Combustion of Packed Pellets of Core-Shell Particle

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combustion-packed-pellet-core-shell-particle

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5.1.1 Detailed Description

Python program to quickly check out and understand QR Factorization method for solving matrix equations

The matrices are printed at each step of factorization to understand the transformation of the matrices

Chapter 6

Class Documentation

6.1 CoreShellCombustionParticle< real_t > Class Template Reference

Class to represent Core-Shell Particle with functions estimate thermodynamic properties for varying composition and temperature.

`#include <Core-Shell-Combustion-Particle.hpp>`

Public Member Functions

- CoreShellCombustionParticle (Substance< real_t > core_material, Substance< real_t > shell_material, Substance< real_t > product_material, real_t diffusivity_pre_exponential_factor, real_t diffusivity_↩ activation_energy)

  Construct a new Core Shell Combustion Particle object.
- real_t getDensity ()

  Get the Density of the Particle.
- real_t getHeatCapacity ()

  Get the Heat Capacity of the particle.
- real_t getHeatConductivity ()

  Get the Heat Conductivity of the particle.
- real_t getEnthalpy (real_t temperature)

  Get the Enthalpy of the particle.
- real_t getDiffusivity (real_t temperature)

  Get the Diffusivity for the interdiffusion of the core and shell material.
- void printProperties (std::ostream &output_stream)

  Print the properties of the substance to the given stream.

Protected Attributes

- real_t mass_fraction_reactant_A

  Mass fraction of reactant A.
- real_t mass_fraction_reactant_B

  Mass fraction of reactant B.
- real_t mass_fraction_product_AB

  Mass fraction of product AB.
- real_t pre_exponential_factor

  Pre exponential factor for Arrhenius Diffusivity model.
- real_t activation_energy

  Activation energy for Arrhenius Diffusivity model.
- Substance< real_t > reactant_A

  Reactant A substance initially present in the core.
- Substance< real_t > reactant_B

  Reactant B substance initially present in the shell.
- Substance< real_t > product_AB

  Product AB substance.

6.1.1 Detailed Description

template<typename real_t>
class CoreShellCombustionParticle< real_t >

Class to represent Core-Shell Particle with functions estimate thermodynamic properties for varying composition and temperature.

Template Parameters

real_t	

Definition at line 28 of file Core-Shell-Combustion-Particle.hpp.

6.1.2 Constructor & Destructor Documentation

6.1.2.1 CoreShellCombustionParticle()

```
template<typename real_t >
CoreShellCombustionParticle< real_t >::CoreShellCombustionParticle (
            Substance< real_t > core_material,
            Substance< real_t > shell_material,
            Substance< real_t > product_material,
            real_t diffusivity_pre_exponential_factor,
            real_t diffusivity_activation_energy )
```

Construct a new Core Shell Combustion Particle object.

Parameters

core_material	Substance that forms the core material
shell_material	Substance that forms the shell material
product_material	Substance that is produced as a result of the reaction of the core and shell material
diffusivity_pre_exponential_factor	Pre-exponential factor in the Arrhenius model for diffusivity
diffusivity_activation_energy	Activation energy in the Arrhenius model for diffusivity

Definition at line 17 of file Core-Shell-Combustion-Particle.cpp.

6.1.3 Member Function Documentation

6.1.3.1 getDensity()

```
template<typename real_t >
real_t CoreShellCombustionParticle< real_t >::getDensity
```

Get the Density of the Particle.

Returns

real_t Density of the particle

Definition at line 59 of file Core-Shell-Combustion-Particle.cpp.

6.1.3.2 getDiffusivity()

```
template<typename real_t >
real_t CoreShellCombustionParticle< real_t >::getDiffusivity (
            real_t temperature )
```

Get the Diffusivity for the interdiffusion of the core and shell material.

Parameters

temperature	Overall temperature of the particle

Returns

real_t Diffusivity for interdiffusion model at the specified temperature

Definition at line 68 of file Core-Shell-Combustion-Particle.cpp.

6.1.3.3 getEnthalpy()

```
template<typename real_t >
real_t CoreShellCombustionParticle< real_t >::getEnthalpy (
            real_t temperature )
```

Get the Enthalpy of the particle.

Parameters

temperature	Overall temperature of the particle

Returns

real_t Enthalpy of the particle at the specified temperature

Definition at line 92 of file Core-Shell-Combustion-Particle.cpp.

6.1.3.4 getHeatCapacity()

```
template<typename real_t >
real_t CoreShellCombustionParticle< real_t >::getHeatCapacity
```

Get the Heat Capacity of the particle.

Returns

real_t Heat capacity of the particle

Definition at line 74 of file Core-Shell-Combustion-Particle.cpp.

6.1.3.5 getHeatConductivity()

```
template<typename real_t >
real_t CoreShellCombustionParticle< real_t >::getHeatConductivity
```

Get the Heat Conductivity of the particle.

Returns

real_t Heat capacity of the particle

Definition at line 83 of file Core-Shell-Combustion-Particle.cpp.

6.1.3.6 printProperties()

```
template<typename real_t >
void CoreShellCombustionParticle< real_t >::printProperties (
            std::ostream & output_stream )
```

Print the properties of the substance to the given stream.

Parameters

output_stream	Stream to which the properties are printed

Definition at line 36 of file Core-Shell-Combustion-Particle.cpp.

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

- include/thermo-physical-properties/Core-Shell-Combustion-Particle.hpp
- src/thermo-physical-properties/Core-Shell-Combustion-Particle.cpp

6.2 GMatrix< real_t > Class Template Reference

Class to implement a memory efficient Givens' Rotation Matrix that can vanish the element $a_{k+1,k}$ of a matrix A.

`#include <G_Matrix.hpp>`

Public Member Functions

- GMatrix (RMatrix< real_t > &matrix, unsigned int index)

  Construct a new Givens Rotation Matrix to vanish the element at position $(k+1,k)$ of R matrix.
- void multiply (RMatrix< real_t > &R)

  Multiplies the Givens Rotation Matrix to the R Matrix and updates the R matrix in place.
- void multiplyLastRow (RMatrix< real_t > &R)

  Multiplies the Givens rotation matrix to the R matrix where the rotation matrix is formed to vanish the sub diagonal element of the last row $(N,N-1)$ of the $N \times N$ R matrix.
- void multiply (QMatrix< real_t > &Q)

  Multiplies the Givens Rotation Matrix to the Q Matrix and updates the Q matrix in place.

Private Attributes

- real_t g_k_k

  Element of Givens Rotation Matrix at position k,k.
- real_t g_k_kp1

  Element of Givens Rotation Matrix at position $k,k+1$.
- real_t g_kp1_k

  Element of Givens Rotation Matrix at position $k+1,k$.
- real_t g_kp1_kp1

  Element of Givens Rotation Matrix at position $k+1,k+1$.
- unsigned int k

  Index k, where we want to vanish the element at position $k+1,k$.

