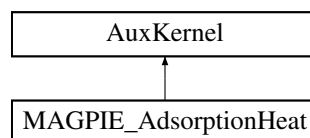
- [MAGPIE_Adsorption.h](#)

4.46 MAGPIE_AdsorptionHeat Class Reference

Magpie Adsorption Heat class inherits from AuxKernel.

```
#include <MAGPIE_AdsorptionHeat.h>
```

Inheritance diagram for MAGPIE_AdsorptionHeat:



Public Member Functions

- [MAGPIE_AdsorptionHeat](#) (const InputParameters ¶meters)
Standard MOOSE public constructor.

Protected Member Functions

- virtual Real [computeValue](#) ()
Required MOOSE function override.

Private Attributes

- unsigned int [_index](#)
Index of the gaseous species to calculate adsorbtion heat for.
- const MaterialProperty
< [MAGPIE_DATA](#) > & [_magpie_dat](#)

Material Property holding the MAGPIE data structure.

- [VariableValue](#) & [_solid_conc](#)

Reference to the adsorbed amount of the given species (AuxVariable)

4.46.1 Detailed Description

Magpie Adsorption Heat class inherits from AuxKernel.

This class object creates an AuxKernel for use in the MOOSE framework. The AuxKernel will calculate the heat of adsorption for a given species in the gas phase based on parameters, variables, and constants set in the MAGPIE object. Those values include temperature, pressure, concentration, and associated equilibrium energy constants. The return value is the heat of adsorption value in J/kg.

Definition at line 63 of file MAGPIE_AdsorptionHeat.h.

4.46.2 Constructor & Destructor Documentation

4.46.2.1 MAGPIE_AdsorptionHeat::MAGPIE_AdsorptionHeat (const InputParameters & parameters)

Standard MOOSE public constructor.

4.46.3 Member Function Documentation

4.46.3.1 virtual Real MAGPIE_AdsorptionHeat::computeValue () [protected], [virtual]

Required MOOSE function override.

This is the function that is called by the MOOSE framework when a calculation of the AuxVariable is needed. You are required to override this function for any inherited AuxKernel.

4.46.4 Member Data Documentation

4.46.4.1 unsigned int MAGPIE_AdsorptionHeat::_index [private]

Index of the gaseous species to calculate adsorbtion heat for.

Definition at line 76 of file MAGPIE_AdsorptionHeat.h.

4.46.4.2 const MaterialProperty< MAGPIE_DATA >& MAGPIE_AdsorptionHeat::_magpie_dat [private]

Material Property holding the MAGPIE data structure.

Definition at line 77 of file MAGPIE_AdsorptionHeat.h.

4.46.4.3 VariableValue& MAGPIE_AdsorptionHeat::_solid_conc [private]

Reference to the adsorbed amount of the given species (AuxVariable)

Definition at line 78 of file MAGPIE_AdsorptionHeat.h.

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

- [MAGPIE_AdsorptionHeat.h](#)

4.47 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`

4.47.1 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.

Definition at line 164 of file `magpie.h`.

4.47.2 Member Data Documentation

4.47.2.1 `std::vector<GPAST_DATA> MAGPIE_DATA::gpast_dat`

Definition at line 168 of file `magpie.h`.

4.47.2.2 `std::vector<GSTA_DATA> MAGPIE_DATA::gsta_dat`

Definition at line 166 of file `magpie.h`.

4.47.2.3 `std::vector<mSPD_DATA> MAGPIE_DATA::mspd_dat`

Definition at line 167 of file `magpie.h`.

4.47.2.4 `SYSTEM_DATA MAGPIE_DATA::sys_dat`

Definition at line 169 of file `magpie.h`.

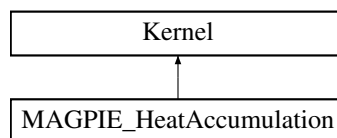
The documentation for this struct was generated from the following file:

- [magpie.h](#)

4.48 MAGPIE_HeatAccumulation Class Reference

```
#include <MAGPIE_HeatAccumulation.h>
```

Inheritance diagram for MAGPIE_HeatAccumulation:



Public Member Functions

- [MAGPIE_HeatAccumulation](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_porosity](#)
- const MaterialProperty< Real > & [_pellet_density](#)
- std::vector< VariableValue * > [_solid_heat](#)
- std::vector< VariableValue * > [_solid_heat_old](#)

4.48.1 Detailed Description

Definition at line 19 of file MAGPIE_HeatAccumulation.h.

4.48.2 Constructor & Destructor Documentation

4.48.2.1 `MAGPIE_HeatAccumulation::MAGPIE_HeatAccumulation (const InputParameters & parameters)`

4.48.3 Member Function Documentation

4.48.3.1 `virtual Real MAGPIE_HeatAccumulation::computeQpJacobian ()` [protected], [virtual]

4.48.3.2 `virtual Real MAGPIE_HeatAccumulation::computeQpResidual ()` [protected], [virtual]

4.48.4 Member Data Documentation

4.48.4.1 `const MaterialProperty<Real>& MAGPIE_HeatAccumulation::_pellet_density` [private]

Definition at line 31 of file MAGPIE_HeatAccumulation.h.

4.48.4.2 `const MaterialProperty<Real>& MAGPIE_HeatAccumulation::_porosity` [private]

Definition at line 30 of file MAGPIE_HeatAccumulation.h.

4.48.4.3 `std::vector<VariableValue*> MAGPIE_HeatAccumulation::_solid_heat` [private]

Definition at line 32 of file MAGPIE_HeatAccumulation.h.

4.48.4.4 `std::vector<VariableValue*> MAGPIE_HeatAccumulation::_solid_heat_old` [private]

Definition at line 33 of file MAGPIE_HeatAccumulation.h.

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

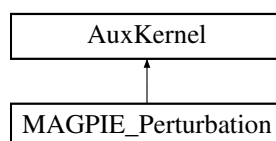
- [MAGPIE_HeatAccumulation.h](#)

4.49 MAGPIE_Perturbation Class Reference

Magpie Perturbation class inherits from AuxKernel.

```
#include <MAGPIE_Perturbation.h>
```

Inheritance diagram for MAGPIE_Perturbation:



Public Member Functions

- [MAGPIE_Perturbation](#) (const InputParameters ¶meters)
Standard MOOSE public constructor.

Protected Member Functions

- virtual Real [computeValue](#) ()
Required MOOSE function override.

Private Attributes

- unsigned int [_index](#)
Index of the gaseous species to calculate equilibria for.
- const MaterialProperty
< [MAGPIE_DATA](#) > & [_magpie_dat](#)
Material Property holding the MAGPIE data structure.

4.49.1 Detailed Description

Magpie Perturbation class inherits from AuxKernel.

This class object creates an AuxKernel for use in the MOOSE framework. The AuxKernel will calculate the perturbed equilibria for a given species in the gas phase based on parameters, variables, and constants set in the MAGPIE object. Those values include temperature, pressure, concentration, and associated equilibrium energy constants. The return value is the adsorption perturbation value in mol/kg.

Definition at line 72 of file MAGPIE_Perturbation.h.

4.49.2 Constructor & Destructor Documentation**4.49.2.1 MAGPIE_Perturbation::MAGPIE_Perturbation (const InputParameters & parameters)**

Standard MOOSE public constructor.

4.49.3 Member Function Documentation**4.49.3.1 virtual Real MAGPIE_Perturbation::computeValue () [protected],[virtual]**

Required MOOSE function override.

This is the function that is called by the MOOSE framework when a calculation of the AuxVariable is needed. You are required to override this function for any inherited AuxKernel.

4.49.4 Member Data Documentation**4.49.4.1 unsigned int MAGPIE_Perturbation::_index [private]**

Index of the gaseous species to calculate equilibria for.

Definition at line 85 of file MAGPIE_Perturbation.h.

4.49.4.2 `const MaterialProperty< MAGPIE_DATA >& MAGPIE_Perturbation::_magpie_dat` [private]

Material Property holding the MAGPIE data structure.

Definition at line 86 of file MAGPIE_Perturbation.h.

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

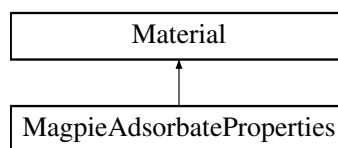
- [MAGPIE_Perturbation.h](#)

4.50 MagpieAdsorbateProperties Class Reference

[MagpieAdsorbateProperties](#) class object inherits from Material object.

```
#include <MagpieAdsorbateProperties.h>
```

Inheritance diagram for MagpieAdsorbateProperties:



Public Member Functions

- [MagpieAdsorbateProperties](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.

Protected Member Functions

- virtual void [computeQpProperties](#) ()
Required function override for Material objects in MOOSE.

Private Attributes

- `std::vector< unsigned int > _index`
Indices for the gas species in the system.
- `VariableValue & _temperature`
Reference to the coupled column temperature.
- `VariableValue & _total_pressure`
Reference to the coupled column pressure.
- `std::vector< VariableValue * > _gas_conc`
Pointer list to the coupled gases.
- `std::vector< int > _num_sites`
List of the number of sites each gas species' isotherm contains.
- `std::vector< Real > _max_capacity`
List of the maximum adsorption capacities of each gas species.
- `std::vector< Real > _molar_volume`
List of the van der Waal's molar volumes of each species.
- `std::vector< Real > _enthalpy_1`
List of the site 1 enthalpies for each gas species.
- `std::vector< Real > _enthalpy_2`
List of the site 2 enthalpies for each gas species.

- `std::vector< Real > _enthalpy_3`
List of the site 3 enthalpies for each gas species.
- `std::vector< Real > _enthalpy_4`
List of the site 4 enthalpies for each gas species.
- `std::vector< Real > _enthalpy_5`
List of the site 5 enthalpies for each gas species.
- `std::vector< Real > _enthalpy_6`
List of the site 6 enthalpies for each gas species.
- `std::vector< Real > _entropy_1`
List of the site 1 entropies for each gas species.
- `std::vector< Real > _entropy_2`
List of the site 2 entropies for each gas species.
- `std::vector< Real > _entropy_3`
List of the site 3 entropies for each gas species.
- `std::vector< Real > _entropy_4`
List of the site 4 entropies for each gas species.
- `std::vector< Real > _entropy_5`
List of the site 5 entropies for each gas species.
- `std::vector< Real > _entropy_6`
List of the site 6 entropies for each gas species.
- `MaterialProperty< MAGPIE_DATA > & _magpie_dat`
MaterialProperty object to hold the MAGPIE_DATA structure and all relevant information.

4.50.1 Detailed Description

[MagpieAdsorbateProperties](#) class object inherits from Material object.

This class object inherits from the Material object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will set up the [MAGPIE_DATA](#) structure (see [magpie.h](#)) based on user provided input from the input file. That information will be used to estimate the adsorption of each species in the system based on temperature, pressure, and concentrations of each species.

Note

The GSTA isotherm model for each species allows upto 6 energetically distinct adsorption sites. If those sites are not used by a particular species, then those energies should be left as zeros in the input files and the number of relevant sites for each species needs to be recorded in the input file. Each species is allowed to have a different number of adsorption sites in a particular adsorbent.

Definition at line 62 of file [MagpieAdsorbateProperties.h](#).

4.50.2 Constructor & Destructor Documentation

4.50.2.1 `MagpieAdsorbateProperties::MagpieAdsorbateProperties (const InputParameters & parameters)`

Required constructor for objects in MOOSE.

4.50.3 Member Function Documentation

4.50.3.1 `virtual void MagpieAdsorbateProperties::computeQpProperties () [protected], [virtual]`

Required function override for Material objects in MOOSE.

This function computes the material properties when they are needed by other MOOSE objects.

4.50.4 Member Data Documentation

4.50.4.1 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_1` [private]

List of the site 1 enthalpies for each gas species.

Definition at line 84 of file MagpieAdsorbateProperties.h.

4.50.4.2 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_2` [private]

List of the site 2 enthalpies for each gas species.

Definition at line 85 of file MagpieAdsorbateProperties.h.

4.50.4.3 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_3` [private]

List of the site 3 enthalpies for each gas species.

Definition at line 86 of file MagpieAdsorbateProperties.h.

4.50.4.4 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_4` [private]

List of the site 4 enthalpies for each gas species.

Definition at line 87 of file MagpieAdsorbateProperties.h.

4.50.4.5 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_5` [private]

List of the site 5 enthalpies for each gas species.

Definition at line 88 of file MagpieAdsorbateProperties.h.

4.50.4.6 `std::vector<Real> MagpieAdsorbateProperties::_enthalpy_6` [private]

List of the site 6 enthalpies for each gas species.

Definition at line 89 of file MagpieAdsorbateProperties.h.

4.50.4.7 `std::vector<Real> MagpieAdsorbateProperties::_entropy_1` [private]

List of the site 1 entropies for each gas species.

Definition at line 91 of file MagpieAdsorbateProperties.h.

4.50.4.8 `std::vector<Real> MagpieAdsorbateProperties::_entropy_2` [private]

List of the site 2 entropies for each gas species.

Definition at line 92 of file MagpieAdsorbateProperties.h.

4.50.4.9 `std::vector<Real> MagpieAdsorbateProperties::_entropy_3` [private]

List of the site 3 entropies for each gas species.

Definition at line 93 of file MagpieAdsorbateProperties.h.

4.50.4.10 `std::vector<Real> MagpieAdsorbateProperties::_entropy_4` [private]

List of the site 4 entropies for each gas species.

Definition at line 94 of file MagpieAdsorbateProperties.h.

4.50.4.11 `std::vector<Real> MagpieAdsorbateProperties::_entropy_5` [private]

List of the site 5 entropies for each gas species.

Definition at line 95 of file MagpieAdsorbateProperties.h.

4.50.4.12 `std::vector<Real> MagpieAdsorbateProperties::_entropy_6` [private]

List of the site 6 entropies for each gas species.

Definition at line 96 of file `MagpieAdsorbateProperties.h`.

4.50.4.13 `std::vector<VariableValue*> MagpieAdsorbateProperties::_gas_conc` [private]

Pointer list to the coupled gases.

Definition at line 78 of file `MagpieAdsorbateProperties.h`.

4.50.4.14 `std::vector<unsigned int> MagpieAdsorbateProperties::_index` [private]

Indices for the gas species in the system.

Definition at line 75 of file `MagpieAdsorbateProperties.h`.

4.50.4.15 `MaterialProperty< MAGPIE_DATA >& MagpieAdsorbateProperties::_magpie_dat` [private]

MaterialProperty object to hold the `MAGPIE_DATA` structure and all relevant information.

This is the object that needs to interface with the MAGPIE functions in order to solve for variable information such as adsorption capacities, mixed gas adsorption equilibria, and heats of adsorption.

Definition at line 102 of file `MagpieAdsorbateProperties.h`.

4.50.4.16 `std::vector<Real> MagpieAdsorbateProperties::_max_capacity` [private]

List of the maximum adsorption capacities of each gas species.

Definition at line 81 of file `MagpieAdsorbateProperties.h`.

4.50.4.17 `std::vector<Real> MagpieAdsorbateProperties::_molar_volume` [private]

List of the van der Waal's molar volumes of each species.

Definition at line 82 of file `MagpieAdsorbateProperties.h`.

4.50.4.18 `std::vector<int> MagpieAdsorbateProperties::_num_sites` [private]

List of the number of sites each gas species' isotherm contains.

Definition at line 80 of file `MagpieAdsorbateProperties.h`.

4.50.4.19 `VariableValue& MagpieAdsorbateProperties::_temperature` [private]

Reference to the coupled column temperature.

Definition at line 76 of file `MagpieAdsorbateProperties.h`.

4.50.4.20 `VariableValue& MagpieAdsorbateProperties::_total_pressure` [private]

Reference to the coupled column pressure.

Definition at line 77 of file `MagpieAdsorbateProperties.h`.

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

- [MagpieAdsorbateProperties.h](#)

4.51 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., $a_{ij} = A(i,j)$)
- 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 Triangular (this->x)
- [Matrix & lowerTriangularSolve](#) (const [Matrix](#) &L, const [Matrix](#) &v)
Function to solve the system $Lx=v$ for x given that L is lower Triangular (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.

4.51.1 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.

Definition at line 53 of file macaw.h.

4.51.2 Constructor & Destructor Documentation**4.51.2.1 `template<class T > Matrix< T >::Matrix (int rows, int columns)`**

Constructor for matrix with given number of rows and columns.

Definition at line 208 of file macaw.h.

4.51.2.2 `template<class T > Matrix< T >::Matrix (const Matrix< T > & M)`

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

Definition at line 247 of file macaw.h.

References `Matrix< T >::Data`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

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

Default constructor for creating an empty matrix.

Definition at line 292 of file macaw.h.

References Matrix< T >::num_cols, and Matrix< T >::num_rows.

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

Default destructor for clearing out memory.

Definition at line 302 of file macaw.h.

4.51.3 Member Function Documentation**4.51.3.1 template<class T > Matrix< T > & Matrix< T >::adjoint (const Matrix< T > & M)**

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

Definition at line 734 of file macaw.h.

References arg_matrix_same, mError, non_square_matrix, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.2 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.

Definition at line 489 of file macaw.h.

References arg_matrix_same, Matrix< T >::Data, Matrix< T >::determinate(), mError, non_square_matrix, Matrix< T >::num_cols, and Matrix< T >::num_rows.

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

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

Definition at line 1774 of file macaw.h.

References matvec_mis_match, mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.4 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.

Definition at line 1644 of file macaw.h.

References arg_matrix_same, mError, and Matrix< T >::num_rows.

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

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.

Definition at line 1344 of file macaw.h.

References arg_matrix_same, dim_mis_match, mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.6 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.

Definition at line 1686 of file macaw.h.

References `arg_matrix_same`, `matvec_mis_match`, `mError`, and `Matrix< T >::num_rows`.

4.51.3.7 `template<class T> int Matrix< T >::columns ()`

Function to return the number of columns in a matrix.

Definition at line 351 of file `macaw.h`.

4.51.3.8 `template<class T> void Matrix< T >::columnShrink ()`

Function to delete the last column of this matrix.

Definition at line 1741 of file `macaw.h`.

References `Matrix< T >::Data`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

4.51.3.9 `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.

Definition at line 1322 of file `macaw.h`.

References `dim_mis_match`, `matvec_mis_match`, and `mError`.

4.51.3.10 `template<class T> Matrix< T > & Matrix< T >::ConstantICFill (const T IC)`

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

Definition at line 1134 of file `macaw.h`.

References `dim_mis_match`, and `mError`.

4.51.3.11 `template<class T> T Matrix< T >::determinate ()`

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

Definition at line 358 of file `macaw.h`.

References `Matrix< T >::Data`, `Matrix< T >::determinate()`, `mError`, `non_square_matrix`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

Referenced by `Matrix< T >::cofactor()`, `Matrix< T >::determinate()`, and `Matrix< T >::inverse()`.

