Combustion of Packed Pellets of Core-Shell Particle

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Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

GivensRotationMatrix< real_t >	
LowerTriangularMatrix< real_t >	9
$\label{lem:total_total_total} \textit{TridiagonalMatrix} < \textit{real_t} > \dots $	1
ORSolver	13

2 Hierarchical Index

Chapter 2

Class Index

2.1 Class List

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

GivensRotationMatrix< real_t >	
Class to implement a memory efficient Givens' Rotation Matrix that can vanish the element	
$a_{k+1,k}$ of a tridiagonal matrix A	7
LowerTriangularMatrix< real_t >	
Class to implement a memory efficient model of Lower Triangular Square Matrix	ç
QRSolver	
Class to implement QR factorization algorithm for solving matrix equations of the $A.x = b$ where	
A is a n x n tridiagonal matrix and x and b are n x 1 vectors	13
TridiagonalMatrix< real_t >	
Class to implement a memory efficient 2D Tridiagonal square matrix	15

4 Class Index

Chapter 3

File Index

3.1 File List

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

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Example to test LowerTriangularMatrix class	21
combustion-packed-pellet-core-shell-particles/examples/QR_Solver_Example.cpp	
Example cpp file to test out QR_Solver functions	22
combustion-packed-pellet-core-shell-particles/examples/Tridiagonal_Matrix_Example.cpp	??
combustion-packed-pellet-core-shell-particles/include/GivensRotationMatrix.hpp	
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	22
combustion-packed-pellet-core-shell-particles/include/Lower_Triangular_Matrix.hpp	
This header file defines a class for memory efficient implementation of lower triangualer square	
matrices	23
combustion-packed-pellet-core-shell-particles/include/QR_Solver.hpp	
This header file defines a class for solving 2D matrix equations of the form $A.x = b$ (where A is	
an $n \times n$ matrix and x and y are y are y are y are the class is	
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combustion-packed-pellet-core-shell-particles/src/QR_Solver.cpp	??
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Chapter 4

Class Documentation

4.1 GivensRotationMatrix< 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 tridiagonal matrix A.

```
#include <GivensRotationMatrix.hpp>
```

Public Member Functions

• GivensRotationMatrix ()

Construct a new Givens Rotation Matrix.

- void setupRotationMatrix (TridiagonalMatrix < real_t > &matrix, unsigned int index)
 - Sets up the Givens Rotation Matrix to vanish the element at position (i+1,i) of tridiagonal matrix.
- void multiply (TridiagonalMatrix < real_t > &matrix)

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

void multiply (LowerTriangularMatrix < real_t > &matrix)

Private Attributes

- real t element i i
- real_t element_i_ip1
- real_t element_ip1_i
- real_t element_ip1_ip1
- unsigned int i

4.1.1 Detailed Description

```
template<typename real_t> class GivensRotationMatrix< real_t >
```

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

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

$$\begin{array}{cccc} 1 & i=j\neq k, k+1\\ \cos\theta & i=j=k, k+1\\ g_{ij}=& \sin\theta & i=k, j=k+1\\ -\sin\theta & i=k+1, j=k\\ 0 & \textbf{otherwise} \end{array} \tag{4.1}$$

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

$$C_{N\times N} = G_{N\times N} \cdot B_{N\times N} \tag{4.2}$$

$$\Rightarrow c_{ij} = \sum_{l=1}^{N} g_{i,l} b_{l,j} \tag{4.3}$$

$$g_{k,k}b_{k,j} + g_{k,k+1}b_{k+1,j} \qquad i = k \\ \Rightarrow c_{ij} = \begin{array}{ccc} g_{k+1,k}b_{k+1,j} + g_{k+1,k+1}b_{k+1,j} & i = k \\ b_{i,j} & \text{otherwise} \end{array}$$

Template Parameters

real←	float, double or long double data types to represent real numbers
_t	

Definition at line 57 of file GivensRotationMatrix.hpp.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 GivensRotationMatrix()

```
\label{template} template < typename real\_t > \\ GivensRotationMatrix < real\_t > :: GivensRotationMatrix ( )
```

Construct a new Givens Rotation Matrix.

4.1.3 Member Function Documentation

4.1.3.1 multiply()

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

Parameters

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

For multiplication with a Tridiagonal matrix

4.1.3.2 setupRotationMatrix()

Sets up the Givens Rotation Matrix to vanish the element at position (i+1,i) of tridiagonal matrix.

