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Chapter 1

Hierarchical Index

1.1 Class Hierarchy

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

hdnum::Banach
hdnum::SparseMatrix< REAL >::builder
hdnum::SparseMatrix< REAL >::column_index_iterator
hdnum::SparseMatrix< REAL >::const_column_index_iterator
hdnum::SparseMatrix< REAL >::const_row_iterator
$\label{localization} \mbox{hdnum::oc::OpCounter} < F > :: Counters \qquad . \qquad 10$
hdnum::DenseMatrix< REAL >
hdnum::DenseMatrix< number_type >
$\label{eq:hdnum::DIRK} \text{hdnum::DIRK} < M, S > \dots \dots$
$\label{eq:hdnum:ee} \mbox{hdnum::EE} < M > \dots $
hdnum::Exception
hdnum::ErrorException
hdnum::IOError
hdnum::InvalidStateException
hdnum::MathError
hdnum::NotImplemented
hdnum::RangeError
hdnum::SystemError
hdnum::OutOfMemoryError
hdnum::TimerError
hdnum::GenericNonlinearProblem< Lambda, Vec >
hdnum::Heun2< M >
hdnum::Heun3< M >
$ hdnum:: IE < M, S > \dots \dots$
hdnum::ImplicitRungeKuttaStepProblem < M >
hdnum::Kutta3< M >
$\label{eq:modifiedEuler} \mbox{hdnum::ModifiedEuler} < M > \ \dots \$
hdnum::Newton
hdnum::oc::OpCounter< F >
$ hdnum :: RE < M, S > \dots $
$\label{eq:hdnum::RKF45} \mbox{hdnum::RKF45} < \mbox{M} > \dots $
hdnum::SparseMatrix< REAL >::row_iterator
$\label{eq:hdnum::RungeKutta} $$ hdnum::RungeKutta < M, S > \dots $
hdnum::RungeKutta4< M >
hdnum::SGrid < N, DF, dimension >

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Class Index

2.1 Class List

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

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hdnum::EE< M >	
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Heun method (order 2 with 2 stages)	36
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hdnum::ImplicitRungeKuttaStepProblem< M >	
Nonlinear problem we need to solve to do one step of an implicit Runge Kutta method	40
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Default exception if a function was called while the object is not in a valid state for that function	41
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Default exception class for I/O errors	41
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hdnum::ModifiedEuler< M >	
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hdnum::Newton	
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hdnum::SGrid< N, DF, dimension >	
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hdnum::SquareRootProblem< N >	
Example class for a nonlinear model $F(x) = 0$;	65
hdnum::StationarySolver< M >	
Stationary problem solver. E.g. for elliptic problmes	66
hdnum::SystemError	
Default exception class for OS errors	67
hdnum::Timer	
A simple stop watch	67
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Exception thrown by the Timer class	68
hdnum::Vector< REAL >	
Class with mathematical vector operations	69

Chapter 3

File Index

3.1 File List

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

src/densematrix.hh
src/exceptions.hh
A few common exception classes
src/lr.hh
This file implements LU decomposition
src/newton.hh
Newton's method with line search
src/ode.hh
Solvers for ordinary differential equations
src/opcounter.hh
This file implements an operator counting class
src/pde.hh
Solvers for partial differential equations
src/precision.hh
Find machine precision for given float type
src/qr.hh
This file implements QR decomposition using Gram-Schmidt method
src/qrhousholder.hh
This file implements QR decomposition using housholder transformation
src/rungekutta.hh
src/sgrid.hh
src/sparsematrix.hh
src/timer.hh
A simple timing class
src/vector.hh

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Chapter 4

Class Documentation

4.1 hdnum::Banach Class Reference

Solve nonlinear problem using a fixed point iteration.

```
#include <newton.hh>
```

Public Member Functions

• Banach ()

constructor stores reference to the model

void set_maxit (size_type n)

maximum number of iterations before giving up

void set_sigma (double sigma_)

damping parameter

• void set_linesearchsteps (size_type n)

maximum number of steps in linesearch before giving up

void set_verbosity (size_type n)

control output given 0=nothing, 1=summary, 2=every step, 3=include line search

void set_abslimit (double I)

basolute limit for defect

void set_reduction (double I)

reduction factor

template < class M >

void solve (const M &model, Vector< typename M::number_type > &x) const
do one step

• bool has_converged () const

4.1.1 Detailed Description

Solve nonlinear problem using a fixed point iteration.

solve
$$F(x) = 0$$
.

$$x = x - \sigma * F(x)$$

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

• src/newton.hh

4.2 hdnum::SparseMatrix < REAL >::builder Class Reference

Public Member Functions

```
    builder (size_type new_m_rows, size_type new_m_cols)
```

- builder (const std::initializer_list< std::initializer_list< REAL > > &v)
- std::pair< typename std::map< size_type, REAL >::iterator, bool > addEntry (size_type i, size_type j, REAL value)
- std::pair< typename std::map< size_type, REAL >::iterator, bool > addEntry (size_type i, size_type j)
- bool operator== (const SparseMatrix::builder &other) const
- bool operator!= (const SparseMatrix::builder &other) const
- size_type colsize () const noexcept
- size_type rowsize () const noexcept
- size_type setNumCols (size_type new_m_cols) noexcept
- size_type setNumRows (size_type new_m_rows)
- void clear () noexcept
- std::string to_string () const
- SparseMatrix build ()

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

· src/sparsematrix.hh

4.3 hdnum::SparseMatrix< REAL >::column_index_iterator Class Reference

Public Types

```
• using self_type = column_index_iterator
```

- using difference_type = std::ptrdiff_t
- using value_type = std::pair<REAL &, size_type const &>
- using pointer = value_type *
- using reference = value_type &
- using iterator_category = std::bidirectional_iterator_tag

Public Member Functions

- column_index_iterator (typename std::vector< REAL >::iterator vallter, std::vector< size_type >::iterator collndicesIter)
- self_type & operator++ ()
- self type & operator++ (int junk)
- value_type operator* ()
- value_type::first_type value ()
- value_type::second_type index ()
- bool operator== (const self_type &other)
- bool operator!= (const self_type &other)

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

· src/sparsematrix.hh

4.4 hdnum::SparseMatrix< REAL >::const_column_index_iterator Class Reference

Public Types

```
    using self_type = const_column_index_iterator
    using difference_type = std::ptrdiff_t
    using value_type = std::pair<REAL const &, size_type const &>
    using pointer = value_type *
    using reference = value_type &
    using iterator_category = std::bidirectional_iterator_tag
```

Public Member Functions

```
    const_column_index_iterator (typename std::vector< REAL >::const_iterator vallter, std::vector< size_type >::const_iterator collndicesIter)
    self_type & operator++ ()
    self_type operator++ (int junk)
    value_type operator* ()
    value_type::first_type value ()
    value_type::second_type index ()
    bool operator== (const self_type &other)
    bool operator!= (const self_type &other)
```

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

src/sparsematrix.hh

4.5 hdnum::SparseMatrix< REAL >::const_row_iterator Class Reference

Public Types

```
using self_type = const_row_iterator
using difference_type = std::ptrdiff_t
using value_type = self_type
using pointer = self_type *
using reference = self_type &
using iterator_category = std::bidirectional_iterator_tag
```

Public Member Functions

- const_row_iterator (std::vector< size_type >::const_iterator rowPtrlter, std::vector< size_type >::const_iterator rowPtrlter, std::vector< size_type >::const_iterator vallter)
- const_column_iterator begin () const
- · const column iterator end () const
- const_column_index_iterator ibegin () const
- · const_column_index_iterator iend () const
- · const column iterator cbegin () const
- · const column iterator cend () const
- self type & operator++ ()
- self_type & operator++ (int junk)
- self_type & operator+= (difference_type offset)
- self type & operator-= (difference type offset)
- self_type operator- (difference_type offset)
- self_type operator+ (difference_type offset)
- reference operator[] (difference type offset)
- bool operator< (const self_type &other)
- bool operator> (const self_type &other)
- self_type & operator* ()
- bool operator== (const self_type &rhs)
- bool operator!= (const self_type &rhs)

Friends

• self_type operator+ (const difference_type &offset, const self_type &sec)

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

· src/sparsematrix.hh

4.6 hdnum::oc::OpCounter< F >::Counters Struct Reference

Struct storing the number of operations.

```
#include <opcounter.hh>
```

Public Member Functions

- void reset ()
- template<typename Stream >

void reportOperations (Stream &os, bool doReset=false)

Report operations to stream object.

size_type totalOperationCount (bool doReset=false)

Get total number of operations.

- Counters & operator+= (const Counters &rhs)
- Counters operator- (const Counters &rhs)

Public Attributes

- size_type addition_count
- size_type multiplication_count
- · size type division count
- size_type exp_count
- size_type pow_count
- size_type sin_count
- size_type sqrt_count
- size_type comparison_count

4.6.1 Detailed Description

```
template<typename F> struct hdnum::oc::OpCounter< F>::Counters
```

Struct storing the number of operations.

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

• src/opcounter.hh

4.7 hdnum::DenseMatrix< REAL > Class Template Reference

Class with mathematical matrix operations.

```
#include <densematrix.hh>
```

Public Types

typedef std::size_t size_type

Type used for array indices.

- typedef std::vector< REAL > VType
- typedef VType::const_iterator ConstVectorIterator
- typedef VType::iterator VectorIterator

Public Member Functions

• DenseMatrix ()

default constructor (empty Matrix)

DenseMatrix (const std::size_t _rows, const std::size_t _cols, const REAL def_val=0)

constructor

• DenseMatrix (const std::initializer_list< std::initializer_list< REAL >> &v)

constructor from initializer list

DenseMatrix (const hdnum::SparseMatrix < REAL > &other)

constructor from hdnum::SparseMatrix

- void addNewRow (const hdnum::Vector < REAL > &rowvector)
- size_t rowsize () const

get number of rows of the matrix

• size_t colsize () const

get number of columns of the matrix

- · bool scientific () const
- · void scientific (bool b) const

Switch between floating point (default=true) and fixed point (false) display.

• std::size t iwidth () const

get index field width for pretty-printing

• std::size_t width () const

get data field width for pretty-printing

• std::size t precision () const

get data precision for pretty-printing

void iwidth (std::size_t i) const

set index field width for pretty-printing

· void width (std::size_t i) const

set data field width for pretty-printing

• void precision (std::size_t i) const

set data precision for pretty-printing

REAL & operator() (const std::size_t row, const std::size_t col)

(i,j)-operator for accessing entries of a (m x n)-matrix directly

• const REAL & operator() (const std::size_t row, const std::size_t col) const

read-access on matrix element A_ij using A(i,j)

const ConstVectorIterator operator[] (const std::size_t row) const

read-access on matrix element A_ij using A[i][j]

VectorIterator operator[] (const std::size_t row)

write-access on matrix element A_ij using A[i][j]

DenseMatrix & operator= (const DenseMatrix &A)

assignment operator

• DenseMatrix & operator= (const REAL value)

assignment from a scalar value

• DenseMatrix sub (size_type i, size_type j, size_type rows, size_type cols)

Submatrix extraction.

• DenseMatrix transpose () const

Transposition.

DenseMatrix & operator+= (const DenseMatrix &B)

Addition assignment.

DenseMatrix & operator-= (const DenseMatrix &B)

Subtraction assignment.

DenseMatrix & operator*= (const REAL s)

```
Scalar multiplication assignment.
```

DenseMatrix & operator/= (const REAL s)

Scalar division assignment.

• void update (const REAL s, const DenseMatrix &B)

Scaled update of a Matrix.

template < class V >

void mv (Vector< V > &y, const Vector< V > &x) const

 $matrix\ vector\ product\ y = A*x$

template < class V >

void umv (Vector< V > &y, const Vector< V > &x) const

update matrix vector product y += A*x

template < class V >

void umv (Vector< V > &y, const V &s, const Vector< V > &x) const

update matrix vector product y += sA*x

void mm (const DenseMatrix< REAL > &A, const DenseMatrix< REAL > &B)

assign to matrix product C = A*B to matrix C

void umm (const DenseMatrix < REAL > &A, const DenseMatrix < REAL > &B)

add matrix product A*B to matrix C

void sc (const Vector < REAL > &x, std::size t k)

set column: make x the k'th column of A

void sr (const Vector < REAL > &x, std::size t k)

set row: make x the k'th row of A

REAL norm_infty () const

compute row sum norm

REAL norm_1 () const

compute column sum norm

Vector< REAL > operator* (const Vector< REAL > &x) const

vector = matrix * vector

DenseMatrix operator* (const DenseMatrix &x) const

matrix = matrix * matrix

• DenseMatrix operator+ (const DenseMatrix &x) const

matrix = matrix + matrix

• DenseMatrix operator- (const DenseMatrix &x) const

matrix = matrix - matrix

Related Symbols

(Note that these are not member symbols.)

```
• template<class T>
```

void identity (DenseMatrix< T > &A)

• template<typename REAL >

void spd (DenseMatrix < REAL > &A)

• template<typename REAL >

void vandermonde (DenseMatrix< REAL> &A, const Vector< REAL> x)

 $\bullet \ \ \text{template}{<} \text{typename REAL} >$

void readMatrixFromFileDat (const std::string &filename, DenseMatrix< REAL > &A)

Read matrix from a text file.

template<typename REAL >

void readMatrixFromFileMatrixMarket (const std::string &filename, DenseMatrix< REAL > &A)

Read matrix from a matrix market file.

4.7.1 Detailed Description

```
template<typename REAL> class hdnum::DenseMatrix< REAL>
```

Class with mathematical matrix operations.

4.7.2 Member Function Documentation

4.7.2.1 colsize()

```
template<typename REAL >
size_t hdnum::DenseMatrix< REAL >::colsize ( ) const [inline]
```

get number of columns of the matrix

Example:

```
hdnum::DenseMatrix<double> A(4,5);
size_t nColumns = A.colsize();
std::cout « "Matrix A has " « nColumns « " columns." « std::endl;
```

Output:

Matrix A has 5 columns.

4.7.2.2 mm()

assign to matrix product C = A*B to matrix C

Implements C = A*B where A and B are matrices

Parameters

in	Α	constant reference to a DenseMatrix
in	В	constant reference to a DenseMatrix

Example:

```
hdnum::DenseMatrix<double> A(2,6,1.0);
hdnum::DenseMatrix<double> B(6,3,-1.0);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(6); // use at least 6 columns for displaying
matrix entries A.precision(3); // display 3 digits behind the point

std::cout « "A =" « A « std::endl;
std::cout « "B =" « B « std::endl;
hdnum::DenseMatrix<double> C(2,3);
C.mm(A,B);
```

```
std::cout « "C = A*B =" « C « std::endl;
```

Output:

```
A =
      1
             2
                    3
0
                            4
  1.000 1.000 1.000 1.000 1.000 1.000
1.000 1.000 1.000 1.000 1.000
      1
             2
0
0 -1.000 -1.000 -1.000
1 -1.000 -1.000 -1.000
2 -1.000 -1.000 -1.000
3 -1.000 -1.000 -1.000
4 -1.000 -1.000 -1.000
5 -1.000 -1.000 -1.000
C = A*B =
0 1 2
0 -6.000 -6.000 -6.000
1 -6.000 -6.000 -6.000
```

4.7.2.3 mv()

matrix vector product y = A*x

Implements y = A*x where x and y are a vectors and A is a matrix

Parameters

ſ	in	У	reference to the resulting Vector
ſ	in	Χ	constant reference to a Vector

Example:

```
hdnum::Vector<double> x(3,10.0);
hdnum::Vector<double> y(2);
hdnum::DenseMatrix<double> A(2,3,1.0);

x.scientific(false); // fixed point representation for all Vector objects
A.scientific(false); // fixed point representation for all DenseMatrix
objects

std::cout « "A =" « A « std::endl;
std::cout « "x =" « x « std::endl;
A.mv(y,x);
std::cout « "y = A*x =" « y « std::endl;
```

Output:

```
x =
[ 0] 10.0000000
[ 1] 10.0000000
[ 2] 10.0000000

y = A*x =
[ 0] 30.0000000
[ 1] 30.0000000
```

4.7.2.4 operator()()

(i,j)-operator for accessing entries of a (m x n)-matrix directly

Parameters

in	row	row index (0m-1)		
in	col	column index (0n-1)		

Example:

```
hdnum::DenseMatrix<double> A(4,4);
A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(3);
identity(A); // Defines the identity matrix of the same dimension
std::cout « "A=" « A « std::endl;
std::cout « "reading A(0,0)=" « A(0,0) « std::endl;
std::cout « "resetting A(0,0) and A(2,3)..." « std::endl;
A(0,0) = 1.234;
A(2,3) = 432.1;
std::cout « "A=" « A « std::endl;
```

Output:

```
0
                        3
                    0.000
            0.000
0
     1.000
                             0.000
1
     0.000
             1.000
                     0.000
                             0.000
2
     0.000
             0.000
                    1.000
                             0.000
     0.000
             0.000
                    0.000
                              1.000
3
reading A(0,0)=1.000
resetting A(0,0) and A(2,3)...
A=
       1
                        3
Λ
0
     1.234
            0.000
                    0.000
                            0.000
1
     0.000
             1.000
                     0.000
                              0.000
                   1.000 432.100
2
     0.000
             0.000
     0.000
             0.000 0.000
                             1.000
```

4.7.2.5 operator*() [1/2]

Parameters

in	X	constant reference to a DenseMatrix	

Example:

```
hdnum::DenseMatrix<double> A(3,3,2.0);
hdnum::DenseMatrix<double> B(3,3,4.0);
hdnum::DenseMatrix<double> C(3,3);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

std::cout « "A=" « A « std::endl;
std::cout « "B=" « B « std::endl;
C=A*B;
std::cout « "C=A*B=" « C « std::endl;
```

Output:

```
A=
0
        1
                2
       2.0
              2.0
                       2.0
0
       2.0
               2.0
1
                        2.0
2
       2.0
               2.0
                        2.0
B=
0
                2
       4.0
              4.0
                       4.0
0
              4.0
1
       4.0
                       4.0
2
       4.0
               4.0
                        4.0
C=A*B=
0
        1
                2
      24.0
             24.0
                      24.0
0
      24.0
             24.0
                     24.0
1
      24.0
              24.0
                       24.0
2.
```

4.7.2.6 operator*() [2/2]

vector = matrix * vector

Parameters

in	X	constant reference to a Vector	
----	---	--------------------------------	--

Example:

```
hdnum::Vector<double> x(3,4.0);
hdnum::DenseMatrix<double> A(3,3,2.0);
hdnum::Vector<double> y(3);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

x.scientific(false); // fixed point representation for all Vector objects
x.width(8);
x.precision(1);

std::cout « "A=" « A « std::endl;
std::cout « "x=" « x « std::endl;
```

```
y=A*x; std::cout « "y=A*x" « y « std::endl;
```

Output:

```
A=
        1
                2
0
                       2.0
       2.0
               2.0
0
       2.0
1
               2.0
                        2.0
2
       2.0
              2.0
                        2.0
x=
[0]
       4.0
[1]
       4.0
[2]
        4.0
y=A*x
       24.0
[0]
[ 1]
       24.0
       24.0
[2]
```

4.7.2.7 operator*=()

Scalar multiplication assignment.