4.51.3.12 `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)

Definition at line 1395 of file `macaw.h`.

References `arg_matrix_same`, `dim_mis_match`, `mError`, `Matrix< T >::num_cols`, `Matrix< T >::num_rows`, and `singular_matrix`.

4.51.3.13 `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.

Definition at line 1369 of file `macaw.h`.

References `dim_mis_match`, and `mError`.

4.51.3.14 `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.

Definition at line 782 of file macaw.h.

References empty_matrix, and mError.

4.51.3.15 `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.

Definition at line 332 of file macaw.h.

References mError, Matrix< T >::operator>(), and out_of_bounds.

Referenced by Matrix< T >::lowerHessenberg2Triangular(), Matrix< T >::operator*(), and Matrix< T >::upperHessenberg2Triangular().

4.51.3.16 `template<class T> T Matrix< T >::inner_product (const Matrix< T > & x)`

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

Definition at line 463 of file macaw.h.

References dim_mis_match, mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.17 `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

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

Definition at line 1182 of file macaw.h.

References dim_mis_match, mError, and qo().

4.51.3.18 `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

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

Definition at line 1242 of file macaw.h.

References dim_mis_match, M_PI, mError, and qo().

4.51.3.19 `template<class T> Matrix< T > & Matrix< T >::inverse (const Matrix< T > & M)`

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

Definition at line 756 of file macaw.h.

References A, arg_matrix_same, Matrix< T >::Data, Matrix< T >::determinate(), mError, non_square_matrix, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.20 `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)

Definition at line 876 of file macaw.h.

References `A`, `arg_matrix_same`, `dim_mis_match`, `mError`, `Matrix< T>::num_cols`, `Matrix< T>::num_rows`, `singular_matrix`, and `unstable_matrix`.

4.51.3.21 `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.

Definition at line 1561 of file macaw.h.

References `arg_matrix_same`, `dim_mis_match`, `Matrix< T>::edit()`, `matrix_too_small`, `mError`, `Matrix< T>::num_cols`, `Matrix< T>::num_rows`, and `singular_matrix`.

4.51.3.22 `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)

Definition at line 1627 of file macaw.h.

References `arg_matrix_same`, `Matrix< T>::Data`, and `mError`.

4.51.3.23 `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 Triangular (this->x)

Definition at line 1471 of file macaw.h.

References `arg_matrix_same`, `dim_mis_match`, `mError`, `Matrix< T>::num_cols`, `Matrix< T>::num_rows`, and `singular_matrix`.

4.51.3.24 `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.

Definition at line 1031 of file macaw.h.

4.51.3.25 `template<class T> T Matrix< T>::norm ()`

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

Definition at line 427 of file macaw.h.

4.51.3.26 `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., $a_{ij} = A(i,j)$)

Definition at line 219 of file macaw.h.

References `mError`, and `out_of_bounds`.

Referenced by `Matrix< T>::edit()`.

4.51.3.27 `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.

Definition at line 232 of file macaw.h.

References mError, and out_of_bounds.

4.51.3.28 `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.

Definition at line 612 of file macaw.h.

References Matrix< T >::Data.

4.51.3.29 `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.

Definition at line 642 of file macaw.h.

References Matrix< T >::Data, dim_mis_match, Matrix< T >::edit(), mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.30 `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.

Definition at line 566 of file macaw.h.

References Matrix< T >::Data, dim_mis_match, mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.31 `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.

Definition at line 589 of file macaw.h.

References Matrix< T >::Data, dim_mis_match, mError, Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.32 `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.

Definition at line 627 of file macaw.h.

References Matrix< T >::Data.

4.51.3.33 `template<class T> Matrix< T > & Matrix< T >::operator= (const Matrix< T > & M)`

Equals operator for setting one matrix equal to another matrix.

Definition at line 264 of file macaw.h.

References Matrix< T >::num_cols, and Matrix< T >::num_rows.

4.51.3.34 `template<class T> void Matrix< T >::rowExtend (const Matrix< T > & v)`

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

Definition at line 1758 of file macaw.h.

References matvec_mis_match, mError, and Matrix< T >::num_cols.

4.51.3.35 `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.

Definition at line 1665 of file macaw.h.

References `arg_matrix_same`, `mError`, and `Matrix< T >::num_cols`.

4.51.3.36 `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*.

Definition at line 1707 of file macaw.h.

References `arg_matrix_same`, `matvec_mis_match`, `mError`, and `Matrix< T >::num_cols`.

4.51.3.37 `template<class T> int Matrix< T >::rows ()`

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

Definition at line 344 of file macaw.h.

4.51.3.38 `template<class T> void Matrix< T >::rowShrink ()`

Function to delete the last row of this matrix.

Definition at line 1728 of file macaw.h.

4.51.3.39 `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.

Definition at line 309 of file macaw.h.

References `invalid_size`, and `mError`.

4.51.3.40 `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.

Definition at line 1153 of file macaw.h.

References `arg_matrix_same`, `Matrix< T >::Data`, `dim_mis_match`, `mError`, and `Matrix< T >::num_rows`.

4.51.3.41 `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

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

Definition at line 1220 of file macaw.h.

References `dim_mis_match`, and `mError`.

4.51.3.42 `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 fill out a column matrix with zeros at all nodes except for the node indicated. That node's value will be the product of the node id with the *coeff* and *variable* values given.

Definition at line 1108 of file macaw.h.

References `dim_mis_match`, and `mError`.

4.51.3.43 `template<class T> T Matrix< T >::sum ()`

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

Definition at line 448 of file macaw.h.

4.51.3.44 `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.

Definition at line 676 of file macaw.h.

References `arg_matrix_same`, `Matrix< T >::Data`, `mError`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

4.51.3.45 `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.

Definition at line 699 of file macaw.h.

References `arg_matrix_same`, `Matrix< T >::Data`, `dim_mis_match`, `mError`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

4.51.3.46 `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.

Definition at line 981 of file macaw.h.

References `mError`, and `non_square_matrix`.

4.51.3.47 `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)

Definition at line 807 of file macaw.h.

References `A`, `arg_matrix_same`, `dim_mis_match`, `mError`, `Matrix< T >::num_cols`, and `Matrix< T >::num_rows`.

4.51.3.48 `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.

Definition at line 1279 of file macaw.h.

References `matvec_mis_match`, `mError`, and `non_square_matrix`.

4.51.3.49 `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.

Definition at line 1512 of file macaw.h.

References `arg_matrix_same`, `dim_mis_match`, `Matrix< T >::edit()`, `matrix_too_small`, `mError`, `Matrix< T >::num_cols`, `Matrix< T >::num_rows`, and `singular_matrix`.

4.51.3.50 `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)

Definition at line 1610 of file macaw.h.

References `arg_matrix_same`, `Matrix< T >::Data`, and `mError`.

4.51.3.51 `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 Triangular (this->x)

Definition at line 1430 of file macaw.h.

References `arg_matrix_same`, `dim_mis_match`, `mError`, `Matrix< T >::num_cols`, `Matrix< T >::num_rows`, and `singular_matrix`.

4.51.3.52 `template<class T> void Matrix< T >::zeros ()`

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

Definition at line 324 of file macaw.h.

4.51.4 Member Data Documentation

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

Storage vector for the elements of the matrix.

Definition at line 203 of file macaw.h.

Referenced by `Matrix< T >::cofactor()`, `Matrix< T >::columnShrink()`, `Matrix< T >::determinate()`, `Matrix< T >::inverse()`, `Matrix< T >::lowerHessenbergSolve()`, `Matrix< T >::Matrix()`, `Matrix< T >::operator*()`, `Matrix< T >::operator+()`, `Matrix< T >::operator-()`, `Matrix< T >::operator/()`, `Matrix< T >::SolnTransform()`, `Matrix< T >::transpose()`, `Matrix< T >::transpose_multiply()`, and `Matrix< T >::upperHessenbergSolve()`.

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

Number of columns of the matrix.

Definition at line 202 of file macaw.h.

Referenced by `Matrix< T >::adjoint()`, `Matrix< T >::cofactor()`, `Matrix< T >::columnExtend()`, `Matrix< T >::columnProjection()`, `Matrix< T >::columnShrink()`, `Matrix< T >::determinate()`, `Matrix< T >::diagonalSolve()`, `Matrix< T >::inner_product()`, `Matrix< T >::inverse()`, `Matrix< T >::ladshawSolve()`, `Matrix< T >::lowerHessenberg2Triangular()`, `Matrix< T >::lowerTriangularSolve()`, `Matrix< T >::Matrix()`, `Matrix< T >::operator*()`, `Matrix< T >::operator+()`, `Matrix< T >::operator-()`, `Matrix< T >::operator=()`, `Matrix< T >::rowExtend()`, `Matrix< T >::rowExtract()`, `Matrix< T >::rowReplace()`, `Matrix< T >::transpose()`, `Matrix< T >::transpose_multiply()`, `Matrix< T >::tridiagonalSolve()`, `Matrix< T >::upperHessenberg2Triangular()`, and `Matrix< T >::upperTriangularSolve()`.

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

Number of rows of the matrix.

Definition at line 201 of file macaw.h.

Referenced by `Matrix< T >::adjoint()`, `Matrix< T >::cofactor()`, `Matrix< T >::columnExtend()`, `Matrix< T >::columnExtract()`, `Matrix< T >::columnProjection()`, `Matrix< T >::columnReplace()`, `Matrix< T >::columnShrink()`, `Matrix< T >::determinate()`, `Matrix< T >::diagonalSolve()`, `Matrix< T >::inner_product()`, `Matrix< T >::inverse()`, `Matrix< T >::ladshawSolve()`, `Matrix< T >::lowerHessenberg2Triangular()`, `Matrix< T >::lowerTriangularSolve()`, `Matrix< T >::Matrix()`, `Matrix< T >::operator*()`, `Matrix< T >::operator+()`, `Matrix< T >::operator-()`, `Matrix< T >::operator=()`, `Matrix< T >::SolnTransform()`, `Matrix< T >::transpose()`, `Matrix< T >::transpose_multiply()`, `Matrix<`

`T >::tridiagonalSolve()`, `Matrix< T >::upperHessenberg2Triangular()`, and `Matrix< T >::upperTriangularSolve()`.

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

- [macaw.h](#)

4.52 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/cm³) {use RE3}.
- `double total_dyn_vis`
Calculated: Total dynamic viscosity (g/cm/s)
- `double kinematic_viscosity`
Calculated: Kinematic viscosity (cm²/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 (cm²/s)
- `std::vector< PURE_GAS > species_dat`
Vector of the pure gas info of all species.

4.52.1 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.

Definition at line 116 of file `egret.h`.

4.52.2 Member Data Documentation

4.52.2.1 `Matrix<double> MIXED_GAS::binary_diffusion`

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

Definition at line 136 of file egret.h.

4.52.2.2 `double MIXED_GAS::char_length`

Given: Characteristic Length (cm)

Definition at line 126 of file egret.h.

4.52.2.3 `bool MIXED_GAS::CheckMolefractions = true`

Given: True = Check Molefractions for errors.

Definition at line 120 of file egret.h.

4.52.2.4 `double MIXED_GAS::gas_temperature`

Given: Gas temperature (K)

Definition at line 124 of file egret.h.

4.52.2.5 `double MIXED_GAS::kinematic_viscosity`

Calculated: Kinematic viscosity (cm^2/s)

Definition at line 132 of file egret.h.

4.52.2.6 `std::vector<double> MIXED_GAS::molefraction`

Given: Gas molefractions of each species (-)

Definition at line 127 of file egret.h.

4.52.2.7 `int MIXED_GAS::N`

Given: Total number of gas species.

Definition at line 119 of file egret.h.

4.52.2.8 `double MIXED_GAS::Reynolds`

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

Definition at line 135 of file egret.h.

4.52.2.9 `std::vector<PURE_GAS> MIXED_GAS::species_dat`

Vector of the pure gas info of all species.

Definition at line 139 of file egret.h.

4.52.2.10 `double MIXED_GAS::total_density`

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

Definition at line 130 of file egret.h.

4.52.2.11 `double MIXED_GAS::total_dyn_vis`

Calculated: Total dynamic viscosity ($\text{g}/\text{cm}/\text{s}$)

Definition at line 131 of file egret.h.

4.52.2.12 double MIXED_GAS::total_molecular_weight

Calculated: Total molecular weight (g/mol)

Definition at line 133 of file egret.h.

4.52.2.13 double MIXED_GAS::total_pressure

Given: Total gas pressure (kPa)

Definition at line 123 of file egret.h.

4.52.2.14 double MIXED_GAS::total_specific_heat

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

Definition at line 134 of file egret.h.

4.52.2.15 double MIXED_GAS::velocity

Given: Gas phase velocity (cm/s)

Definition at line 125 of file egret.h.

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

- [egret.h](#)

4.53 mSPD_DATA Struct Reference

MSPD Data Structure.

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

Public Attributes

- double [s](#)
Area shape factor.
- double [v](#)
van der Waals Volume (cm³/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.

4.53.1 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.

Definition at line 110 of file magpie.h.

4.53.2 Member Data Documentation

4.53.2.1 double mSPD_DATA::eMax

Maximum lateral interaction energy (J/mol)

Definition at line 114 of file magpie.h.

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

Binary interaction parameter matrix (i,j)

Definition at line 115 of file magpie.h.

4.53.2.3 double mSPD_DATA::gama

Activity coefficient calculated from mSPD.

Definition at line 116 of file magpie.h.

4.53.2.4 double mSPD_DATA::s

Area shape factor.

Definition at line 112 of file magpie.h.

4.53.2.5 double mSPD_DATA::v

van der Waals Volume (cm³/mol)

Definition at line 113 of file magpie.h.

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

- [magpie.h](#)

4.54 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.

4.54.1 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.

Definition at line 569 of file lark.h.

4.54.2 Member Data Documentation

4.54.2.1 **Matrix**<double> NUM_JAC_DATA::dxj

Vector of perturbed x values.

Definition at line 574 of file lark.h.

4.54.2.2 **double** NUM_JAC_DATA::eps = sqrt(DBL_EPSILON)

Perturbation value.

Definition at line 571 of file lark.h.

4.54.2.3 **Matrix**<double> NUM_JAC_DATA::Fx

Vector of function evaluations at x.

Definition at line 572 of file lark.h.

4.54.2.4 **Matrix**<double> NUM_JAC_DATA::Fxp

Vector of function evaluations at x+eps.

Definition at line 573 of file lark.h.

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

- [lark.h](#)

4.55 OPTRANS_DATA Struct Reference

Data structure for implementation of linear operator transposition.

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

Public Attributes

- **Matrix**< double > **li**
The ith column vector of the identity operator.
- **Matrix**< double > **Ai**
The ith column vector of the user's linear operator.

4.55.1 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.

Definition at line 324 of file lark.h.

4.55.2 Member Data Documentation

4.55.2.1 **Matrix**<double> OPTRANS_DATA::Ai

The ith column vector of the user's linear operator.

Definition at line 327 of file lark.h.

4.55.2.2 Matrix<double> OPTRANS_DATA::li

The ith column vector of the identity operator.

Definition at line 326 of file lark.h.

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

- [lark.h](#)

4.56 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
Absolute 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.

4.56.1 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.

Definition at line 217 of file lark.h.

4.56.2 Member Data Documentation

4.56.2.1 double PCG_DATA::alpha

Step size for new solution.

Definition at line 222 of file lark.h.

4.56.2.2 **Matrix**<double> PCG_DATA::Ap

Result of matrix-vector multiplication.

Definition at line 240 of file lark.h.

4.56.2.3 double PCG_DATA::bestres

Best found residual norm.

Definition at line 229 of file lark.h.

4.56.2.4 **Matrix**<double> PCG_DATA::bestx

Best found solution to the linear system.

Definition at line 234 of file lark.h.

4.56.2.5 double PCG_DATA::beta

Step size for new search direction.

Definition at line 223 of file lark.h.

4.56.2.6 int PCG_DATA::iter = 0

Actual number of iterations taken.

Definition at line 220 of file lark.h.

4.56.2.7 int PCG_DATA::maxit = 0

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

Definition at line 219 of file lark.h.

4.56.2.8 bool PCG_DATA::Output = true

True = print messages to console.

Definition at line 231 of file lark.h.

4.56.2.9 **Matrix**<double> PCG_DATA::p

Search direction.

Definition at line 239 of file lark.h.

4.56.2.10 **Matrix**<double> PCG_DATA::r

Residual vector for the linear system.

Definition at line 235 of file lark.h.

4.56.2.11 **Matrix**<double> PCG_DATA::r_old

Previous residual vector.

Definition at line 236 of file lark.h.

4.56.2.12 **double** PCG_DATA::relres

Relative residual norm.

Definition at line 227 of file lark.h.

4.56.2.13 **double** PCG_DATA::relres_base

Initial residual norm.

Definition at line 228 of file lark.h.

4.56.2.14 **double** PCG_DATA::res

Absolute residual norm.

Definition at line 226 of file lark.h.

4.56.2.15 **double** PCG_DATA::tol_abs = 1e-6

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

Definition at line 225 of file lark.h.

4.56.2.16 **double** PCG_DATA::tol_rel = 1e-6

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

Definition at line 224 of file lark.h.

4.56.2.17 **Matrix**<double> PCG_DATA::x

Current solution to the linear system.

Definition at line 233 of file lark.h.

4.56.2.18 **Matrix**<double> PCG_DATA::z

Preconditioned residual vector (result of precon function)

Definition at line 237 of file lark.h.

4.56.2.19 **Matrix**<double> PCG_DATA::z_old

Previous preconditioned residual vector.

Definition at line 238 of file lark.h.

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

- [lark.h](#)

4.57 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.

4.57.1 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.

Definition at line 449 of file lark.h.

4.57.2 Member Data Documentation

4.57.2.1 double PICARD_DATA::bestres

Best found residual norm.

Definition at line 459 of file lark.h.

4.57.2.2 Matrix<double> PICARD_DATA::bestx

Best found solution vector.

Definition at line 464 of file lark.h.

4.57.2.3 int PICARD_DATA::iter = 0

Actual number of iterations.

Definition at line 452 of file lark.h.

4.57.2.4 int PICARD_DATA::maxit = 0

Maximum allowable iterations - default = min(3*vec_size,1000)

Definition at line 451 of file lark.h.

4.57.2.5 bool PICARD_DATA::Output = true

True = print messages to console.

Definition at line 461 of file lark.h.

4.57.2.6 Matrix<double> PICARD_DATA::r

Residual of the non-linear system.

Definition at line 465 of file lark.h.

4.57.2.7 double PICARD_DATA::relres

Relative residual norm of the iterate.

Definition at line 457 of file lark.h.

4.57.2.8 double PICARD_DATA::relres_base

Initial residual norm.

Definition at line 458 of file lark.h.

4.57.2.9 double PICARD_DATA::res

Residual norm of the iterate.

Definition at line 456 of file lark.h.