Parameters

matrix	Tridiagonal matrix whose element at position $\left(i+1,i\right)$ needs to be vanished
index	i

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

• combustion-packed-pellet-core-shell-particles/include/GivensRotationMatrix.hpp

4.2 LowerTriangularMatrix< real_t > Class Template Reference

Class to implement a memory efficient model of Lower Triangular Square Matrix.

```
#include <Lower_Triangular_Matrix.hpp>
```

Public Member Functions

LowerTriangularMatrix (unsigned int n)

Construct a new Lower Triangular Matrix object.

∼LowerTriangularMatrix ()

Destroy the Lower Triangular Matrix object.

real_t getElement (unsigned int row_index, unsigned int column_index)

Get the i,j th element of the Lower Triangular 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 Lower Triangular Matrix.

void printMatrix ()

Prints the Lower Triangular Matrix in form of a 2D array.

Private Member Functions

• unsigned int getIndex (unsigned int row_index, unsigned int column_index)

Get the index of i,j th element of lower triangular matrix.

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 lower triangular matrix.

Private Attributes

real_t * array

One dimensional array to store only non zero elements of the lower triangular matrix.

const unsigned int N

Size of main diagonal of $N \times N$ square matrix.

4.2.1 Detailed Description

```
template<typename real_t> class LowerTriangularMatrix< real_t >
```

Class to implement a memory efficient model of Lower Triangular Square Matrix.

Template Parameters

```
real

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

_t
```

Definition at line 23 of file Lower_Triangular_Matrix.hpp.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 LowerTriangularMatrix()

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

Construct a new Lower Triangular Matrix object.

Parameters

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

Definition at line 17 of file Lower_Triangular_Matrix.cpp.

4.2.2.2 ∼LowerTriangularMatrix()

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

Destroy the Lower Triangular Matrix object.

Definition at line 30 of file Lower Triangular Matrix.cpp.

4.2.3 Member Function Documentation

4.2.3.1 getElement()

Get the i,j th element of the Lower Triangular Matrix.

Parameters

row_index	Row index i
column_index	Column index j

Returns

Value of the i,j th element of the Lower Triangular Matrix

Definition at line 58 of file Lower_Triangular_Matrix.cpp.

4.2.3.2 getIndex()

Get the index of i,j th element of lower triangular matrix.

Parameters

row_index	Row index i
column_index	Column index j

Returns

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

Definition at line 37 of file Lower_Triangular_Matrix.cpp.

4.2.3.3 indexOfZeroElement()

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

Parameters

row_index	Row index i
column_index	Column index j

Returns

true if i,j are indices of zero elements in a lower triangular matrix false if i,j are indices of non zero elements in a lower triangular matrix

Definition at line 48 of file Lower_Triangular_Matrix.cpp.

4.2.3.4 printMatrix()

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

Prints the Lower Triangular Matrix in form of a 2D array.

Definition at line 97 of file Lower_Triangular_Matrix.cpp.

4.2.3.5 setElement()

```
template<typename real_t >
void LowerTriangularMatrix< 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 Lower Triangular 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 76 of file Lower_Triangular_Matrix.cpp.

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

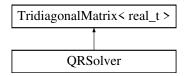
- combustion-packed-pellet-core-shell-particles/include/Lower_Triangular_Matrix.hpp
- combustion-packed-pellet-core-shell-particles/src/Lower_Triangular_Matrix.cpp

4.3 QRSolver Class Reference

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

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

Inheritance diagram for QRSolver:



Public Member Functions

QRSolver (unsigned int N)

Construct a new QRSolver object.

∼QRSolver ()

Destroy the QRSolver object.

- · void QRfactorize ()
- void initQ ()

Private Member Functions

void loadR ()

Loads the values of R matrix that will change during multiplication with Givens' rotation matrix to temporary variables.

void setupGivensRotationMatrix ()

Setup Givens' rotation matrix.

· void multiplyGivensMatrixWithR ()

Multiplies the Givens rotation matrix with R matrix and updates its value.

void multiplyGivensMatrixWithQ ()

Multiplies the Givens rotation matrix with R matrix and updates its value.

unsigned int getIndex (unsigned int row_index, unsigned int column_index)

Get the index in a flattened linear array representation of a 2D matrix.

Private Attributes

- real_t * Q
- real_t G_k_k
- real t G k kp1
- real_t G_kp1_k
- real_t G_kp1_kp1
- real_t R_k_k
- real_t R_k_kp1
- · real t R kp1 k
- real_t R_kp1_kp1
- real_t R_kp1_kp2
- · unsigned int k

4.3.1 Detailed Description

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

Definition at line 27 of file QR_Solver.hpp.

4.3.2 Constructor & Destructor Documentation

4.3.2.1 QRSolver()