Implements A *= s where s is a scalar

Parameters

in	S	scalar value to multiply with

Example:

```
double s = 0.5;
hdnum::DenseMatrix<double> A(2,3,1.0);
std::cout « "A=" « A « std::endl;
A *= s;
std::cout « "A=" « A « std::endl;
```

Output:

```
A=
0 1 2
0 1.000e+00 1.000e+00 1.000e+00
1 1.000e+00 1.000e+00 1.000e+00

0.5*A =
0 1 2
0 5.000e-01 5.000e-01 5.000e-01
1 5.000e-01 5.000e-01 5.000e-01
```

4.7.2.8 operator+()

matrix = matrix + matrix

Parameters

in x constant reference to a DenseMa	rix
--------------------------------------	-----

Example:

```
hdnum::DenseMatrix<double> A(3,3,2.0);
hdnum::DenseMatrix<double> B(3,3,4.0);
hdnum::DenseMatrix<double> C(3,3);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

std::cout « "A=" « A « std::endl;
std::cout « "B=" « B « std::endl;
C=A+B;
std::cout « "C=A+B=" « C « std::endl;
```

Output:

```
A=
0
       1
0
       2.0
             2.0
                     2.0
              2.0
       2.0
                      2.0
1
2
       2.0
               2.0
                       2.0
B=
0
               2
             4.0
       4.0
                     4.0
0
             4.0
1
       4.0
                      4.0
2
       4.0
              4.0
                       4.0
C=A+B=
0
       1
               2
             6.0
      6.0
                     6.0
0
       6.0
             6.0
                      6.0
       6.0
                       6.0
2.
              6.0
```

4.7.2.9 operator+=()

Addition assignment.

Implements A += B matrix addition

Parameters

in B	another Matrix
------	----------------

4.7.2.10 operator-()

Parameters

in	X	constant reference to a DenseMatrix	
----	---	-------------------------------------	--

Example:

```
hdnum::DenseMatrix<double> A(3,3,2.0);
hdnum::DenseMatrix<double> B(3,3,4.0);
hdnum::DenseMatrix<double> C(3,3);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

std::cout « "A=" « A « std::endl;
std::cout « "B=" « B « std::endl;
C=A-B;
std::cout « "C=A-B=" « C « std::endl;
```

Output:

```
A=
0
        1
                 2
0
        2.0
                2.0
                        2.0
        2.0
                2.0
                          2.0
1
2
        2.0
                2.0
                          2.0
B=
0
                 2
        4.0
                4.0
                        4.0
0
1
        4.0
                4.0
                         4.0
2
        4.0
                4.0
                         4.0
C=A-B=
0
        1
                 2
      -2.0
               -2.0
                        -2.0
0
1
       -2.0
                -2.0
                        -2.0
       -2.0
               -2.0
                        -2.0
2.
```

4.7.2.11 operator-=()

Subtraction assignment.

Implements A -= B matrix subtraction

Parameters

```
in B another matrix
```

4.7.2.12 operator/=()

Scalar division assignment.

Implements A /= s where s is a scalar

Parameters

in	s	scalar value to multiply with
----	---	-------------------------------

Example:

```
double s = 0.5;
hdnum::DenseMatrix<double> A(2,3,1.0);
std::cout « "A=" « A « std::endl;
A /= s;
std::cout « "A=" « A « std::endl;
```

Output:

4.7.2.13 operator=() [1/2]

assignment operator

Example:

```
hdnum::DenseMatrix<double> A(4,4);
spd(A);
hdnum::DenseMatrix<double> B(4,4);
B = A;
std::cout « "B=" « B « std::endl;
```

Output:

4.7.2.14 operator=() [2/2]

assignment from a scalar value

Example:

```
hdnum::DenseMatrix<double> A(2,3);
A = 5.432;
A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(3); std::cout « "A=" « A « std::endl;
```

Output:

```
A=
0 1 2
0 5.432 5.432 5.432
1 5.432 5.432 5.432
```

4.7.2.15 rowsize()

```
template<typename REAL >
size_t hdnum::DenseMatrix< REAL >::rowsize ( ) const [inline]
```

get number of rows of the matrix

Example:

```
hdnum::DenseMatrix<double> A(4,5);
size_t nRows = A.rowsize();
std::cout « "Matrix A has " « nRows « " rows." « std::endl;
```

Output:

Matrix A has 4 rows.

4.7.2.16 sc()

set column: make x the k'th column of A

Parameters

	in	X	constant reference to a Vector
Ī	in	k	number of the column of A to be set

Example:

```
hdnum::Vector<double> x(2,434.0);
hdnum::DenseMatrix<double> A(2,6);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

std::cout « "original A=" « A « std::endl;
A.sc(x,3); // redefine fourth column of the matrix
std::cout « "modified A=" « A « std::endl;
```

Output:

origi 0 0	nal A= 1 0.0 0.0	2 0.0 0.0	3 0.0 0.0	4 0.0 0.0	5 0.0 0.0	0.0			
Τ.	0.0	0.0	0.0	0.0	0.0	0.0			
modif	modified A=								
0	1	2	3	4	5				
0	0.0	0.0	0.0	434.0	0.0	0.0			
1	0.0	0.0	0.0	434.0	0.0	0.0			

4.7.2.17 scientific()

Switch between floating point (default=true) and fixed point (false) display.

Example:

```
\label{lem:decomposition} $$ \begin{array}{ll} hdnum::DenseMatrix < double > A(4,4); \\ A.scientific(false); // fixed point representation for all DenseMatrix objects A.width(8); A.precision(3); identity(A); // Defines the identity matrix of the same dimension std::cout & "A=" & A & std::endl; \\ \end{array}
```

Output:

```
A=
0
                        3
                   0.000
0
     1.000
           0.000
                             0.000
                   0.000
     0.000
             1.000
                            0.000
1
2
     0.000
             0.000
                     1.000
                             0.000
                   0.000
3
     0.000
             0.000
                             1.000
```

4.7.2.18 sr()

set row: make x the k'th row of A

Parameters

in	Х	constant reference to a Vector
in	k	number of the row of A to be set

Example:

```
hdnum::Vector<double> x(3,434.0);
hdnum::DenseMatrix<double> A(3,3);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(8); A.precision(1);

std::cout « "original A=" « A « std::endl;
A.sr(x,1); // redefine second row of the matrix
std::cout « "modified A=" « A « std::endl;
```

Output:

```
original A=
    1
               2
Ω
0
      0.0
              0.0
                      0.0
1
      0.0
             0.0
                      0.0
2
      0.0
             0.0
                      0.0
modified A=
0
      1
               2
             0.0
0
      0.0
                     0.0
                    434.0
1
     434.0
            434.0
2
      0.0
              0.0
                      0.0
```

4.7.2.19 sub()

```
template<typename REAL >
DenseMatrix hdnum::DenseMatrix< REAL >::sub (
```

```
size_type i,
size_type j,
size_type rows,
size_type cols ) [inline]
```

Submatrix extraction.

Returns a new matrix that is a subset of the components of the given matrix.

Parameters

	in	i	first row index of the new matrix
	in	j	first column index of the new matrix
Ī	in	rows	row size of the new matrix, i.e. it has components [i,i+rows-1]
Ī	in	cols	column size of the new matrix, i.e. it has components [j,j+cols-1]

4.7.2.20 transpose()

```
template<typename REAL >
DenseMatrix hdnum::DenseMatrix< REAL >::transpose ( ) const [inline]
```

Transposition.

Return the transposed as a new matrix.

4.7.2.21 umm()

add matrix product A*B to matrix C

Implements C += A*B where A, B and C are matrices

Parameters

ir	l	Α	constant reference to a DenseMatrix
ir	1	В	constant reference to a DenseMatrix

Example:

```
hdnum::DenseMatrix<double> A(2,6,1.0);
hdnum::DenseMatrix<double> B(6,3,-1.0);
hdnum::DenseMatrix<double> C(2,3,0.5);

A.scientific(false); // fixed point representation for all DenseMatrix
objects A.width(6); A.precision(3);

std::cout « "C =" « C « std::endl;
std::cout « "A =" « A « std::endl;
std::cout « "B =" « B « std::endl;
c.umm(A,B);
std::cout « "C + A*B =" « C « std::endl;
```

Output:

```
C =
0
     1
            2
0
   0.500 0.500 0.500
   0.500 0.500 0.500
1
A =
     1
            2
                   3
0
                           4
  1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000
0
B =
     1
            2
0
0 -1.000 -1.000 -1.000
1 -1.000 -1.000 -1.000
2 -1.000 -1.000 -1.000
3 -1.000 -1.000 -1.000
4 -1.000 -1.000 -1.000
5 -1.000 -1.000 -1.000
C + A*B =
0 1
0 -5.500 -5.500 -5.500
1 -5.500 -5.500 -5.500
```

4.7.2.22 umv() [1/2]

update matrix vector product y += sA*x

Implements y += sA*x where s is a scalar value, x and y are a vectors and A is a matrix

Parameters

-			
	in	У	reference to the resulting Vector
	in	s	constant reference to a number type
	in	Х	constant reference to a Vector

Example:

```
double s=0.5;
hdnum::Vector<double> x(3,10.0);
hdnum::Vector<double> y(2,5.0);
hdnum::DenseMatrix<double> A(2,3,1.0);
x.scientific(false); // fixed point representation for all Vector objects
A.scientific(false); // fixed point representation for all DenseMatrix
objects
std::cout « "y =" « y « std::endl;
std::cout « "A =" « A « std::endl;
std::cout « "x =" « x « std::endl;
A.umv(y,s,x);
std::cout « "y = s*A*x =" « y « std::endl;
```

Output:

```
у =
[0]
         5.0000000
         5.0000000
[ 1]
A =
         1
                    2
0
0
        1.000
                   1.000
                               1.000
                  1.000
1
        1.000
                               1.000
x =
       10.0000000
[0]
[1]
       10.0000000
        10.0000000
[2]
y = s \star A \star x =
[ 0] 20.0000000
[ 1] 20.0000000
```

4.7.2.23 umv() [2/2]

update matrix vector product y += A*x

Implements y += A*x where x and y are a vectors and A is a matrix

Parameters

in	У	reference to the resulting Vector	
in	Х	constant reference to a Vector	

Example:

```
hdnum::Vector<double> x(3,10.0);
hdnum::Vector<double> y(2,5.0);
hdnum::DenseMatrix<double> A(2,3,1.0);

x.scientific(false); // fixed point representation for all Vector objects
A.scientific(false); // fixed point representation for all DenseMatrix
objects

std::cout « "y =" « y « std::endl;
std::cout « "A =" « A « std::endl;
std::cout « "x =" « x « std::endl;
A.umv(y,x);
std::cout « "y = A*x =" « y « std::endl;
```

Output:

```
[ 0]
       5.0000000
        5.0000000
[ 1]
A =
         1
0
                   2.
0
       1.000
                 1.000
                          1.000
                       1.000
1
       1.000
                1.000
x =
       10.0000000
[0]
```

```
[ 1] 10.0000000
[ 2] 10.0000000
y + A*x =
[ 0] 35.0000000
[ 1] 35.0000000
```

4.7.2.24 update()

Scaled update of a Matrix.

Implements A += s*B where s is a scalar and B a matrix

Parameters

i	n	s	scalar value to multiply with
i	n	В	another matrix

Example:

```
double s = 0.5;
hdnum::DenseMatrix<double> A(2,3,1.0);
hdnum::DenseMatrix<double> B(2,3,2.0);
A.update(s,B);
std::cout « "A + s*B = " « A « std::endl;
```

Output:

```
A + s*B = 0 1 2 0 1.500 1.500 1.500 1.500
```

4.7.3 Friends And Related Symbol Documentation

4.7.3.1 identity()

```
template<class T >  \label{eq:class} \mbox{void identity (} \\ \mbox{DenseMatrix< T > & A ) [related]
```

Function: make identity matrix

```
template<class T>
inline void identity (DenseMatrix<T> &A)
```

Parameters

in	Α	reference to a DenseMatrix that shall be filled with entries

Example:

```
hdnum::DenseMatrix<double> A(4,4);
identity(A);

A.scientific(false); // fixed point representation for all DenseMatrix objects
A.width(10);
A.precision(5);

std::cout « "A=" « A « std::endl;
```

Output:

```
A=
0
           1
                      2.
                                  3
               0.00000 0.00000
0
      1.00000
                                        0.00000
      0.00000 1.00000 0.00000 0.00000
1
      0.00000 0.00000 1.00000 0.00000
0.00000 0.00000 0.00000 1.00000
2
3
      0.00000
                 0.00000
                            0.00000
                                        1.00000
```

4.7.3.2 readMatrixFromFileDat()

Read matrix from a text file.

Parameters

in	filename	name of the text file
in,out	Α	reference to a DenseMatrix

Example:

```
hdnum::DenseMatrix<number> L;
readMatrixFromFile("matrixL.dat", L );
std::cout « "L=" « L « std::endl;
```

Contents of "matrixL.dat":

Output:

```
1.000e+00 0.000e+00 0.000e+00

2.000e+00 1.000e+00 0.000e+00

3.000e+00 2.000e+00 1.000e+00

would give:

L=

0 1 2

0 1.000e+00 0.000e+00 0.000e+00

1 2.000e+00 1.000e+00 0.000e+00

2 3.000e+00 2.000e+00 1.000e+00
```

4.7.3.3 readMatrixFromFileMatrixMarket()

Read matrix from a matrix market file.

Parameters

in	filename	name of the text file
in,out	Α	reference to a DenseMatrix

Example:

```
hdnum::DenseMatrix<number> L;
readMatrixFromFile("matrixL.mtx", L );
std::cout « "L=" « L « std::endl;
```

Output:

4.7.3.4 spd()

Function: make a symmetric and positive definite matrix

```
template<typename REAL>
inline void spd (DenseMatrix<REAL> &A)
```

Parameters

Example:

```
hdnum::DenseMatrix<double> A(4,4);
spd(A);

A.scientific(false); // fixed point representation for all DenseMatrix objects
A.width(10);
A.precision(5);

std::cout « "A=" « A « std::endl;
```

Output:

```
A= 0 1 2 3 0 4.00000 -1.00000 -0.25000 -0.11111 1 -1.00000 4.00000 -1.00000 -0.25000 2 -0.25000 -1.00000 4.00000 3 -0.11111 -0.25000 -1.00000 4.00000
```

4.7.3.5 vandermonde()

Function: make a vandermonde matrix

```
template<typename REAL>
inline void vandermonde (DenseMatrix<REAL> &A, const Vector<REAL> x)
```

Parameters

in	Α	reference to a DenseMatrix that shall be filled with entries
in	X	constant reference to a Vector

Example:

```
hdnum::Vector<double> x(4);
fill(x,2.0,1.0);
hdnum::DenseMatrix<double> A(4,4);
vandermonde(A,x);

A.scientific(false); // fixed point representation for all DenseMatrix objects
A.width(10);
A.precision(5);

x.scientific(false); // fixed point representation for all Vector objects
x.width(10);
x.precision(5);

std::cout « "x=" « x « std::endl;
std::cout « "A=" « A « std::endl;
```

Output:

```
X=
[ 0]
       2.00000
[ 1]
       3.00000
[2]
       4.00000
[3]
     5.00000
A=
               2.00000 4.00000
3.00000 9.00000
     1.00000
0
                                       8.00000
1
      1.00000
                                       27.00000
                 4.00000 16.00000 64.00000
2
      1.00000
      1.00000
                 5.00000 25.00000 125.00000
```

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

src/densematrix.hh

4.8 hdnum::DIRK< M, S> Class Template Reference

Implementation of a general Diagonal Implicit Runge-Kutta method.

```
#include <ode.hh>
```

Public Types

```
• typedef M::size_type size_type
     export size type

    typedef M::time_type time_type

     export time_type
• typedef M::number_type number_type
     export number_type

    typedef DenseMatrix< number_type > ButcherTableau

     the type of a Butcher tableau
```

Public Member Functions

```
    DIRK (const M &model_, const S &newton_, const ButcherTableau &butcher_, const int order_)

• DIRK (const M &model_, const S &newton_, const std::string method)
• void set dt (time type dt )
```

void set_verbosity (size_type verbosity_)

set time step for subsequent steps

set verbosity level

• void step ()

do one step

• bool get_error () const

get current state

void set state (time type t , const Vector< number type > &u)

set current state

const Vector < number_type > & get_state () const

get current state

time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

• void get info () const

print some information

4.8.1 Detailed Description

```
template < class M, class S>
class hdnum::DIRK< M, S>
```

Implementation of a general Diagonal Implicit Runge-Kutta method.