4.57.2.10 double PICARD_DATA::tol_abs = 1e-6

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

Definition at line 455 of file lark.h.

4.57.2.11 double PICARD_DATA::tol_rel = 1e-6

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

Definition at line 454 of file lark.h.

4.57.2.12 Matrix<double> PICARD_DATA::x0

Previous iterate solution vector.

Definition at line 463 of file lark.h.

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

- [lark.h](#)

4.58 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 [fun_call](#) = 0
Actual number of function calls made.
- 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.

4.58.1 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.

Definition at line 511 of file `lark.h`.

4.58.2 Member Data Documentation

4.58.2.1 BACKTRACK_DATA PJFNK_DATA::backtrack_dat

Data structure for the Backtracking Linesearch algorithm.

Definition at line 550 of file `lark.h`.

4.58.2.2 Matrix<double> PJFNK_DATA::bestx

Best found solution vector to the non-linear system.

Definition at line 538 of file `lark.h`.

4.58.2.3 BiCGSTAB_DATA PJFNK_DATA::bicgstab_dat

Data structure for the BiCGSTAB method.

Definition at line 543 of file lark.h.

4.58.2.4 bool PJFNK_DATA::Bounce = false

True = allow Linesearch to go outside local well, False = Strict local convergence.

Definition at line 532 of file lark.h.

4.58.2.5 CGS_DATA PJFNK_DATA::cgs_dat

Data structure for the CGS method.

Definition at line 544 of file lark.h.

4.58.2.6 double PJFNK_DATA::eps =sqrt(DBL_EPSILON)

Value of epsilon used jacvec - default = sqrt(DBL_EPSILON)

Definition at line 527 of file lark.h.

4.58.2.7 Matrix<double> PJFNK_DATA::F

Stored fuction evaluation at x (also the residual)

Definition at line 534 of file lark.h.

4.58.2.8 int PJFNK_DATA::fun_call = 0

Actual number of function calls made.

Definition at line 515 of file lark.h.

4.58.2.9 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.

Definition at line 559 of file lark.h.

4.58.2.10 Matrix<double> PJFNK_DATA::Fv

Stored function evaluation at x+eps*v.

Definition at line 535 of file lark.h.

4.58.2.11 GCR_DATA PJFNK_DATA::gcr_dat

Data structure for the GCR method.

Definition at line 546 of file lark.h.

4.58.2.12 GMRESLP_DATA PJFNK_DATA::gmreslp_dat

Data structure for the GMRESLP method.

Definition at line 541 of file lark.h.

4.58.2.13 GMRESR_DATA PJFNK_DATA::gmresr_dat

Data structure for the GMRESR method.

Definition at line 547 of file lark.h.

4.58.2.14 GMRESRP_DATA PJFNK_DATA::gmresrp_dat

Data structure for the GMRESRP method.

Definition at line 545 of file lark.h.

4.58.2.15 int PJFNK_DATA::l_iter = 0

Number of linear iterations.

Definition at line 514 of file lark.h.

4.58.2.16 bool PJFNK_DATA::L_Output = false

True = print Linear messages to console.

Definition at line 530 of file lark.h.

4.58.2.17 double PJFNK_DATA::lin_tol_abs = 1e-6

Absolute tolerance of the linear solver - default = 1e-6.

Definition at line 522 of file lark.h.

4.58.2.18 double PJFNK_DATA::lin_tol_rel = 1e-6

Relative tolerance of the linear solver - default = 1e-6.

Definition at line 521 of file lark.h.

4.58.2.19 int PJFNK_DATA::linear_solver = -1

Flag to denote which linear solver to use - default = PJFNK Chooses.

Definition at line 517 of file lark.h.

4.58.2.20 bool PJFNK_DATA::LineSearch = false

True = use Backtracking Linesearch for global convergence.

Definition at line 531 of file lark.h.

4.58.2.21 double PJFNK_DATA::nl_bestres

Best found residual norm.

Definition at line 526 of file lark.h.

4.58.2.22 int PJFNK_DATA::nl_iter = 0

Number of non-linear iterations.

Definition at line 513 of file lark.h.

4.58.2.23 int PJFNK_DATA::nl_maxit = 0

Maximum allowable non-linear steps.

Definition at line 516 of file lark.h.

4.58.2.24 bool PJFNK_DATA::NL_Output = true

True = print PJFNK messages to console.

Definition at line 529 of file lark.h.

4.58.2.25 double PJFNK_DATA::nl_relres

Relative residual for the non-linear system.

Definition at line 524 of file lark.h.

4.58.2.26 double PJFNK_DATA::nl_res

Absolute residual norm for the non-linear system.

Definition at line 523 of file lark.h.

4.58.2.27 double PJFNK_DATA::nl_res_base

Initial residual norm for the non-linear system.

Definition at line 525 of file lark.h.

4.58.2.28 double PJFNK_DATA::nl_tol_abs = 1e-6

Absolute Convergence tolerance for non-linear system - default = 1e-6.

Definition at line 519 of file lark.h.

4.58.2.29 double PJFNK_DATA::nl_tol_rel = 1e-6

Relative Convergence tol for the non-linear system - default = 1e-6.

Definition at line 520 of file lark.h.

4.58.2.30 PCG_DATA PJFNK_DATA::pcg_dat

Data structure for the PCG method.

Definition at line 542 of file lark.h.

4.58.2.31 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.

Definition at line 561 of file lark.h.

4.58.2.32 const void* PJFNK_DATA::precon_data

Data structure pointer for user's preconditioning data.

Definition at line 557 of file lark.h.

4.58.2.33 const void* PJFNK_DATA::res_data

Data structure pointer for user's residual data.

Definition at line 555 of file lark.h.

4.58.2.34 Matrix<double> PJFNK_DATA::v

Stored vector of $x + \epsilon v$.

Definition at line 536 of file lark.h.

4.58.2.35 Matrix<double> PJFNK_DATA::x

Current solution vector for the non-linear system.

Definition at line 537 of file lark.h.

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

- [lark.h](#)

4.59 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 (cm²/s)
- double [dynamic_viscosity](#)
Calculated: dynamic viscosities (g/cm/s)
- double [density](#)
Calculated: gas densities (g/cm³) {use RE3}.
- double [Schmidt](#)
Calculated: Value of the Schmidt number (-)

4.59.1 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.

Definition at line 95 of file egret.h.

4.59.2 Member Data Documentation

4.59.2.1 double PURE_GAS::density

Calculated: gas densities (g/cm³) {use RE3}.

Definition at line 107 of file egret.h.

4.59.2.2 double PURE_GAS::dynamic_viscosity

Calculated: dynamic viscosities (g/cm/s)

Definition at line 106 of file egret.h.

4.59.2.3 double PURE_GAS::molecular_diffusion

Calculated: molecular diffusivities (cm^2/s)

Definition at line 105 of file egret.h.

4.59.2.4 double PURE_GAS::molecular_weight

Given: molecular weights (g/mol)

Definition at line 98 of file egret.h.

4.59.2.5 double PURE_GAS::Schmidt

Calculated: Value of the Schmidt number (-)

Definition at line 108 of file egret.h.

4.59.2.6 double PURE_GAS::specific_heat

Given: Specific heat of the gas (J/g/K)

Definition at line 102 of file egret.h.

4.59.2.7 double PURE_GAS::Sutherland_Const

Given: Sutherland's Constant (K)

Definition at line 100 of file egret.h.

4.59.2.8 double PURE_GAS::Sutherland_Temp

Given: Sutherland's Reference Temperature (K)

Definition at line 99 of file egret.h.

4.59.2.9 double PURE_GAS::Sutherland_Viscosity

Given: Sutherland's Reference Viscosity (g/cm/s)

Definition at line 101 of file egret.h.

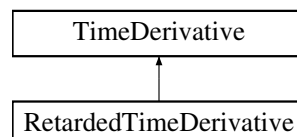
The documentation for this struct was generated from the following file:

- [egret.h](#)

4.60 RetardedTimeDerivative Class Reference

```
#include <RetardedTimeDerivative.h>
```

Inheritance diagram for RetardedTimeDerivative:

**Public Member Functions**

- [RetardedTimeDerivative](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- int [_index](#)
- const MaterialProperty
< std::vector< Real > > & [_retardation](#)

4.60.1 Detailed Description

Definition at line 12 of file RetardedTimeDerivative.h.

4.60.2 Constructor & Destructor Documentation

4.60.2.1 RetardedTimeDerivative::RetardedTimeDerivative (const InputParameters & *parameters*)

4.60.3 Member Function Documentation

4.60.3.1 virtual Real RetardedTimeDerivative::computeQpJacobian () [protected], [virtual]

4.60.3.2 virtual Real RetardedTimeDerivative::computeQpResidual () [protected], [virtual]

4.60.4 Member Data Documentation

4.60.4.1 int RetardedTimeDerivative::_index [private]

Definition at line 23 of file RetardedTimeDerivative.h.

4.60.4.2 const MaterialProperty<std::vector<Real>>& RetardedTimeDerivative::_retardation [private]

Definition at line 24 of file RetardedTimeDerivative.h.

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

- [RetardedTimeDerivative.h](#)

4.61 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 around 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 cm²) - only if pellet is not spherical.
- double `char_micro`
Characteristic size for micro scale (um or um²) - 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 (cm²/hr)*
- double(* [eval_surfDiff](#))(int i, int l, const void *[user_data](#))
- Function pointer for evaluating surface diffusion (um²/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)*

4.61.1 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 simplify 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.

Definition at line 92 of file scopsowl.h.

4.61.2 Member Data Documentation

4.61.2.1 double SCOPSOWL_DATA::binder_fraction

Volume of binder per total volume of pellet (-)

Definition at line 116 of file scopsowl.h.

4.61.2.2 double SCOPSOWL_DATA::binder_poresize

Nominal radius of the binder pores (cm)

Definition at line 118 of file scopsowl.h.

4.61.2.3 double SCOPSOWL_DATA::binder_porosity

Volume of pores per volume of binder (-)

Definition at line 117 of file scopsowl.h.

4.61.2.4 double SCOPSOWL_DATA::char_macro

Characteristic size for macro scale (cm or cm^2) - only if pellet is not spherical.

Definition at line 114 of file scopsowl.h.

4.61.2.5 double SCOPSOWL_DATA::char_micro

Characteristic size for micro scale (μm or μm^2) - only if crystal is not spherical.

Definition at line 115 of file scopsowl.h.

4.61.2.6 int SCOPSOWL_DATA::coord_macro

Coordinate system for large pellet.

Definition at line 95 of file scopsowl.h.

4.61.2.7 int SCOPSOWL_DATA::coord_micro

Coordinate system for small crystal (if any)

Definition at line 96 of file scopsowl.h.

4.61.2.8 double SCOPSOWL_DATA::crystal_radius

Nominal radius of the crystal - microscale domain (μm)

Definition at line 113 of file scopsowl.h.

4.61.2.9 bool SCOPSOWL_DATA::DirichletBC = false

True = Dirichlet BC; False = Neumann BC.

Definition at line 121 of file scopsowl.h.

4.61.2.10 double(* SCOPSOWL_DATA::eval_ads)(int i, int l, const void *user_data)

Function pointer for evaluating adsorption (mol/kg)

Definition at line 127 of file scopsowl.h.

4.61.2.11 double(* SCOPSOWL_DATA::eval_diff)(int i, int l, const void *user_data)

Function pointer for evaluating pore diffusion (cm^2/hr)

Definition at line 129 of file scopsowl.h.

4.61.2.12 double(* SCOPSOWL_DATA::eval_kf)(int i, const void *user_data)

Function pointer for evaluating film mass transfer (cm/hr)

Definition at line 131 of file scopsowl.h.

4.61.2.13 double(* SCOPSOWL_DATA::eval_retard)(int i, int l, const void *user_data)

Function pointer for evaluating retardation (-)

Definition at line 128 of file scopsowl.h.

4.61.2.14 double(* SCOPSOWL_DATA::eval_surfDiff)(int i, int l, const void *user_data)

Function pointer for evaluating surface diffusion ($\mu\text{m}^2/\text{hr}$)

Definition at line 130 of file scopsowl.h.

4.61.2.15 `std::vector<FINCH_DATA> SCOPSOWL_DATA::finch_dat`

Data structure for pore adsorption kinetics for all species (u in mol/L)

Definition at line 136 of file scopsowl.h.

4.61.2.16 `MIXED_GAS* SCOPSOWL_DATA::gas_dat`

Pointer to the [MIXED_GAS](#) data structure (may or may not be used)

Definition at line 134 of file scopsowl.h.

4.61.2.17 `double SCOPSOWL_DATA::gas_temperature`

Gas phase temperature (K)

Definition at line 111 of file scopsowl.h.

4.61.2.18 `double SCOPSOWL_DATA::gas_velocity`

Superficial Gas Velocity around pellet (cm/s)

Definition at line 109 of file scopsowl.h.

4.61.2.19 `bool SCOPSOWL_DATA::Heterogeneous = true`

True = pellet is made of binder and crystals, False = all one phase.

Definition at line 107 of file scopsowl.h.

4.61.2.20 `int SCOPSOWL_DATA::level = 2`

Level of coupling between the different scales (default = 2)

Definition at line 97 of file scopsowl.h.

4.61.2.21 `MAGPIE_DATA SCOPSOWL_DATA::magpie_dat`

Data structure for a magpie problem (to be used if not using skua)

Definition at line 135 of file scopsowl.h.

4.61.2.22 `bool SCOPSOWL_DATA::NonLinear = true`

True = Non-linear solver; False = Linear solver.

Definition at line 122 of file scopsowl.h.

4.61.2.23 `FILE* SCOPSOWL_DATA::OutputFile`

Output file pointer to the output file for postprocesses.

Definition at line 126 of file scopsowl.h.

4.61.2.24 `std::vector<SCOPSOWL_PARAM_DATA> SCOPSOWL_DATA::param_dat`

Data structure for parameter info for all species.

Definition at line 137 of file scopsowl.h.

4.61.2.25 `double SCOPSOWL_DATA::pellet_density`

Mass of the pellet per volume of pellet (kg/L)

Definition at line 119 of file scopsowl.h.

4.61.2.26 double SCOPSOWL_DATA::pellet_radius

Nominal radius of the pellet - macroscale domain (cm)

Definition at line 112 of file scopsowl.h.

4.61.2.27 bool SCOPSOWL_DATA::Print2Console = true

True = results to console; False = no printing.

Definition at line 105 of file scopsowl.h.

4.61.2.28 bool SCOPSOWL_DATA::Print2File = true

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

Definition at line 104 of file scopsowl.h.

4.61.2.29 double SCOPSOWL_DATA::sim_time

Stopping time for the simulation (hrs)

Definition at line 98 of file scopsowl.h.

4.61.2.30 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)

Definition at line 139 of file scopsowl.h.

4.61.2.31 bool SCOPSOWL_DATA::SurfDiff = true

True = includes SKUA simulation if Heterogeneous; False = only uses MAGPIE.

Definition at line 106 of file scopsowl.h.

4.61.2.32 double SCOPSOWL_DATA::t

Current time of the simulations (hrs)

Definition at line 100 of file scopsowl.h.

4.61.2.33 double SCOPSOWL_DATA::t_counter = 0.0

Counter for the time output.

Definition at line 101 of file scopsowl.h.

4.61.2.34 double SCOPSOWL_DATA::t_old

Old time of the simulations (hrs)

Definition at line 99 of file scopsowl.h.

4.61.2.35 double SCOPSOWL_DATA::t_print

Print output at every t_print time (hrs)

Definition at line 102 of file scopsowl.h.

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

Temporary place holder for gas mole fractions in other locations (-)

Definition at line 124 of file scopsowl.h.

4.61.2.37 double SCOPSOWL_DATA::total_pressure

Gas phase total pressure (kPa)

Definition at line 110 of file scopsowl.h.

4.61.2.38 unsigned long int SCOPSOWL_DATA::total_steps

Running total of all calculation steps.

Definition at line 94 of file scopsowl.h.

4.61.2.39 const void* SCOPSOWL_DATA::user_data

Data structure for users info to calculate parameters.

Definition at line 133 of file scopsowl.h.

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

Outside mole fractions of each component (-)

Definition at line 123 of file scopsowl.h.

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

- [scopsowl.h](#)

4.62 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 Dirichlet BCs (L/kg)*
- double [pore_diffusion](#)
- Value for constant pore diffusion (cm²/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 (um²/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.*

4.62.1 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 SCOPSOWL functions.

Definition at line 44 of file scopsowl.h.

4.62.2 Member Data Documentation

4.62.2.1 double SCOPSOWL_PARAM_DATA::activation_energy

Activation energy for surface diffusion (J/mol)

Definition at line 69 of file scopsowl.h.

4.62.2.2 bool SCOPSOWL_PARAM_DATA::Adsorbable

True = species can adsorb; False = species cannot adsorb.

Definition at line 75 of file scopsowl.h.

4.62.2.3 double SCOPSOWL_PARAM_DATA::affinity

Affinity parameter used in empirical adjustments (-)

Definition at line 72 of file scopsowl.h.

4.62.2.4 Matrix<double> SCOPSOWL_PARAM_DATA::dq_dc

Storage vector for current adsorption slope/strength (dq/dc) (L/kg)

Definition at line 52 of file scopsowl.h.

4.62.2.5 double SCOPSOWL_PARAM_DATA::dq_dco

Boundary value of adsorption slope for Dirichelt BCs (L/kg)

Definition at line 64 of file scopsowl.h.

4.62.2.6 double SCOPSOWL_PARAM_DATA::film_transfer

Value for constant film mass transfer (cm/hr)

Definition at line 67 of file scopsowl.h.

4.62.2.7 double SCOPSOWL_PARAM_DATA::pore_diffusion

Value for constant pore diffusion (cm^2/hr)

Definition at line 66 of file scopsowl.h.

4.62.2.8 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg

Average adsorbed amount for a species at each node (mol/kg)

Definition at line 46 of file scopsowl.h.

4.62.2.9 Matrix<double> SCOPSOWL_PARAM_DATA::qAvg_old

Old Average adsorbed amount for a species at each node (mol/kg)

Definition at line 47 of file scopsowl.h.

4.62.2.10 double SCOPSOWL_PARAM_DATA::qIntegralAvg

Integral average of adsorption over the entire pellet (mol/kg)

Definition at line 56 of file scopsowl.h.

4.62.2.11 double SCOPSOWL_PARAM_DATA::qIntegralAvg_old

Old Integral average of adsorption over the entire pellet (mol/kg)

Definition at line 57 of file scopsowl.h.

4.62.2.12 double SCOPSOWL_PARAM_DATA::qo

Boundary value of adsorption if using Dirichlet BCs (mol/kg)

Definition at line 62 of file scopsowl.h.

4.62.2.13 Matrix<double> SCOPSOWL_PARAM_DATA::Qst

Heat of adsorption for all nodes (J/mol)

Definition at line 49 of file scopsowl.h.