```
QRSolver::QRSolver ( \label{eq:QRSolver} \mbox{unsigned int $N$} \mbox{ } \mbox{)}
```

Construct a new QRSolver object.

Parameters



Definition at line 5 of file QR_Solver.cpp.

4.3.2.2 \sim QRSolver()

```
QRSolver::\simQRSolver ( )
```

Destroy the QRSolver object.

Definition at line 14 of file QR_Solver.cpp.

4.3.3 Member Function Documentation

4.3.3.1 getIndex()

Get the index in a flattened linear array representation of a 2D matrix.

Parameters

row_index	Row index i of the desired element
column_index	Column index j of the desired element

Returns

Index in a linear array of the i,j element of a 2D matrix implemented using the linear array

Definition at line 87 of file QR_Solver.hpp.

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

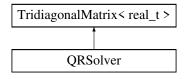
- combustion-packed-pellet-core-shell-particles/include/QR_Solver.hpp
- combustion-packed-pellet-core-shell-particles/src/QR_Solver.cpp

4.4 TridiagonalMatrix< real_t > Class Template Reference

Class to implement a memory efficient 2D Tridiagonal square matrix.

```
#include <Tridiagonal_Matrix.hpp>
```

Inheritance diagram for TridiagonalMatrix< real t>:



Public Member Functions

• TridiagonalMatrix (unsigned int n)

Construct a new Tridiagonal Matrix.

∼TridiagonalMatrix ()

Destroy the Tridiagonal Matrix.

• real t getElement (unsigned int row index, unsigned int column index)

Get the i,j th element of 2D Tridiagonal Matrix.

• void setElement (unsigned int row_index, unsigned int column_index, real_t value)

Set the value of the i,j th element of 2D Tridiagonal Matrix.

void printMatrix ()

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

• void print ()

Prints the Triadiagonal 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 Tridiagonal 2D Matrix.

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 tridiagonal matrix.

Private Attributes

real t * array

Flattened array of size 4 * N to represent 2D Tridiagonal matrix of size $N \times N$.

const unsigned int N

Size of main diagonal of the $N \times N$ 2D Tridiagonal Matrix.

4.4.1 Detailed Description

```
template<typename real_t> class TridiagonalMatrix< real_t >
```

Class to implement a memory efficient 2D Tridiagonal square 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 accessible for this matrix

Definition at line 30 of file Tridiagonal_Matrix.hpp.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 TridiagonalMatrix()

Construct a new Tridiagonal Matrix.

Parameters

```
n \mid Size of main diagonal of the N \times N 2D Tridiagonal Matrix
```

Definition at line 17 of file Tridiagonal_Matrix.cpp.

4.4.2.2 ∼TridiagonalMatrix()

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

Destroy the Tridiagonal Matrix.

Definition at line 28 of file Tridiagonal_Matrix.cpp.

4.4.3 Member Function Documentation

4.4.3.1 getElement()

Get the i,j th element of 2D Tridiagonal Matrix.

Parameters

row_index	Row index i	
column_index	Column index j	

Returns

Value of the i,j th element of a 2D Tridiagonal Matrix

Definition at line 35 of file Tridiagonal_Matrix.cpp.

4.4.3.2 getIndex()

```
template<typename real_t >
unsigned int TridiagonalMatrix< real_t >::getIndex (
```

```
unsigned int row_index,
unsigned int column_index ) [private]
```

Get the index of the i,j th element of Tridiagonal 2D Matrix.

Parameters

row_index	Row index i	
column_index	Column index j	

Returns

Returns the index in the the flattened array used to represent the 2D Tridiagonal Matrix

Definition at line 108 of file Tridiagonal_Matrix.cpp.

4.4.3.3 indexOfZeroElement()

```
template<typename real_t >
bool TridiagonalMatrix< 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 tridiagonal matrix.

Parameters

row_index	
column_index	

Returns

true if i,j are indices of zero elements in a Tridiagonal matrix false if i,j are indicess of non-zero elements in a Tridiagonal matrix

Definition at line 124 of file Tridiagonal_Matrix.cpp.

4.4.3.4 print()

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

Prints the Triadiagonal Matrix in form of a flattened array.

Definition at line 93 of file Tridiagonal_Matrix.cpp.

4.4.3.5 printMatrix()

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

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

Definition at line 74 of file Tridiagonal Matrix.cpp.