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

М	the model type
S	nonlinear solver

4.8.2 Constructor & Destructor Documentation

4.8.2.1 DIRK() [1/2]

constructor stores reference to the model and requires a butcher tableau

4.8.2.2 DIRK() [2/2]

constructor stores reference to the model and sets the default butcher tableau corresponding to the given order

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

• src/ode.hh

4.9 hdnum::EE< M > Class Template Reference

Explicit Euler method as an example for an ODE solver.

```
#include <ode.hh>
```

Public Types

```
    typedef M::size_type size_type
        export size_type
    typedef M::time_type time_type
        export time_type
    typedef M::number_type number_type
        export number_type
```

Public Member Functions

EE (const M &model_)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

· void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

4.9.1 Detailed Description

template < class M > class hdnum::EE < M >

Explicit Euler method as an example for an ODE solver.

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

• src/ode.hh

4.10 hdnum::ErrorException Class Reference

General Error.

#include <exceptions.hh>

Inheritance diagram for hdnum::ErrorException:

hdnum::Exception
hdnum::ErrorException

Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 - store string in internal message buffer
- const std::string & what () const

output internal message buffer

4.10.1 Detailed Description

General Error.

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

· src/exceptions.hh

4.11 hdnum::Exception Class Reference

Base class for Exceptions.

#include <exceptions.hh>

Inheritance diagram for hdnum::Exception:



Public Member Functions

- void message (const std::string &message)
 - store string in internal message buffer
- const std::string & what () const

output internal message buffer

4.11.1 Detailed Description

Base class for Exceptions.

all HDNUM exceptions are derived from this class via trivial subclassing:

```
class MyException : public Dune::Exception {};
```

You should not throw a Dune::Exception directly but use the macro DUNE_THROW() instead which fills the message-buffer of the exception in a standard way and features a way to pass the result in the operator <<-style

See also

HDNUM_THROW, IOError, MathError

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

src/exceptions.hh

4.12 hdnum::GenericNonlinearProblem< Lambda, Vec > Class Template Reference

A generic problem class that can be set up with a lambda defining F(x)=0.

```
#include <newton.hh>
```

Public Types

typedef std::size_t size_type

export size_type

typedef Vec::value_type number_type

export number_type

Public Member Functions

• GenericNonlinearProblem (const Lambda &l_, const Vec &x_, number_type eps_=1e-7)

constructor stores parameter lambda

• std::size_t size () const

return number of componentes for the model

void F (const Vec &x, Vec &result) const

model evaluation

void F_x (const Vec &x, DenseMatrix< number_type > &result) const

jacobian evaluation needed for implicit solvers

4.12.1 Detailed Description

```
template<typename Lambda, typename Vec>
class hdnum::GenericNonlinearProblem< Lambda, Vec>
```

A generic problem class that can be set up with a lambda defining F(x)=0.

Template Parameters

Lambda	mapping a Vector to a Vector
Vec	the type for the Vector

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

• src/newton.hh

4.13 hdnum::Heun2 M > Class Template Reference

Heun method (order 2 with 2 stages)

```
#include <ode.hh>
```

Public Types

```
• typedef M::size_type size_type
```

export size_type

• typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

• Heun2 (const M &model)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

time_type get_time () const

get current time

time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

4.13.1 Detailed Description

template<class M>
class hdnum::Heun2< M >

Heun method (order 2 with 2 stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

• src/ode.hh

4.14 hdnum::Heun3 < M > Class Template Reference

Heun method (order 3 with 3 stages)

```
#include <ode.hh>
```

Public Types

```
    typedef M::size_type size_type
    export size_type
```

• typedef M::time_type time_type

export time_type

typedef M::number_type number_type

export number_type

Public Member Functions

```
• Heun3 (const M &model_)
```

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

• void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

4.14.1 Detailed Description

```
template < class M> class hdnum::Heun3< M>
```

Heun method (order 3 with 3 stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

src/ode.hh

4.15 hdnum::IE< M, S > Class Template Reference

Implicit Euler using Newton's method to solve nonlinear system.

```
#include <ode.hh>
```

Public Types

```
• typedef M::size_type size_type
```

export size_type

typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

```
    IE (const M &model_, const S &newton_)
```

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

void set_verbosity (size_type verbosity_)

set verbosity level

• void step ()

do one step

bool get_error () const

get current state

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

void get_info () const

print some information

4.15.1 Detailed Description

```
template < class M, class S> class hdnum::IE< M, S>
```

Implicit Euler using Newton's method to solve nonlinear system.

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

М	the model type
S	nonlinear solver

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

src/ode.hh

4.16 hdnum::ImplicitRungeKuttaStepProblem< M > Class Template Reference

Nonlinear problem we need to solve to do one step of an implicit Runge Kutta method.

```
#include <rungekutta.hh>
```

Public Types

typedef M::size_type size_type

export size type

typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

• ImplicitRungeKuttaStepProblem (const M &model_, DenseMatrix< number_type > A_, Vector< number_type > b_, Vector< number_type > c_, time_type t_, Vector< number_type > u_, time_type dt_)

constructor stores parameter lambda

std::size_t size () const

return number of componentes for the model

- void ${\bf F}$ (const Vector< number_type > &x, Vector< number_type > &result) const

model evaluation

void F_x (const Vector< number_type > &x, DenseMatrix< number_type > &result) const

jacobian evaluation needed for newton in implicite solvers

4.16.1 Detailed Description

```
template < class M > class hdnum::ImplicitRungeKuttaStepProblem < M >
```

Nonlinear problem we need to solve to do one step of an implicit Runge Kutta method.

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

• src/rungekutta.hh

4.17 hdnum::InvalidStateException Class Reference

Default exception if a function was called while the object is not in a valid state for that function.

#include <exceptions.hh>

Inheritance diagram for hdnum::InvalidStateException:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 store string in internal message buffer
- const std::string & what () const output internal message buffer

4.17.1 Detailed Description

Default exception if a function was called while the object is not in a valid state for that function.

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

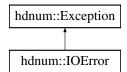
• src/exceptions.hh

4.18 hdnum::IOError Class Reference

Default exception class for I/O errors.

#include <exceptions.hh>

Inheritance diagram for hdnum::IOError:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

• void message (const std::string &message)

store string in internal message buffer

• const std::string & what () const

output internal message buffer

4.18.1 Detailed Description

Default exception class for I/O errors.

This is a superclass for any errors dealing with file/socket I/O problems like

- · file not found
- · could not write file
- · could not connect to remote socket

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

· src/exceptions.hh

4.19 hdnum::Kutta3< M > Class Template Reference

Kutta method (order 3 with 3 stages)

```
#include <ode.hh>
```

Public Types

• typedef M::size_type size_type

export size_type

• typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

Kutta3 (const M &model_)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

· void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

size_type get_order () const

return consistency order of the method

4.19.1 Detailed Description

template < class M > class hdnum::Kutta3 < M >

Kutta method (order 3 with 3 stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

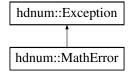
• src/ode.hh

4.20 hdnum::MathError Class Reference

Default exception class for mathematical errors.

#include <exceptions.hh>

Inheritance diagram for hdnum::MathError:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

• void message (const std::string &message)

store string in internal message buffer

• const std::string & what () const

output internal message buffer

4.20.1 Detailed Description

Default exception class for mathematical errors.

This is the superclass for all errors which are caused by mathematical problems like

- · matrix not invertible
- · not convergent

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

• src/exceptions.hh

4.21 hdnum::ModifiedEuler < M > Class Template Reference

Modified Euler method (order 2 with 2 stages)

```
#include <ode.hh>
```

Public Types

• typedef M::size_type size_type

export size_type

• typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

ModifiedEuler (const M &model_)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

· void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

4.21.1 Detailed Description

template < class M > class hdnum::ModifiedEuler < M >

Modified Euler method (order 2 with 2 stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

src/ode.hh

4.22 hdnum::Newton Class Reference

Solve nonlinear problem using a damped Newton method.

#include <newton.hh>

Public Member Functions

· Newton ()

constructor stores reference to the model

void set_maxit (size_type n)

maximum number of iterations before giving up

- void set_sigma (double sigma_)
- void set linesearchsteps (size type n)

maximum number of steps in linesearch before giving up

void set_verbosity (size_type n)

control output given 0=nothing, 1=summary, 2=every step, 3=include line search

void set_abslimit (double I)

basolute limit for defect

void set_reduction (double I)

reduction factor

template < class M >

 $\mbox{void } \mbox{\bf solve} \mbox{ (const M \&model, Vector$<$ typename M::number_type $> \&x) const}$

do one step

- · bool has_converged () const
- size_type iterations () const

4.22.1 Detailed Description

Solve nonlinear problem using a damped Newton method.

The Newton solver is parametrized by a model. The model also exports all relevant types for types.

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

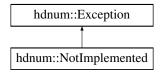
src/newton.hh

4.23 hdnum::NotImplemented Class Reference

Default exception for dummy implementations.

```
#include <exceptions.hh>
```

Inheritance diagram for hdnum::NotImplemented:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 - store string in internal message buffer
- const std::string & what () const

output internal message buffer

4.23.1 Detailed Description

Default exception for dummy implementations.

This exception can be used for functions/methods

- · that have to be implemented but should never be called
- · that are missing

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

· src/exceptions.hh

4.24 hdnum::oc::OpCounter< F > Class Template Reference

```
#include <opcounter.hh>
```

Classes

struct Counters

Struct storing the number of operations.

Public Types

- using size_type = std::size_t
- using value_type = F

Public Member Functions

```
• template<typename T >
```

OpCounter (const T &t, typename std::enable_if< std::is_same< T, int >::value and !std::is_same< F, int >::value >::type *=nullptr)

- OpCounter (const F &f)
- OpCounter (F &&f)
- OpCounter (const char *s)
- OpCounter & operator= (const char *s)
- operator F () const
- OpCounter & operator= (const F &f)
- OpCounter & operator= (F &&f)
- F * data ()
- const F * data () const

Static Public Member Functions

- static void additions (std::size t n)
- static void multiplications (std::size_t n)
- static void divisions (std::size_t n)
- static void reset ()
- template<typename Stream >

static void reportOperations (Stream &os, bool doReset=false)

Report operations to stream object.

• static size_type totalOperationCount (bool doReset=false)

Return total number of operations.

Public Attributes

F_v

Static Public Attributes

• static Counters counters

Friends

- std::ostream & operator<< (std::ostream &os, const OpCounter &f)
- std::istringstream & operator>> (std::istringstream &iss, OpCounter &f)

4.24.1 Detailed Description

template<typename F> class hdnum::oc::OpCounter< F >

Class counting operations

This is done by overloading operations and storing the numbers in a static class member.

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

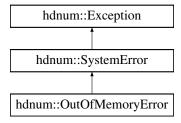
· src/opcounter.hh

4.25 hdnum::OutOfMemoryError Class Reference

Default exception if memory allocation fails.

#include <exceptions.hh>

Inheritance diagram for hdnum::OutOfMemoryError:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 - store string in internal message buffer
- const std::string & what () const output internal message buffer

4.25.1 Detailed Description

Default exception if memory allocation fails.

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

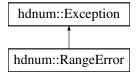
· src/exceptions.hh

4.26 hdnum::RangeError Class Reference

Default exception class for range errors.

#include <exceptions.hh>

Inheritance diagram for hdnum::RangeError:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 - store string in internal message buffer
- const std::string & what () const
 - output internal message buffer

4.26.1 Detailed Description

Default exception class for range errors.

This is the superclass for all errors which are caused because the user tries to access data that was not allocated before. These can be problems like

- · accessing array entries behind the last entry
- · adding the fourth non zero entry in a sparse matrix with only three non zero entries per row

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

• src/exceptions.hh

4.27 hdnum::RE< M, S > Class Template Reference

Adaptive one-step method using Richardson extrapolation.

```
#include <ode.hh>
```

Public Types

```
• typedef M::size_type size_type
```

export size_type

• typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

```
    RE (const M &model_, S &solver_)
```

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

void set_TOL (time_type TOL_)

set tolerance for adaptive computation

• void step ()

do one step

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

void get_info () const

print some information

4.27.1 Detailed Description

```
template < class M, class S> class hdnum::RE< M, S>
```

Adaptive one-step method using Richardson extrapolation.

Template Parameters

М	a model
S	any of the (non-adaptive) one step methods (solving model M)

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

• src/ode.hh

4.28 hdnum::RKF45< M > Class Template Reference

Adaptive Runge-Kutta-Fehlberg method.

```
#include <ode.hh>
```

Public Types

```
    typedef M::size_type size_type
    export size_type
```

• typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

```
• RKF45 (const M &model_)
```

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

void set_TOL (time_type TOL_)

set tolerance for adaptive computation

• void step ()

do one step

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

• size_type get_order () const

return consistency order of the method

void get_info () const

print some information

4.28.1 Detailed Description

```
template < class M > class hdnum::RKF45 < M >
```

Adaptive Runge-Kutta-Fehlberg method.

Template Parameters

```
M the model type
```

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

· src/ode.hh

4.29 hdnum::SparseMatrix< REAL >::row_iterator Class Reference

Public Types

```
using self_type = row_iterator
using difference_type = std::ptrdiff_t
using value_type = self_type
using pointer = self_type *
using reference = self_type &
using iterator_category = std::random_access_iterator_tag
```

Public Member Functions

```
• row_iterator (std::vector< size_type >::iterator rowPtrlter, std::vector< size_type >::iterator colIndicesIter,
  typename std::vector< REAL >::iterator vallter)
• column_iterator begin ()

    column iterator end ()

• column_index_iterator ibegin ()
· column index iterator iend ()
• self type & operator++ ()

    self_type operator++ (int junk)

    self_type & operator+= (difference_type offset)

• self_type & operator-= (difference_type offset)
• self type operator- (difference type offset)
• self type operator+ (difference type offset)
• reference operator[] (difference_type offset)

    bool operator< (const self_type &other)</li>

    bool operator> (const self_type &other)

self_type & operator* ()

    bool operator== (const self_type &rhs)

bool operator!= (const self_type &rhs)
```

Friends

• self_type operator+ (const difference_type &offset, const self_type &sec)

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

· src/sparsematrix.hh

4.30 hdnum::RungeKutta < M, S > Class Template Reference

classical Runge-Kutta method (order n with n stages)

```
#include <rungekutta.hh>
```

Public Types

```
• typedef M::size_type size_type
```

export size_type

• typedef M::time_type time_type

export time_type

typedef M::number type number_type

export number_type

Public Member Functions

RungeKutta (const M &model_, DenseMatrix< number_type > A_, Vector< number_type > b_, Vector< number type > c)

constructor stores reference to the model

RungeKutta (const M &model_, DenseMatrix< number_type > A_, Vector< number_type > b_, Vector<
 number_type > c_, number_type sigma_)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

bool check_explicit ()

test if method is explicit

• void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

• time_type get_dt () const

get dt used in last step (i.e. to compute current state)

void set_verbosity (int verbosity_)

how much should the ODE solver talk

4.30.1 Detailed Description

```
template<class M, class S = Newton>
class hdnum::RungeKutta< M, S >
```

classical Runge-Kutta method (order n with n stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

М	The model type
S	(Nonlinear) solver (default is Newton)

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

• src/rungekutta.hh

4.31 hdnum::RungeKutta4< M > Class Template Reference

```
classical Runge-Kutta method (order 4 with 4 stages)
```

```
#include <ode.hh>
```

Public Types

• typedef M::size_type size_type

export size_type

• typedef M::time_type time_type

export time_type

typedef M::number_type number_type

export number_type

Public Member Functions

RungeKutta4 (const M &model_)

constructor stores reference to the model

void set_dt (time_type dt_)

set time step for subsequent steps

• void step ()

do one step

void set_state (time_type t_, const Vector< number_type > &u_)

set current state

const Vector< number_type > & get_state () const

get current state

• time_type get_time () const

get current time

time_type get_dt () const

get dt used in last step (i.e. to compute current state)

size_type get_order () const

return consistency order of the method

4.31.1 Detailed Description

```
template < class M >
```

class hdnum::RungeKutta4< M >

classical Runge-Kutta method (order 4 with 4 stages)

The ODE solver is parametrized by a model. The model also exports all relevant types for time and states. The ODE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

• src/ode.hh

4.32 hdnum::SGrid < N, DF, dimension > Class Template Reference

Structured Grid for Finite Differences.

```
#include <sgrid.hh>
```

Public Types

- enum { dim = dimension }
- typedef std::size_t size_type

Export size type.

typedef N number_type

Export number type.

typedef DF DomainFunction

Type of the function defining the domain.

Public Member Functions

 SGrid (const Vector< number_type > extent_, const Vector< size_type > size_, const DomainFunction &df_)

Constructor.

- size_type getNeighborIndex (const size_type In, const size_type n_dim, const int n_side, const int k=1) const Provides the index of the k-th neighbor of the node with index In.
- bool isBoundaryNode (const size_type In) const

Returns true if the node is on the boundary of the discrete computational domain.

size_type getNumberOfNodes () const

Returns the number of nodes which are in the computaional domain.

- Vector < size_type > getGridSize () const
- $\bullet \ \ \text{Vector} < \text{number_type} > \textbf{getCellWidth} \ () \ \text{const} \\$

Returns the cell width h of the structured grid.

Vector< number_type > getCoordinates (const size_type In) const

Returns the world coordinates of the node with the given node index.

Public Attributes

const size_type invalid_node

The value which is returned to indicate an invalid node.

Static Public Attributes

```
    static const int positive = 1
        Side definitions for usage in getNeighborIndex(..)
    static const int negative = -1
```

4.32.1 Detailed Description

```
template<class N, class DF, int dimension> class hdnum::SGrid< N, DF, dimension>
```

Structured Grid for Finite Differences.