4.62.2.14 Matrix<double> SCOPSOWL_PARAM_DATA::Qst_old

Old Heat of adsorption for all nodes (J/mol)

Definition at line 50 of file scopsowl.h.

4.62.2.15 double SCOPSOWL_PARAM_DATA::QstAvg

Integral average heat of adsorption (J/mol)

Definition at line 59 of file scopsowl.h.

4.62.2.16 double SCOPSOWL_PARAM_DATA::QstAvg_old

Old integral average heat of adsorption (J/mol)

Definition at line 60 of file scopsowl.h.

4.62.2.17 double SCOPSOWL_PARAM_DATA::Qsto

Boundary value of adsorption heat if using Dirichlet BCs (J/mol)

Definition at line 63 of file scopsowl.h.

4.62.2.18 double SCOPSOWL_PARAM_DATA::ref_diffusion

Reference state surface diffusivity (um^2/hr)

Definition at line 70 of file scopsowl.h.

4.62.2.19 double SCOPSOWL_PARAM_DATA::ref_pressure

Definition at line 73 of file scopsowl.h.

4.62.2.20 double SCOPSOWL_PARAM_DATA::ref_temperature

Reference temperature for empirical adjustments (K)

Definition at line 71 of file scopsowl.h.

4.62.2.21 std::string SCOPSOWL_PARAM_DATA::speciesName

String to hold the name of each species.

Definition at line 77 of file scopsowl.h.

4.62.2.22 double SCOPSOWL_PARAM_DATA::xIC

Initial conditions for adsorbed molefractions.

Definition at line 54 of file scopsowl.h.

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

- [scopsowl.h](#)

4.63 SKUA_DATA Struct Reference

Data structure for all simulation information in SKUA.

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

Public Attributes

- unsigned long int [total_steps](#)
Running total of all calculation steps.
- int [coord](#)
Used to determine the coordinates of the problem.
- 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
- Counts for print times for output (hrs)*
- double `t_print`
- Prints out every t_print time (hrs)*
- double `qTn`
- Old total amounts adsorbed (mol/kg)*
- double `qTnp1`
- New total amounts adsorbed (mol/kg)*
- bool `Print2File` = true
- True = results to .txt; False = no printing.*
- bool `Print2Console` = true
- True = results to console; False = no printing.*
- double `gas_velocity`
- Superficial Gas Velocity around pellet (cm/s)*
- double `pellet_radius`
- Nominal radius of the pellet/crystal (um)*
- double `char_measure`
- Length or Area if in Cylindrical or Cartesian coordinates (um or um²)*
- bool `DirichletBC` = true
- 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 (-)*
- FILE * `OutputFile`
- Output file pointer to the output file.*
- double(* `eval_diff`)(int i, int l, const void *`user_data`)
- Function pointer for evaluating surface diffusivity.*
- double(* `eval_kf`)(int i, const void *`user_data`)
- Function pointer for evaluating film mass transfer.*
- const void * `user_data`
- Data structure for user's information needed in parameter functions.*
- `MAGPIE_DATA` `magpie_dat`
- Data structure for adsorption equilibria (see [magpie.h](#))*
- `MIXED_GAS` * `gas_dat`
- Pointer to the `MIXED_GAS` data structure (see [egret.h](#))*
- `std::vector< FINCH_DATA > finch_dat`
- Data structure for adsorption kinetics (see [finch.h](#))*
- `std::vector< SKUA_PARAM > param_dat`
- Data structure for SKUA specific parameters.*

4.63.1 Detailed Description

Data structure for all simulation information in SKUA.

C-style object holding all data, functions, and other objects needed to successfully run a SKUA simulation. This object holds system information, such as boundary condition type, adsorbent size, and total adsorption, and also contains structure for EGRET ([egret.h](#)), FINCH ([finch.h](#)), and MAGPIE ([magpie.h](#)) calculations. Function pointers for evaluation of the surface diffusivity and film mass transfer coefficients can be overridden by the user to change the behavior of the SKUA simulation. However, defaults are also provided for these functions.

Definition at line 84 of file `skua.h`.

4.63.2 Member Data Documentation

4.63.2.1 double SKUA_DATA::char_measure

Length or Area if in Cylindrical or Cartesian coordinates (um or um²)

Definition at line 100 of file skua.h.

4.63.2.2 int SKUA_DATA::coord

Used to determine the coordinates of the problem.

Definition at line 87 of file skua.h.

4.63.2.3 bool SKUA_DATA::DirichletBC = true

True = Dirichlet BC; False = Neumann BC.

Definition at line 101 of file skua.h.

4.63.2.4 double(* SKUA_DATA::eval_diff)(int i, int l, const void *user_data)

Function pointer for evaluating surface diffusivity.

Definition at line 106 of file skua.h.

4.63.2.5 double(* SKUA_DATA::eval_kf)(int i, const void *user_data)

Function pointer for evaluating film mass transfer.

Definition at line 107 of file skua.h.

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

Data structure for adsorption kinetics (see [finch.h](#))

Definition at line 111 of file skua.h.

4.63.2.7 MIXED_GAS* SKUA_DATA::gas_dat

Pointer to the [MIXED_GAS](#) data structure (see [egret.h](#))

Definition at line 110 of file skua.h.

4.63.2.8 double SKUA_DATA::gas_velocity

Superficial Gas Velocity around pellet (cm/s)

Definition at line 98 of file skua.h.

4.63.2.9 MAGPIE_DATA SKUA_DATA::magpie_dat

Data structure for adsorption equilibria (see [magpie.h](#))

Definition at line 109 of file skua.h.

4.63.2.10 bool SKUA_DATA::NonLinear = true

True = Non-linear solver; False = Linear solver.

Definition at line 102 of file skua.h.

4.63.2.11 FILE* SKUA_DATA::OutputFile

Output file pointer to the output file.

Definition at line 105 of file skua.h.

4.63.2.12 `std::vector<SKUA_PARAM> SKUA_DATA::param_dat`

Data structure for SKUA specific parameters.

Definition at line 112 of file skua.h.

4.63.2.13 `double SKUA_DATA::pellet_radius`

Nominal radius of the pellet/crystal (um)

Definition at line 99 of file skua.h.

4.63.2.14 `bool SKUA_DATA::Print2Console = true`

True = results to console; False = no printing.

Definition at line 96 of file skua.h.

4.63.2.15 `bool SKUA_DATA::Print2File = true`

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

Definition at line 95 of file skua.h.

4.63.2.16 `double SKUA_DATA::qTn`

Old total amounts adsorbed (mol/kg)

Definition at line 93 of file skua.h.

4.63.2.17 `double SKUA_DATA::qTnp1`

New total amounts adsorbed (mol/kg)

Definition at line 94 of file skua.h.

4.63.2.18 `double SKUA_DATA::sim_time`

Stopping time for the simulation (hrs)

Definition at line 88 of file skua.h.

4.63.2.19 `double SKUA_DATA::t`

Current time of the simulations (hrs)

Definition at line 90 of file skua.h.

4.63.2.20 `double SKUA_DATA::t_counter = 0.0`

Counts for print times for output (hrs)

Definition at line 91 of file skua.h.

4.63.2.21 `double SKUA_DATA::t_old`

Old time of the simulations (hrs)

Definition at line 89 of file skua.h.

4.63.2.22 `double SKUA_DATA::t_print`

Prints out every t_print time (hrs)

Definition at line 92 of file skua.h.

4.63.2.23 unsigned long int SKUA_DATA::total_steps

Running total of all calculation steps.

Definition at line 86 of file skua.h.

4.63.2.24 const void* SKUA_DATA::user_data

Data structure for user's information needed in parameter functions.

Definition at line 108 of file skua.h.

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

Outside mole fractions of each component (-)

Definition at line 103 of file skua.h.

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

- [skua.h](#)

4.64 SKUA_PARAM Struct Reference

Data structure for species' parameters in SKUA.

```
#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](#)

4.64.1 Detailed Description

Data structure for species' parameters in SKUA.

C-style object holding data and parameters associated with the gas/solid species in the overall SKUA system. These parameters are used in to modify surface diffusivity with temperature, establish film mass transfer coefficients, formulate the initial conditions, and store solution results for heat of adsorption and adsorbed mole fractions. One of these objects will be created for each species in the gas system.

Definition at line 56 of file skua.h.

4.64.2 Member Data Documentation

4.64.2.1 double SKUA_PARAM::activation_energy

Definition at line 58 of file skua.h.

4.64.2.2 bool SKUA_PARAM::Adsorbable

Definition at line 73 of file skua.h.

4.64.2.3 double SKUA_PARAM::affinity

Definition at line 61 of file skua.h.

4.64.2.4 double SKUA_PARAM::film_transfer

Definition at line 63 of file skua.h.

4.64.2.5 double SKUA_PARAM::Qstn

Definition at line 68 of file skua.h.

4.64.2.6 double SKUA_PARAM::Qstnp1

Definition at line 69 of file skua.h.

4.64.2.7 double SKUA_PARAM::ref_diffusion

Definition at line 59 of file skua.h.

4.64.2.8 double SKUA_PARAM::ref_pressure

Definition at line 62 of file skua.h.

4.64.2.9 double SKUA_PARAM::ref_temperature

Definition at line 60 of file skua.h.

4.64.2.10 std::string SKUA_PARAM::speciesName

Definition at line 75 of file skua.h.

4.64.2.11 double SKUA_PARAM::xIC

Definition at line 65 of file skua.h.

4.64.2.12 double SKUA_PARAM::xn

Definition at line 70 of file skua.h.

4.64.2.13 double SKUA_PARAM::xnp1

Definition at line 71 of file skua.h.

4.64.2.14 double SKUA_PARAM::y_eff

Definition at line 66 of file skua.h.

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

- [skua.h](#)

4.65 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/m²)
- double [As](#)
Specific surface area of adsorbent (m²/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).

4.65.1 Detailed Description

System Data Structure.

C-style object holding all the data associated with the overall system to be modeled.

Definition at line 139 of file magpie.h.

4.65.2 Member Data Documentation

4.65.2.1 double SYSTEM_DATA::As

Specific surface area of adsorbent (m^2/kg)

Definition at line 146 of file magpie.h.

4.65.2.2 double SYSTEM_DATA::avg_norm

Used to store all norms from evaluations then average at end of run.

Definition at line 150 of file magpie.h.

4.65.2.3 bool SYSTEM_DATA::Carrier

If there is an inert carrier gas, Carrier == true.

Definition at line 155 of file magpie.h.

4.65.2.4 int SYSTEM_DATA::I

Definition at line 148 of file magpie.h.

4.65.2.5 bool SYSTEM_DATA::Ideal

If the behavior of the system is determined to be ideal, then Ideal == true.

Definition at line 156 of file magpie.h.

4.65.2.6 int SYSTEM_DATA::J

Definition at line 148 of file magpie.h.

4.65.2.7 int SYSTEM_DATA::K

Special indices used to keep track of sub-systems.

Definition at line 148 of file magpie.h.

4.65.2.8 double SYSTEM_DATA::max_norm

Used to store the maximum e.norm calculated from non-linear iterations.

Definition at line 151 of file magpie.h.

4.65.2.9 int SYSTEM_DATA::N

Total Number of Components.

Definition at line 147 of file magpie.h.

4.65.2.10 bool SYSTEM_DATA::Output

Boolean to suppress output if desired (true = display, false = no display).

Definition at line 157 of file magpie.h.

4.65.2.11 int SYSTEM_DATA::Par

Number of binary parameters to solve for.

Definition at line 153 of file magpie.h.

4.65.2.12 double SYSTEM_DATA::PI

Total Lumped Spreading Pressure (mol/kg)

Definition at line 144 of file magpie.h.

4.65.2.13 double SYSTEM_DATA::pi

Actual Spreading pressure (J/m²)

Definition at line 145 of file magpie.h.

4.65.2.14 double SYSTEM_DATA::PT

Total Pressure (kPa)

Definition at line 142 of file magpie.h.

4.65.2.15 double SYSTEM_DATA::qT

Total Amount adsorbed (mol/kg)

Definition at line 143 of file magpie.h.

4.65.2.16 bool SYSTEM_DATA::Recover

If Recover == false, standard GPAST using y's as knowns.

Definition at line 154 of file magpie.h.

4.65.2.17 int SYSTEM_DATA::Sys

Number of sub-systems to solve.

Definition at line 152 of file magpie.h.

4.65.2.18 double SYSTEM_DATA::T

System Temperature (K)

Definition at line 141 of file magpie.h.

4.65.2.19 unsigned long int SYSTEM_DATA::total_eval

Counter to keep track of total number of non-linear steps.

Definition at line 149 of file magpie.h.

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

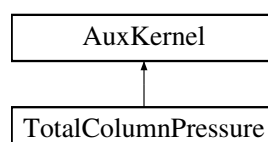
- [magpie.h](#)

4.66 TotalColumnPressure Class Reference

Total Column Pressure class inherits from AuxKernel.

```
#include <TotalColumnPressure.h>
```

Inheritance diagram for TotalColumnPressure:



Public Member Functions

- [TotalColumnPressure](#) (const InputParameters ¶meters)
Standard MOOSE public constructor.

Protected Member Functions

- virtual Real [computeValue](#) ()
Required MOOSE function override.

Private Attributes

- VariableValue & [_temperature](#)
Reference to the temperature non-linear variable.
- std::vector< unsigned int > [_index](#)
Indices of the gaseous species coupled to the object.
- std::vector< VariableValue * > [_gas_conc](#)
Pointer list for the non-linear concentration variables.

4.66.1 Detailed Description

Total Column Pressure class inherits from AuxKernel.

This class object creates an AuxKernel for use in the MOOSE framework. The AuxKernel will calculate the total column pressure (in kPa) based on the non-linear variables of temperature and concentration of each species in the gas phase. Total pressure is calculated based on the ideal gas law.

Definition at line 54 of file TotalColumnPressure.h.

4.66.2 Constructor & Destructor Documentation

4.66.2.1 TotalColumnPressure::TotalColumnPressure (const InputParameters & parameters)

Standard MOOSE public constructor.

4.66.3 Member Function Documentation

4.66.3.1 virtual Real TotalColumnPressure::computeValue () [protected],[virtual]

Required MOOSE function override.

This is the function that is called by the MOOSE framework when a calculation of the total system pressure is needed. You are required to override this function for any inherited AuxKernel.

4.66.4 Member Data Documentation

4.66.4.1 std::vector<VariableValue*> TotalColumnPressure::_gas_conc [private]

Pointer list for the non-linear concentration variables.

Definition at line 70 of file TotalColumnPressure.h.

4.66.4.2 std::vector<unsigned int> TotalColumnPressure::_index [private]

Indices of the gaseous species coupled to the object.

Definition at line 69 of file TotalColumnPressure.h.

4.66.4.3 VariableValue& TotalColumnPressure::temperature [private]

Reference to the temperature non-linear variable.

Definition at line 68 of file TotalColumnPressure.h.

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

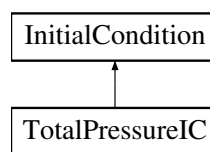
- [TotalColumnPressure.h](#)

4.67 TotalPressureIC Class Reference

[TotalPressureIC](#) class object inherits from InitialCondition object.

```
#include <TotalPressureIC.h>
```

Inheritance diagram for TotalPressureIC:



Public Member Functions

- [TotalPressureIC](#) (const InputParameters ¶meters)
Required constructor for objects in MOOSE.
- virtual Real [value](#) (const Point &p)
Required function override for setting the value of the non-linear variable at a given point.

Private Attributes

- Real [_PT_IC](#)
Initial condition for the total pressure in the column (kPa)

4.67.1 Detailed Description

[TotalPressureIC](#) class object inherits from InitialCondition object.

This class object inherits from the InitialCondition object in the MOOSE framework. All public and protected members of this class are required function overrides. The object will establish the initial conditions for total pressure as constant throughout the domain.

Note

You can have the non-linear variable vary spatially in the domain by inheriting from and or modifying this file to do so.

Definition at line 58 of file TotalPressureIC.h.

4.67.2 Constructor & Destructor Documentation

4.67.2.1 TotalPressureIC::TotalPressureIC (const InputParameters & parameters)

Required constructor for objects in MOOSE.

4.67.3 Member Function Documentation

4.67.3.1 virtual Real TotalPressureIC::value (const Point & p) [virtual]

Required function override for setting the value of the non-linear variable at a given point.

This function passes a point p as an argument. The return value will be the value of the non-linear variable at that point. That information is used to establish the spatially varying initial condition for the given non-linear variable.

4.67.4 Member Data Documentation

4.67.4.1 Real TotalPressureIC::_PT_IC [private]

Initial condition for the total pressure in the column (kPa)

Definition at line 70 of file TotalPressureIC.h.

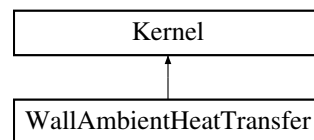
The documentation for this class was generated from the following file:

- [TotalPressureIC.h](#)

4.68 WallAmbientHeatTransfer Class Reference

```
#include <WallAmbientHeatTransfer.h>
```

Inheritance diagram for WallAmbientHeatTransfer:



Public Member Functions

- [WallAmbientHeatTransfer](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_wall_exterior_transfer_coeff](#)
- const MaterialProperty< Real > & [_inner_dia](#)
- const MaterialProperty< Real > & [_outer_dia](#)
- VariableValue & [_ambient_temp](#)

4.68.1 Detailed Description

Definition at line 11 of file WallAmbientHeatTransfer.h.

4.68.2 Constructor & Destructor Documentation

4.68.2.1 WallAmbientHeatTransfer::WallAmbientHeatTransfer (const InputParameters & *parameters*)

4.68.3 Member Function Documentation

4.68.3.1 virtual Real WallAmbientHeatTransfer::computeQpJacobian () [protected],[virtual]

4.68.3.2 virtual Real WallAmbientHeatTransfer::computeQpResidual () [protected],[virtual]

4.68.4 Member Data Documentation

4.68.4.1 VariableValue& WallAmbientHeatTransfer::_ambient_temp [private]

Definition at line 25 of file WallAmbientHeatTransfer.h.

4.68.4.2 const MaterialProperty<Real>& WallAmbientHeatTransfer::_inner_dia [private]

Definition at line 22 of file WallAmbientHeatTransfer.h.

4.68.4.3 const MaterialProperty<Real>& WallAmbientHeatTransfer::_outer_dia [private]

Definition at line 23 of file WallAmbientHeatTransfer.h.

4.68.4.4 const MaterialProperty<Real>& WallAmbientHeatTransfer::_wall_exterior_transfer_coeff [private]

Definition at line 21 of file WallAmbientHeatTransfer.h.

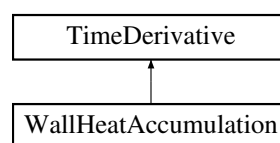
The documentation for this class was generated from the following file:

- [WallAmbientHeatTransfer.h](#)

4.69 WallHeatAccumulation Class Reference

#include <WallHeatAccumulation.h>

Inheritance diagram for WallHeatAccumulation:



Public Member Functions

- [WallHeatAccumulation](#) (const InputParameters ¶meters)

Protected Member Functions

- virtual Real [computeQpResidual](#) ()
- virtual Real [computeQpJacobian](#) ()

Private Attributes

- const MaterialProperty< Real > & [_wall_density](#)
- const MaterialProperty< Real > & [_wall_heat_capacity](#)

4.69.1 Detailed Description

Definition at line 12 of file WallHeatAccumulation.h.

4.69.2 Constructor & Destructor Documentation

4.69.2.1 WallHeatAccumulation::WallHeatAccumulation (const InputParameters & *parameters*)

4.69.3 Member Function Documentation

4.69.3.1 virtual Real WallHeatAccumulation::computeQpJacobian () [protected],[virtual]

4.69.3.2 virtual Real WallHeatAccumulation::computeQpResidual () [protected],[virtual]

4.69.4 Member Data Documentation

4.69.4.1 const MaterialProperty<Real>& WallHeatAccumulation::_wall_density [private]

Definition at line 23 of file WallHeatAccumulation.h.

4.69.4.2 const MaterialProperty<Real>& WallHeatAccumulation::_wall_heat_capacity [private]

Definition at line 24 of file WallHeatAccumulation.h.

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

- [WallHeatAccumulation.h](#)

5 File Documentation

5.1 AdsorbentProperties.h File Reference

Material Properties kernel that will setup and hold all information associated with the adsorbent.