6.2.1 Detailed Description

template<typename real_t>
class GMatrix< real_t >

Class to implement a memory efficient Givens' Rotation Matrix that can vanish the element $a_{k+1,k}$ of a matrix A.

A Givens rotation matrix is an orthogonal such that $G_{N\times N} = [g_{ij}]_{N\times N}$ where

$$g_{ij} = \begin{cases} 1 & i = j \neq k, k+1 \\ \cos\theta & i = j = k, k+1 \\ \sin\theta & i = k, j = k+1 \\ -\sin\theta & i = k+1, j = k \\ 0 & \text{otherwise} \end{cases} \tag{6.1}$$

When the Givens Rotation Matrix is multiplied to another matrix $B_{N\times N} = [b_{i,j}]_{N\times N}$

$$C_{N\times N} = G_{N\times N} \cdot B_{N\times N} \tag{6.2}$$

$$\Rightarrow c_{ij} = \sum_{l=1}^{N} g_{i,l} b_{l,j} \tag{6.3}$$

$$\Rightarrow c_{ij} = \begin{cases} g_{k,k}b_{k,j} + g_{k,k+1}b_{k+1,j} & i = k \\ g_{k+1,k}b_{k,j} + g_{k+1,k+1}b_{k+1,j} & i = k+1 \\ b_{i,j} & \text{otherwise} \end{cases} \tag{6.4}$$

Template Parameters

real_t	float, double or long double data types to represent real numbers

Definition at line 58 of file G_Matrix.hpp.

6.2.2 Constructor & Destructor Documentation

6.2.2.1 GMatrix()

```
template<typename real_t >
GMatrix< real_t >::GMatrix (
            RMatrix< real_t > & matrix,
            unsigned int index )
```

Construct a new Givens Rotation Matrix to vanish the element at position $(k+1, k)$ of R matrix.

Parameters

R	R matrix whose element at position $(k+1, k)$ needs to be vanished
index	k

Definition at line 18 of file G_Matrix.cpp.

6.2.3 Member Function Documentation

6.2.3.1 multiply() [1/2]

```
template<typename real_t >
void GMatrix< real_t >::multiply (
            QMatrix< real_t > & Q )
```

Multiplies the Givens Rotation Matrix to the Q Matrix and updates the Q matrix in place.

Parameters

Q	Q Matrix passed as reference

Q matrix may be represented as $Q_{N\times N} = [q_{i,j}]_{N\times N}$ where

$$q_{i,j} = 0, \quad j > i$$

Thus, when a rotation matrix is multiplied to Q matrix

$$C_{N\times N} = G_{N\times N} \cdot Q_{N\times N} \tag{6.5}$$

$$\Rightarrow c_{ij} = \sum_{l=1}^{N} g_{i,l} q_{l,j} \tag{6.6}$$

$$\Rightarrow c_{ij} = \begin{cases} g_{k,k} l_{k,j} + g_{k,k+1} q_{k+1,j} & i = k \\ g_{k+1,k} l_{k,j} + g_{k+1,k+1} q_{k+1,j} & i = k+1 \\ q_{i,j} & \text{otherwise} \end{cases} \tag{6.7}$$

Definition at line 49 of file G_Matrix.cpp.

6.2.3.2 multiply() [2/2]

```
template<typename real_t >
void GMatrix< real_t >::multiply (
            RMatrix< real_t > & R )
```

Multiplies the Givens Rotation Matrix to the R Matrix and updates the R matrix in place.

Parameters

R	R Matrix that will be converted into upper tridiagonal matrix after multiplication

R matrix can be represented as $R_{N\times N} = [r_{i,j}]_{N\times N}$ where

$$r_{i,j} = \quad 0 \quad \text{if} \quad j < i-1 \quad \text{or} \quad j > i+1 \tag{6.8}$$

Thus, upon multiplying the R matrix with the rotation matrix, we get matrix $C_{N\times N}$

$$c_{ij} = \begin{array}{ll} g_{k,k}r_{k,j} + g_{k,k+1}r_{k+1,j} & i = k \\ g_{k+1,k}r_{k,j} + g_{k+1,k+1}r_{k+1,j} & i = k+1 \\ r_{i,j} & \text{otherwise} \end{array} \tag{6.9}$$

$$\Rightarrow c_{ij} = \begin{array}{lll} g_{k,k}r_{k,k-1} & i = k & j = k-1 \\ g_{k,k}r_{k,k} + g_{k,k+1}r_{k+1,k} & i = k & j = k \\ g_{k,k}r_{k,k+1} + g_{k,k+1}r_{k+1,k+1} & i = k & j = k+1 \\ g_{k,k+1}r_{k+1,k+2} & i = k & j = k+2 \\ g_{k+1,k}r_{k,k-1} & i = k+1 & j = k-1 \\ g_{k+1,k}r_{k,k} + g_{k+1,k+1}r_{k+1,k} & i = k+1 & j = k \\ g_{k+1,k}r_{k,k+1} + g_{k+1,k+1}r_{k+1,k+1} & i = k+1 & j = k+1 \\ g_{k+1,k+1}r_{k+1,k+2} & i = k+1 & j = k+2 \\ r_{i,j} & \text{otherwise} & \end{array} \tag{6.10}$$

But as we iterate over k and multiply the corresponding rotation marix, the sub-diagonal ($r_{i,i-1}$) becomes zero and the super-super-diagonal ($r_{i,i+2}$) fills up with non-zero values.

$$\Rightarrow c_{ij} = \begin{array}{lll} 0 & i = k & j = k-1 \\ g_{k,k}r_{k,k} + g_{k,k+1}r_{k+1,k} & i = k & j = k \\ g_{k,k}r_{k,k+1} + g_{k,k+1}r_{k+1,k+1} & i = k & j = k+1 \\ g_{k,k+1}r_{k+1,k+2} & i = k & j = k+2 \\ 0 & i = k+1 & j = k-1 \\ 0 & i = k+1 & j = k \\ g_{k+1,k}r_{k,k+1} + g_{k+1,k+1}r_{k+1,k+1} & i = k+1 & j = k+1 \\ g_{k+1,k+1}r_{k+1,k+2} & i = k+1 & j = k+2 \\ r_{i,j} & \text{otherwise} & \end{array} \tag{6.11}$$

Definition at line 80 of file G_Matrix.cpp.

6.2.3.3 multiplyLastRow()

```
template<typename real_t >
void GMatrix< real_t >::multiplyLastRow (
            RMatrix< real_t > & R )
```

Multiplies the Givens rotation matrix to the R matrix where the rotation matrix is formed to vanish the sub diagonal element of the last row $(N, N-1)$ of the $N \times N$ R matrix.

$$\Rightarrow c_{ij} = \begin{array}{lll} 0 & i = k & j = k-1 \\ g_{N-1,N-1}r_{N-1,N-1} + g_{N-1,N}r_{N,N-1} & i = k & j = k \\ g_{N-1,N-1}r_{N-1,N} + g_{N-1,N}r_{N,N} & i = k & j = k+1 \\ 0 & i = k+1 & j = k-1 \\ 0 & i = k+1 & j = k \\ g_{N,N-1}r_{N-1,N} + g_{N,N}r_{N,N} & i = k+1 & j = k+1 \\ r_{i,j} & \text{otherwise} & \end{array} \tag{6.12}$$

Parameters

R	R Matrix that will be converted into upper tridiagonal matrix after multiplication

Definition at line 135 of file G_Matrix.cpp.