Template Parameters

N	A continuous type representing coordinate values.
DF	A boolean function which defines the domain.
dimension	The grid dimension.

4.32.2 Constructor & Destructor Documentation

4.32.2.1 SGrid()

```
template<class N , class DF , int dimension> hdnum::SGrid< N, DF, dimension>::SGrid ( const Vector< number_type > extent_, const Vector< size_type > size_, const DomainFunction & df_-) [inline]
```

Constructor.

Parameters

in	extent← –	The extent of the grid domain. The actual computational domain may be smaller and is defined by the domain function df
in	size⊷	The number of nodes in each grid dimension.
	_	
in	df_	The domain function. It has to provide a boolean function evaluate(Vector $<$ number_type $>$ x) which returns true if the node which is positioned at the coordinates of x is within the computational domain.

4.32.3 Member Function Documentation

4.32.3.1 getNeighborIndex()

```
template<class N , class DF , int dimension>
size_type hdnum::SGrid< N, DF, dimension >::getNeighborIndex (
```

```
const size_type ln,
const size_type n_dim,
const int n_side,
const int k = 1 ) const [inline]
```

Provides the index of the k-th neighbor of the node with index In.

Parameters

in	In	Index of the node whose neighbor is to be determined.
in	n_dim	The axes which connects the node and its neighbor (e.g. n_dim = 0 for a neighbor in the direction of the x-axes
in	n_side	Determines whether the neighbor is in positive of negative direction of the given axes. Should be either SGrid::positive or SGrid::negative.
in	k	For k=1 it will return the direct neighbor. Higher values will give distant nodes in the given direction. If the indicated node is not within the grid any more, then invalid_node will be returned. For k=0 it will simply return In.

Returns

size_type The index of the neighbor node.

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

· src/sgrid.hh

4.33 hdnum::SparseMatrix< REAL > Class Template Reference

Sparse matrix Class with mathematical matrix operations.

```
#include <sparsematrix.hh>
```

Classes

- · class builder
- class column_index_iterator
- · class const_column_index_iterator
- class const_row_iterator
- · class row_iterator

Public Types

• using size_type = std::size_t

Types used for array indices.

• using column_iterator = typename std::vector<REAL>::iterator

type of a regular column iterator (no access to indices)

• using const_column_iterator = typename std::vector<REAL>::const_iterator

type of a const regular column iterator (no access to indices)

Public Member Functions

• SparseMatrix ()=default

default constructor (empty SparseMatrix)

SparseMatrix (const size_type _rows, const size_type _cols)

constructor with added dimensions and columns

size_type rowsize () const

get number of rows of the matrix

· size type colsize () const

get number of columns of the matrix

• bool scientific () const

pretty-print output properties

row_iterator begin ()

get a (possibly modifying) row iterator for the sparse matrix

• row_iterator end ()

get a (possibly modifying) row iterator for the sparse matrix

· const row iterator cbegin () const

get a (non modifying) row iterator for the sparse matrix

· const_row_iterator cend () const

get a (non modifying) row iterator for the sparse matrix

- const_row_iterator begin () const
- · const row iterator end () const
- · void scientific (bool b) const

Switch between floating point (default=true) and fixed point (false) display.

• size_type iwidth () const

get index field width for pretty-printing

• size_type width () const

get data field width for pretty-printing

• size type precision () const

get data precision for pretty-printing

• void iwidth (size_type i) const

set index field width for pretty-printing

· void width (size type i) const

set data field width for pretty-printing

void precision (size_type i) const

set data precision for pretty-printing

- column_iterator find (const size_type row_index, const size_type col_index) const
- bool exists (const size_type row_index, const size_type col_index) const
- REAL & get (const size_type row_index, const size_type col_index)

write access on matrix element A_ij using A.get(i,j)

const REAL & operator() (const size_type row_index, const size_type col_index) const

read-access on matrix element A_ij using A(i,j)

• bool operator== (const SparseMatrix &other) const

checks whether two matricies are equal based on values and dimension

bool operator!= (const SparseMatrix &other) const

checks whether two matricies are unequal based on values and dimension

- bool operator< (const SparseMatrix &other)=delete
- bool operator> (const SparseMatrix &other)=delete
- bool operator<= (const SparseMatrix &other)=delete
- bool operator>= (const SparseMatrix &other)=delete
- SparseMatrix transpose () const
- SparseMatrix operator*= (const REAL scalar)

- SparseMatrix operator/= (const REAL scalar)
- template < class V >

void mv (Vector< V > &result, const Vector< V > &x) const

matrix vector product y = A*x

- Vector < REAL > operator* (const Vector < REAL > &x) const matrix vector product A*x
- template<class V >

void umv (Vector< V >&result, const Vector< V >&x) const

update matrix vector product y += A*x

· auto norm_infty () const

calculate row sum norm

- std::string to_string () const noexcept
- void print () const noexcept
- SparseMatrix< REAL > matchingIdentity () const

creates a matching identity

Static Public Member Functions

static SparseMatrix identity (const size_type dimN)
 identity for the matrix

Related Symbols

(Note that these are not member symbols.)

template < class REAL > void identity (SparseMatrix < REAL > &A)

4.33.1 Detailed Description

```
template<typename REAL> class hdnum::SparseMatrix< REAL >
```

Sparse matrix Class with mathematical matrix operations.

4.33.2 Constructor & Destructor Documentation

4.33.2.1 SparseMatrix()

```
template<typename REAL >
hdnum::SparseMatrix< REAL >::SparseMatrix ( ) [default]
```

default constructor (empty SparseMatrix)

Example:

```
hdnum::SparseMatrix<double> A();
auto nRows = A.rowsize();
std::cout « "Matrix A has " « nRows « " rows." « std::endl;
```

Output:

Matrix A has 0 rows.

4.33.3 Member Function Documentation

4.33.3.1 begin() [1/2]

```
template<typename REAL >
row_iterator hdnum::SparseMatrix< REAL >::begin ( ) [inline]
```

get a (possibly modifying) row iterator for the sparse matrix

The iterator points to the first row in the matrix.

Example:

```
// A is of type hdnum::SparseMatrix<int> and contains some values
// the deduced variable type for row_it is
// hdnum::SparseMatrix<int>::row_iterator
// but thats way to long to type out ;)
for(auto row_it = A.begin(); row_it != A.end(); row_it++) {
    for(auto val_it = row_it.begin(); val_it != row_it.end(); val_it++) {
        *val_it = 1;
    }
}
```

4.33.3.2 begin() [2/2]

```
template<typename REAL >
const_row_iterator hdnum::SparseMatrix< REAL >::begin ( ) const [inline]
```

See also

cbegin() const

4.33.3.3 cbegin()

```
template<typename REAL >
const_row_iterator hdnum::SparseMatrix< REAL >::cbegin ( ) const [inline]
```

get a (non modifying) row iterator for the sparse matrix

The iterator points to the first row in the matrix.

4.33.3.4 cend()

```
template<typename REAL >
const_row_iterator hdnum::SparseMatrix< REAL >::cend ( ) const [inline]
```

get a (non modifying) row iterator for the sparse matrix

The iterator points to the row one after the last one.

```
4.33.3.5 colsize()
```

```
template < typename REAL >
size_type hdnum::SparseMatrix< REAL >::colsize ( ) const [inline]
get number of columns of the matrix
Example:
hdnum::SparseMatrix<double> A(4,5);
auto nRows = A.colsize();
std::cout « "Matrix A has " « nRows « " rows." « std::endl;
Output:
Matrix A has 4 rows.
4.33.3.6 end() [1/2]
template<typename REAL >
row_iterator hdnum::SparseMatrix< REAL >::end ( ) [inline]
get a (possibly modifying) row iterator for the sparse matrix
The iterator points to the row one after the last one.
// A is of type hdnum::SparseMatrix<int> and contains some values
// the deduced variable type for row_it is
// hdnum::SparseMatrix<int>::row_iterator
// but thats way to long to type out ;)
for(auto row_it = A.begin(); row_it != A.end(); row_it++) {
    for(auto val_it = row_it.begin(); val_it != row_it.end(); val_it++) {
        *val_it = 1;
    }
}
4.33.3.7 end() [2/2]
{\tt template}{<}{\tt typename}~{\tt REAL}~>
const_row_iterator hdnum::SparseMatrix< REAL >::end ( ) const [inline]
See also
      cend() const
4.33.3.8 identity()
template<typename REAL >
static SparseMatrix hdnum::SparseMatrix< REAL >::identity (
                 const size_type dimN ) [inline], [static]
identity for the matrix
Example:
auto A = hdnum::SparseMatrix<double>::identity(4);
// fixed point representation for all SparseMatrix objects
A.scientific(false);
A.width(8);
A.precision(3);
std::cout « "A=" « A « std::endl;
```

```
A=
        1
                 2.
                          3
0
0
     1.000
              0.000
                      0.000
                                0.000
1
     0.000
              1.000
                     0.000
                                0.000
     0.000
              0.000
                      1.000
                                 0.000
2
3
      0.000
              0.000
                       0.000
                                 1.000
```

Output:

4.33.3.9 matchingldentity()

```
template<typename REAL >
SparseMatrix< REAL > hdnum::SparseMatrix< REAL >::matchingIdentity ( ) const [inline]
```

creates a matching identity

Example:

```
auto A = hdnum::SparseMatrix<double>(4, 5);
auto B = A.matchingIdentity();
// fixed point representation for all SparseMatrix objects
A.scientific(false);
A.width(8);
A.precision(3);
std::cout « "A=" « A « std::endl;
```

Output:

```
A =
0
       1
                2
                        3
0
     1.000
             0.000
                     0.000
                              0.000
                     0.000
                              0.000
1
     0.000
             1.000
     0.000
             0.000 1.000
                             0.000
     0.000
             0.000
                    0.000
                              1.000
```

4.33.3.10 mv()

matrix vector product y = A*x

Implements y = A*x where x and y are a vectors and A is a matrix

Parameters

in	result	reference to the resulting Vector
in	X	constant reference to a Vector

4.33.3.11 norm_infty()

```
template<typename REAL >
auto hdnum::SparseMatrix< REAL >::norm_infty ( ) const [inline]
```

calculate row sum norm

$$||A||_{\infty} = \max_{i=1...m} \sum_{j=1}^{n} |a_{ij}|$$

4.33.3.12 operator*()

matrix vector product A*x

Implements A*x where x is a vectors and A is a matrix

Parameters

```
in x constant reference to a Vector
```

4.33.3.13 operator*=()

Element-wise multiplication of the matrix

Parameters

	in	scalar	with same type as the matrix elements	1
--	----	--------	---------------------------------------	---

4.33.3.14 operator/=()

Element-wise division of the matrix

Parameters

in	scalar	with same type as the matrix elements
----	--------	---------------------------------------

4.33.3.15 rowsize()

```
template<typename REAL >
size_type hdnum::SparseMatrix< REAL >::rowsize ( ) const [inline]
```

get number of rows of the matrix

Example:

```
hdnum::SparseMatrix<double> A(4,5);
auto nRows = A.rowsize();
std::cout « "Matrix A has " « nRows « " rows." « std::endl;
```

Output:

Matrix A has 4 rows.

4.33.3.16 scientific()

Switch between floating point (default=true) and fixed point (false) display.

Example:

```
hdnum::SparseMatrix<double> A(4,4);

// fixed point representation for all SparseMatrix objects objects
A.scientific(false);
A.width(8); A.precision(3); identity(A);

// Defines the identity matrix of the same dimension
std::cout « "A=" « A « std::endl;
```

Output:

```
A=
0
                       3
    1.000
                   0.000
           0.000
                            0.000
0
1
    0.000
           1.000 0.000
                           0.000
                  1.000
                            0.000
2
     0.000
            0.000
     0.000
            0.000
                            1.000
```

4.33.3.17 umv()

update matrix vector product y += A*x

Implements y += A*x where x and y are a vectors and A is a matrix

Parameters

in	result	reference to the resulting Vector
in	X	constant reference to a Vector

4.33.4 Friends And Related Symbol Documentation

4.33.4.1 identity()

Function: make identity matrix

```
template<class T>
inline void identity (SparseMatrix<T> &A)
```

Parameters

i	.n	Α	reference to a SparseMatrix that shall be filled with entries
---	----	---	---

Example:

```
hdnum::SparseMatrix<double> A(4,4);
identity(A);
// fixed point representation for all DenseMatrix objects
A.scientific(false);
A.width(10);
A.precision(5);
std::cout « "A=" « A « std::endl;
```

Output:

Α=				
0	1	2	3	
0	1.00000	0.00000	0.00000	0.00000
1	0.00000	1.00000	0.00000	0.00000
2	0.00000	0.00000	1.00000	0.00000
3	0.00000	0.00000	0.00000	1.00000

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

- · src/densematrix.hh
- · src/sparsematrix.hh

4.34 hdnum::SquareRootProblem< N > Class Template Reference

Example class for a nonlinear model F(x) = 0;.

```
#include <newton.hh>
```

Public Types

- typedef std::size_t size_type
 export size_type
- typedef N number_type

export number_type

Public Member Functions

• SquareRootProblem (number_type a_)

constructor stores parameter lambda

• std::size_t size () const

return number of componentes for the model

void F (const Vector < N > &x, Vector < N > &result) const

model evaluation

void F_x (const Vector < N > &x, DenseMatrix < N > &result) const

jacobian evaluation needed for implicit solvers

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4.34.1 Detailed Description

```
template < class N > class hdnum::SquareRootProblem < N > Example class for a nonlinear model F(x) = 0;. This example solves F(x) = x*x - a = 0 Template Parameters
```

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

a type representing x and F components

• src/newton.hh

4.35 hdnum::StationarySolver< M > Class Template Reference

Stationary problem solver. E.g. for elliptic problmes.

```
#include <pde.hh>
```

Public Types

typedef M::size_type size_type

export size_type

typedef M::time_type time_type

export time_type

• typedef M::number_type number_type

export number_type

Public Member Functions

StationarySolver (const M &model_)

constructor stores reference to the model

• void solve ()

do one step

- const Vector< number_type > & get_state () const

get current state

• size_type get_order () const

return consistency order of the method

4.35.1 Detailed Description

```
template < class M > class hdnum::StationarySolver < M >
```

Stationary problem solver. E.g. for elliptic problmes.

The PDE solver is parametrized by a model. The model also exports all relevant types for the solution. The PDE solver encapsulates the states needed for the computation.

Template Parameters

M the model type

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

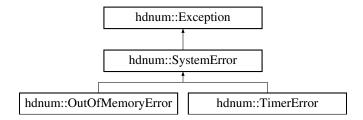
• src/pde.hh

4.36 hdnum::SystemError Class Reference

Default exception class for OS errors.

#include <exceptions.hh>

Inheritance diagram for hdnum::SystemError:



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

- void message (const std::string &message)
 store string in internal message buffer
- const std::string & what () const output internal message buffer

4.36.1 Detailed Description

Default exception class for OS errors.

This class is thrown when a system-call is used and returns an error.

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

• src/exceptions.hh

4.37 hdnum::Timer Class Reference

A simple stop watch.

#include <timer.hh>

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Public Member Functions

• Timer ()

A new timer, start immediately.

void reset ()

Reset timer.

• double elapsed () const

Get elapsed user-time in seconds.

4.37.1 Detailed Description

A simple stop watch.

This class reports the elapsed user-time, i.e. time spent computing, after the last call to Timer::reset(). The results are seconds and fractional seconds. Note that the resolution of the timing depends on your OS kernel which should be somewhere in the milisecond range.

The class is basically a wrapper for the libc-function getrusage()

Taken from the DUNE project www.dune-project.org

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

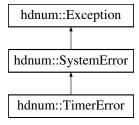
· src/timer.hh

4.38 hdnum::TimerError Class Reference

Exception thrown by the Timer class

```
#include <timer.hh>
```

 $Inheritance\ diagram\ for\ hdnum:: Timer Error:$



Additional Inherited Members

Public Member Functions inherited from hdnum::Exception

void message (const std::string &message)

store string in internal message buffer

· const std::string & what () const

output internal message buffer

4.38.1 Detailed Description

Exception thrown by the Timer class

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

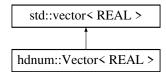
· src/timer.hh

4.39 hdnum::Vector < REAL > Class Template Reference

Class with mathematical vector operations.

```
#include <vector.hh>
```

Inheritance diagram for hdnum::Vector< REAL >:



Public Types

typedef std::size_t size_type

Type used for array indices.

Public Member Functions

• Vector ()

default constructor, also inherited from the STL vector default constructor

Vector (const size_t size, const REAL defaultvalue_=0)

another constructor, with arguments, setting the default value for all entries of the vector of given size

• Vector (const std::initializer_list< REAL > &v)

constructor from initializer list

Vector & operator= (const REAL value)

Assign all values of the Vector from one scalar value: x = value.

Vector sub (size_type i, size_type m)

Subvector extraction.

Vector & operator*= (const REAL value)

Multiplication by a scalar value (x *= value)

Vector & operator/= (const REAL value)

Division by a scalar value (x /= value)

Vector & operator+= (const Vector &y)

Add another vector (x += y)

Vector & operator-= (const Vector &y)

Subtract another vector (x -= y)

Vector & update (const REAL alpha, const Vector &y)

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Update vector by addition of a scaled vector (x += a y)

REAL operator* (Vector &x) const
 Inner product with another vector.