4.4.3.6 setElement()

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

Set the value of the i,j th element of 2D Tridiagonal 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 53 of file Tridiagonal_Matrix.cpp.

4.4.4 Member Data Documentation

4.4.4.1 array

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

Flattened array of size 4 * N to represent 2D Tridiagonal matrix of size $N \times N$.

Definition at line 93 of file Tridiagonal Matrix.hpp.

4.4.4.2 N

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

Size of main diagonal of the $N \times N$ 2D Tridiagonal Matrix.

Definition at line 100 of file Tridiagonal_Matrix.hpp.

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

- combustion-packed-pellet-core-shell-particles/include/Tridiagonal Matrix.hpp
- combustion-packed-pellet-core-shell-particles/src/Tridiagonal_Matrix.cpp

Chapter 5

File Documentation

5.1 combustion-packed-pellet-core-shell-particles/examples/Lower_←
Triangular_Matrix_Example.cpp File
Reference

Example to test LowerTriangularMatrix class.

```
#include <iostream>
#include <stdexcept>
#include "Lower_Triangular_Matrix.hpp"
```

Functions

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

5.1.1 Detailed Description

Example to test LowerTriangularMatrix class.

```
Author
```

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

Version

0.1

Date

2021-06-27

Copyright

Copyright (c) 2021

22 File Documentation

5.2 combustion-packed-pellet-core-shell-particles/examples/QR_← Solver_Example.cpp File Reference

Example cpp file to test out QR_Solver functions.

```
#include "QR_Solver.hpp"
```

Functions

- QR_Solver my_solver (5)
- int main (int argc, char const *argv[])

Variables

• real t A [3 *5]

5.2.1 Detailed Description

Example cpp file to test out QR_Solver functions.

Author

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

Version

0.1

Date

2021-06-24

Copyright

Copyright (c) 2021

5.3 combustion-packed-pellet-core-shell-particles/include/Givens⊸ RotationMatrix.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 <Tridiagonal_Matrix.hpp>
#include <Lower_Triangular_Matrix.hpp>
```

Classes

class GivensRotationMatrix< real t >

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

5.3.1 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
```

combustion-packed-pellet-core-shell-particles/include/Lower_ Triangular Matrix.hpp File Reference

This header file defines a class for memory efficient implementation of lower triangualer square matrices.

Classes

class LowerTriangularMatrix< real t >

Class to implement a memory efficient model of Lower Triangular Square Matrix.

5.4.1 Detailed Description

This header file defines a class for memory efficient implementation of lower triangualer square matrices.

Author

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

Version

0.1

Date

2021-06-25

Copyright

Copyright (c) 2021

24 File Documentation

5.5 combustion-packed-pellet-core-shell-particles/include/QR_← Solver.hpp File Reference

This header file defines a class for solving 2D matrix equations of the form A.x = b (where A is an n x n matrix and x and b are n x 1 vectors) using QR factorization technique. Also the class is implemented in such a way that it may be parallelized easily using openmp constructs.

```
#include "Tridiagonal_Matrix.hpp"
```

Classes

class QRSolver

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

5.5.1 Detailed Description

This header file defines a class for solving 2D matrix equations of the form A.x = b (where A is an n x n matrix and x and b are n x 1 vectors) using QR factorization technique. Also the class is implemented in such a way that it may be parallelized easily using openmp constructs.

```
Author
```

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

Version

0.1

Date

2021-06-23

Copyright

Copyright (c) 2021

5.6 combustion-packed-pellet-core-shell-particles/include/Tridiagonal_← Matrix.hpp File Reference

This header file serves the definition of an implementation for a Tridiagonal Matrix.

Classes

class TridiagonalMatrix < real_t >

Class to implement a memory efficient 2D Tridiagonal square matrix.

5.6.1 Detailed Description

This header file serves the definition of an implementation for a Tridiagonal Matrix.

Author

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

Version

0.1

Date

2021-06-24

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5.7 combustion-packed-pellet-core-shell-particles/src/Lower_← Triangular_Matrix.cpp File Reference

```
#include "Lower_Triangular_Matrix.hpp"
#include "stdexcept"
```

5.7.1 Detailed Description

Author

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

Version

0.1

Date

2021-06-25

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26 File Documentation

5.8 combustion-packed-pellet-core-shell-particles/src/Tridiagonal_← Matrix.cpp File Reference

Implementation of Tridiagonal Matrix.

```
#include "Tridiagonal_Matrix.hpp"
#include <stdexcept>
```

5.8.1 Detailed Description

Implementation of Tridiagonal Matrix.

Author

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Version

0.1

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