```
#include "Material.h"
```

Classes

- class [AdsorbentProperties](#)
AdsorbentProperties class object inherits from Material object.

Functions

- template<>
InputParameters [validParams](#)< [AdsorbentProperties](#) > ()

5.1.1 Detailed Description

Material Properties kernel that will setup and hold all information associated with the adsorbent. Material Properties kernel that will setup and hold all information associated with the fixed-bed.

This file creates a material property object for various properties of a given adsorbent. These properties are then used in other material property files and/or kernels to calculate information such as linear velocity, mechanical dispersion, or any adsorption kinetic parameters.

Note

Currently, we do not couple with adsorption kinetics, so this file is only used in conjunction with the linear velocity and mechanical dispersion properties.

Warning

THIS KERNEL IS INCOMPLETE! ONLY USED FOR DATA STORAGE FOR PELLET DENSITY AND HEAT CAPACITY!

Author

Austin Ladshaw

Date

11/20/2015

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This file creates a material property object for various properties of the fixed bed. Those properties are used in conjunction with other kernels and materials to establish information such as heat transfer coefficients, conductivities, and size parameters.

Warning

THIS KERNEL IS INCOMPLETE! ONLY USED FOR DATA STORAGE FOR VARIOUS BED PARAMETERS!

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [AdsorbentProperties.h](#).

5.1.2 Function Documentation

5.1.2.1 `template<> InputParameters validParams< AdsorbentProperties > ()`

5.2 BedHeatAccumulation.h File Reference

```
#include "TimeDerivative.h"
```

Classes

- class [BedHeatAccumulation](#)

Functions

- `template<> InputParameters validParams< BedHeatAccumulation > ()`

5.2.1 Function Documentation

5.2.1.1 `template<> InputParameters validParams< BedHeatAccumulation > ()`

5.3 BedProperties.h File Reference

```
#include "Material.h"
```

Classes

- class [BedProperties](#)
BedProperties class object inherits from Material object.

Functions

- `template<> InputParameters validParams< BedProperties > ()`

5.3.1 Function Documentation

5.3.1.1 `template<> InputParameters validParams< BedProperties > ()`

5.4 BedWallHeatTransfer.h File Reference

```
#include "Kernel.h"
```

Classes

- class [BedWallHeatTransfer](#)

Functions

- `template<>`
`InputParameters validParams< BedWallHeatTransfer > ()`

5.4.1 Function Documentation

5.4.1.1 `template<> InputParameters validParams< BedWallHeatTransfer > ()`

5.5 ColumnTemperatureIC.h File Reference

Initial Condition kernel for initial temperature in a fixed-bed column.

```
#include "InitialCondition.h"
```

Classes

- class `ColumnTemperatureIC`
`ColumnTemperatureIC` class object inherits from `InitialCondition` object.

Functions

- `template<>`
`InputParameters validParams< ColumnTemperatureIC > ()`

5.5.1 Detailed Description

Initial Condition kernel for initial temperature in a fixed-bed column. This file creates an initial condition for the temperature in the bed. The initial condition for temperature is assumed a constant value at all points in the bed. However, this can be modified later to include spatially varying initial conditions for temperature.

Note

If you want to have spatially varying initial conditions, you will need to modify the virtual value function of this kernel. Otherwise, it is assumed that the non-linear variable is initially constant at all points in the domain.

Author

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Date

11/20/2015

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Definition in file `ColumnTemperatureIC.h`.

5.5.2 Function Documentation

5.5.2.1 `template<> InputParameters validParams< ColumnTemperatureIC > ()`

5.6 ConcentrationIC.h File Reference

Initial Condition kernel for initial concentration of a species in a fixed-bed column.

```
#include "InitialCondition.h"
```

Classes

- class [ConcentrationIC](#)
[ConcentrationIC](#) class object inherits from [InitialCondition](#) object.

Functions

- `template<>`
`InputParameters validParams< ConcentrationIC > \(\)`

5.6.1 Detailed Description

Initial Condition kernel for initial concentration of a species in a fixed-bed column. This file creates an initial condition for the concentration of a species in the bed. The initial condition for concentration is assumed a constant value at all points in the bed. However, this can be modified later to include varying initial conditions.

Note

If you want to have spatially varying initial conditions, you will need to modify the virtual value function of this kernel. Otherwise, it is assumed that the non-linear variable is initially constant at all points in the domain.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [ConcentrationIC.h](#).

5.6.2 Function Documentation

5.6.2.1 `template<> InputParameters validParams< ConcentrationIC > ()`

5.7 DGAdvection.h File Reference

Discontinuous Galerkin kernel for advection.

```
#include "DGKernel.h"
#include <cmath>
```

Classes

- class [DGAdvection](#)
[DGAdvection](#) class object inherits from [DGKernel](#) object.

Functions

- `template<>`
`InputParameters validParams< DGAdvection > \(\)`

5.7.1 Detailed Description

Discontinuous Galerkin kernel for advection. This file creates a discontinuous Galerkin kernel for advection physics in a given domain. It is a generic advection kernel that is meant to be inherited from to make a more specific kernel for a given problem. The physical parameter in this kernel's formulation is a velocity vector. That vector can be built piecewise by the respective x, y, and z components of a velocity field at a given quadrature point.

Note

Any DG kernel under DGOSPREY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

Author

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Date

11/20/2015

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Definition in file [DGAdvection.h](#).

5.7.2 Function Documentation

5.7.2.1 `template<> InputParameters validParams< DGAdvection > ()`

5.8 DGAnisotropicDiffusion.h File Reference

Discontinuous Galerkin kernel for anisotropic diffusion.

```
#include "DGKernel.h"
#include <cmath>
```

Classes

- class [DGAnisotropicDiffusion](#)
[DGAnisotropicDiffusion](#) class object inherits from [DGKernel](#) object.

Functions

- `template<>`
`InputParameters validParams< DGAnisotropicDiffusion > \(\)`

5.8.1 Detailed Description

Discontinuous Galerkin kernel for anisotropic diffusion. This file creates a discontinuous Galerkin kernel for anisotropic diffusion in a given domain. It is a generic diffusion kernel that is meant to be inherited from to make a more specific kernel for a given problem. The physical parameter in this kernel's formulation is a diffusion tensor. That tensor can be built piecewise by the respective components of the tensor at a given quadrature point.

Note

Any DG kernel under DGOSPREY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

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Date

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Definition in file [DGAnisotropicDiffusion.h](#).

5.8.2 Function Documentation

5.8.2.1 `template<> InputParameters validParams< DGAnisotropicDiffusion > ()`

5.9 DGColumnHeatAdvection.h File Reference

Discontinuous Galerkin kernel for energy advection in a fixed-bed column.

```
#include "DGAdvection.h"
```

Classes

- class [DGColumnHeatAdvection](#)
DGColumnHeatAdvection class object inherits from DGAdvection object.

Macros

- `#define` [DGCOLUMNHEATADVECTION_H](#)

Functions

- `template<>`
`InputParameters` [validParams< DGColumnHeatAdvection > \(\)](#)

5.9.1 Detailed Description

Discontinuous Galerkin kernel for energy advection in a fixed-bed column. This file creates a discontinuous Galerkin kernel for the advective heat transfer in a fixed-bed column. The advection portion of the energy transport equations involves the linear velocity in the system, as well as the gas density and gas heat capacity. Those parameters are given as material properties for the system.

Note

Any DG kernel under DGOSPREY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

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Date

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Definition in file [DGColumnHeatAdvection.h](#).

5.9.2 Macro Definition Documentation

5.9.2.1 #define DGCOLUMNHEATADVECTION_H

Definition at line 47 of file DGColumnHeatAdvection.h.

5.9.3 Function Documentation

5.9.3.1 template<> InputParameters validParams< DGColumnHeatAdvection > ()

5.10 DGColumnHeatDispersion.h File Reference

Discontinuous Galerkin kernel for energy dispersion in a fixed-bed column.

```
#include "DGAnisotropicDiffusion.h"
```

Classes

- class [DGColumnHeatDispersion](#)
DGColumnHeatDispersion class object inherits from *DGAnisotropicDiffusion* object.

Macros

- #define [DGCOLUMNHEATDISPERSION_H](#)

Functions

- template<>
 InputParameters [validParams< DGColumnHeatDispersion > \(\)](#)

5.10.1 Detailed Description

Discontinuous Galerkin kernel for energy dispersion in a fixed-bed column. This file creates a discontinuous Galerkin kernel for the dispersive heat transfer in a fixed-bed column. The dispersion portion of the energy transport equations involves the thermal conductivity in the system. That parameter is calculated in a material properties file and passed into this object for use the construction of residuals and Jacobians.

Note

Any DG kernel under DGOSPREY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

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Definition in file [DGColumnHeatDispersion.h](#).

5.10.2 Macro Definition Documentation

5.10.2.1 #define DGCOLUMNHEATDISPERSION_H

Definition at line 47 of file DGColumnHeatDispersion.h.

5.10.3 Function Documentation

5.10.3.1 template<> InputParameters validParams< DGColumnHeatDispersion > ()

5.11 DGColumnMassAdvection.h File Reference

Discontinuous Galerkin kernel for mass advection in a fixed-bed column.

```
#include "DGAdvection.h"
```

Classes

- class [DGColumnMassAdvection](#)
[DGColumnMassAdvection](#) class object inherits from [DGAdvection](#) object.

Functions

- template<>
InputParameters [validParams< DGColumnMassAdvection >](#) ()

5.11.1 Detailed Description

Discontinuous Galerkin kernel for mass advection in a fixed-bed column. This file creates a discontinuous Galerkin kernel for the advective mass transfer in a fixed-bed column. The advection portion of the mass transport equations involves the linear velocity in the system. That parameter is given as material property.

Note

Any DG kernel under DGOSPREY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [DGColumnMassAdvection.h](#).

5.11.2 Function Documentation

5.11.2.1 `template<> InputParameters validParams< DGColumnMassAdvection > ()`

5.12 DGColumnMassDispersion.h File Reference

Discontinuous Galerkin kernel for mass dispersion in a fixed-bed column.

```
#include "DGAnisotropicDiffusion.h"
```

Classes

- class [DGColumnMassDispersion](#)
[DGColumnMassDispersion](#) class object inherits from [DGAnisotropicDiffusion](#) object.

Functions

- `template<> InputParameters validParams< DGColumnMassDispersion > ()`

5.12.1 Detailed Description

Discontinuous Galerkin kernel for mass dispersion in a fixed-bed column. This file creates a discontinuous Galerkin kernel for the dispersive mass transfer in a fixed-bed column. The dispersion portion of the mass transport equations involves the molecular diffusivity of a species in the system, as well as the overall axial dispersion of material caused by mechanical mixing and molecular diffusion. Those parameters are calculated in a material properties file and passed into this object for use the construction of residuals and Jacobians.

Note

Any DG kernel under DGOSPNEY will have a cooresponding G kernel (usually of same name) that must be included with the DG kernel in the input file. This is because the DG finite element method breaks into several different residual pieces, only a handful of which are handled by the DG kernel system and the other parts must be handled by the standard Galerkin system. This my be due to some legacy code in MOOSE. I am not sure if it is possible to lump all of these actions into a single DG kernel.

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Definition in file [DGColumnMassDispersion.h](#).

5.12.2 Function Documentation

5.12.2.1 `template<> InputParameters validParams< DGColumnMassDispersion > ()`

5.13 DGColumnWallHeatFluxBC.h File Reference

Boundary Condition kernel for the heat flux across the wall of the fixed-bed column.

```
#include "DGFluxBC.h"
```

Classes

- class [DGColumnWallHeatFluxBC](#)
DGColumnWallHeatFluxBC class object inherits from [DGFluxBC](#) object.

Functions

- `template<> InputParameters validParams< DGColumnWallHeatFluxBC > \(\)`

5.13.1 Detailed Description

Boundary Condition kernel for the heat flux across the wall of the fixed-bed column. This file creates a boundary condition kernel for the heat flux across the boundary of the walls of the column in the fixed-bed adsorber. It inherits from the [DGFluxBC](#), which acts as a generic flux BC module. This kernel is coupled to the wall temperature variable, as well as the material properties for thermal conductivity and the bed-wall heat transfer coefficient.

This type of boundary condition for DG kernels applies the true flux boundary condition. Alternatively, you can use the "FluxLimitedBC" to impose a Dirichlet boundary condition on the system. Although, in true finite volumes or DG methods, there is no Dirichlet boundary conditions, because the solutions are based on fluxes into and out of cells in a domain.

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11/20/2015

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Definition in file [DGColumnWallHeatFluxBC.h](#).

5.13.2 Function Documentation

5.13.2.1 `template<> InputParameters validParams< DGColumnWallHeatFluxBC > ()`

5.14 DGColumnWallHeatFluxLimitedBC.h File Reference

Boundary Condition kernel for a dirichlet-like boundary condition of heat on the column wall.

```
#include "DGFluxLimitedBC.h"
```

Classes

- class [DGColumnWallHeatFluxLimitedBC](#)
[DGColumnWallHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

Functions

- `template<> InputParameters validParams< DGColumnWallHeatFluxLimitedBC > \(\)`

5.14.1 Detailed Description

Boundary Condition kernel for a dirichlet-like boundary condition of heat on the column wall. This file creates a boundary condition that mimics a Dirichlet boundary condition for the heat of the column at the wall. A true Dirichlet boundary condition does not exist in DG methods. However, this will create a weak form that imposes a constraint that the solution must be of a certain value at the boundary.

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Definition in file [DGColumnWallHeatFluxLimitedBC.h](#).

5.14.2 Function Documentation

5.14.2.1 `template<> InputParameters validParams< DGColumnWallHeatFluxLimitedBC > ()`

5.15 DGFluxBC.h File Reference

Boundary Condition kernel for the flux across a boundary of the domain.

```
#include "IntegratedBC.h"
#include "libmesh/vector_value.h"
```

Classes

- class [DGFluxBC](#)
[DGFluxBC](#) class object inherits from [IntegratedBC](#) object.

Functions

- `template<>`
`InputParameters validParams< DGFluxBC > \(\)`

5.15.1 Detailed Description

Boundary Condition kernel for the flux across a boundary of the domain. This file creates a generic boundary condition kernel for the flux of material accross a boundary. The flux is based on a diffusivity tensor and a velocity vector and is valid in all directions and all boundaries of a DG method. Since the DG method's flux boundary conditions are essitally the same for input and ouput boundaries, this kernel will check the sign of the flux normal to the boundary and determine automattically whether it is an output or input boundary, then apply the appropriate conditions.

This type of boundary condition for DG kernels applies the true flux boundary condition. Alternatively, you can use the "FluxLimitedBC" to impose a Dirichlet boundary condition on the system. Although, in true finite volumes or DG methods, there is no Dirichlet boundary conditions, because the solutions are based on fluxes into and out of cells in a domain.

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Definition in file [DGFluxBC.h](#).

5.15.2 Function Documentation

5.15.2.1 `template<> InputParameters validParams< DGFluxBC > ()`

5.16 DGFluxLimitedBC.h File Reference

Boundary Condition kernel to mimic a Dirichlet BC for DG methods.

```
#include "IntegratedBC.h"
#include "libmesh/vector_value.h"
```

Classes

- class [DGFluxLimitedBC](#)
[DGFluxLimitedBC](#) class object inherits from [IntegratedBC](#) object.

Functions

- `template<> InputParameters validParams< DGFluxLimitedBC > \(\)`

5.16.1 Detailed Description

Boundary Condition kernel to mimic a Dirichlet BC for DG methods. This file creates a boundary condition kernel to impose a dirichlet-like boundary condition in DG methods. True DG methods do not have Dirichlet boundary conditions, so this kernel seeks to impose a constraint on the inlet of a boundary that is met if the value of a variable at the inlet boundary is equal to the finite element solution at that boundary. When the condition is not met, the residuals get penalized until the condition is met.

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Definition in file [DGFluxLimitedBC.h](#).

5.16.2 Function Documentation

5.16.2.1 `template<> InputParameters validParams< DGFluxLimitedBC > ()`

5.17 DGHeatFluxBC.h File Reference

Boundary Condition kernel for the heat flux in and out of the ends of the fixed-bed column.

```
#include "DGFluxBC.h"
```

Classes

- class [DGHeatFluxBC](#)
[DGHeatFluxBC](#) class object inherits from [DGFluxBC](#) object.

Functions

- template<>
 InputParameters [validParams](#)< [DGHeatFluxBC](#) > ()

5.17.1 Detailed Description

Boundary Condition kernel for the heat flux in and out of the ends of the fixed-bed column. This file creates a boundary condition kernel for the heat flux across the boundary of the ends of the column in the fixed-bed adsorber. It inherits from the [DGFluxBC](#), which acts as a generic flux BC module. This kernel is coupled to the column temperature variable, as well as the material properties for thermal conductivity, gas density and heat capacity, and the velocity in the domain.

This type of boundary condition for DG kernels applies the true flux boundary condition. Alternatively, you can use the "FluxLimitedBC" to impose a Dirichlet boundary condition on the system. Although, in true finite volumes or DG methods, there is no Dirichlet boundary conditions, because the solutions are based on fluxes into and out of cells in a domain.

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Definition in file [DGHeatFluxBC.h](#).

5.17.2 Function Documentation

5.17.2.1 template<> InputParameters validParams< [DGHeatFluxBC](#) > ()

5.18 DGHeatFluxLimitedBC.h File Reference

Boundary Condition kernel to mimic a dirichlet boundary condition at the column inlet.