 Vector operator+ (Vector &x) const

```
Adding two vectors x+y.
    · Vector operator- (Vector &x) const
           vector subtraction x-y

    REAL two norm 2 () const

           Square of the Euclidean norm.
    • REAL two_norm () const
          Euclidean norm of a vector.
    · bool scientific () const
          pretty-print output property: true = scientific, false = fixed point representation
    · void scientific (bool b) const
           scientific(true) is the default, scientific(false) switches to the fixed point representation
    • std::size t iwidth () const
          get index field width for pretty-printing
    • std::size t width () const
          get data field width for pretty-printing

    std::size_t precision () const

          get data precision for pretty-printing
    · void iwidth (std::size_t i) const
          set index field width for pretty-printing

    void width (std::size_t i) const

          set data field width for pretty-printing

    void precision (std::size_t i) const

           set data precision for pretty-printing
Related Symbols
(Note that these are not member symbols.)
    • template<typename REAL >
       std::ostream & operator<< (std::ostream &os, const Vector< REAL > &x)
           Output operator for Vector.
    • template<typename REAL >
       void gnuplot (const std::string &fname, const Vector< REAL > x)
           Output contents of a Vector x to a text file named fname.

    template<typename REAL >

       void readVectorFromFile (const std::string &filename, Vector < REAL > &vector)
           Read vector from a text file.

    template < class REAL >

       void fill (Vector< REAL > &x, const REAL &t, const REAL &dt)
           Fill vector, with entries starting at t, consecutively shifted by dt.
    • template < class REAL >
       void unitvector (Vector< REAL > &x, std::size_t j)
           Defines j-th unitvector (j=0,...,n-1) where n = length of the vector.
```

4.39.1 Detailed Description

```
template<typename REAL> class hdnum::Vector< REAL>
```

Class with mathematical vector operations.

4.39.2 Member Function Documentation

4.39.2.1 operator*()

Inner product with another vector.

Example:

```
hdnum::Vector<double> x(2);
x.scientific(false); // set fixed point display mode
x[0] = 12.0;
x[1] = 3.0;
std::cout « "x=" « x « std::endl;
hdnum::Vector<double> y(2);
y[0] = 4.0;
y[1] = -1.0;
std::cout « "y=" « y « std::endl;
double s = x*y;
std::cout « "s = x*y = " « s « std::endl;
```

Output:

```
x = 
[ 0] 12.0000000
[ 1] 3.0000000

y = 
[ 0] 4.0000000
[ 1] -1.0000000

s = x * y = 45.0000000
```

4.39.2.2 operator+()

Adding two vectors x+y.

Example:

```
hdnum::Vector<double> x(2);
x.scientific(false); // set fixed point display mode
x[0] = 12.0;
x[1] = 3.0;
std::cout « "x=" « x « std::endl;
hdnum::Vector<double> y(2);
y[0] = 4.0;
y[1] = -1.0;
std::cout « "y=" « y « std::endl;
std::cout « "x+y = " « x+y « std::endl;
```

Output:

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4.39.2.3 operator-()

vector subtraction x-y

Example:

```
hdnum::Vector<double> x(2);
x.scientific(false); // set fixed point display mode
x[0] = 12.0;
x[1] = 3.0;
std::cout « "x=" « x « std::endl;
hdnum::Vector<double> y(2);
y[0] = 4.0;
y[1] = -1.0;
std::cout « "y=" « y « std::endl;
std::cout « "x-y = " « x-y « std::endl;
```

Output:

```
x=
[ 0] 12.0000000
[ 1] 3.0000000

y=
[ 0] 4.0000000
[ 1] -1.0000000

x-y =
[ 0] 8.0000000
[ 1] 4.0000000
```

4.39.2.4 operator=()

Assign all values of the Vector from one scalar value: x = value.

Parameters

Example:

```
hdnum::Vector<double> x(4);
x = 1.23;
std::cout « "x=" « x « std::endl;
```

Output:

```
x=
[ 0] 1.2340000e+00
[ 1] 1.2340000e+00
[ 2] 1.2340000e+00
[ 3] 1.2340000e+00
```

4.39.2.5 scientific()

scientific(true) is the default, scientific(false) switches to the fixed point representation

Example:

```
hdnum::Vector<double> x(3);
x[0] = 2.0;
x[1] = 2.0;
x[2] = 1.0;
std::cout « "x=" « x « std::endl;
x.scientific(false); // set fixed point display mode
std::cout « "x=" « x « std::endl;
```

Output:

```
[ 0] 2.0000000e+00
[ 1] 2.0000000e+00
[ 2] 1.0000000e+00

x=
[ 0] 2.000000
[ 1] 2.000000
[ 2] 1.0000000
```

4.39.2.6 sub()

Subvector extraction.

Returns a new vector that is a subset of the components of the given vector.

Parameters

in	i	first index of the new vector
in	m	size of the new vector, i.e. it has components [i,i+m-1]

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4.39.2.7 two_norm()

```
template<typename REAL >
REAL hdnum::Vector< REAL >::two_norm ( ) const [inline]
```

Euclidean norm of a vector.

Example:

```
hdnum::Vector<double> x(3);
x.scientific(false); // set fixed point display mode
x[0] = 2.0;
x[1] = 2.0;
x[2] = 1.0;
x[2] = 1.0;
xd::cout « "x=" « x « std::endl;
std::cout « "euclidean norm of x = " « x.two_norm() « std::endl;
```

Output:

4.39.3 Friends And Related Symbol Documentation

4.39.3.1 fill()

Fill vector, with entries starting at t, consecutively shifted by dt.

Example:

```
hdnum::Vector<double> x(5);
fill(x,2.01,0.1);
x.scientific(false); // set fixed point display mode
std::cout « "x=" « x « std::endl;
```

Output:

4.39.3.2 gnuplot()

Output contents of a Vector x to a text file named fname.

Example:

```
hdnum::Vector<double> x(5);
unitvector(x,3);
x.scientific(false); // set fixed point display mode
gnuplot("test.dat",x);
```

Output:

4.39.3.3 operator << ()

Output operator for Vector.

Example:

```
hdnum::Vector<double> x(3);
x[0] = 2.0;
x[1] = 2.0;
x[2] = 1.0;
std::cout « "x=" « x « std::endl;
```

Output:

```
x=
[ 0] 2.0000000e+00
[ 1] 2.0000000e+00
[ 2] 1.0000000e+00
```

4.39.3.4 readVectorFromFile()

Read vector from a text file.

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Parameters

in	filename	name of the text file
in,out	vector	reference to a Vector

Example:

```
hdnum::Vector<number> x;
readVectorFromFile("x.dat", x );
std::cout « "x=" « x « std::endl;
```

Output:

```
Contents of "x.dat":
1.0
2.0
3.0

would give:
x=
[ 0] 1.0000000e+00
[ 1] 2.0000000e+00
[ 2] 3.0000000e+00
```

4.39.3.5 unitvector()

Defines j-th unitvector (j=0,...,n-1) where n = length of the vector.

Example:

```
hadnum::Vector<double> x(5);
unitvector(x,3);
x.scientific(false); // set fixed point display mode
std::cout « "x=" « x « std::endl;
```

Output:

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

• src/vector.hh

Chapter 5

File Documentation

5.1 densematrix.hh

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil; c-basic-offset: 2 -*-
00003 \star File: densematrix.hh
00004 * Author: ngo
00005 *
00006 * Created on April 15, 2011
00007 */
80000
00009 #ifndef DENSEMATRIX_HH
00010 #define DENSEMATRIX_HH
00011
00012 #include <cstdlib>
00013 #include <fstream>
00014 #include <iomanip>
00015 #include <iostream>
00016 #include <sstream>
00017 #include <string>
00018
00019 #include "exceptions.hh"
00020 #include "sparsematrix.hh"
00021 #include "vector.hh"
00022
00023 namespace hdnum {
00024
00025 // forward-declare the sparse matrix template to make the transforming
00026 // constructor from hdnum::SparseMatrix -> hdnum::DenseMatrix working
00027 template <typename REAL>
00028 class SparseMatrix;
00029
00032 template <typename REAL>
00033 class DenseMatrix {
00034 public:
00036
        typedef std::size_t size_type;
00037
           typedef typename std::vector<REAL> VType;
00038
          typedef typename VType::const_iterator ConstVectorIterator;
00039
          typedef typename VType::iterator VectorIterator;
00040
00041 private:
          VType m_data; // Matrix data is stored in an STL vector! std::size_t m_rows; // Number of Matrix rows std::size_t m_cols; // Number of Matrix columns
00043
00044
00045
          static bool bScientific;
00046
          static std::size_t nIndexWidth;
static std::size_t nValueWidth;
00047
00048
00049
           static std::size_t nValuePrecision;
00050
           REAL myabs(REAL x) const {
00052
00053
             if (x >= REAL(0))
00054
                    return x;
00055
               else
00056
00057
00058
00060
           inline REAL& at(const std::size_t row, const std::size_t col) {
00061
               return m_data[row * m_cols + col];
00062
```

```
inline const REAL& at(const std::size_t row, const std::size_t col) const {
00066
             return m_data[row * m_cols + col];
00067
00068
00069 public:
00071
          DenseMatrix() : m_data(0, 0), m_rows(0), m_cols(0) {}
00072
00074
          DenseMatrix(const std::size_t _rows, const std::size_t _cols,
00075
                      const REAL def_val = 0)
00076
              : m_data(_rows * _cols, def_val), m_rows(_rows), m_cols(_cols) {}
00077
00079
          DenseMatrix(const std::initializer_list<std::initializer_list<REAL>& v) {
08000
              m_rows = v.size();
m_cols = v.begin()->size();
00081
00082
              for (auto row : v) {
00083
                  if (row.size() != m_cols) {
                      std::cout « "Zeilen der Matrix nicht gleich lang" « std::endl;
00084
00085
                      exit(1);
00086
00087
                  for (auto elem : row) m_data.push_back(elem);
00088
              }
00089
          }
00090
00092
          DenseMatrix(const hdnum::SparseMatrix<REAL>& other)
00093
              : m_data(other.rowsize() * other.colsize()), m_rows(other.rowsize()),
                m_cols(other.colsize()) {
00094
00095
              using counter_type = typename hdnum::SparseMatrix<REAL>::size_type;
00096
              counter_type row_index {};
00097
              for (auto& row : other) {
                  for (auto it = row.ibegin(); it != row.iend(); it++) {
00098
00099
                      this->operator[](row_index)[it.index()] = it.value();
00100
00101
                  row_index++;
00102
              }
00103
          }
00104
00105
          void addNewRow(const hdnum::Vector<REAL>& rowvector) {
00106
              m_rows++;
00107
              m_cols = rowvector.size();
00108
              for (std::size_t i = 0; i < m_cols; i++) m_data.push_back(rowvector[i]);</pre>
00109
          }
00110
00111
00112
          // copy constructor (not needed, since it inherits from the STL vector)
          DenseMatrix( const DenseMatrix& A )
00113
00114
00115
          this->m_data = A.m_data;
00116
          m_rows = A.m_rows;
          m_cols = A.m_cols;
00117
00118
00119
          */
00120
00136
          size_t rowsize() const { return m_rows; }
00137
          size_t colsize() const { return m_cols; }
00153
00154
00155
          // pretty-print output properties
00156
          bool scientific() const { return bScientific; }
00157
00179
          void scientific(bool b) const { bScientific = b; }
00180
00182
          std::size t iwidth() const { return nIndexWidth; }
00183
00185
          std::size_t width() const { return nValueWidth; }
00186
00188
          std::size_t precision() const { return nValuePrecision; }
00189
00191
          void iwidth(std::size t i) const { nIndexWidth = i; }
00192
00194
          void width(std::size_t i) const { nValueWidth = i; }
00195
00197
          void precision(std::size_t i) const { nValuePrecision = i; }
00198
00242
          // overloaded element access operators
00243
          // write access on matrix element A ij using A(i,j)
00244
          inline REAL& operator()(const std::size_t row, const std::size_t col) {
00245
              assert(row < m_rows || col < m_cols);</pre>
00246
              return at(row, col);
00247
00248
00250
          inline const REAL& operator()(const std::size_t row,
00251
                                         const std::size_t col) const {
00252
              assert(row < m_rows || col < m_cols);</pre>
00253
              return at(row, col);
00254
          }
00255
00257
          const ConstVectorIterator operator[](const std::size t row) const {
```

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```
assert (row < m_rows);
00259
                return m_data.begin() + row * m_cols;
00260
           }
00261
           VectorIterator operator[](const std::size_t row) {
00263
00264
                assert (row < m_rows);
00265
                return m_data.begin() + row * m_cols;
00266
00267
00290
           DenseMatrix& operator=(const DenseMatrix& A) {
               m_data = A.m_data;
00291
                m_rows = A.m_rows;
00292
00293
                m_cols = A.m_cols;
00294
               return *this;
00295
           }
00296
00316
           DenseMatrix& operator=(const REAL value) {
                for (std::size_t i = 0; i < rowsize(); i++)
    for (std::size_t j = 0; j < colsize(); j++) (*this)(i, j) = value;</pre>
00317
00318
00319
                return *this;
00320
00321
00334
           DenseMatrix sub(size_type i, size_type j, size_type rows, size_type cols) {
00335
                DenseMatrix A(rows, cols);
DenseMatrix& self = *this;
00336
                for (size_type k1 = 0; k1 < rows; k1++) {</pre>
00337
00338
                     for (size_type k2 = 0; k2 < cols; k2++) {</pre>
00339
                         A[k1][k2] = self[k1 + i][k2 + j];
00340
00341
                }
00342
                return A:
00343
           }
00344
00350
           DenseMatrix transpose() const {
                DenseMatrix A(m_cols, m_rows);
for (size_type i = 0; i < m_rows; i++) {
    for (size_type j = 0; j < m_cols; j++) {</pre>
00351
00352
00353
00354
                         A[j][i] = this->operator[](i)[j];
00355
00356
00357
                return A;
00358
           }
00359
00360
           // Basic Matrix Operations
00361
00369
           DenseMatrix& operator+=(const DenseMatrix& B) {
                for (size_type i = 0; i < rowsize(); ++i) {
    for (size_type j = 0; j < colsize(); ++j) {
        (*this)(i, j) += B(i, j);
    }
}</pre>
00370
00371
00372
00373
00374
00375
                return *this;
00376
00377
00385
           DenseMatrix& operator = (const DenseMatrix& B) {
               00386
00388
                          (*this)(i, j) -= B(i, j);
00389
                return *this;
00390
           }
00391
00421
           DenseMatrix& operator *= (const REAL s) {
00422
                for (std::size_t i = 0; i < rowsize(); ++i)</pre>
00423
                     for (std::size_t j = 0; j < colsize(); ++j) (*this)(i, j) *= s;</pre>
00424
                return *this;
00425
           }
00426
00457
           DenseMatrix& operator/=(const REAL s) {
00458
                for (std::size_t i = 0; i < rowsize(); ++i)</pre>
                     for (std::size_t j = 0; j < colsize(); ++j) (*this)(i, j) /= s;</pre>
00459
00460
00461
           }
00462
           void update(const REAL s, const DenseMatrix& B) {
   for (std::size_t i = 0; i < rowsize(); ++i)
      for (std::size_t j = 0; j < colsize(); ++j)</pre>
00489
00490
00491
00492
                         (*this)(i, j) += s * B(i, j);
00493
00494
00537
           template <class V>
           void mv(Vector<V>& y, const Vector<V>& x) const {
   if (this->rowsize() != y.size())
00538
00540
                     HDNUM_ERROR("mv: size of A and y do not match");
00541
                if (this->colsize() != x.size())
                     HDNUM_ERROR("mv: size of A and x do not match");
00542
00543
                for (std::size_t i = 0; i < rowsize(); ++i) {</pre>
00544
                    y[i] = 0;
```

```
for (std::size_t j = 0; j < colsize(); ++j)</pre>
00546
                       y[i] += (*this)(i, j) * x[j];
00547
               }
00548
          }
00549
00597
           template <class V>
           void umv(Vector<V>& y, const Vector<V>& x) const {
00598
00599
               if (this->rowsize() != y.size())
00600
                   HDNUM_ERROR("mv: size of A and y do not match");
00601
               if (this->colsize() != x.size())
                   HDNUM_ERROR("mv: size of A and x do not match");
00602
               for (std::size_t j = 0; j < colsize(); ++j) {
    for (std::size_t j = 0; j < colsize(); ++j)
00603
00604
00605
                       y[i] += (*this)(i, j) * x[j];
00606
               }
00607
          }
00608
00659
           template <class V>
00660
           void umv(Vector<V>& y, const V& s, const Vector<V>& x) const {
               if (this->rowsize() != y.size())
00661
00662
                    HDNUM_ERROR("mv: size of A and y do not match");
               if (this->colsize() != x.size())
   HDNUM_ERROR("mv: size of A and x do not match");
00663
00664
               for (std::size_t i = 0; i < rowsize(); ++i) {
    for (std::size_t j = 0; j < colsize(); ++j)</pre>
00665
00666
                      y[i] += s * (*this)(i, j) * x[j];
00668
00669
          }
00670
          void mm(const DenseMatrix<REAL>& A, const DenseMatrix<REAL>& B) {
00719
               if (this->rowsize() != A.rowsize())
00720
00721
                    HDNUM_ERROR("mm: size incompatible");
00722
               if (this->colsize() != B.colsize())
00723
                   HDNUM_ERROR("mm: size incompatible");
00724
               if (A.colsize() != B.rowsize()) HDNUM_ERROR("mm: size incompatible");
00725
00726
               for (std::size_t i = 0; i < rowsize(); i++)</pre>
                    for (std::size_t j = 0; j < colsize(); j++) {</pre>
00728
                        (*this)(i, j) = 0;
00729
                        for (std::size_t k = 0; k < A.colsize(); k++)</pre>
00730
                             (*this)(i, j) += A(i, k) * B(k, j);
00731
                   }
00732
          }
00733
00787
           void umm(const DenseMatrix<REAL>& A, const DenseMatrix<REAL>& B) {
00788
               if (this->rowsize() != A.rowsize())
00789
                   HDNUM_ERROR("mm: size incompatible");
00790
               if (this->colsize() != B.colsize())
                    HDNUM_ERROR("mm: size incompatible");
00791
00792
               if (A.colsize() != B.rowsize()) HDNUM_ERROR("mm: size incompatible");
00793
00794
               for (std::size_t i = 0; i < rowsize(); i++)</pre>
                    for (std::size_t j = 0; j < colsize(); j++)
    for (std::size_t k = 0; k < A.colsize(); k++)
        (*this)(i, j) += A(i, k) * B(k, j);</pre>
00795
00796
00797
00798
          }
00799
00833
           void sc(const Vector<REAL>& x, std::size_t k) {
00834
              if (this->rowsize() != x.size()) HDNUM_ERROR("cc: size incompatible");
00835
00836
               for (std::size t i = 0; i < rowsize(); i++) (*this)(i, k) = x[i];
00837
          }
00838
00874
           void sr(const Vector<REAL>& x, std::size_t k) {
00875
               if (this->colsize() != x.size()) HDNUM_ERROR("cc: size incompatible");
00876
00877
               for (std::size t i = 0; i < colsize(); i++) (*this)(k, i) = x[i];
00878
           }
00879
00881
           REAL norm_infty() const {
00882
               REAL norm(0.0);
00883
               for (std::size_t i = 0; i < rowsize(); i++) {</pre>
00884
                   REAL sum(0.0);
                    for (std::size_t j = 0; j < colsize(); j++)</pre>
00885
                        sum += myabs((*this)(i, j));
00886
                    if (sum > norm) norm = sum;
00887
00888
00889
               return norm;
00890
           }
00891
00893
           REAL norm 1() const {
00894
               REAL norm(0.0);
00895
               for (std::size_t j = 0; j < colsize(); j++) {</pre>
00896
                   REAL sum(0.0);
00897
                   for (std::size_t i = 0; i < rowsize(); i++)</pre>
                        sum += myabs((*this)(i, j));
00898
00899
                    if (sum > norm) norm = sum;
```