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

- include/qrsolver/G_Matrix.hpp
- src/qrsolver/G_Matrix.cpp

6.3 QMatrix< real_t > Class Template Reference

Class to implement a memory efficient model of $N \times N$ Q Matrix.

`#include <Q_Matrix.hpp>`

Public Member Functions

- QMatrix (unsigned int n)
  Construct a new Q Matrix.
- ~QMatrix ()
  Destroy the Q Matrix object.
- real_t getElement (unsigned int row_index, unsigned int column_index)
  Get the i,j th element of the Q Matrix.
- void setElement (unsigned int row_index, unsigned int column_index, real_t value)
  Set the value of the i,j th element of the Q Matrix.
- void printMatrix ()
  Prints the Q Matrix in form of a 2D array.
- void identity ()
  Makes Q matrix an identity matrix.
- void multiply (real_t *b, real_t *x)
  Multiplies the Q matrix with the column vector b and stores the result in the column vector x.

Private Member Functions

- unsigned int getIndex (unsigned int row_index, unsigned int column_index)
  Get the index of i,j th element of Q matrix in the flattened array.
- bool indexOfZeroElement (unsigned int row_index, unsigned int column_index)
  Checks if the row index i and the column index j belong to a zero element of the Q matrix.

Private Attributes

- real_t * array
  One dimensional array to store only non zero elements of the lower triangular matrix.
- const unsigned int N
  Number of rows in a $N \times N$ square matrix.

6.3.1 Detailed Description

template<typename real_t>
class QMatrix< real_t >

Class to implement a memory efficient model of $N \times N$ Q Matrix.

Template Parameters

real_t	float, double or long double data types to represent real numbers

Definition at line 25 of file Q_Matrix.hpp.

6.3.2 Constructor & Destructor Documentation

6.3.2.1 QMatrix()

```
template<typename real_t >
QMatrix< real_t >::QMatrix (
            unsigned int n )
```

Construct a new Q Matrix.

Parameters

n	Number of rows in the $N \times N$ square matrix

Definition at line 21 of file Q_Matrix.cpp.

6.3.3 Member Function Documentation

6.3.3.1 getElement()

```
template<typename real_t >
real_t QMatrix< real_t >::getElement (
            unsigned int row_index,
            unsigned int column_index )
```

Get the i,j th element of the Q Matrix.

Parameters

row_index	Row index i
column_index	Column index j

Returns

Value of the i,j th element of the Q Matrix

Definition at line 62 of file Q_Matrix.cpp.

6.3.3.2 getIndex()

```
template<typename real_t >
unsigned int QMatrix< real_t >::getIndex (
            unsigned int row_index,
            unsigned int column_index )  [private]
```

Get the index of i,j th element of Q matrix in the flattened array.

Parameters

row_index	Row index i
column_index	Column index j

Returns

Index of the i,j th element in the flattened array

Definition at line 41 of file Q_Matrix.cpp.

6.3.3.3 indexOfZeroElement()

```
template<typename real_t >
bool QMatrix< real_t >::indexOfZeroElement (
            unsigned int row_index,
            unsigned int column_index )  [private]
```

Checks if the row index i and the column index j belong to a zero element of the Q matrix.

Parameters

row_index	Row index i
column_index	Column index j

Returns

true if i,j are indices of zero elements in a Q matrix

false if i,j are indices of non zero elements in a Q matrix

Definition at line 52 of file Q_Matrix.cpp.

6.3.3.4 multiply()

```
template<typename real_t >
void QMatrix< real_t >::multiply (
             real_t * b,
             real_t * x )
```

Multiplies the Q matrix with the column vector b and stores the result in the column vector x.

Parameters

b	
x	

Definition at line 132 of file Q_Matrix.cpp.

6.3.3.5 setElement()

```
template<typename real_t >
void QMatrix< real_t >::setElement (
             unsigned int row_index,
             unsigned int column_index,
             real_t value )
```

Set the value of the i,j th element of the Q Matrix.

Parameters

row_index	Row index i
column_index	Column index j
value	Value to be set at the i,j th position

Definition at line 80 of file Q_Matrix.cpp.

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

- include/qrsolver/Q_Matrix.hpp
- src/qrsolver/Q_Matrix.cpp

6.4 QRSolver< real_t > Class Template Reference

Class to implement QR factorization algorithm for solving matrix equations of the $A \cdot x = b$ where A is a $N \times N$ tridiagonal matrix and x and b are $N \times 1$ vectors.

```
#include <QR_Solver.hpp>
```

Public Member Functions

- QRSolver (unsigned int N)

  Construct a new QRSolver object.
- ~QRSolver ()

  Destroy the QRSolver object.
- void setEquation (unsigned int index, real_t e, real_t f, real_t g, real_t b)

  Set up equation represented by ith row of the matrix equation $ex_{i-1} + fx_i + gx_{i+1} = b$.
- void setEquationFirstRow (real_t f, real_t g, real_t b)

  Set up equation represented by the first row of the matrix equation $fx_i + gx_{i+1} = b$.
- void setEquationLastRow (real_t e, real_t f, real_t b)

  up equation represented by the last row of the matrix equation $ex_{i-1}fx_i = b$
- void printMatrixEquation ()

  Prints the matrix A *and vector* b.
- void printQRMatrices ()

  Prints the factorized matrices $Q \cdot R$.
- void getSolution (real_t *x)

  Finds the solution to matrix equation and saves it to array x.

Private Member Functions

- void QRFactorize ()

  Factorizes the tridiagonal A *matrix stored in R to* $Q \cdot R$.

Private Attributes

- QMatrix< real_t > Q

  Q *matrix for QR Factorization*
- RMatrix< real_t > R

  R *matrix for QR Factorization*
- const unsigned int N

  Number of rows N *of the matrix* A.
- real_t * b

  One dimensional array to store $N \times N$ *vector* b.
- unsigned int k

  Iterator.

6.4.1 Detailed Description

template<typename real_t>
class QRSolver< real_t >

Class to implement QR factorization algorithm for solving matrix equations of the $A \cdot x = b$ where A is a $N \times N$ tridiagonal matrix and x and b are $N \times 1$ vectors.

Template Parameters

real_t	

Definition at line 32 of file QR_Solver.hpp.

6.4.2 Constructor & Destructor Documentation

6.4.2.1 QRSolver()

```
template<typename real_t >
QRSolver< real_t >::QRSolver (
            unsigned int N )
```

Construct a new QRSolver object.