```
#include "DGFluxLimitedBC.h"
```

Classes

- class [DGHeatFluxLimitedBC](#)
[DGHeatFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

Functions

- `template<>`
`InputParameters validParams< DGHeatFluxLimitedBC > ()`

5.18.1 Detailed Description

Boundary Condition kernel to mimic a dirichlet boundary condition at the column inlet. This file creates a dirichlet-like boundary condition kernel for the column temperature at the inlet of the system. The outlet boundary condition would remain unchanged from the standard DG form of the boundaries. Only the inlet BC is affected by this file. See [FluxLimitedBC.h](#) for more details.

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Definition in file [DGHeatFluxLimitedBC.h](#).

5.18.2 Function Documentation

5.18.2.1 `template<> InputParameters validParams< DGHeatFluxLimitedBC > ()`

5.19 DGMassFluxBC.h File Reference

Boundary Condition kernel for the mass flux in and out of the ends of the fixed-bed column.

```
#include "DGFluxBC.h"
```

Classes

- class [DGMassFluxBC](#)
[DGMassFluxBC](#) class object inherits from [DGFluxBC](#) object.

Functions

- `template<>`
`InputParameters validParams< DGMassFluxBC > ()`

5.19.1 Detailed Description

Boundary Condition kernel for the mass flux in and out of the ends of the fixed-bed column. This file creates a boundary condition kernel for the mass flux across the boundary of the ends of the column in the fixed-bed adsorber. It inherits from the [DGFluxBC](#), which acts as a generic flux BC module. This kernel is coupled to the column temperature variable, as well as the material properties for thermal conductivity, gas density and heat capacity, and the velocity in the domain.

This type of boundary condition for DG kernels applies the true flux boundary condition. Alternatively, you can use the "FluxLimitedBC" to impose a Dirichlet boundary condition on the system. Although, in true finite volumes or DG methods, there is no Dirichlet boundary conditions, because the solutions are based on fluxes into and out of cells in a domain.

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Definition in file [DGMassFluxBC.h](#).

5.19.2 Function Documentation

5.19.2.1 `template<> InputParameters validParams< DGMassFluxBC > ()`

5.20 DGMassFluxLimitedBC.h File Reference

Boundary Condition kernel to mimic a dirichlet boundary condition at the column inlet.

```
#include "DGFluxLimitedBC.h"
```

Classes

- class [DGMassFluxLimitedBC](#)
[DGMassFluxLimitedBC](#) class object inherits from [DGFluxLimitedBC](#) object.

Functions

- `template<> InputParameters validParams< DGMassFluxLimitedBC > ()`

5.20.1 Detailed Description

Boundary Condition kernel to mimic a dirichlet boundary condition at the column inlet. This file creates a dirichlet-like boundary condition kernel for the gas species concentration at the inlet of the system. The outlet boundary condition would remain unchanged from the standard DG form of the boundaries. Only the inlet BC is affected by this file. See FluxLimitedBC.h for more details.

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Definition in file [DGMassFluxLimitedBC.h](#).

5.20.2 Function Documentation

5.20.2.1 `template<> InputParameters validParams< DGMassFluxLimitedBC > ()`

5.21 DgospreyApp.h File Reference

Registration object for creating a registering DGOSPNEY kernels.

```
#include "MooseApp.h"
```

Classes

- class [DgospreyApp](#)
DgospreyApp inherits from the MooseApp object.

Functions

- `template<> InputParameters validParams< DgospreyApp > ()`

5.21.1 Detailed Description

Registration object for creating a registering DGOSPNEY kernels. This file is responsible for registering all DGOSPNEY kernels in the MOOSE framework. Any additional kernel developed under DGOSPNEY must be included and registered in this structure. This structure is required by MOOSE in order to have the DGOSPNEY objects interact with the underlying MOOSE solvers and finite element framework.

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Definition in file [DgospreyApp.h](#).

5.21.2 Function Documentation

5.21.2.1 `template<> InputParameters validParams< DgospreyApp > ()`

5.22 DgospreyRevision.h File Reference**Macros**

- `#define DGOSPNEY_REVISION "git commit 9890b6c on 2014-09-24"`

5.22.1 Macro Definition Documentation

5.22.1.1 `#define DGOSPNEY_REVISION "git commit 9890b6c on 2014-09-24"`

Definition at line 6 of file base/DgospreyRevision.h.

5.23 DgospreyRevision.h File Reference**Macros**

- `#define DGOSPNEY_REVISION "git commit 5a076c0 on 2015-08-31"`

5.23.1 Macro Definition Documentation

5.23.1.1 `#define DGOSPNEY_REVISION "git commit 5a076c0 on 2015-08-31"`

Definition at line 6 of file DgospreyRevision.h.

5.24 Dispersion.h File Reference

```
#include "Kernel.h"
```

Classes

- class [Dispersion](#)

Functions

- `template<>`
InputParameters `validParams< Dispersion > ()`

5.24.1 Function Documentation

5.24.1.1 `template<> InputParameters validParams< Dispersion > ()`

5.25 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 species.
- struct `MIXED_GAS`
Data structure holding information necessary for computing mixed gas properties.

Macros

- `#define EGRET_HPP_`
- `#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 cm³*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/cm³)
- `#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/cm³)
- `#define Nu(mu, rho) ((mu)/(rho))`
Calculation of kinematic viscosity from dynamic viscosity and density (cm²/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 (cm²/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 (cm²/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)` ($u \cdot L / \text{nu}$)
- Calculation of the Reynold's Number (-)*
- #define `ScNum(nu, D)` (nu / D)
- Calculation of the Schmidt Number (-)*
- #define `FilmMTCoeff(D, L, Re, Sc)` ($(D/L) \cdot (2.0 + (1.1 \cdot \text{pow}(\text{Re}, 0.6) \cdot \text{pow}(\text{Sc}, 0.3)))$)
- 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`.*

5.25.1 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 empirical models that were developed to account for changes in density and viscosity with changes in temperature between standard temperatures and up to 1000 K.

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01/29/2015

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Definition in file [egret.h](#).

5.25.2 Macro Definition Documentation

5.25.2.1 #define `CE3(p, T)` ($(p)/(R \cdot T)$)

Calculation of concentration/density from partial pressure ($\text{CE3} = \text{mol}/\text{cm}^3$)

Definition at line 42 of file egret.h.

5.25.2.2 #define `Cstd(p, T)` ($(p)/(R \cdot T)$)

Calculation of concentration/density from partial pressure ($\text{Cstd} = \text{mol/L}$)

Definition at line 38 of file egret.h.

5.25.2.3 `#define D_ii(rhoi, mui) (1.385*mui/rhoi)`

Calculation of self-diffusivity (cm^2/s)

Definition at line 74 of file egret.h.

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

Calculation of binary diffusion based on MW, density, and viscosity info (cm^2/s)

Definition at line 66 of file egret.h.

5.25.2.5 `#define Dp_ij(Dij, PT) ((PT*Dij)/Po)`

Calculation of the corrected binary diffusivity (cm^2/s)

Definition at line 62 of file egret.h.

5.25.2.6 `#define EGRET_HPP_`

Definition at line 23 of file egret.h.

5.25.2.7 `#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)

Definition at line 86 of file egret.h.

5.25.2.8 `#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)

Definition at line 70 of file egret.h.

5.25.2.9 `#define Nu(mu, rho) ((mu)/(rho))`

Calculation of kinematic viscosity from dynamic viscosity and density (cm^2/s)

Definition at line 54 of file egret.h.

5.25.2.10 `#define PE3(c, T) ((c)*RE3*T)`

Calculation of partial pressure from concentration/density ($c = \text{mol}/\text{cm}^3$)

Definition at line 50 of file egret.h.

5.25.2.11 `#define Po 100.0`

Standard state pressure (kPa)

Definition at line 34 of file egret.h.

5.25.2.12 `#define PSI(T) (0.873143 + (0.000072375*T))`

Calculation of temperature correction factor for dynamic viscosity.

Definition at line 58 of file egret.h.

5.25.2.13 `#define Pstd(c, T) ((c)*Rstd*T)`

Calculation of partial pressure from concentration/density ($c = \text{mol/L}$)

Definition at line 46 of file egret.h.

5.25.2.14 `#define RE3 8.3144621E+3`

Gas Constant in $\text{cm}^3 \cdot \text{kPa} / \text{K} \cdot \text{mol}$ (Convenient for density calculations)

Definition at line 30 of file egret.h.

5.25.2.15 `#define ReNum(u, L, nu) (u*L/nu)`

Calculation of the Reynold's Number (-)

Definition at line 78 of file egret.h.

5.25.2.16 `#define Rstd 8.3144621`

Gas Constant in $\text{J} / \text{K} \cdot \text{mol}$ (or) $\text{L} \cdot \text{kPa} / \text{K} \cdot \text{mol}$ (Standard Units)

Definition at line 26 of file egret.h.

5.25.2.17 `#define ScNum(nu, D) (nu/D)`

Calculation of the Schmidt Number (-)

Definition at line 82 of file egret.h.

5.25.3 Function Documentation

5.25.3.1 `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.

5.25.3.2 `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.

5.25.3.3 `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

<i>PT</i>	total gas pressure in kPa
<i>T</i>	gas temperature in K
<i>us</i>	gas velocity in cm/s
<i>L</i>	characteristic length in cm (this depends on the particular system)
<i>y</i>	vector of gas mole fractions of each species in the mixture
<i>gas_dat</i>	pointer to the MIXED_GAS data structure

5.26 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.

5.26.1 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 occurred.

Author

Austin Ladshaw

Date

04/28/2014

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Definition in file [error.h](#).

5.26.2 Macro Definition Documentation

5.26.2.1 #define mError(i)

Value:

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

Definition at line 22 of file error.h.

Referenced by Matrix< T >::adjoint(), Matrix< T >::cofactor(), Matrix< T >::columnExtend(), Matrix< T >::columnExtract(), Matrix< T >::columnProjection(), Matrix< T >::columnReplace(), Matrix< T >::columnVectorFill(), Matrix< T >::ConstantICFill(), Matrix< T >::determinate(), Matrix< T >::diagonalSolve(), Matrix< T >::dirichletBCFill(), Matrix< T >::Display(), Matrix< T >::edit(), Matrix< T >::inner_product(), Matrix< T >::IntegralAvg(), Matrix< T >::IntegralTotal(), Matrix< T >::inverse(), Matrix< T >::ladshawSolve(), Matrix< T >::lowerHessenberg2Triangular(), Matrix< T >::lowerHessenbergSolve(), Matrix< T >::lowerTriangularSolve(), Matrix< T >::operator*(), Matrix< T >::operator*(), Matrix< T >::operator+(), Matrix< T >::operator-(), Matrix< T >::rowExtend(), Matrix< T >::rowExtract(), Matrix< T >::rowReplace(), Matrix< T >::set_size(), Matrix< T >::SolnTransform(), Matrix< T >::sphericalAvg(), Matrix< T >::sphericalBCFill(), Matrix< T >::transpose(), Matrix< T >::transpose_multiply(), Matrix< T >::tridiagonalFill(), Matrix< T >::tridiagonalSolve(), Matrix< T >::tridiagonalVectorFill(), Matrix< T >::upperHessenberg2Triangular(), Matrix< T >::upperHessenbergSolve(), and Matrix< T >::upperTriangularSolve().

5.26.3 Enumeration Type Documentation

5.26.3.1 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

Definition at line 28 of file error.h.

5.26.4 Function Documentation

5.26.4.1 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 occurred.

5.27 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 return 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.

5.27.1 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 Tadmor (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...

$$z^d \frac{d}{dz} (R \frac{du}{dt}) = \frac{d}{dz} (z^d D \frac{du}{dz}) - \frac{d}{dz} (z^d v * u) - z^d k * u + z^d S$$

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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Definition in file [finch.h](#).

5.27.2 Enumeration Type Documentation

5.27.2.1 enum finch_coord_type

List of enum options to define the coordinate system in FINCH.

Enumerator

Cartesian

Cylindrical

Spherical

Definition at line 65 of file finch.h.

5.27.2.2 enum finch_solve_type

List of enum options to define the solver type in FINCH.

Enumerator

FINCH_Picard

LARK_Picard

LARK_PJFNK

Definition at line 62 of file finch.h.

5.27.3 Function Documentation

5.27.3.1 `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.

5.27.3.2 `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.

5.27.3.3 `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.

5.27.3.4 `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.

5.27.3.5 `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.

5.27.3.6 `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.

5.27.3.7 `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.

5.27.3.8 `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.

5.27.3.9 `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.

5.27.3.10 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.

5.27.3.11 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.

5.27.3.12 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.

5.27.3.13 int l_direct (FINCH_DATA * dat)

Function solves the discretized FINCH problem directly by assuming it is linear.

5.27.3.14 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)

5.27.3.15 double max (std::vector< double > & values)

Function returns the maximum in a list of values.

5.27.3.16 double min (std::vector< double > & values)

Function returns the minimum in a list of values.

5.27.3.17 double minmod (std::vector< double > & values)

Function returns the result of the minmod function acting on a list of values.

5.27.3.18 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.

5.27.3.19 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.

5.27.3.20 `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.

5.27.3.21 `void print2file_dim_header (FILE * Output, FINCH_DATA * dat)`

Function will print out a dimension header for FINCH output.

5.27.3.22 `void print2file_newline (FILE * Output, FINCH_DATA * dat)`

Function will force print out a blank line.

5.27.3.23 `void print2file_result_new (FILE * Output, FINCH_DATA * dat)`

Function will print out the new results to the variable u.

5.27.3.24 `void print2file_result_old (FILE * Output, FINCH_DATA * dat)`

Function will print out the old results to the variable u.

5.27.3.25 `void print2file_tab (FILE * Output, FINCH_DATA * dat)`

Function will force print out a tab.

5.27.3.26 `void print2file_time_header (FILE * Output, FINCH_DATA * dat)`

Function will print out a time header for FINCH output.

5.27.3.27 `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

<code>user_callroutine</code>	function pointer the the call routine function
<code>user_setic</code>	function pointer to set initial conditions for problem
<code>user_timestep</code>	function pointer to set the next time step
<code>user_preprocess</code>	function pointer to setup a preprocess operation
<code>user_solve</code>	function pointer to solve the system of equations

<i>user_setparams</i>	function pointer to set the parameters in the problem (always override this)
<i>user_discretize</i>	function pointer to select discretization scheme for the problem
<i>user_bcs</i>	function pointer to evaluate boundary conditions for the problem
<i>user_res</i>	function pointer to evaluate non-linear residuals for the problem
<i>user_precon</i>	function pointer to perform a linear preconditioning operation
<i>user_postprocess</i>	function pointer to setup a postprocess operation
<i>user_reset</i>	function pointer to reset stateful data for next simulation
<i>dat</i>	pointer to the FINCH_DATA structure
<i>param_data</i>	user supplied pointer to a data structure needed in <i>user_setparams</i>

5.27.3.28 int uAverage ([FINCH_DATA](#) * *dat*)

Function integrates the conserved quantity to return it's average in the domain.

5.27.3.29 int uTotal ([FINCH_DATA](#) * *dat*)

Function integrates the conserved quantity to return it's total in the domain.

5.27.3.30 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.

5.28 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 "magpie.h"
```

5.28.1 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](#) [magpie.h](#)

Author

Austin Ladshaw

Date

04/28/2014

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Definition in file [flock.h](#).

5.29 FlowProperties.h File Reference

Material Properties kernel that will setup and calculate gas flow properties based on physical characteristics.

```
#include "Material.h"
#include "flock.h"
```

Classes

- class [FlowProperties](#)
FlowProperties class object inherits from Material object.

Macros

- #define [_gas_const](#) 8.3144621
Gas Law Constant - J/K/mol.

Functions

- template<>
InputParameters [validParams< FlowProperties >\(\)](#)

5.29.1 Detailed Description

Material Properties kernel that will setup and calculate gas flow properties based on physical characteristics. This file creates a material property object for the flow properties in the fixed-bed column. The flow properties are calculated based on some dimensional analysis, empirical relationships, and kinetic theory of gases. Those properties are then coupled the with mass and energy kernels in the domain to simulate the dynamic and non-linear behavior in the system.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [FlowProperties.h](#).

5.29.2 Macro Definition Documentation

5.29.2.1 `#define _gas_const 8.3144621`

Gas Law Constant - J/K/mol.

Definition at line 45 of file FlowProperties.h.

5.29.3 Function Documentation

5.29.3.1 `template<> InputParameters validParams< FlowProperties > ()`

5.30 FluidHeatTransfer.h File Reference

```
#include "Kernel.h"
```

Classes

- class [FluidHeatTransfer](#)

Functions

- `template<> InputParameters validParams< FluidHeatTransfer > \(\)`

5.30.1 Function Documentation

5.30.1.1 `template<> InputParameters validParams< FluidHeatTransfer > ()`

5.31 GAdvection.h File Reference

```
#include "Kernel.h"
```

Classes

- class [GAdvection](#)

Functions

- `template<> InputParameters validParams< GAdvection > \(\)`

5.31.1 Function Documentation

5.31.1.1 `template<> InputParameters validParams< GAdvection > ()`

5.32 GAnisotropicDiffusion.h File Reference

```
#include "Kernel.h"
```


Classes

- class [GAnisotropicDiffusion](#)

Functions

- template<>
InputParameters [validParams< GAnisotropicDiffusion >](#) ()

5.32.1 Function Documentation

5.32.1.1 [template<> InputParameters validParams< GAnisotropicDiffusion >](#) ()

5.33 GColumnHeatAdvection.h File Reference

```
#include "GAdvection.h"
```

Classes

- class [GColumnHeatAdvection](#)

Functions

- template<>
InputParameters [validParams< GColumnHeatAdvection >](#) ()

5.33.1 Function Documentation

5.33.1.1 [template<> InputParameters validParams< GColumnHeatAdvection >](#) ()

5.34 GColumnHeatDispersion.h File Reference

```
#include "GAnisotropicDiffusion.h"
```

Classes

- class [GColumnHeatDispersion](#)

Functions

- template<>
InputParameters [validParams< GColumnHeatDispersion >](#) ()

5.34.1 Function Documentation

5.34.1.1 [template<> InputParameters validParams< GColumnHeatDispersion >](#) ()

5.35 GColumnMassAdvection.h File Reference

```
#include "GAdvection.h"
```

Classes

- class [GColumnMassAdvection](#)

Functions

- template<>
InputParameters [validParams< GColumnMassAdvection >](#) ()

5.35.1 Function Documentation

5.35.1.1 [template<> InputParameters validParams< GColumnMassAdvection >](#) ()

5.36 GColumnMassDispersion.h File Reference

```
#include "GAnisotropicDiffusion.h"
```

Classes

- class [GColumnMassDispersion](#)

Functions

- template<>
InputParameters [validParams< GColumnMassDispersion >](#) ()

5.36.1 Function Documentation

5.36.1.1 [template<> InputParameters validParams< GColumnMassDispersion >](#) ()

5.37 HeatConductivity.h File Reference

```
#include "Kernel.h"
```

Classes

- class [HeatConductivity](#)

Functions

- template<>
InputParameters [validParams< HeatConductivity >](#) ()

5.37.1 Function Documentation

5.37.1.1 [template<> InputParameters validParams< HeatConductivity >](#) ()

5.38 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 *bicgstab_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 $A^{\wedge T}r=u$.
- `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 gmresPreconditioner (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.