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```
00901
               return norm;
00902
          }
00903
00949
          Vector<REAL> operator*(const Vector<REAL>& x) const {
00950
              assert(x.size() == colsize());
00952
               Vector<REAL> y(rowsize());
               for (std::size_t r = 0; r < rowsize(); ++r) {
    for (std::size_t c = 0; c < colsize(); ++c) {</pre>
00953
00954
                       y[r] += at(r, c) * x[c];
00955
00956
00957
00958
00959
          }
00960
01003
          DenseMatrix operator*(const DenseMatrix& x) const {
01004
               assert(colsize() == x.rowsize());
01005
01006
               const std::size_t out_rows = rowsize();
01007
               const std::size_t out_cols = x.colsize();
01008
               DenseMatrix y(out_rows, out_cols, 0.0);
               for (std::size_t r = 0; r < out_rows; ++r)
    for (std::size_t c = 0; c < out_cols; ++c)
        for (std::size_t i = 0; i < colsize(); ++i)</pre>
01009
01010
01011
01012
                           y(r, c) += at(r, i) * x(i, c);
01013
01014
               return y;
01015
          }
01016
01059
          DenseMatrix operator+(const DenseMatrix& x) const {
01060
               assert(colsize() == x.colsize());
01061
               assert(rowsize() == x.rowsize());
01062
               const std::size_t out_rows = rowsize();
const std::size_t out_cols = x.colsize();
DenseMatrix y(out_rows, out_cols, 0.0);
01063
01064
01065
01066
               y = *this;
01067
               y += x;
01068
               return y;
01069
          }
01070
          DenseMatrix operator-(const DenseMatrix& x) const {
01113
01114
              assert(colsize() == x.colsize());
              assert(rowsize() == x.rowsize());
01115
01116
01117
               const std::size_t out_rows = rowsize();
               const std::size_t out_cols = x.colsize();
01118
               DenseMatrix y(out_rows, out_cols, 0.0);
01119
01120
               v = *this;
               y -= x;
01121
01122
               return y;
01123
          }
01124 };
01125
01126 template <typename REAL>
01127 bool DenseMatrix<REAL>::bScientific = true;
01128 template <typename REAL>
01129 std::size_t DenseMatrix<REAL>::nIndexWidth = 10;
01130 template <typename REAL>
01131 std::size_t DenseMatrix<REAL>::nValueWidth = 10;
01132 template <typename REAL>
01133 std::size_t DenseMatrix<REAL>::nValuePrecision = 3;
01134
01158 template <typename REAL>
s « std::endl:
01160
            s « " " « std::setw(A.iwidth()) « " "
« " ";
          s « "
01161
01162
01163
          for (typename DenseMatrix<REAL>::size_type j = 0; j < A.colsize(); ++j)</pre>
01164
              s « std::setw(A.width()) « j « " ";
01165
          s « std::endl;
01166
          for (typename DenseMatrix<REAL>::size_type i = 0; i < A.rowsize(); ++i) {
    s « " " « std::setw(A.iwidth()) « i « " ";</pre>
01167
              s « "
01168
               for (typename DenseMatrix<REAL>::size_type j = 0; j < A.colsize();</pre>
01169
01170
                     ++j) {
01171
                    if (A.scientific()) {
                        s « std::setw(A.width()) « std::scientific « std::showpoint
01172
01173
                         « std::setprecision(A.precision()) « A[i][j] « "
01174
                    } else {
01175
                       s « std::setw(A.width()) « std::fixed « std::showpoint
01176
                          « std::setprecision(A.precision()) « A[i][j] «
01177
                    }
01178
01179
               s « std::endl;
01180
```

```
01181
          return s;
01182 }
01183
01190 template <typename REAL>
01191 inline void fill(DenseMatrix<REAL>& A, const REAL& t) {
          for (typename DenseMatrix<REAL>::size_type i = 0; i < A.rowsize(); ++i)</pre>
01192
               for (typename DenseMatrix<REAL>::size_type j = 0; j < A.colsize(); ++j)</pre>
01193
01194
                   A[i][j] = t;
01195 }
01196
01198 template <typename REAL>
01199 inline void zero(DenseMatrix<REAL>& A) {
         for (std::size_t i = 0; i < A.rowsize(); ++i)
    for (std::size_t j = 0; j < A.colsize(); ++j) A(i, j) = REAL(0);</pre>
01200
01201
01202 }
01203
01237 template <class T>
01238 inline void identity(DenseMatrix<T>& A) {
          for (typename DenseMatrix<T>::size_type i = 0; i < A.rowsize(); ++i)</pre>
01240
               for (typename DenseMatrix<T>::size_type j = 0; j < A.colsize(); ++j)</pre>
01241
                    if (i == j)
01242
                        A[i][i] = T(1);
                    else
01243
01244
                       A[i][j] = T(0);
01245 }
01246
01282 template <typename REAL>
01283 inline void spd(DenseMatrix<REAL>& A) {
        if (A.rowsize() != A.colsize() || A.rowsize() == 0)
01284
               HDNUM_ERROR("need square and nonempty matrix");
01285
           for (std::size_t i = 0; i < A.rowsize(); ++i)
    for (std::size_t j = 0; j < A.colsize(); ++j)</pre>
01286
01287
01288
                   <u>if</u> (<u>i</u> == <u>j</u>)
01289
                        A(i, i) = REAL(4.0);
01290
                   else
                        A(i, j) = -REAL(1.0) / ((i - j) * (i - j));
01291
01292 }
01293
01343 template <typename REAL>
01344 inline void vandermonde (DenseMatrix<REAL>& A, const Vector<REAL> x) {
01345
           if (A.rowsize() != A.colsize() || A.rowsize() == 0)
           HDNUM_ERROR("need square and nonempty matrix");
if (A.rowsize() != x.size()) HDNUM_ERROR("need A and x of same size");
01346
01347
01348
           for (typename DenseMatrix<REAL>::size_type i = 0; i < A.rowsize(); ++i) {</pre>
              REAL p(1.0);
01349
               for (typename DenseMatrix<REAL>::size_type j = 0; j < A.colsize();</pre>
01350
                   ++j) {
A[i][j] = p;
01351
01352
                   p *= x[i];
01353
01354
               }
01355
          }
01356 }
01357
01359 template <typename REAL>
01360 inline void gnuplot(const std::string& fname, const DenseMatrix<REAL>& A) {
          std::fstream f(fname.c_str(), std::ios::out);
for (typename DenseMatrix<REAL>::size_type i = 0; i < A.rowsize(); ++i) {</pre>
01361
01362
01363
               for (typename DenseMatrix<REAL>::size_type j = 0; j < A.colsize();</pre>
01364
                     ++j) {
01365
                    if (A.scientific()) {
                        f « std::setw(A.width()) « std::scientific « std::showpoint
01366
01367
                         « std::setprecision(A.precision()) « A[i][j];
01368
                    } else {
01369
                       f « std::setw(A.width()) « std::fixed « std::showpoint
01370
                          « std::setprecision(A.precision()) « A[i][j];
01371
                    }
01372
01373
               f « std::endl;
01374
01375
           f.close();
01376 }
01377
01407 template <typename REAL>
01408 inline void readMatrixFromFileDat(const std::string& filename,
01409
                                            DenseMatrix<REAL>& A) {
01410
           std::string buffer;
01411
           std::ifstream fin(filename.c_str());
           std::size_t i = 0;
std::size_t j = 0;
01412
01413
01414
           if (fin.is_open()) {
               while (std::getline(fin, buffer)) {
01415
01416
                   std::istringstream iss(buffer);
                    hdnum::Vector<REAL> rowvector;
01417
01418
                    while (iss) {
01419
                       std::string sub;
01420
                        iss » sub;
01421
                        // std::cout « " sub = " « sub.c_str() « ": ";
```

```
if (sub.length() > 0) {
01423
                            REAL a = atof(sub.c_str());
01424
                            // std::cout « std::fixed « std::setw(10) «
                            // std::setprecision(5) « a;
01425
01426
                            rowvector.push_back(a);
01427
01428
01429
01430
                   if (rowvector.size() > 0) {
01431
                        A.addNewRow(rowvector);
01432
                        // std::cout « std::endl;
01433
01434
                   }
01435
01436
               fin.close();
01437
          } else {
               HDNUM_ERROR("Could not open file!");
01438
01439
          }
01440 }
01475 template <typename REAL>
01476 inline void readMatrixFromFileMatrixMarket(const std::string& filename,
01477
                                                    DenseMatrix<REAL>& A) {
01478
          std::string buffer;
01479
          std::ifstream fin(filename.c_str());
01480
          std::size_t i = 0;
01481
01482
          if (fin.is_open()) {
              // ignore all comments from the file (starting with %) while (fin.peek() == '%') fin.ignore(2048, '\n');
01483
01484
01485
01486
              std::getline(fin, buffer);
01487
              std::istringstream first_line(buffer);
01488
               first_line » i » j;
01489
               DenseMatrix<REAL> A_temp(i, j);
01490
01491
               while (std::getline(fin, buffer)) {
01492
                   std::istringstream iss(buffer);
01493
01494
                   REAL value {};
                   iss » i » j » value; // i-1, j-1, because matrix market does not use zero based indexing A_temp(i - 1, j - 1) = value;
01495
01496
01497
01498
01499
               A = A_{temp};
01500
               fin.close();
01501
          } else {
               HDNUM_ERROR("Could not open file! \"" + filename + "\"");
01502
          }
01503
01504 }
01505
01506 } // namespace hdnum
01507
01508 #endif // DENSEMATRIX HH
```

5.2 src/exceptions.hh File Reference

A few common exception classes.

```
#include <string>
#include <sstream>
```

Classes

· class hdnum::Exception

Base class for Exceptions.

class hdnum::IOError

Default exception class for I/O errors.

· class hdnum::MathError

Default exception class for mathematical errors.

· class hdnum::RangeError

Default exception class for range errors.

· class hdnum::NotImplemented

Default exception for dummy implementations.

· class hdnum::SystemError

Default exception class for OS errors.

class hdnum::OutOfMemoryError

Default exception if memory allocation fails.

· class hdnum::InvalidStateException

Default exception if a function was called while the object is not in a valid state for that function.

· class hdnum::ErrorException

General Error.

Macros

- #define THROWSPEC(E) #E << ": "
- #define HDNUM_THROW(E, m)
- #define HDNUM_ERROR(m)

Functions

std::ostream & hdnum::operator<< (std::ostream &stream, const Exception &e)

5.2.1 Detailed Description

A few common exception classes.

This file defines a common framework for generating exception subclasses and to throw them in a simple manner. Taken from the DUNE project www.dune-project.org

5.2.2 Macro Definition Documentation

5.2.2.1 HDNUM_ERROR

5.2.2.2 HDNUM THROW

Macro to throw an exception

5.3 exceptions.hh 85

Parameters

Ε	exception class derived from Dune::Exception
m	reason for this exception in ostream-notation

```
Example:
    if (filehandle == 0)
DUNE_THROW(FileError, "Could not open " « filename « " for reading!")
```

DUNE_THROW automatically adds information about the exception thrown to the text. If DUNE_DEVEL_MODE is defined more detail about the function where the exception happened is included. This mode can be activated via the --enable-dunedevel switch of ./configure

5.3 exceptions.hh

Go to the documentation of this file.

```
00001 #ifndef HDNUM_EXCEPTIONS_HH
00002 #define HDNUM_EXCEPTIONS_HH
00003
00004 #include <string>
00005 #include <sstream>
00006
00007 namespace hdnum {
80000
00035
        class Exception {
00036
        public:
00037
               void message(const std::string &message);
00038
               const std::string& what() const;
00039
        private:
00040
               std::string _message;
00041
00042
00043
        inline void Exception::message(const std::string &message)
00044
        {
00045
               _message = message;
00046
00047
00048
         inline const std::string& Exception::what() const
00049
00050
               return _message;
00051
00052
00053
         inline std::ostream& operator«(std::ostream &stream, const Exception &e)
00054
00055
               return stream « e.what();
00056
00058
        // the "format" the exception-type gets printed.
00059 // _LINE_ are standard C-defines, the GNU cpp-infofile claims that 00060 // C99 defines _func_ as well. _FUNCTION_ is a GNU-extension 00061 #ifdef HDNUM_DEVEL_MODE
00062  # define THROWSPEC(E)  #E « " [" « __func__ « ":" « __FILE__ « ":" « __LINE__ « "]: "
00063 #else
00064 # define THROWSPEC(E) #E « ": "
00065 #endif
00066
00084
         // this is the magic: use the usual do { \dots } while (0) trick, create
00085 // the full message via a string stream and throw the created object 00086 #define HDNUM_THROW(E, m) do { E th_ex; std::ostringstream th_out;
00087
               th_out « THROWSPEC(E) « m; th_ex.message(th_out.str()); throw th_ex;
00088
00089
00099
        class IOError : public Exception {};
00100
00109
        class MathError : public Exception {};
00110
00122
         class RangeError : public Exception {};
00123
00131
         class NotImplemented : public Exception {};
00132
00139
        class SystemError : public Exception {};
00140
00144
         class OutOfMemoryError : public SystemError {};
00145
```

```
class InvalidStateException : public Exception {};
00150
00153
       class ErrorException : public Exception {};
00154
       // throw {\tt ErrorException} with message
00155
00156 #define HDNUM_ERROR(m) do { hdnum::ErrorException th_ex; std::ostringstream th_out;
              th_out « THROWSPEC (hdnum::ErrorException) « m; \
00157
00158
              th__ex.message(th__out.str());
00159
              std::cout « th__ex.what() « std::endl; \
             throw th__ex;
00160
       } while (0)
00161
00162
00163 } // end namespace
00164
00165 #endif
```

5.4 src/lr.hh File Reference

This file implements LU decomposition.