Parameters

N	Size of the matrix equations

Definition at line 20 of file QR_Solver.cpp.

6.4.3 Member Function Documentation

6.4.3.1 getSolution()

```
template<typename real_t >
void QRSolver< real_t >::getSolution (
            real_t * x )
```

Finds the solution to matrix equation and saves it to array x.

Parameters

x	Array to store the solution of the matrix equation

Definition at line 154 of file QR_Solver.cpp.

6.4.3.2 printMatrixEquation()

```
template<typename real_t >
void QRSolver< real_t >::printMatrixEquation
```

Prints the matrix A and vector b.

To be used before QR factorization is performed in getSolution

Definition at line 94 of file QR_Solver.cpp.

6.4.3.3 printQRMatrices()

```
template<typename real_t >
void QRSolver< real_t >::printQRMatrices
```

Prints the factorized matrices $Q \cdot R$.

To be used after QR factorization is performed in getSolution

Definition at line 140 of file QR_Solver.cpp.

6.4.3.4 setEquation()

```
template<typename real_t >
void QRSolver< real_t >::setEquation (
            unsigned int index,
            real_t e,
            real_t f,
            real_t g,
            real_t b )
```

Set up equation represented by ith row of the matrix equation $ex_{i-1} + fx_i + gx_{i+1} = b$.

Parameters

index	i
e	Coefficient to x_{i-1}
f	Coefficient to x_i
g	Coefficient to x_{i+1}
b	Constant

Definition at line 39 of file QR_Solver.cpp.

6.4.3.5 setEquationFirstRow()

```
template<typename real_t >
void QRSolver< real_t >::setEquationFirstRow (
            real_t f,
            real_t g,
            real_t b )
```

Set up equation represented by the first row of the matrix equation $fx_i + gx_{i+1} = b$.

Parameters

f	Coefficient to x_i
g	Coefficient to x_{i+1}
b	Constant

Definition at line 60 of file QR_Solver.cpp.

6.4.3.6 setEquationLastRow()

```
template<typename real_t >
void QRSolver< real_t >::setEquationLastRow (
            real_t e,
            real_t f,
            real_t b )
```

up equation represented by the last row of the matrix equation $ex_{i-1}fx_i = b$

Parameters

e	Coefficient to x_{i-1}
f	Coefficient to x_i
b	Constant

Definition at line 77 of file QR_Solver.cpp.

6.4.4 Member Data Documentation

6.4.4.1 R

```
template<typename real_t >
RMatrix<real_t> QRSolver< real_t >::R  [private]
```

R matrix for QR Factorization

The R matrix also serves as the initial tridiagonal A matrix to save memory and more important reduce redundant memory copy operations

Definition at line 48 of file QR_Solver.hpp.

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

- include/qrsolver/QR_Solver.hpp
- src/qrsolver/QR_Solver.cpp

6.5 RMatrix< real_t > Class Template Reference

Class to implement a memory efficient $N \times N$ R matrix.

`#include <R_Matrix.hpp>`

Public Member Functions

- RMatrix (unsigned int n)
  Construct a new R Matrix.
- ~RMatrix ()
  Destroy the R Matrix.
- real_t getElement (unsigned int row_index, unsigned int column_index)
  Get the i,j th element of R Matrix.
- void setElement (unsigned int row_index, unsigned int column_index, real_t value)
  Set the value of the i,j th element of R Matrix.
- void printMatrix ()
  Prints the R Matrix in form of a 2D array.
- void print ()
  Prints the R Matrix in form of a flattened array.

Private Member Functions

- unsigned int getIndex (unsigned int row_index, unsigned int column_index)
  Get the index of the i,j th element of R Matrix in the flattened array.
- bool indexOfZeroElement (unsigned int row_index, unsigned int column_index)
  Checks if the row index i and the column index j belong to a zero element of the R matrix.

Private Attributes

- real_t * array
  *Flattened array of size 4 * N to represent R matrix of size $N \times N$.*
- const unsigned int N
  Size of main diagonal of the $N \times N$ R Matrix.

6.5.1 Detailed Description

template<typename real_t>
class RMatrix< real_t >

Class to implement a memory efficient $N \times N$ R matrix.

The class is specifically built for implementation in a QR factorization algorithm for solving matrix equations of the form $A \cdot x = b$. The QR algo converts a normal tridiagonal matrix (a matrix with non zero entries only at indices $(i, i-1)$, (i, i) and $(i, i+1)$) to an upper tridiagonal matrix (a matrix with non zero entries only at indices (i, i), $(i, i+1)$ and $(i, i+2)$). Thus only indices $(i, i-1)$, (i, i), $(i, i+1)$ and $(i, i+2)$ are stored in memory for this matrix

Definition at line 30 of file R_Matrix.hpp.

6.5.2 Constructor & Destructor Documentation

6.5.2.1 RMatrix()

```
template<typename real_t >
RMatrix< real_t >::RMatrix (
            unsigned int n )
```

Construct a new R Matrix.

Parameters

n	Size of main diagonal of the $N \times N$ R Matrix

Definition at line 18 of file R_Matrix.cpp.

6.5.2.2 ~RMatrix()

```
template<typename real_t >
RMatrix< real_t >::~RMatrix
```

Destroy the R Matrix.

Definition at line 29 of file R_Matrix.cpp.

6.5.3 Member Function Documentation

6.5.3.1 getElement()

```
template<typename real_t >
real_t RMatrix< real_t >::getElement (
            unsigned int row_index,
            unsigned int column_index )
```

Get the i,j th element of R Matrix.

Parameters

row_index	Row index i
column_index	Column index j

Returns

Value of the i,j th element of a R Matrix

Definition at line 36 of file R_Matrix.cpp.

6.5.3.2 getIndex()

```
template<typename real_t >
unsigned int RMatrix< real_t >::getIndex (
            unsigned int row_index,
            unsigned int column_index )  [private]
```

Get the index of the i,j th element of R Matrix in the flattened array.

Parameters

row_index	Row index i
column_index	Column index j

Returns

Returns the index in the the flattened array

Definition at line 109 of file R_Matrix.cpp.

6.5.3.3 indexOfZeroElement()

```
template<typename real_t >
bool RMatrix< real_t >::indexOfZeroElement (
            unsigned int row_index,
            unsigned int column_index )  [private]
```

Checks if the row index i and the column index j belong to a zero element of the R matrix.

Parameters

row_index	
column_index	

Returns

true if i,j are indices of zero elements in a R matrix

false if i,j are indicess of non-zero elements in a R matrix

Definition at line 125 of file R_Matrix.cpp.

6.5.3.4 print()

```
template<typename real_t >
void RMatrix< real_t >::print
```

Prints the R Matrix in form of a flattened array.

Definition at line 94 of file R_Matrix.cpp.

6.5.3.5 printMatrix()

```
template<typename real_t >
void RMatrix< real_t >::printMatrix
```

Prints the R Matrix in form of a 2D array.