5.38.1 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 Orthogonalization 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 to 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 its 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 preconditioners with more GMRES steps. This can result in 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

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Date

10/14/2014

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Definition in file [lark.h](#).

5.38.2 Macro Definition Documentation

5.38.2.1 `#define MIN_TOL 1e-15`

Minimum Allowable Tolerance for linear and non-linear problems.

Definition at line 111 of file lark.h.

5.38.3 Enumeration Type Documentation

5.38.3.1 `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

Definition at line 492 of file lark.h.

5.38.4 Function Documentation

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

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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>r0</i>	user supplied vector to serve as the first basis vector in the orthonormal basis
<i>arnoldi_dat</i>	pointer to the ARNOLDI_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

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

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

<i>feval</i>	user supplied residual function for the non-linear system
<i>Fkp1</i>	vector holding the residuals for the next non-linear step
<i>xkp1</i>	vector holding the solution for the next non-linear step
<i>pk</i>	vector holding the current non-linear search direction
<i>normFk</i>	value of the current non-linear residual
<i>backtrack_dat</i>	pointer to the BACKTRACK_DATA data structure
<i>feval_data</i>	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.

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

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 occasionally breakdown and fail. Most common failures are caused by poor preconditioning. Works very well for grid-based linear systems.

Parameters

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system Ax=b
<i>bicg_dat</i>	pointer to the BICGSTAB_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

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

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 well for grid-based linear systems.

Parameters

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>cgs_dat</i>	pointer to the CGS_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.5 `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 (FOM). 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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>gmreslp_dat</i>	pointer to the GMRESLP_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.6 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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>gcr_dat</i>	pointer to the GCR_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.7 `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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system Ax=b
<i>gmreslp_dat</i>	pointer to the GMRESLP_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.8 `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 significantly 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

<i>matvec</i>	user supplied linear operator given as an int function
<i>terminal_precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>gmresr_dat</i>	pointer to the GMRESR_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>term_precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.9 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 GMRESLP. 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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>gmresrp_dat</i>	pointer to the GMRESRP_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.10 `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

<i>r</i>	vector supplied to the preconditioner to operate on
<i>Mr</i>	vector to hold the result of the preconditioning operation
<i>data</i>	void pointer to the GMRESR_DATA data structure

5.38.4.11 `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

<i>v</i>	vector to be multiplied by the Jacobian matrix
<i>Jv</i>	storage vector for the result of the Jacobi-vector product
<i>data</i>	void pointer to the PJFNK_DATA data structure holding solver information

5.38.4.12 `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

<i>r</i>	vector supplied to the preconditioner to operate on
<i>Mr</i>	vector to hold the result of the preconditioning operation
<i>data</i>	void pointer to the KMS_DATA data structure

5.38.4.13 `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 its `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

<i>matvec</i>	user supplied linear operator given as an int function
<i>terminal_precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>kms_dat</i>	pointer to the KMS_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>term_precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.14 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

<i>Func</i>	user supplied function for evaluation of the non-linear system
<i>x</i>	matrix holding the current value of the non-linear variables
<i>J</i>	matrix that will store the numerical Jacobian result
<i>Nx</i>	number of non-linear variables in the system
<i>Nf</i>	number of non-linear functions in the system
<i>jac_dat</i>	pointer to the NUM_JAC_DATA data structure
<i>user_data</i>	user supplied void pointer to a data structure used in the non-linear function

5.38.4.15 `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 accomplished by reordering the transpose operator and multiplying the non-transposed operator by a complete set of orthonormal vectors. The end result gives the i th component of the vector u for each operation ($u_i = r^T A^T e_i$). Here, e_i is a vector made from the i th column of the identity matrix. If the linear system is sufficiently large, then this operation may take some time.

Parameters

<i>matvec</i>	user supplied linear operator given as an int function
<i>r</i>	vector to be multiplied by the transpose of the operator
<i>u</i>	vector to store the result of the operator transposition ($u = A^T r$)
<i>transpose_dat</i>	pointer to the OPTRANS_DATA data structure
<i>matvec_data</i>	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.

5.38.4.16 `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

<i>matvec</i>	user supplied linear operator given as an int function
<i>precon</i>	user supplied preconditioning operator given as an int function
<i>b</i>	matrix of boundary conditions in the linear system $Ax=b$
<i>pcg_dat</i>	pointer to the PCG_DATA data structure
<i>matvec_data</i>	user supplied void pointer to a data structure needed for the linear operator
<i>precon_data</i>	user supplied void pointer to a data structure needed for the preconditioning 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.

5.38.4.17 `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 matrix 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

<i>res</i>	user supplied function for the non-linear residuals of the system
<i>evalx</i>	user supplied function for the weak form to estimate the next solution
<i>x</i>	user supplied matrix holding the initial guess to the non-linear system
<i>picard_dat</i>	pointer to the PICARD_DATA data structure
<i>res_data</i>	user supplied void pointer to a data structure used for residual evaluations
<i>evalx_data</i>	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: $x = 1 - x0^2$ Rearrange residual to form a weak solution

5.38.4.18 `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 (PJFNK) 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 $x_{k+1} = x_k + s_k$

Parameters

<i>res</i>	user supplied residual function for the non-linear system
<i>precon</i>	user supplied preconditioning function for the linear sub-problems
<i>x</i>	user supplied initial guess and storage location of the solution
<i>pjfnk_dat</i>	pointer to the PJFNK_DATA data structure
<i>res_data</i>	user supplied void pointer to data structure used in residual function
<i>precon_data</i>	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.

5.38.4.19 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

<i>x</i>	matrix that will hold the new updated solution to the linear system
<i>x0</i>	matrix that holds the previous solution to the linear system
<i>arnoldi_dat</i>	pointer to the ARNOLDI_DATA data structure

5.39 LinearDrivingForce.h File Reference

```
#include "Kernel.h"
```

Classes

- class [LinearDrivingForce](#)

Functions

- `template<>`
`InputParameters validParams< LinearDrivingForce > ()`

5.39.1 Function Documentation

5.39.1.1 `template<> InputParameters validParams< LinearDrivingForce > ()`

5.40 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.

5.40.1 Detailed Description

MAtrix CAlculation Workspace. macaw.cpp

This is a small C++ library that facilitates 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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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.

Definition in file [macaw.h](#).

5.40.2 Macro Definition Documentation**5.40.2.1 #define M_PI 3.14159265358979323846264338327950288**

Value of PI with double precision.

Definition at line 43 of file macaw.h.

Referenced by `Matrix< T >::IntegralTotal()`.

5.41 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: $\text{J}/(\text{K} \cdot \text{mol}) = k_B \cdot N_A$.
- `#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 Imfit 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 Imfit 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 Imfit 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 Imfit 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 Imfit 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.

5.41.1 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 explanation 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, wherein the isotherm for each species is represented 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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Definition in file [magpie.h](#).

5.41.2 Macro Definition Documentation

5.41.2.1 `#define A 3.13E+09`

Corresponding van der Waals standard area for our coordination number (cm^2/mol)

Definition at line 56 of file [magpie.h](#).

Referenced by `Matrix< T >::inverse()`, `Matrix< T >::ladshawSolve()`, and `Matrix< T >::tridiagonalSolve()`.

5.41.2.2 `#define DBL_EPSILON 2.2204460492503131e-016`

Machine precision value used for approximating gradients.

Definition at line 48 of file [magpie.h](#).

5.41.2.3 `#define He(qm, K1, m)(qm * K1) / (m * Po)`

This macro calculates the Henry's Coefficient for the *ith* component.

Definition at line 91 of file [magpie.h](#).

5.41.2.4 `#define kB 1.3806488E-23`

Boltzmann's Constant - Units: J/K.

Definition at line 76 of file magpie.h.

5.41.2.5 `#define lnKo(H, S, T) -(H / (R * T)) + (S / R)`

This macro calculates the natural log of the dimensionless isotherm parameter.

Definition at line 86 of file magpie.h.

5.41.2.6 `#define Na 6.0221413E+23`

Avagadro's Number - Units: molecules/mol.

Definition at line 72 of file magpie.h.

5.41.2.7 `#define Po 100.0`

Standard State Pressure - Units: kPa.

Definition at line 64 of file magpie.h.

5.41.2.8 `#define R 8.3144621`

Gas Constant - Units: J/(K*mol) = kB * Na.

Definition at line 68 of file magpie.h.

5.41.2.9 `#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.

Definition at line 81 of file magpie.h.

5.41.2.10 `#define V 18.92`

Corresponding van der Waals standard volume for our coordination number (cm³/mol)

Definition at line 60 of file magpie.h.

5.41.2.11 `#define Z 10.0`

Surface coordination number used in the MSPD activity model.

Definition at line 52 of file magpie.h.

5.41.3 Function Documentation

5.41.3.1 `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

<i>p</i>	partial pressure in kPa at which to evaluate the GSTA model
<i>data</i>	void pointer to the MAGPIE_DATA data structure
<i>i</i>	index of the gas species for which the GSTA model is being evaluated

5.41.3.2 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.

5.41.3.3 void eval_eta (const double * par, int m_dat, const void * data, double * fvec, int * info)

Function used with Imfit 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 use when evaluating the activity coefficients for the overall mixture. User does not need to call this function. GPAST will call automatically when needed.

Parameters

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>m_dat</i>	number of functions/variables in the GPAST system of equations
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>fvec</i>	list of residuals formed by the functions in GPAST
<i>info</i>	integer flag variable used in the Imfit routine

5.41.3.4 void eval_GPAST (const double * par, int m_dat, const void * data, double * fvec, int * info)

Function used with Imfit 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>m_dat</i>	number of functions/variables in the GPAST system of equations
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>fvec</i>	list of residuals formed by the functions in GPAST
<i>info</i>	integer flag variable used in the Imfit routine

5.41.3.5 void eval_po (const double * par, int m_dat, const void * data, double * fvec, int * info)

Function used with Imfit 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>m_dat</i>	number of functions/variables in the GPAST system of equations
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>fvec</i>	list of residuals formed by the functions in GPAST
<i>info</i>	integer flag variable used in the Imfit routine

5.41.3.6 void eval_po_PI (const double * par, int m_dat, const void * data, double * fvec, int * info)

Function used with Imfit 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>m_dat</i>	number of functions/variables in the GPAST system of equations
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>fvec</i>	list of residuals formed by the functions in GPAST
<i>info</i>	integer flag variable used in the Imfit routine

5.41.3.7 void eval_po_qo (const double * *par*, int *m_dat*, const void * *data*, double * *fvec*, int * *info*)

Function used with Imfit 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>m_dat</i>	number of functions/variables in the GPAST system of equations
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>fvec</i>	list of residuals formed by the functions in GPAST
<i>info</i>	integer flag variable used in the Imfit routine

5.41.3.8 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>i</i>	ith species for which we will approximate the activity model gradient

5.41.3.9 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>data</i>	void pointer for the MAGPIE_DATA data structure

5.41.3.10 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

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>data</i>	void pointer for the MAGPIE_DATA data structure
<i>i</i>	ith species that we want to calculate the activity coefficient for
<i>PI</i>	lumped spreading pressure term used in gradient estimations

5.41.3.11 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 initialize 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

<i>data</i>	void pointer for the MAGPIE_DATA data structure holding all necessary information
-------------	---

5.41.3.12 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

<i>po</i>	partial pressure in kPa at which to evaluate the lumped spreading pressure
<i>data</i>	void pointer to the MAGPIE_DATA data structure
<i>i</i>	index of the gas species for which the GSTA model is being evaluated

5.41.3.13 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

<i>p</i>	partial pressure in kPa at which to evaluate the GSTA model
<i>data</i>	void pointer to the MAGPIE_DATA data structure
<i>i</i>	index of the gas species for which the GSTA model is being evaluated

5.41.3.14 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

<i>po</i>	partial pressure in kPa at which to evaluate the GSTA model
<i>data</i>	void pointer to the MAGPIE_DATA data structure
<i>i</i>	index of the gas species for which the GSTA model is being evaluated

Referenced by `Matrix< T >::IntegralAvg()`, and `Matrix< T >::IntegralTotal()`.

5.41.3.15 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

<i>po</i>	partial pressure in kPa at which to evaluate the heat of adsorption
<i>data</i>	void pointer to the MAGPIE_DATA data structure
<i>i</i>	index of the gas species for which the GSTA model is being evaluated

5.41.3.16 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 use 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 [SYSTEM_DATA](#) structure.

Parameters

<i>par</i>	list of parameters representing variables to be solved for in GPAST
<i>data</i>	void pointer for the MAGPIE_DATA data structure

5.42 MAGPIE_Adsorption.h File Reference

Auxillary kernel to calculate adsorption equilibria of a particular gas species in the system.

```
#include "AuxKernel.h"
#include "flock.h"
```

Classes

- class [MAGPIE_Adsorption](#)
Magpie Adsorption class inherits from AuxKernel.

Functions

- `template<> InputParameters validParams< MAGPIE_Adsorption > ()`

5.42.1 Detailed Description

Auxillary kernel to calculate adsorption equilibria of a particular gas species in the system. This file is responsible for calculating the adsorption equilibria of a particular species in the system. The MAGPIE object is stored as a material property whose constants are set in the corresponding material property file (see [MagpieAdsorbateProperties.h](#)). That information is then used to call the MAGPIE routine to calculate the mixed gas adsorption for a specific species of interest.

Unfortunately, the material property system has recently changed in MOOSE, making this operation much less efficient. Under the new system, all material properties are declared as constants when outside of their respective material property files. This means that in order for me to call the MAGPIE subroutine, which edits values in the MAGPIE object, I have to create a copy of the entire object and have the subroutine act on that copy.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [MAGPIE_Adsorption.h](#).

5.42.2 Function Documentation

5.42.2.1 `template<> InputParameters validParams< MAGPIE_Adsorption > ()`

5.43 MAGPIE_AdsorptionHeat.h File Reference

Auxillary kernel to calculate heat of adsorption of a particular gas species in the system.

```
#include "AuxKernel.h"
#include "flock.h"
```

Classes

- class [MAGPIE_AdsorptionHeat](#)
Magpie Adsorption Heat class inherits from AuxKernel.

Functions

- template<>
InputParameters [validParams< MAGPIE_AdsorptionHeat > \(\)](#)

5.43.1 Detailed Description

Auxillary kernel to calculate heat of adsorption of a particular gas species in the system. This file is responsible for calculating the heat of adsorption of a particular species in the system. The MAGPIE object is stored as a material property whose constants are set in the corresponding material property file (see [MagpieAdsorbateProperties.h](#)). That information is then used to call the MAGPIE routine to calculate the mixed gas adsorption for a specific species of interest.

Unfortunately, the material property system has recently changed in MOOSE, making this operation much less efficient. Under the new system, all material properties are declared as constants when outside of their respective material property files. This means that in order for me to call the MAGPIE subroutine, which edits values in the MAGPIE object, I have to create a copy of the entire object and have the subroutine act on that copy.

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Definition in file [MAGPIE_AdsorptionHeat.h](#).

5.43.2 Function Documentation

5.43.2.1 `template<> InputParameters validParams< MAGPIE_AdsorptionHeat > ()`

5.44 MAGPIE_HeatAccumulation.h File Reference

```
#include "Kernel.h"
```

Classes

- class [MAGPIE_HeatAccumulation](#)

Functions

- template<>
InputParameters [validParams< MAGPIE_HeatAccumulation >\(\)](#)

5.44.1 Function Documentation

5.44.1.1 template<> InputParameters validParams< MAGPIE_HeatAccumulation > ()

5.45 MAGPIE_Perturbation.h File Reference

Auxillary kernel to calculate the perturbed adsorption equilibria of a particular gas species in the system.

```
#include "AuxKernel.h"
#include "flock.h"
```

Classes

- class [MAGPIE_Perturbation](#)
Magpie Perturbation class inherits from AuxKernel.

Functions

- template<>
InputParameters [validParams< MAGPIE_Perturbation >\(\)](#)

5.45.1 Detailed Description

Auxillary kernel to calculate the perturbed adsorption equilibria of a particular gas species in the system. This file is responsible for calculating the perturbed adsorption equilibria of a particular species in the system. The MAGPIE object is stored as a material property whose constants are set in the corresponding material property file (see [MagpieAdsorbateProperties.h](#)). That information is then used to call the MAGPIE routine to calculate the mixed gas perturbed adsorption for a specific species of interest.

The perturbation is used to approximate the strength of adsorption via first order finite difference. That adsorption strength is then loosely coupled to the gaseous species non-linear variable through a retardation coefficient in the mass transport equations. We use loose coupling to improve the efficiency of the solutions for this multi-scale mass transfer problem. Full coupling would result in significant losses in efficiency, or even complete failure to converge. DO NOT TRY FULL COUPLING!

Unfortunately, the material property system has recently changed in MOOSE, making this operation much less efficient. Under the new system, all material properties are declared as constants when outside of their respective material property files. This means that in order for me to call the MAGPIE subroutine, which edits values in the MAGPIE object, I have to create a copy of the entire object and have the subroutine act on that copy.

Note

We will only use this kernel to approximate the retardation effect of adsorption IF we are neglecting the micro-scale kinetics of adsorption/mass transfer into the adsorbent pellets. Kinetics coupling will be accomplished in another kernel.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [MAGPIE_Perturbation.h](#).

5.45.2 Function Documentation

5.45.2.1 `template<> InputParameters validParams< MAGPIE_Perturbation > ()`

5.46 MagpieAdsorbateProperties.h File Reference

Material Properties kernel that will setup and hold all information associated with MAGPIE simulations.

```
#include "Material.h"
#include "flock.h"
```

Classes

- class [MagpieAdsorbateProperties](#)
[MagpieAdsorbateProperties](#) class object inherits from Material object.

Functions

- `template<>`
`InputParameters validParams< MagpieAdsorbateProperties > \(\)`

5.46.1 Detailed Description

Material Properties kernel that will setup and hold all information associated with MAGPIE simulations. This file creates a material property object for the MAGPIE data structure and associated constants. That information is used in conjunction with the MAGPIE simulation functions (see [magpie.h](#)) in order to approximate the adsorption capacities and adsorbed amounts of each gas species in a given system for a given adsorbent.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [MagpieAdsorbateProperties.h](#).