```
#include "vector.hh"
#include "densematrix.hh"
```

Functions

```
template < class T >
  void hdnum::Ir (DenseMatrix< T > &A, Vector< std::size t > &p)
     compute Ir decomposition of A with first nonzero pivoting
• template<class T >
  T hdnum::abs (const T &t)
     our own abs class that works also for multiprecision types
• template<class T >
  void hdnum::Ir_partialpivot (DenseMatrix< T > &A, Vector< std::size_t > &p)
     Ir decomposition of A with column pivoting

    template < class T >

  void hdnum::Ir_fullpivot (DenseMatrix< T > &A, Vector< std::size_t > &p, Vector< std::size_t > &q)
     Ir decomposition of A with full pivoting
  void hdnum::permute forward (const Vector < std::size t > &p, Vector < T > &b)
     apply permutations to a right hand side vector
• template<class T >
  void hdnum::permute_backward (const Vector < std::size t > &q, Vector < T > &z)
     apply permutations to a solution vector
• template<class T >
  void hdnum::row_equilibrate (DenseMatrix< T > &A, Vector< T > &s)
     perform a row equilibration of a matrix; return scaling for later use
• template<class T >
  void hdnum::apply_equilibrate (Vector< T > &s, Vector< T > &b)
     apply row equilibration to right hand side vector
  void hdnum::solveL (const DenseMatrix< T > &A, Vector< T > &x, const Vector< T > &b)
     Assume L = lower triangle of A with Lii=1, solve L x = b.
template < class T >
  void hdnum::solveR (const DenseMatrix< T > &A, Vector< T > &x, const Vector< T > &b)
     Assume R = upper triangle of A and solve R x = b.
• template<class T >
  void hdnum::linsolve (DenseMatrix< T > &A, Vector< T > &x, Vector< T > &b)
     a complete solver; Note A, x and b are modified!
```

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5.4.1 Detailed Description

This file implements LU decomposition.

5.5 lr.hh

```
Go to the documentation of this file.
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*- 00002 #ifndef HDNUM_LR_HH
00003 #define HDNUM LR HH
00004
00005 #include "vector.hh"
00006 #include "densematrix.hh"
00007
00012 namespace hdnum {
00013
00015
        template<class T>
00016
        void lr (DenseMatrix<T>& A, Vector<std::size_t>& p)
00017
00018
           if (A.rowsize()!=A.colsize() || A.rowsize()==0)
00019
             HDNUM_ERROR("need square and nonempty matrix");
00020
           if (A.rowsize()!=p.size())
00021
             HDNUM_ERROR("permutation vector incompatible with matrix");
00022
00023
           // transformation to upper triangular
00024
           for (std::size_t k=0; k<A.rowsize()-1; ++k)</pre>
00025
00026
               \ensuremath{//} find pivot element and exchange rows
               for (std::size_t r=k; r<A.rowsize(); ++r)
00027
00028
                 if (A[r][k]!=0)
                     p[k] = r; // store permutation in step k if (r>k) // exchange complete row if r!=k
00030
00031
00032
                        for (std::size_t j=0; j<A.colsize(); ++j)</pre>
00033
00034
                            T temp(A[k][j]);
                            A[k][j] = A[r][j];
A[r][j] = temp;
00035
00036
00037
00038
                      break;
00039
00040
               if (A[k][k]==0) HDNUM_ERROR("matrix is singular");
00041
00042
               // modification
00043
               for (std::size_t i=k+1; i<A.rowsize(); ++i)</pre>
00044
                   T qik(A[i][k]/A[k][k]);
00045
00046
                   A[i][k] = qik;
                   for (std::size_t j=k+1; j<A.colsize(); ++j)
   A[i][j] -= qik * A[k][j];</pre>
00047
00048
00049
00050
             }
00051
00052
00054
        template<class T>
00055
         T abs (const T& t)
00056
00057
           if (t<0.0)
00058
            return -t;
          else
00059
00060
             return t:
00061
00062
00064
        template<class T>
00065
         void lr_partialpivot (DenseMatrix<T>& A, Vector<std::size_t>& p)
00066
              (A.rowsize()!=A.colsize() || A.rowsize()==0)
00067
            HDNUM_ERROR("need square and nonempty matrix");
00068
00069
           if (A.rowsize()!=p.size())
00070
             HDNUM_ERROR("permutation vector incompatible with matrix");
00071
00072
           // initialize permutation
00073
           for (std::size_t k=0; k<A.rowsize(); ++k)</pre>
00074
            p[k] = k;
00075
00076
           // transformation to upper triangular
00077
           for (std::size_t k=0; k<A.rowsize()-1; ++k)</pre>
00078
               // find pivot element
00079
```

```
08000
               for (std::size_t r=k+1; r<A.rowsize(); ++r)</pre>
00081
                if (abs(A[r][k])>abs(A[k][k]))
00082
                   p[k] = r; // store permutation in step k
00083
               if (p[k]>k) // exchange complete row if r!=k
00084
00085
                 for (std::size_t j=0; j<A.colsize(); ++j)</pre>
00086
00087
                      T temp(A[k][j]);
00088
                     A[k][j] = A[p[k]][j];
00089
                     A[p[k]][j] = temp;
                   }
00090
00091
00092
               if (A[k][k]==0) HDNUM_ERROR("matrix is singular");
00093
00094
               // modification
00095
               for (std::size_t i=k+1; i<A.rowsize(); ++i)</pre>
00096
00097
                   T qik(A[i][k]/A[k][k]);
00098
                   A[i][k] = qik;
00099
                   for (std::size_t j=k+1; j<A.colsize(); ++j)</pre>
00100
                     A[i][j] = qik * A[k][j];
00101
                 }
00102
            }
00103
        1
00104
00106
        template<class T>
00107
        void lr_fullpivot (DenseMatrix<T>& A, Vector<std::size_t>& p, Vector<std::size_t>& q)
00108
          if (A.rowsize()!=A.colsize() || A.rowsize()==0)
00109
00110
            HDNUM_ERROR("need square and nonempty matrix");
           if (A.rowsize()!=p.size())
00111
00112
             HDNUM_ERROR("permutation vector incompatible with matrix");
00113
00114
           \label{eq:condition} \ensuremath{\text{//}}\ initialize\ permutation}
00115
          for (std::size_t k=0; k<A.rowsize(); ++k)</pre>
00116
            p[k] = q[k] = k;
00117
00118
           // transformation to upper triangular
00119
           for (std::size_t k=0; k<A.rowsize()-1; ++k)</pre>
00120
00121
               // find pivot element
               for (std::size_t r=k; r<A.rowsize(); ++r)
for (std::size_t s=k; s<A.colsize(); ++s)</pre>
00122
00123
00124
                   if (abs(A[r][s])>abs(A[k][k]))
00125
00126
                       p[k] = r; // store permutation in step k
00127
                       q[k] = s;
00128
00129
00130
               if (p[k]>k) // exchange complete row if r!=k
                 for (std::size_t j=0; j<A.colsize(); ++j)</pre>
00131
00132
00133
                      T temp(A[k][j]);
                     A[k][j] = A[p[k]][j];
A[p[k]][j] = temp;
00134
00135
00136
               if (q[k]>k) // exchange complete column if s!=k
00137
00138
                 for (std::size_t i=0; i<A.rowsize(); ++i)</pre>
00139
00140
                      T temp(A[i][k]);
                     A[i][k] = A[i][q[k]];
A[i][q[k]] = temp;
00141
00142
00143
00144
00145
               if (std::abs(A[k][k])==0) HDNUM_ERROR("matrix is singular");
00146
               // modification
00147
               for (std::size_t i=k+1; i<A.rowsize(); ++i)</pre>
00148
00149
00150
                     qik(A[i][k]/A[k][k]);
00151
                   A[i][k] = qik;
                    for (std::size_t j=k+1; j<A.colsize(); ++j)</pre>
00152
00153
                     A[i][j] = qik * A[k][j];
00154
                 }
             }
00155
00156
00157
00159
        template<class T>
00160
        void permute_forward (const Vector<std::size_t>& p, Vector<T>& b)
00161
00162
          if (b.size()!=p.size())
00163
             HDNUM_ERROR("permutation vector incompatible with rhs");
00164
00165
           for (std::size_t k=0; k<b.size()-1; ++k)</pre>
00166
            if (p[k]!=k) std::swap(b[k],b[p[k]]);
00167
00168
```

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```
template<class T>
00171
        void permute_backward (const Vector<std::size_t>& q, Vector<T>& z)
00172
00173
          if (z.size()!=q.size())
00174
            HDNUM ERROR ("permutation vector incompatible with z");
00175
00176
          for (int k=z.size()-2; k>=0; --k)
00177
             if (q[k]!=std::size_t(k)) std::swap(z[k],z[q[k]]);
00178
00179
00181
        template<class T>
        void row_equilibrate (DenseMatrix<T>& A, Vector<T>& s)
00182
00183
00184
          if (A.rowsize()*A.colsize()==0)
            HDNUM_ERROR("need nonempty matrix");
00185
00186
           if (A.rowsize()!=s.size())
00187
            HDNUM_ERROR("scaling vector incompatible with matrix");
00188
00189
          // equilibrate row sums
00190
          for (std::size_t k=0; k<A.rowsize(); ++k)</pre>
00191
00192
               s[k] = T(0.0);
               for (std::size_t j=0; j<A.colsize(); ++j)</pre>
00193
                s[k] += abs(A[k][j]);
00194
               if (std::abs(s[k])==0) HDNUM_ERROR("row sum is zero");
for (std::size_t j=0; j<A.colsize(); ++j)
00195
00196
00197
                 A[k][j] /= s[k];
00198
00199
        }
00200
00202
        template<class T>
00203
        void apply_equilibrate (Vector<T>& s, Vector<T>& b)
00204
00205
          if (s.size()!=b.size())
00206
            HDNUM_ERROR("s and b incompatible");
00207
00208
          // equilibrate row sums
          for (std::size_t k=0; k<b.size(); ++k)</pre>
00210
            b[k] /= s[k];
00211
00212
00214
        template<class T>
        void solveL (const DenseMatrix<T>& A, Vector<T>& x, const Vector<T>& b)
00215
00216
00217
          if (A.rowsize()!=A.colsize() || A.rowsize()==0)
00218
            HDNUM_ERROR("need square and nonempty matrix");
00219
          if (A.rowsize()!=b.size())
00220
            HDNUM_ERROR("right hand side incompatible with matrix");
00221
00222
          for (std::size t i=0; i<A.rowsize(); ++i)</pre>
00223
              T rhs(b[i]);
00224
00225
               for (std::size_t j=0; j<i; j++)</pre>
              rhs -= A[i][j] * x[j];
x[i] = rhs;
00226
00227
00228
            }
00229
00230
00232
        template<class T>
00233
        \label{eq:const_def} \mbox{void solveR (const_DenseMatrix<T>& A, Vector<T>& x, const_Vector<T>& b)}
00234
00235
             (A.rowsize()!=A.colsize() || A.rowsize()==0)
00236
            HDNUM_ERROR("need square and nonempty matrix");
00237
             (A.rowsize()!=b.size())
00238
            HDNUM_ERROR("right hand side incompatible with matrix");
00239
00240
          for (int i=A.rowsize()-1; i>=0; --i)
00241
              T rhs(b[i]);
00242
00243
               for (std::size_t j=i+1; j<A.colsize(); j++)</pre>
00244
                 rhs -= A[i][j] * x[j];
              x[i] = rhs/A[i][i];
00245
            }
00246
00247
00248
00250
        template<class T>
00251
        void linsolve (DenseMatrix<T>& A, Vector<T>& x, Vector<T>& b)
00252
00253
          if (A.rowsize()!=A.colsize() || A.rowsize()==0)
            HDNUM_ERROR("need square and nonempty matrix");
00254
00255
           if (A.rowsize()!=b.size())
00256
            HDNUM_ERROR("right hand side incompatible with matrix");
00257
00258
          Vector<T> s(x.size());
          Vector<std::size_t> p(x.size());
Vector<std::size_t> q(x.size());
00259
00260
00261
          row equilibrate (A.s);
```

5.6 src/newton.hh File Reference

Newton's method with line search.

```
#include "lr.hh"
#include <type_traits>
```

Classes

class hdnum::SquareRootProblem< N >

Example class for a nonlinear model F(x) = 0;

class hdnum::GenericNonlinearProblem< Lambda, Vec >

A generic problem class that can be set up with a lambda defining F(x)=0.

· class hdnum::Newton

Solve nonlinear problem using a damped Newton method.

· class hdnum::Banach

Solve nonlinear problem using a fixed point iteration.

Functions

template<typename F, typename X >
 GenericNonlinearProblem< F, X > hdnum::getNonlinearProblem (const F &f, const X &x, typename X
 ::value_type eps=1e-7)

A function returning a problem class.

5.6.1 Detailed Description

Newton's method with line search.

5.6.2 Function Documentation

5.6.2.1 getNonlinearProblem()

A function returning a problem class.

Automatic template parameter extraction makes fiddling with types unnecessary.

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Template Parameters

-1		a lambda mapping a Vector to a Vector		
	Χ	the type for the Vector		

5.7 newton.hh

```
Go to the documentation of this file.
```

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*- 00002 #ifndef HDNUM_NEWTON_HH
00003 #define HDNUM_NEWTON_HH
00004
00005 #include "lr.hh"
00006 #include <type_traits>
00007
00012 namespace hdnum {
00013
00020
        template<class N>
00021
        class SquareRootProblem
00022
00023
        public:
          typedef std::size_t size_type;
00025
00026
00028
          typedef N number_type;
00029
00031
          SquareRootProblem (number_type a_)
00032
          : a(a_)
{}
00033
00034
00036
          std::size_t size () const
00037
00038
            return 1;
00039
          }
00040
00042
          void F (const Vector<N>& x, Vector<N>& result) const
00043
00044
            result[0] = x[0] * x[0] - a;
00045
00046
00048
          void F_x (const Vector<N>& x, DenseMatrix<N>& result) const
00049
00050
            result[0][0] = number_type(2.0)*x[0];
00051
00052
00053
        private:
00054
          number_type a;
00055
00056
00057
00063
        template<typename Lambda, typename Vec>
00064
        class GenericNonlinearProble
00065
00066
          Lambda lambda; // lambda defining the problem "lambda(x)=0"
00067
          size_t s;
00068
          typename Vec::value_type eps;
00069
        public:
00070
00072
          typedef std::size_t size_type;
00073
00075
          typedef typename Vec::value_type number_type;
00076
00078
          GenericNonlinearProblem (const Lambda& l_, const Vec& x_, number_type eps_ = 1e-7)
00079
            : lambda(l_{-}), s(x_{-}.size()), eps(eps_)
          { }
08000
00081
00083
          std::size_t size () const
00084
00085
            return s;
00086
00087
00089
          void F (const Vec& x, Vec& result) const
00090
00091
            result = lambda(x);
00092
00093
00095
          void F_x (const Vec& x, DenseMatrix<number_type>& result) const
00096
```