Definition at line 75 of file R_Matrix.cpp.

6.5.3.6 setElement()

```
template<typename real_t >
void RMatrix< real_t >::setElement (
            unsigned int row_index,
            unsigned int column_index,
            real_t value )
```

Set the value of the i,j th element of R Matrix.

Parameters

row_index	Row index i
column_index	Column index j
value	Value to be set at the i,j th element

Definition at line 54 of file R_Matrix.cpp.

6.5.4 Member Data Documentation

6.5.4.1 array

```
template<typename real_t >
real_t* RMatrix< real_t >::array  [private]
```

Flattened array of size 4 $*$ N to represent R matrix of size $N \times N$.

Definition at line 93 of file R_Matrix.hpp.

6.5.4.2 N

```
template<typename real_t >
const unsigned int RMatrix< real_t >::N  [private]
```

Size of main diagonal of the $N \times N$ R Matrix.

Definition at line 100 of file R_Matrix.hpp.

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

- include/qrsolver/R_Matrix.hpp
- src/qrsolver/R_Matrix.cpp

6.6 Substance< real_t > Class Template Reference

Class to represent a pure substance.

```
#include <Substance.hpp>
```

Public Member Functions

- Substance (real_t density, real_t heat_capacity, real_t molecular_weight, real_t heat_conductivity, real_t standard_enthalpy_of_formation=0)

  Construct a new Substance.
- real_t getDensity ()

  Get the Density in.
- real_t getHeatCapacity ()

  Get the Heat Capacity.
- real_t getMolecularWeight ()

  Get the Molecular Weight.
- real_t getHeatConductivity ()

  Get the Heat Conductivity.
- real_t getStandardEnthalpyOfFormation ()

  Get the Standard Enthalpy Of Formation.
- real_t getEnthalpy (real_t Temperature)

  Get the Enthalpy of the substance with respect to the T_REF.
- void printProperties (std::ostream &output_stream)

  Print the properties of the substance to the given stream.

Private Attributes

- const real_t _density

  Density of the substance.
- const real_t _heat_capacity

  Heat capacity of the substance.
- const real_t _molecular_weight

  Molecular Weight of the substance.
- const real_t _heat_conductivity

  Heat Conductivity of the substance.
- const real_t _std_enthalpy_formation

  Standard Enthalpy of Formation of the substance.

6.6.1 Detailed Description

template<typename real_t>
class Substance< real_t >

Class to represent a pure substance.

Template Parameters

real_t	

Definition at line 27 of file Substance.hpp.

6.6.2 Constructor & Destructor Documentation

6.6.2.1 Substance()

```
template<typename real_t >
Substance< real_t >::Substance (
            real_t density,
            real_t heat_capacity,
            real_t molecular_weight,
            real_t heat_conductivity,
            real_t standard_enthalpy_of_formation = 0 )  [inline]
```

Construct a new Substance.

Parameters

density	Density of the substance in kg/m^3
heat_capacity	Heat capacity of the substance in $J/kg - K$
molecular_weight	Molecular weight of the substance in kg/mol
heat_conductivity	Heat conductivity of the substance in W/m
standard_enthalpy_of_formation	Standard enthalpy of formation of the substance at 298 K in J/kg

Definition at line 40 of file Substance.hpp.

6.6.3 Member Function Documentation

6.6.3.1 getDensity()

```
template<typename real_t >
real_t Substance< real_t >::getDensity ( )  [inline]
```

Get the Density in.

Returns

real_t Density of the substance

Definition at line 58 of file Substance.hpp.

6.6.3.2 getEnthalpy()

```
template<typename real_t >
real_t Substance< real_t >::getEnthalpy (
            real_t Temperature )  [inline]
```

Get the Enthalpy of the substance with respect to the T_REF.

Parameters

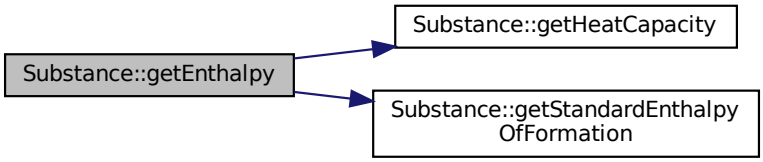
Temperature	Temperature at which enthalpy of the object needs to be evaluated

Returns

real_t Enthalpy of the substance in J / kg

Definition at line 94 of file Substance.hpp.

Here is the call graph for this function:



6.6.3.3 getHeatCapacity()

```
template<typename real_t >
real_t Substance< real_t >::getHeatCapacity ( )  [inline]
```

Get the Heat Capacity.

Returns

real_t Heat Capacity of the substance

Definition at line 65 of file Substance.hpp.

6.6.3.4 getHeatConductivity()

```
template<typename real_t >
real_t Substance< real_t >::getHeatConductivity ( )  [inline]
```

Get the Heat Conductivity.

Returns

real_t Heat Conductivity of the substance

Definition at line 79 of file Substance.hpp.

6.6.3.5 getMolecularWeight()

```
template<typename real_t >
real_t Substance< real_t >::getMolecularWeight ( )  [inline]
```

Get the Molecular Weight.

Returns

real_t Molecular Weight of the substance

Definition at line 72 of file Substance.hpp.

6.6.3.6 getStandardEnthalpyOfFormation()

```
template<typename real_t >
real_t Substance< real_t >::getStandardEnthalpyOfFormation ( )  [inline]
```

Get the Standard Enthalpy Of Formation.

Returns

real_t Standard Enthalpy of Formation of the substance

Definition at line 86 of file Substance.hpp.

6.6.3.7 printProperties()

```
template<typename real_t >
void Substance< real_t >::printProperties (
            std::ostream & output_stream )  [inline]
```

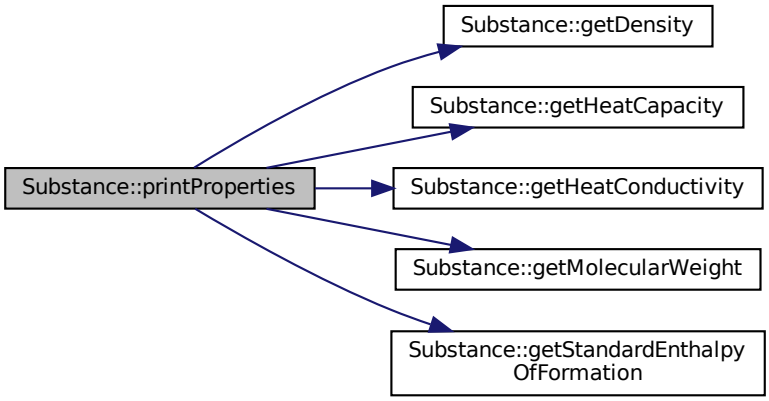
Print the properties of the substance to the given stream.

Parameters

output_stream	Stream to which the properties are printed

Definition at line 104 of file Substance.hpp.