5.46.2 Function Documentation

5.46.2.1 `template<> InputParameters validParams< MagpieAdsorbateProperties > ()`

5.47 RetardedTimeDerivative.h File Reference

```
#include "TimeDerivative.h"
```

Classes

- class [RetardedTimeDerivative](#)

Functions

- `template<> InputParameters validParams< RetardedTimeDerivative > ()`

5.47.1 Function Documentation

5.47.1.1 `template<> InputParameters validParams< RetardedTimeDerivative > ()`

5.48 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 (cm²/s)

- `#define Dk(rp, T, MW) (9700.0*rp*pow((T/MW),0.5))`
Estimate of Knudsen Diffusivity (cm²/s)
- `#define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)), -1.0))`
Estimate of Average Pore Diffusion (cm²/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.

5.48.1 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

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Definition in file [scopsowl.h](#).

5.48.2 Macro Definition Documentation

5.48.2.1 `#define avgDp(Dp, Dk) (pow(((1/Dp)+(1/Dk)),-1.0))`

Estimate of Average Pore Diffusion (cm^2/s)

Definition at line 37 of file scopsowl.h.

5.48.2.2 `#define Dk(rp, T, MW) (9700.0*rp*pow((T/MW),0.5))`

Estimate of Knudsen Diffusivity (cm^2/s)

Definition at line 33 of file scopsowl.h.

5.48.2.3 `#define Dp(Dm, ep) (ep*ep*Dm)`

Estimate of Pore Diffusivity (cm^2/s)

Definition at line 29 of file scopsowl.h.

5.48.2.4 `#define SCOPSOWL_HPP_`

Definition at line 26 of file scopsowl.h.

5.48.3 Function Documentation

5.48.3.1 `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>i</i>	index for the <i>i</i> th species in the system
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.2 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.3 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.4 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.5 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>i</i>	index for the <i>i</i> th species in the system
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.6 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.7 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.8 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>i</i>	index for the <i>i</i> th species in the system
<i>l</i>	index for the <i>l</i> th node in the macro-scale domain
<i>user_data</i>	pointer for the SCOSPOWL_DATA structure

5.48.3.9 void print2file_SCOPSOWL_header (SCOPSOWL_DATA * *owl_dat*)

Function to call the species and time header functions.

5.48.3.10 void print2file_SCOPSOWL_result_new (SCOPSOWL_DATA * *owl_dat*)

Function to print out the new time results to the output file.

5.48.3.11 void print2file_SCOPSOWL_result_old (SCOPSOWL_DATA * *owl_dat*)

Function to print out the old time results to the output file.

5.48.3.12 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.

5.48.3.13 void print2file_species_header (FILE * *Output*, SCOPSOWL_DATA * *owl_dat*, int *i*)

Function to print out the main header for the output file.

5.48.3.14 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.15 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.16 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.17 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.18 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.19 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.20 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

<i>user_data</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
------------------	--

5.48.3.21 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

<i>owl_dat</i>	pointer to the SCOPSOWL_DATA structure (must be initialized)
----------------	--

5.48.3.22 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

<i>file</i>	pointer to the output file to print out results
<i>eval_sorption</i>	pointer to the adsorption evaluation function
<i>eval_retardation</i>	pointer to the retardation evaluation function
<i>eval_pore_diff</i>	pointer to the pore diffusion function
<i>eval_filmMT</i>	pointer to the film mass transfer function
<i>eval_surface_diff</i>	pointer to the surface diffusion function (required)
<i>user_data</i>	pointer to the user's data structure used for the parameter functions
<i>gas_data</i>	pointer to the MIXED_GAS structure used to evaluate kinetic gas theory
<i>owl_data</i>	pointer to the SCOPSOWL_DATA structure

5.49 skua.h File Reference

Surface Kinetics for Uptake by Adsorption.

```
#include "finch.h"
#include "magpie.h"
#include "egret.h"
```

Classes

- struct [SKUA_PARAM](#)
Data structure for species' parameters in SKUA.
- struct [SKUA_DATA](#)
Data structure for all simulation information in SKUA.

Macros

- #define [SKUA_HPP_](#)
- #define [D_inf](#)(Dref, Tref, B, p, T) (Dref * pow(p+sqrt([DBL_EPSILON](#)),(Tref/T)-B))
Empirical correction of diffusivity (um^2/hr)
- #define [D_o](#)(Diff, E, T) (Diff * exp(-E/([Rstd](#)*T)))
Arrhenius Rate Expression for Diffusivity (um^2/hr)
- #define [D_c](#)(Diff, phi) (Diff * (1.0/((1.0+1.1E-6)-phi)))
Approximate Darken Diffusivity Equation (um^2/hr)

Functions

- void [print2file_species_header](#) (FILE *Output, [SKUA_DATA](#) *skua_dat, int i)
Function to print out the species' headers to output file.
- void [print2file_SKUA_time_header](#) (FILE *Output, [SKUA_DATA](#) *skua_dat, int i)
Function to print out time and space headers to output file.
- void [print2file_SKUA_header](#) ([SKUA_DATA](#) *skua_dat)
Function calls the other header functions to establish output file structure.
- void [print2file_SKUA_results_old](#) ([SKUA_DATA](#) *skua_dat)
Function to print out the old time step simulation results to the output file.
- void [print2file_SKUA_results_new](#) ([SKUA_DATA](#) *skua_dat)
Function to print out the new time step simulation results to the output file.
- double [default_Dc](#) (int i, int l, const void *data)
Default function for surface diffusivity.
- double [default_kf](#) (int i, const void *data)
Default function for film mass transfer coefficient.
- double [const_Dc](#) (int i, int l, const void *data)
Constant surface diffusivity function.
- double [simple_darken_Dc](#) (int i, int l, const void *data)
Simple Darken model for surface diffusivity.
- double [theoretical_darken_Dc](#) (int i, int l, const void *data)
Theoretical Darken model for surface diffusivity.
- double [empirical_kf](#) (int i, const void *data)
Empirical function for film mass transfer coefficient.
- double [const_kf](#) (int i, const void *data)
Constant function for film mass transfer coefficient.

- int [molefractionCheck](#) (SKUA_DATA *skua_dat)
Function to check mole fractions in gas and solid phases for errors.
- 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)
Function to setup the function pointers and vector objects in memory to setup the SKUA simulation.
- int [SKUA_Executioner](#) (SKUA_DATA *skua_dat)
Function to execute preprocesses, solvers, and postprocesses for a SKUA simulation.
- int [set_SKUA_ICs](#) (SKUA_DATA *skua_dat)
Function to establish the initial conditions of adsorption in the adsorbent.
- int [set_SKUA_timestep](#) (SKUA_DATA *skua_dat)
Function to establish the time step for the current simulation.
- int [SKUA_preprocesses](#) (SKUA_DATA *skua_dat)
Function to perform the necessary preprocess operations before a solve.
- int [set_SKUA_params](#) (const void *user_data)
Function to call the diffusivity function during the solve.
- int [SKUA_postprocesses](#) (SKUA_DATA *skua_dat)
Function to perform the necessary postprocess operations after a solve.
- int [SKUA_reset](#) (SKUA_DATA *skua_dat)
Function to reset the stateful information in SKUA after a simulation.
- int [SKUA](#) (SKUA_DATA *skua_dat)
Function to iteratively call all execution steps to evolve a simulation through time.

5.49.1 Detailed Description

Surface Kinetics for Uptake by Adsorption. skua.cpp

This file contains structures and functions associated with solving the surface diffusion partial differential equations for adsorption kinetics in spherical and/or cylindrical adsorbents. For this system, it is assumed that the pore size is so small that all molecules are confined to movement exclusively on the surface area of the adsorbent. The total amount of adsorption for each species is drive by the MAGPIE model for non-ideal mixed gas adsorption. Spatial and temporal variance in adsorption is caused by a combination of different kinetics between adsorbing species and different adsorption affinities for the surface.

The function for surface diffusion involves four parameters, although not all of these parameters are required to be used. Surface diffusion theoretically varies with temperature according to the Arrhenius rate expression, but we also add in an empirical correction term to account for variations in diffusivity with the partial pressure of the species in the gas phase.

$$D_{\text{surf}} = D_{\text{ref}} * \exp(-E / (R*T)) * \text{pow}(p, (T_{\text{ref}}/T) - B)$$

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.

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Date

01/26/2015

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Definition in file [skua.h](#).

5.49.2 Macro Definition Documentation

5.49.2.1 `#define D_c(Diff, phi) (Diff * (1.0/((1.0+1.1E-6)-phi)))`

Approximate Darken Diffusivity Equation (um^2/hr)

Definition at line 48 of file skua.h.

5.49.2.2 `#define D_inf(Dref, Tref, B, p, T) (Dref * pow(p+sqrt(DBL_EPSILON),(Tref/T)-B))`

Empirical correction of diffusivity (um^2/hr)

Definition at line 40 of file skua.h.

5.49.2.3 `#define D_o(Diff, E, T) (Diff * exp(-E/(Rstd*T)))`

Arrhenius Rate Expression for Diffusivity (um^2/hr)

Definition at line 44 of file skua.h.

5.49.2.4 `#define SKUA_HPP_`

Definition at line 37 of file skua.h.

5.49.3 Function Documentation

5.49.3.1 `double const_Dc (int i, int l, const void * data)`

Constant surface diffusivity function.

This function allows the user to specify just a single constant value for surface diffusivity. The value of diffusivity applied at all nodes will be the ref_diffusion parameter in [SKUA_PARAM](#).

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>l</i>	index of the node in the spatial discretization that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.2 `double const_kf (int i, const void * data)`

Constant function for film mass transfer coefficient.

This function allows the user to specify a constant value for the film mass transfer coefficient. The value of the film mass transfer coefficient will be the value of film_transfer given in the [SKUA_PARAM](#) data structure.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.3 `double default_Dc (int i, int l, const void * data)`

Default function for surface diffusivity.

This is the default function provided by SKUA for the calculation of the surface diffusivity parameter. The diffusivity is calculated based on the Arrhenius rate expression, then corrected for using the empirical correction term with the outside partial pressure of the gas species.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>l</i>	index of the node in the spatial discretization that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.4 double default_kf (int *i*, const void * *data*)

Default function for film mass transfer coefficient.

This is the default function provided by SKUA for the calculation of the film mass transfer parameter. By default, we are usually going to couple the SKUA model with a pore diffusion model (see [scopsowl.h](#)). Therefore, the film mass transfer coefficient would be zero, because we would only consider a Dirichlet boundary condition for this sub-problem.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.5 double empirical_kf (int *i*, const void * *data*)

Empirical function for film mass transfer coefficient.

This function provides an empirical estimate of the mass transfer coefficient using the gas velocity, molecular diffusivities, and dimensionless numbers (see [egret.h](#)). It is used as the default film mass transfer function IF the boundary condition is specified to be a Neumann type boundary by the user.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.6 int molefractionCheck (SKUA_DATA * *skua_dat*)

Function to check mole fractions in gas and solid phases for errors.

This function is called after reading input and before calling the primary solution routines. It will force an error and quit the program if there are inconsistencies in the mole fractions it was given. All mole fractions must sum to 1, otherwise there is missing information.

5.49.3.7 void print2file_SKUA_header (SKUA_DATA * *skua_dat*)

Function calls the other header functions to establish output file structure.

5.49.3.8 void print2file_SKUA_results_new (SKUA_DATA * *skua_dat*)

Function to print out the new time step simulation results to the output file.

5.49.3.9 void print2file_SKUA_results_old (SKUA_DATA * *skua_dat*)

Function to print out the old time step simulation results to the output file.

5.49.3.10 void print2file_SKUA_time_header (FILE * *Output*, SKUA_DATA * *skua_dat*, int *i*)

Function to print out time and space headers to output file.

5.49.3.11 void print2file_species_header (FILE * *Output*, SKUA_DATA * *skua_dat*, int *i*)

Function to print out the species' headers to output file.

5.49.3.12 `int set_SKUA_ICs (SKUA_DATA * skua_dat)`

Function to establish the initial conditions of adsorption in the adsorbent.

This function needs to be called before doing any simulation or execution of a time step, but only once per simulation. It sets the value of adsorption for each adsorbable species to the specified initial values given via qT and xIC in [SKUA_DATA](#).

5.49.3.13 `int set_SKUA_params (const void * user_data)`

Function to call the diffusivity function during the solve.

This is the function passed into FINCH to be called during the FINCH solver (see [finch.h](#)). It will call the diffusion functions set by the user in the setup function above. This is not overridable.

5.49.3.14 `int set_SKUA_timestep (SKUA_DATA * skua_dat)`

Function to establish the time step for the current simulation.

This function is called to set a time step value for a particular simulation step. By default, the time step is set to (1/4)x space step size. If you need to change the step size, you must do so manually.

5.49.3.15 `int setup_SKUA_DATA (FILE * file, double(*)(int i, int l, const void *user_data) eval_Dc, double(*)(int i, const void *user_data) eval_Kf, const void * user_data, MIXED_GAS * gas_data, SKUA_DATA * skua_dat)`

Function to setup the function pointers and vector objects in memory to setup the SKUA simulation.

This function is called to setup the SKUA problem in memory and set function pointers to either defaults or user specified functions. It must be called prior to calling any other SKUA function and will report an error if the object was not setup properly.

Parameters

<i>file</i>	pointer to the output file for SKUA simulations
<i>eval_Dc</i>	pointer to the function to evaluate the surface diffusivity
<i>eval_Kf</i>	pointer to the function to evaluate the film mass transfer coefficient
<i>user_data</i>	pointer to a user defined data structure used in the calculation the the parameters
<i>gas_data</i>	pointer to the MIXED_GAS data structure for egret.h calculations
<i>skua_dat</i>	pointer to the SKUA_DATA data structure

5.49.3.16 `double simple_darken_Dc (int i, int l, const void * data)`

Simple Darken model for surface diffusivity.

This function uses an approximation to Darken's model for surface diffusion. The approximation is exact if the isotherm for adsorption takes the form of the Langmuir model, but is only approximate if the isotherm is heterogeneous. Forming the approximation in this manner is significantly cheaper than forming the true Darken model expression for the GSTA isotherm.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>l</i>	index of the node in the spatial discretization that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.49.3.17 `int SKUA (SKUA_DATA * skua_dat)`

Function to iteratively call all execution steps to evolve a simulation through time.

This function is used in conjunction with the scenario call from the UI to numerically solve the adsorption kinetics problem in time. It will call the initial conditions function once, then iteratively call the reset, time step, and executioner functions for SKUA to push the simulation forward in time. This function will be called from the SKUA_SCENARIOS

function.

5.49.3.18 int SKUA_Executioner (SKUA_DATA * skua_dat)

Function to execute preprocesses, solvers, and postprocesses for a SKUA simulation.

This function calls the preprocess, solver, and postprocess functions to complete a single time step in a SKUA simulation. User's will want to call this function whenever a time step simulation result is needed. This is used primarily when coupling with other models (see [scopsowl.h](#)).

5.49.3.19 int SKUA_postprocesses (SKUA_DATA * skua_dat)

Function to perform the necessary postprocess operations after a solve.

This function performs postprocess operations after a solve was completed successfully. Those operations include estimating average total adsorption, average adsorbed mole fractions, and heat of adsorption for each species. Results are then printed to the output file.

5.49.3.20 int SKUA_preprocesses (SKUA_DATA * skua_dat)

Function to perform the necessary preprocess operations before a solve.

This function performs preprocess operations prior to calling the solver routine. Those preprocesses include establishing boundary conditions and performing a MAGPIE simulation for the adsorption on the surface (see [magpie.h](#)).

5.49.3.21 int SKUA_reset (SKUA_DATA * skua_dat)

Function to reset the stateful information in SKUA after a simulation.

This function sets all the old state data to the newly formed state data. It needs to be called after a successful execution of the simulation step and before calling for the next time step to be solved. Do not call out of turn, otherwise information will be lost.

5.49.3.22 double theoretical_darken_Dc (int i, int l, const void * data)

Theoretical Darken model for surface diffusivity.

This function uses the full theoretical expression of the Darken's diffusion model to calculate the surface diffusivity. This calculation involves formulating the reference state pressures for the adsorbed amount at every node, then calculating derivatives of the adsorption isotherm for each species. It is more accurate than the simple Darken model function, but costs significantly more computational time.

Parameters

<i>i</i>	index of the gas/adsorbed phase species that this function acts on
<i>l</i>	index of the node in the spatial discretization that this function acts on
<i>data</i>	pointer to the SKUA_DATA structure

5.50 TotalColumnPressure.h File Reference

Auxillary kernel to calculate total column pressure based on temperature and concentrations.

```
#include "AuxKernel.h"
```

Classes

- class [TotalColumnPressure](#)

Total Column Pressure class inherits from AuxKernel.

Functions

- `template<>`
`InputParameters validParams< TotalColumnPressure > ()`

5.50.1 Detailed Description

Auxillary kernel to calculate total column pressure based on temperature and concentrations. This file is responsible for calculating the total column pressure in a fixed-bed adsorber given the temperature and the concentrations of all species in the gas phase. The gas phase is assumed to behave ideally and ideal gas law is employed to estimate the pressure.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [TotalColumnPressure.h](#).

5.50.2 Function Documentation

5.50.2.1 `template<> InputParameters validParams< TotalColumnPressure > ()`

5.51 TotalPressureIC.h File Reference

Initial Condition kernel for initial temperature in a fixed-bed column.

```
#include "InitialCondition.h"
```

Classes

- class [TotalPressureIC](#)
TotalPressureIC class object inherits from InitialCondition object.

Functions

- `template<>`
`InputParameters validParams< TotalPressureIC > ()`

5.51.1 Detailed Description

Initial Condition kernel for initial temperature in a fixed-bed column. This file creates an initial condition for the temperature in the bed. The initial condition for temperature is assumed a constant value at all points in the bed. However, this can be modified later to include spatially varying initial conditions for temperature.

Note

If you want to have spatially varying initial conditions, you will need to modify the virtual value function of this kernel. Otherwise, it is assumed that the non-linear variable is initially constant at all points in the domain.

Author

Austin Ladshaw

Date

11/20/2015

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Definition in file [TotalPressureIC.h](#).

5.51.2 Function Documentation

5.51.2.1 `template<> InputParameters validParams< TotalPressureIC > ()`

5.52 WallAmbientHeatTransfer.h File Reference

```
#include "Kernel.h"
```

Classes

- class [WallAmbientHeatTransfer](#)

Functions

- `template<> InputParameters validParams< WallAmbientHeatTransfer > ()`

5.52.1 Function Documentation

5.52.1.1 `template<> InputParameters validParams< WallAmbientHeatTransfer > ()`

5.53 WallHeatAccumulation.h File Reference

```
#include "TimeDerivative.h"
```

Classes

- class [WallHeatAccumulation](#)

Functions

- `template<>`
InputParameters [validParams< WallHeatAccumulation >\(\)](#)

5.53.1 Function Documentation

5.53.1.1 `template<> InputParameters validParams< WallHeatAccumulation >()`

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