Here is the call graph for this function:



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

- include/thermo-physical-properties/Substance.hpp

Chapter 7

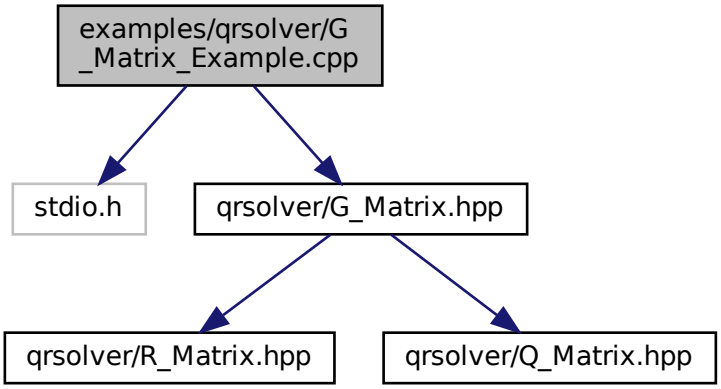
File Documentation

7.1 examples/qrsolver/G_Matrix_Example.cpp File Reference

Example to test out GMatrix class.

```
#include <stdio.h>
#include "qrsolver/G_Matrix.hpp"
```

Include dependency graph for G_Matrix_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

7.1.1 Detailed Description

Example to test out GMatrix class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-01

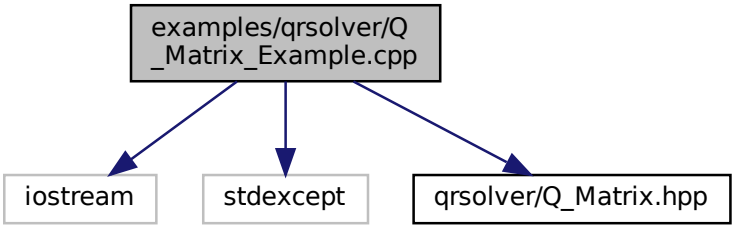
Copyright

7.2 examples/qrsolver/Q_Matrix_Example.cpp File Reference

Example to test QMatrix class.

```
#include <iostream>
#include <stdexcept>
#include "qrsolver/Q_Matrix.hpp"
```

Include dependency graph for Q_Matrix_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

7.2.1 Detailed Description

Example to test QMatrix class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-27

Copyright

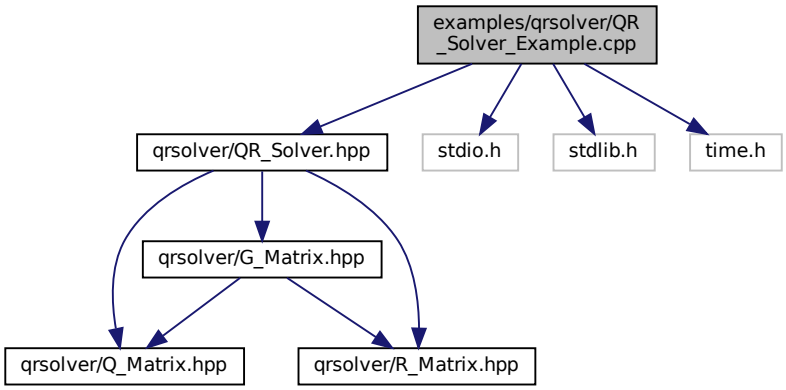
Copyright (c) 2021

7.3 examples/qrsolver/QR_Solver_Example.cpp File Reference

Example cpp file to test out QRSolver class.

```
#include "qrsolver/QR_Solver.hpp"
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
```

Include dependency graph for QR_Solver_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

7.3.1 Detailed Description

Example cpp file to test out QRSolver class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-24

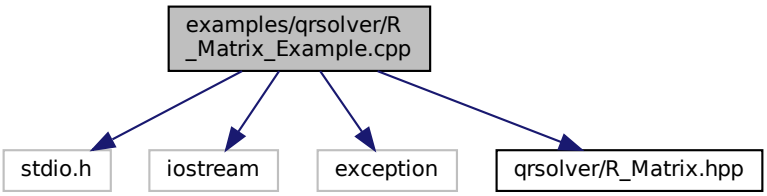
Copyright

7.4 examples/qrsolver/R_Matrix_Example.cpp File Reference

An example cpp program to test the RMatrix class.

```
#include <stdio.h>
#include <iostream>
#include <exception>
#include "qrsolver/R_Matrix.hpp"
```

Include dependency graph for R_Matrix_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

7.4.1 Detailed Description

An example cpp program to test the RMatrix class.

Author

Souritra Garai (you@domain.com)

Version

0.1

Date

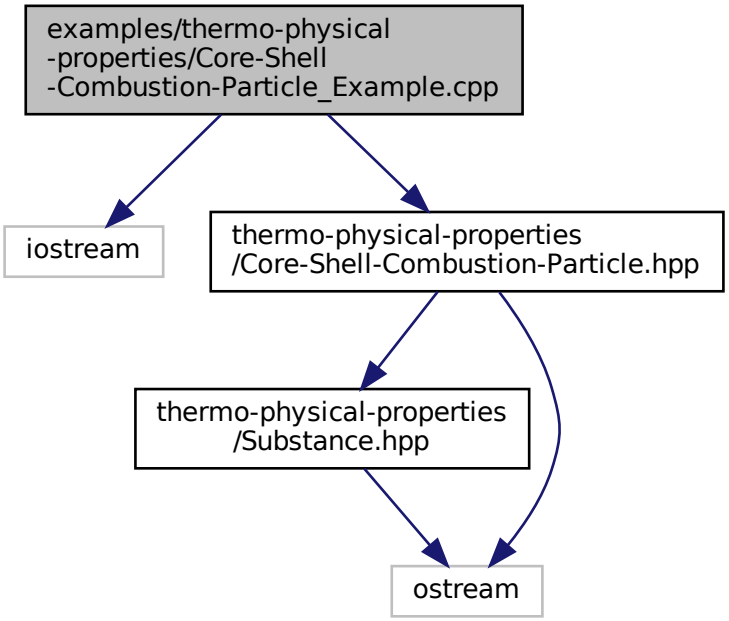
2021-06-24

Copyright

7.5 examples/thermo-physical-properties/Core-Shell-Combustion-Particle_Example.cpp File Reference

```
#include <iostream>
#include "thermo-physical-properties/Core-Shell-Combustion-Particle.hpp"
```

Include dependency graph for Core-Shell-Combustion-Particle_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

Variables

- Substance< float > **A** (10, 10, 10, 10)
- Substance< float > **B** (10, 10, 10, 10)
- Substance< float > **AB** (10, 10, 10, 10, -120)
- CoreShellCombustionParticle< float > **AB_particle** (A, B, AB, 10, 10)

7.5.1 Detailed Description

Author

your name (you@domain.com)

Version

0.1

Date

2021-07-09

Copyright

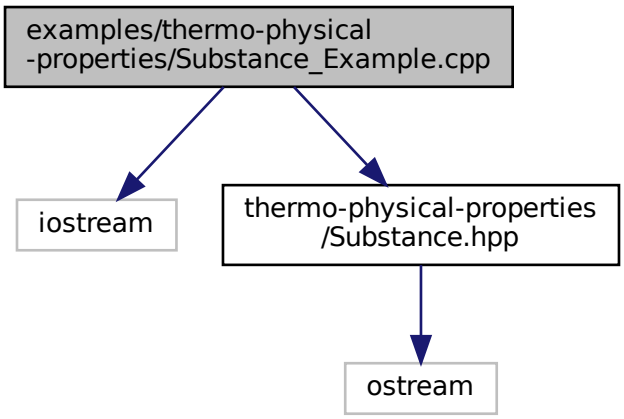
Copyright (c) 2021

7.6 examples/thermo-physical-properties/Substance_Example.cpp File Reference

Example to test functions of Substance class.

```
#include <iostream>
#include "thermo-physical-properties/Substance.hpp"
```

Include dependency graph for Substance_Example.cpp:



Functions

- int **main** (int argc, char const ∗argv[ ])

Variables

- Substance< float > **Water** (1000, 4180, 18E-3, 10)

7.6.1 Detailed Description

Example to test functions of Substance class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-06

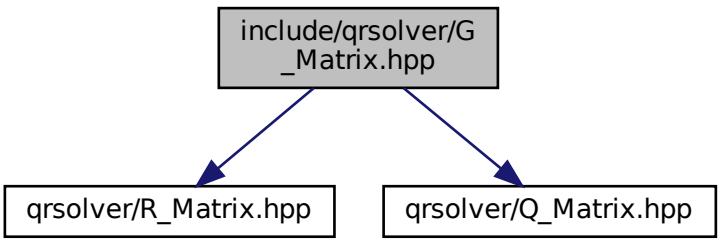
Copyright

7.7 include/qrsolver/G_Matrix.hpp File Reference

This header serves the definition of an implementation of Givens' Rotation matrix. The rotation matrix is used to solve matrix equations through QR factorization method, particularly tridiagonal matrix equation.

```
#include "qrsolver/R_Matrix.hpp"
#include "qrsolver/Q_Matrix.hpp"
```

Include dependency graph for G_Matrix.hpp:



Classes

- class GMatrix< real_t >

  Class to implement a memory efficient Givens' Rotation Matrix that can vanish the element $a_{k+1,k}$ of a matrix A.

7.7.1 Detailed Description

This header serves the definition of an implementation of Givens' Rotation matrix. The rotation matrix is used to solve matrix equations through QR factorization method, particularly tridiagonal matrix equation.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-28

Copyright

Copyright (c) 2021

7.8 include/qrsolver/Q_Matrix.hpp File Reference

This header file defines a class for memory efficient implementation of Q matrix used for QR factorisation of tridiagonal matrix using Givens rotation matrix.

Classes

- class QMatrix< real_t >

  Class to implement a memory efficient model of $N \times N$ Q Matrix.

7.8.1 Detailed Description

This header file defines a class for memory efficient implementation of Q matrix used for QR factorisation of tridiagonal matrix using Givens rotation matrix.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-25

Copyright

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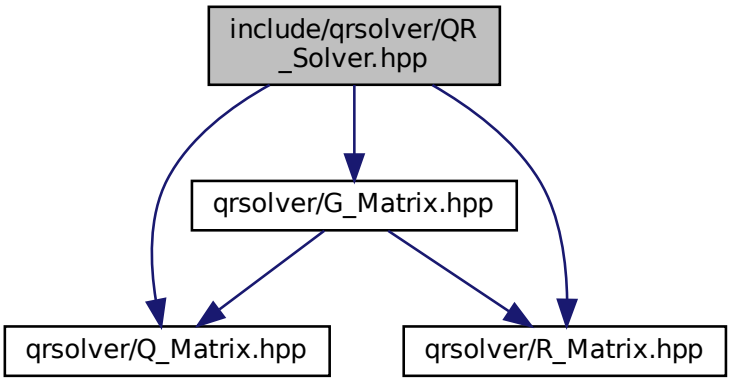
7.9 include/qrsolver/QR_Solver.hpp File Reference

This header file defines a class for solving 2D matrix equations of the form $A \cdot x = b$ (where A is an $N \times N$ matrix and x and b are $N \times 1$ vectors) using QR factorization technique.

```
#include "qrsolver/Q_Matrix.hpp"
#include "qrsolver/R_Matrix.hpp"
#include "qrsolver/G_Matrix.hpp"
```

Include dependency graph for QR_Solver.hpp:



Classes

- class QRSolver< real_t >

  Class to implement QR factorization algorithm for solving matrix equations of the $A \cdot x = b$ where A is a $N \times N$ tridiagonal matrix and x and b are $N \times 1$ vectors.

7.9.1 Detailed Description

This header file defines a class for solving 2D matrix equations of the form $A \cdot x = b$ (where A is an $N \times N$ matrix and x and b are $N \times 1$ vectors) using QR factorization technique.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-23

Copyright

7.10 include/qrsolver/R_Matrix.hpp File Reference

This header file defines a class for memory efficient implementation of R matrix used for QR factorisation of tridiagonal matrix.

Classes

- class RMatrix< real_t >

  Class to implement a memory efficient $N \times N$ R matrix.

7.10.1 Detailed Description

This header file defines a class for memory efficient implementation of R matrix used for QR factorisation of tridiagonal matrix.

Author

Souritra Gari (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-24

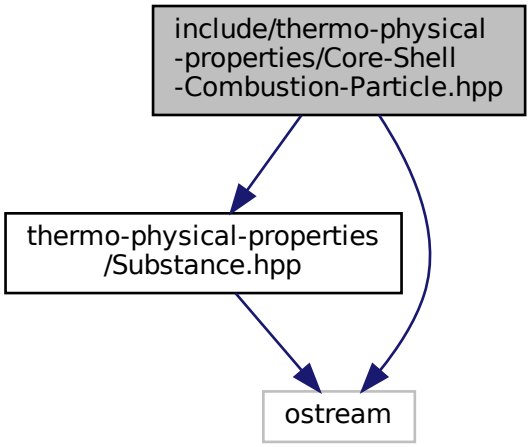
Copyright

7.11 include/thermo-physical-properties/Core-Shell-Combustion-↩ Particle.hpp File Reference

This header defines a class for core shell particle.

```
#include "thermo-physical-properties/Substance.hpp"
#include <ostream>
```

Include dependency graph for Core-Shell-Combustion-Particle.hpp:



Classes

- class CoreShellCombustionParticle< real_t >

  Class to represent Core-Shell Particle with functions estimate thermodynamic properties for varying composition and temperature.

7.11.1 Detailed Description

This header defines a class for core shell particle.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

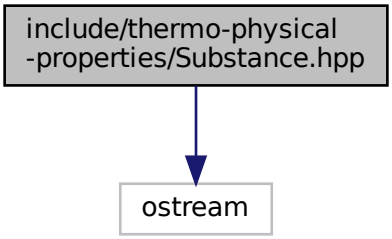
2021-07-08

Copyright

7.12 include/thermo-physical-properties/Substance.hpp File Reference

This header defines a class to represent pure substances with their thermodynamic properties like density, heat capacity etc.

`#include <ostream>`
Include dependency graph for Substance.hpp:



Classes

- class Substance< real_t >

  Class to represent a pure substance.

Macros

- #define **T_REF** 298.15

7.12.1 Detailed Description

This header defines a class to represent pure substances with their thermodynamic properties like density, heat capacity etc.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-06

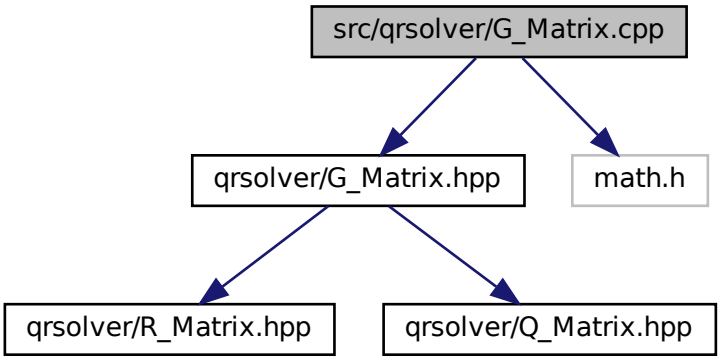
Copyright

7.13 src/qrsolver/G_Matrix.cpp File Reference

Member function definitions for GMatrix class.

```
#include "qrsolver/G_Matrix.hpp"
#include <math.h>
```

Include dependency graph for G_Matrix.cpp:



7.13.1 Detailed Description

Member function definitions for GMatrix class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-01

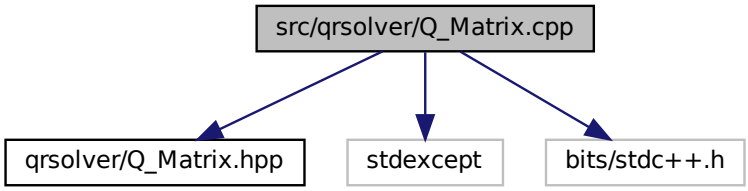
Copyright

7.14 src/qrsolver/Q_Matrix.cpp File Reference

Member function definitions for QMatrix class.

```
#include "qrsolver/Q_Matrix.hpp"
#include <stdexcept>
#include <bits/stdc++.h>
```

Include dependency graph for Q_Matrix.cpp:



7.14.1 Detailed Description

Member function definitions for QMatrix class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-06-25

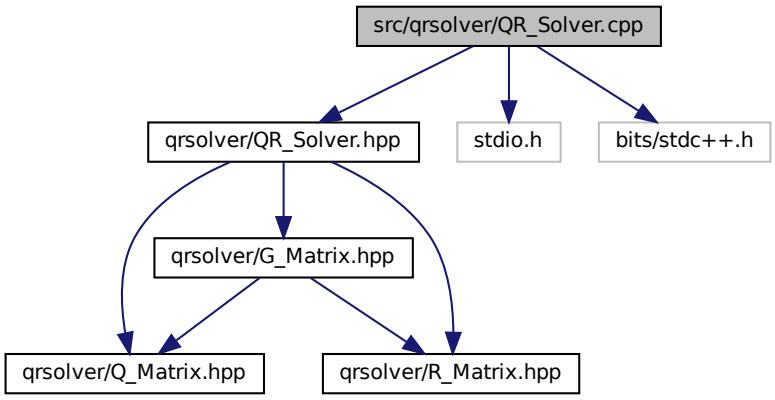
Copyright

7.15 src/qrsolver/QR_Solver.cpp File Reference

Member function definitions for QRSolver class.

```
#include "qrsolver/QR_Solver.hpp"
#include <stdio.h>
#include <bits/stdc++.h>
```

Include dependency graph for QR_Solver.cpp:



7.15.1 Detailed Description

Member function definitions for QRSolver class.

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-01

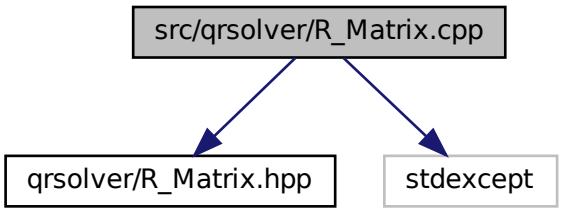
Copyright

7.16 src/qrsolver/R_Matrix.cpp File Reference

Member function definitions for RMatrix class.

```
#include "qrsolver/R_Matrix.hpp"
#include <stdexcept>
```

Include dependency graph for R_Matrix.cpp:



7.16.1 Detailed Description

Member function definitions for RMatrix class.

Author

Souritra Gari (souritra.garai@iitgn.ac.in)

Version

0.1

Date

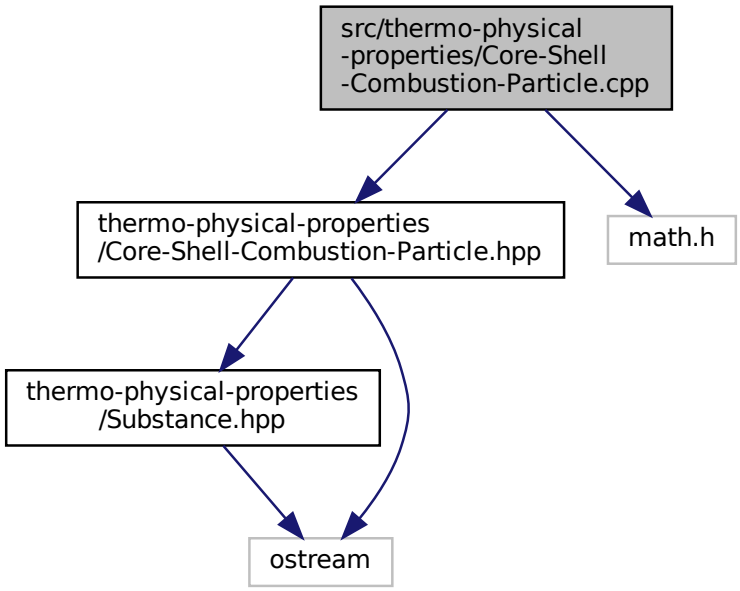
2021-06-24

Copyright

7.17 src/thermo-physical-properties/Core-Shell-Combustion-Particle.cpp File Reference

```
#include "thermo-physical-properties/Core-Shell-Combustion-Particle.hpp"
#include <math.h>
```

Include dependency graph for Core-Shell-Combustion-Particle.cpp:



7.17.1 Detailed Description

Author

Souritra Garai (souritra.garai@iitgn.ac.in)

Version

0.1

Date

2021-07-08

Copyright

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