```
Vec Fx(x.size());
00098
            F(x,Fx);
00099
            Vec z(x);
00100
            Vec Fz(x.size());
00101
00102
             // numerische Jacobimatrix
             for (int j=0; j<result.colsize(); ++j)</pre>
00103
00104
                auto zj = z[j];
auto dz = (1.0+abs(zj))*eps;
00105
00106
                 z[j] += dz;
00107
00108
                 F(z,Fz);
00109
                for (int i=0; i<result.rowsize(); i++)</pre>
00110
                   result[i][j] = (Fz[i]-Fx[i])/dz;
00111
                 z[j] = zj;
00112
              }
00113
          }
00114
        };
00115
00123
        template<typename F, typename X>
        GenericNonlinearProblem<F,X> getNonlinearProblem (const F& f, const X& x, typename X::value_type eps
00124
     = 1e-7)
00125
00126
          return GenericNonlinearProblem<F, X>(f, x, eps);
00127
00128
00135
        class Newton
00136
00137
          typedef std::size_t size_type;
00138
00139
        public:
00141
          Newton ()
00142
           : maxit(25), linesearchsteps(10), verbosity(0),
00143
              reduction(1e-14), abslimit(1e-30), converged(false)
00144
00145
00147
          void set_maxit (size_type n)
00148
00149
            maxit = n;
00150
00151
00152
          void set_sigma (double sigma_)
00153
00154
00155
00156
00158
          void set_linesearchsteps (size_type n)
00159
00160
            linesearchsteps = n;
00161
00162
00164
          void set_verbosity (size_type n)
00165
00166
            verbosity = n;
00167
00168
00170
          void set_abslimit (double 1)
00171
00172
            abslimit = 1;
00173
00174
00176
          void set reduction (double 1)
00177
00178
            reduction = 1;
00179
00180
00182
          template<class M>
          void solve (const M& model, Vector<typename M::number_type> & x) const
00183
00184
00185
             typedef typename M::number_type N;
00186
             // In complex case, we still need to use real valued numbers for residual norms etc.
00187
            using Real = typename std::conditional<std::is_same<std::complex<double>, N>::value, double,
     N>::type;
00188
             Vector<N> r(model.size());
                                                       // residual
00189
             DenseMatrix<N> A(model.size(), model.size()); // Jacobian matrix
00190
             Vector<N> y (model.size());
                                                       // temporary solution in line search
             Vector<N> z (model.size());
00191
                                                       // solution of linear system
00192
             Vector<N> s(model.size());
                                                       // scaling factors
            Vector<size_type> p (model.size());
Vector<size_type> q (model.size());
                                                                   // row permutations
// column permutations
00193
00194
00195
00196
            model.F(x,r);
                                                                  // compute nonlinear residual
00197
             Real R0(std::abs(norm(r)));
                                                                     // norm of initial residual
00198
             Real R(R0);
                                                         // current residual norm
00199
             if (verbosity>=1)
00200
00201
                 std::cout « "Newton "
```

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```
00202
                                 norm=" « std::scientific « std::showpoint
                           « std::setprecision(4) « R0
00203
                           « std::endl;
00204
00205
              }
00206
00207
            converged = false;
            for (size_type i=1; i<=maxit; i++)</pre>
00208
                                                               // do Newton iterations
00209
00210
                 // check absolute size of residual
00211
                 if (R<=abslimit)</pre>
00212
                  {
00213
                    converged = true;
00214
                    return;
00215
00216
                // solve Jacobian system for update
00217
                                                                 // compute Jacobian matrix
00218
                model.F_x(x,A);
00219
                                                                 // equilibrate rows
                 row_equilibrate(A,s);
                 lr_fullpivot(A,p,q);
                                                                 // LR decomposition of A
00220
00221
                                                                 // clear solution
                z = N(0.0);
00222
                apply_equilibrate(s,r);
                                                                  // equilibration of right hand side
00223
                permute_forward(p,r);
                                                                 // permutation of right hand side
                                                                 // forward substitution
00224
                solveL(A,r,r);
                solveR(A, z, r);
                                                                 // backward substitution
00225
00226
                                                                 // backward permutation
                permute_backward(q,z);
00227
00228
00229
                Real lambda(1.0);
                                                          // start with lambda=1
                 for (size_type k=0; k<linesearchsteps; k++)</pre>
00230
00231
00232
                    y = x;
00233
                     y.update(-lambda,z);
                                                                   // y = x+lambda*z
00234
                     model.F(y,r);
                                                                 // r = F(y)
00235
                     Real newR(std::abs(norm(r)));
                                                                    // compute norm
00236
                     if (verbosity>=3)
00237
                                   « " line search " « std::setw(2) « k
« " lambda=" « std::scientific « std::showpoint
00238
                         std::cout « "
00239
00240
                                    « std::setprecision(4) « lambda
00241
                                    « " norm=" « std::scientific « std::showpoint
00242
                                    « std::setprecision(4) « newR
                                    « " red=" « std::scientific « std::showpoint
00243
                                    « std::setprecision(4) « newR/R
00244
00245
                                    « std::endl;
00246
00247
                     if (newR < (1.0-0.25 * lambda) * R)
                                                               // check convergence
00248
00249
                         if (verbosity>=2)
00250
                           {
                             std::cout « " step" « std::setw(3) « i
00251
                                       « " norm=" « std::scientific « std::showpoint
00252
00253
                                        « std::setprecision(4) « newR
00254
                                        « " red=" « std::scientific « std::showpoint
                                        « std::setprecision(4) « newR/R
00255
00256
                                        « std::endl;
00257
                           }
00258
                         x = y;
00259
                         R = newR;
00260
                         break;
                                                                 // continue with Newton loop
00261
                     else lambda \star=0.5:
00262
                                                                 // reduce damping factor
00263
                     if (k==linesearchsteps-1)
00264
                       {
00265
                         if (verbosity>=3)
00266
                           std::cout « "
                                            line search not converged within " « linesearchsteps « " steps" «
     std::endl;
00267
                         return;
00268
                      }
00269
                  }
00270
00271
                 // check convergence
00272
                if (R<=reduction*R0)</pre>
00273
                   {
00274
                     if (verbosity>=1)
00275
                      {
00276
                         std::cout « "Newton converged in " « i « " steps"
                                   « " reduction=" « std::scientific « std::showpoint
00277
00278
                                    \ll std::setprecision(4) \ll R/R0
00279
                                   « std::endl;
00280
                     iterations_taken = i;
00281
00282
                     converged = true;
00283
                     return;
00284
00285
                if (i==maxit)
00286
00287
                     iterations_taken = i;
```

```
if (verbosity>=1)
00289
                       std::cout "Newton not converged within " " maxit " iterations " " std::endl;
00290
                   }
00291
              }
00292
          }
00293
00294
          bool has_converged () const
00295
00296
            return converged;
00297
00298
          size_type iterations() const {
00299
            return iterations_taken;
00300
00301
00302
00303
        private:
00304
          size_type maxit;
00305
          mutable size_type iterations_taken = -1;
size_type linesearchsteps;
00306
00307
          size_type verbosity;
00308
          double reduction;
00309
          double abslimit;
00310
          mutable bool converged;
00311
        };
00312
00313
00314
00315
00323
        class Banach
00324
00325
          typedef std::size_t size_type;
00326
00327
        public:
00329
         Banach ()
           : maxit(25), linesearchsteps(10), verbosity(0), reduction(1e-14), abslimit(1e-30), sigma(1.0), converged(false)
00330
00331
00332
00333
00335
          void set_maxit (size_type n)
00336
00337
            maxit = n;
00338
          }
00339
00341
          void set_sigma (double sigma_)
00342
00343
            sigma = sigma_;
00344
00345
00347
          void set_linesearchsteps (size_type n)
00348
00349
            linesearchsteps = n;
00350
00351
00353
          void set_verbosity (size_type n)
00354
00355
            verbosity = n;
00356
00357
00359
          void set_abslimit (double 1)
00360
00361
            abslimit = 1:
00362
00363
00365
          void set_reduction (double 1)
00366
00367
            reduction = 1;
00368
00369
00371
          template<class M>
00372
           void solve (const M& model, Vector<typename M::number_type>& x) const
00373
00374
             typedef typename M::number_type N;
            Vector<N> r (model.size());
Vector<N> y (model.size());
00375
                                                        // residual
                                                        // temporary solution in line search
00376
00377
00378
            model.F(x,r);
                                                        // compute nonlinear residual
00379
            N R0 (norm(r));
                                                        // norm of initial residual
                                                        // current residual norm
00380
            N R(R0);
00381
             if (verbosity>=1)
00382
              {
00383
                 std::cout « "Banach "
                           « " norm=" « std::scientific « std::showpoint
00384
00385
                            « std::setprecision(4) « R0
00386
                            « std::endl;
00387
               }
00388
00389
            converged = false;
```

```
for (size_type i=1; i<=maxit; i++)</pre>
                                                             // do iterations
00391
                // check absolute size of residual
00392
00393
                if (R<=abslimit)</pre>
00394
00395
                   converged = true;
00396
                    return;
00397
                 }
00398
                // next iterate
00399
00400
                y = x;
                                                          // y = x+lambda*z
// r = F(y)
00401
                y.update(-sigma,r);
                model.F(y,r);
00402
00403
                N newR(norm(r));
                                                // compute norm
00404
                if (verbosity>=2)
00405
                   00406
00407
00408
                              « std::setprecision(4) « newR
00409
                              « " red=" « std::scientific « std::showpoint
00410
                              « std::setprecision(4) « newR/R
00411
                              « std::endl;
00412
                 }
                x = y;
                                                      // accept new iterate
00413
00414
                R = newR;
                                                      // remember new norm
00415
00416
                // check convergence
00417
                if (R<=reduction*R0 || R<=abslimit)</pre>
00418
                    if (verbosity>=1)
00419
00420
00421
                        std::cout « "Banach converged in " « i « " steps"
00422
                                  « " reduction=" « std::scientific « std::showpoint
00423
                                  \mbox{\tt w} std::setprecision(4) \mbox{\tt w} R/R0
00424
                                  « std::endl;
00425
00426
                   converged = true;
                    return;
00428
00429
00430
         }
00431
00432
         bool has converged () const
00433
00434
            return converged;
00435
00436
00437
       private:
        size_type maxit;
00438
00439
         size_type linesearchsteps;
         size_type verbosity;
00440
00441
         double reduction;
00442
         double abslimit;
00443
         double sigma;
00444
         mutable bool converged;
00445
       };
00447 } // namespace hdnum
00448
00449 #endif
```

5.8 src/ode.hh File Reference

solvers for ordinary differential equations

```
#include <vector>
#include "newton.hh"
```

Classes

class hdnum::EE< M >

Explicit Euler method as an example for an ODE solver.

class hdnum::ModifiedEuler< M >

Modified Euler method (order 2 with 2 stages)

class hdnum::Heun2< M >

Heun method (order 2 with 2 stages)

class hdnum::Heun3< M >

Heun method (order 3 with 3 stages)

class hdnum::Kutta3< M >

Kutta method (order 3 with 3 stages)

class hdnum::RungeKutta4< M >

classical Runge-Kutta method (order 4 with 4 stages)

class hdnum::RKF45< M >

Adaptive Runge-Kutta-Fehlberg method.

class hdnum::RE< M, S >

Adaptive one-step method using Richardson extrapolation.

class hdnum::IE< M, S >

Implicit Euler using Newton's method to solve nonlinear system.

class hdnum::DIRK< M, S >

Implementation of a general Diagonal Implicit Runge-Kutta method.

Functions

gnuplot output for time and state sequence

gnuplot output for time and state sequence

5.8.1 Detailed Description

solvers for ordinary differential equations

5.9 ode.hh

Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*- 00002 #ifndef HDNUM_ODE_HH
00003 #define HDNUM_ODE_HH
00004
00005 #include<vector>
00006 #include "newton.hh"
00007
00012 namespace hdnum {
00013
00022
        template<class M>
00023
        class EE
00024
00025
        public:
00027
          typedef typename M::size_type size_type;
00028
00030
          typedef typename M::time_type time_type;
00031
00033
          typedef typename M::number_type number_type;
00034
00036
          EE (const M& model_)
```

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```
00037
           : model(model_), u(model.size()), f(model.size())
00038
00039
            model.initialize(t,u);
00040
           dt = 0.1;
00041
00042
00044
          void set_dt (time_type dt_)
00045
00046
           dt = dt_{;}
00047
00048
00050
          void step ()
00051
00052
           model.f(t,u,f);
                              // evaluate model
00053
            u.update(dt,f);
                              // advance state
           t += dt;
                              // advance time
00054
00055
00056
00058
          void set_state (time_type t_, const Vector<number_type>& u_)
00059
          {
00060
00061
           u = u_;
00062
          }
00063
00065
          const Vector<number_type>& get_state () const
00066
00067
00068
00069
00071
          time_type get_time () const
00072
00073
           return t;
00074
00075
00077
          time_type get_dt () const
00078
00079
           return dt;
08000
00081
00083
          size_type get_order () const
00084
00085
           return 1;
00086
00087
00088
        private:
00089
          const M& model;
00090
          time_type t, dt;
00091
          Vector<number_type> u;
00092
          Vector<number_type> f;
00093
00094
00103
        template<class M>
00104
        class ModifiedEuler
00105
        public:
00106
00108
          typedef typename M::size_type size_type;
00109
00111
          typedef typename M::time_type time_type;
00112
00114
          typedef typename M::number_type number_type;
00115
          ModifiedEuler (const M& model_)
00117
00118
           : model(model_), u(model.size()), w(model.size()), k1(model.size()), k2(model.size())
00119
00120
           c2 = 0.5;
00121
            a21 = 0.5;
           b2 = 1.0;
00122
00123
            model.initialize(t,u);
00124
           dt = 0.1;
00125
00126
00128
          void set_dt (time_type dt_)
00129
           dt = dt_;
00130
00131
          }
00132
00134
          void step ()
00135
            // stage 1
00136
            model.f(t,u,k1);
00137
00138
00139
            // stage 2
00140
00141
            w.update(dt*a21,k1);
00142
            model.f(t+c2*dt,w,k2);
00143
00144
            // final
```

```
00145
           u.update(dt*b2,k2);
00146
           t += dt;
00147
00148
00150
          void set_state (time_type t_, const Vector<number_type>& u_)
00151
00152
00153
00154
00155
00157
          const Vector<number_type>& get_state () const
00158
00159
            return u;
00160
00161
00163
          time_type get_time () const
00164
00165
            return t;
00166
00167
00169
          time_type get_dt () const
00170
00171
           return dt;
00172
00173
00175
          size_type get_order () const
00176
00177
            return 2;
00178
00179
00180
        private:
00181
          const M& model;
00182
          time_type t, dt;
00183
          time_type c2,a21,b2;
          Vector<number_type> u,w;
Vector<number_type> k1,k2;
00184
00185
00186
       };
00187
00188
00197
        template<class M>
00198
        class Heun2
00199
        public:
00200
00202
          typedef typename M::size_type size_type;
00203
00205
          typedef typename M::time_type time_type;
00206
00208
          typedef typename M::number_type number_type;
00209
00211
          Heun2 (const M& model_)
00212
            : model(model_), u(model.size()), w(model.size()), k1(model.size()), k2(model.size())
00213
00214
            c2 = 1.0;
            a21 = 1.0;
00215
           b1 = 0.5;

b2 = 0.5;
00216
00217
00218
            model.initialize(t,u);
00219
            dt = 0.1;
00220
00221
          void set_dt (time_type dt_)
00223
00224
          {
00225
            dt = dt_{;}
00226
00227
00229
          void step ()
          {
    // stage 1
00230
00231
00232
            model.f(t,u,k1);
00233
00234
            // stage 2
00235
            w.update(dt*a21,k1);
00236
00237
            model.f(t+c2*dt,w,k2);
00238
00239
00240
            u.update(dt*b1,k1);
00241
            u.update(dt*b2,k2);
00242
            t += dt;
00243
          }
00244
00246
          void set_state (time_type t_, const Vector<number_type>& u_)
00247
          {
           t = t_;
00248
00249
           u = u_;
00250
00251
```

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```
const Vector<number_type>& get_state () const
00254
00255
            return u;
00256
          }
00257
00259
          time_type get_time () const
00260
00261
            return t;
00262
00263
00265
          time_type get_dt () const
00266
00267
            return dt;
00268
00269
00271
          size_type get_order () const
00272
00273
            return 2;
00274
00275
00276
        private:
00277
          const M& model;
00278
          time_type t, dt;
time_type c2,a21,b1,b2;
00279
00280
          Vector<number_type> u,w;
00281
          Vector<number_type> k1,k2;
00282
00283
00284
00293
        template<class M>
00294
        class Heun3
00295
00296
        public:
00298
          typedef typename M::size_type size_type;
00299
00301
          typedef typename M::time_type time_type;
00302
00304
          typedef typename M::number_type number_type;
00305
00307
          Heun3 (const M& model_)
00308
            : model(model_), u(model.size()), w(model.size()), kl(model.size()),
              k2(model.size()), k3(model.size())
00309
00310
00311
            c2 = time_type(1.0)/time_type(3.0);
00312
            c3 = time_type(2.0)/time_type(3.0);
00313
            a21 = time_type(1.0)/time_type(3.0);
00314
            a32 = time_type(2.0)/time_type(3.0);
            b1 = 0.25;
00315
            b2 = 0.0;
00316
00317
            b3 = 0.75;
00318
            model.initialize(t,u);
00319
            dt = 0.1;
00320
00321
00323
          void set_dt (time_type dt_)
00324
00325
            dt = dt_{;}
00326
00327
00329
          void step ()
00330
            // stage 1
00331
00332
            model.f(t,u,k1);
00333
00334
            // stage 2
00335
            w = u;
00336
            w.update(dt*a21,k1);
            model.f(t+c2*dt,w,k2);
00337
00338
00339
            // stage 3
00340
00341
            w.update(dt*a32,k2);
00342
            model.f(t+c3*dt,w,k3);
00343
00344
            // final
00345
            u.update(dt*b1,k1);
00346
            u.update(dt*b3,k3);
00347
            t += dt;
00348
00349
00351
          void set_state (time_type t_, const Vector<number_type>& u_)
00352
          {
00353
00354
            u = u_;
00355
          }
00356
00358
          const Vector<number type>& get state () const
```

```
{
00360
            return u;
00361
00362
00364
          time_type get_time () const
00365
00366
           return t;
00367
00368
00370
          time_type get_dt () const
00371
00372
            return dt;
00373
00374
00376
          size_type get_order () const
00377
00378
            return 3;
00379
          }
00380
00381
        private:
00382
         const M& model;
00383
          time_type t, dt;
          time_type c2,c3,a21,a31,a32,b1,b2,b3;
00384
          Vector<number_type> u,w;
Vector<number_type> k1,k2,k3;
00385
00386
00387
00388
00397
        template<class M>
00398
        class Kutta3
00399
00400
        public:
00402
          typedef typename M::size_type size_type;
00403
00405
          typedef typename M::time_type time_type;
00406
00408
          typedef typename M::number_type number_type;
00409
00411
          Kutta3 (const M& model_)
00412
            : model(model_), u(model.size()), w(model.size()), k1(model.size()),
00413
              k2(model.size()), k3(model.size())
00414
            c2 = 0.5;
00415
            c3 = 1.0;
00416
            a21 = 0.5;
00417
00418
            a31 = -1.0;
            a32 = 2.0;
00419
00420
            b1 = time_type(1.0)/time_type(6.0);
            b2 = time_type(4.0)/time_type(6.0);
b3 = time_type(1.0)/time_type(6.0);
00421
00422
00423
            model.initialize(t,u);
00424
            dt = 0.1;
00425
00426
00428
          void set_dt (time_type dt_)
00429
00430
            dt = dt_{;}
00431
00432
00434
          void step ()
          {
    // stage 1
00435
00436
00437
            model.f(t,u,k1);
00438
00439
            // stage 2
00440
            w.update(dt*a21,k1);
00441
00442
            model.f(t+c2*dt,w,k2);
00443
00444
            // stage 3
00445
            w = u;
00446
            w.update(dt*a31,k1);
00447
            w.update(dt*a32,k2);
00448
            model.f(t+c3*dt,w,k3);
00449
00450
            // final
00451
            u.update(dt*b1,k1);
00452
            u.update(dt*b2,k2);
00453
            u.update(dt*b3,k3);
00454
            t += dt;
00455
00456
00458
          void set_state (time_type t_, const Vector<number_type>& u_)
00459
          {
            t = t_;
00460
00461
           u = u_;
00462
00463
```

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```
const Vector<number_type>& get_state () const
00466
00467
            return u;
00468
          }
00469
00471
          time_type get_time () const
00472
00473
            return t;
00474
00475
00477
          time_type get_dt () const
00478
00479
            return dt;
00480
00481
00483
          size_type get_order () const
00484
00485
            return 3;
00486
00487
        private:
00488
00489
          const M& model;
          time_type t, dt;
time_type c2,c3,a21,a31,a32,b1,b2,b3;
00490
00491
          Vector<number_type> u,w;
Vector<number_type> k1,k2,k3;
00492
00493
00494
00495
00504
        template<class M>
00505
        class RungeKutta4
00506
00507
        public:
00509
          typedef typename M::size_type size_type;
00510
00512
          typedef typename M::time_type time_type;
00513
00515
          typedef typename M::number_type number_type;
00518
          RungeKutta4 (const M& model_)
00519
            : model(model_), u(model.size()), w(model.size()), k1(model.size()),
00520
               k2(model.size()), k3(model.size()), k4(model.size())
00521
            c2 = 0.5;
00522
            c3 = 0.5;
00523
00524
            c4 = 1.0;
00525
             a21 = 0.5;
00526
             a32 = 0.5;
             a43 = 1.0;
00527
            b1 = time_type(1.0)/time_type(6.0);
00528
            b2 = time_type(2.0)/time_type(6.0);
b3 = time_type(2.0)/time_type(6.0);
00529
00531
            b4 = time_type(1.0)/time_type(6.0);
00532
            model.initialize(t,u);
00533
            dt = 0.1;
00534
00535
          void set_dt (time_type dt_)
00538
00539
            dt = dt_;
00540
00541
00543
          void step ()
00544
          {
00545
            // stage 1
00546
            model.f(t,u,k1);
00547
00548
            // stage 2
00549
            w = u:
            w.update(dt*a21,k1);
00550
00551
            model.f(t+c2*dt,w,k2);
00552
00553
             // stage 3
00554
            w = u;
            w.update(dt*a32,k2);
00555
00556
            model.f(t+c3*dt,w,k3);
00557
00558
             // stage 4
00559
            w.update(dt*a43,k3);
00560
00561
            model.f(t+c4*dt,w,k4);
00562
00563
             // final
00564
             u.update(dt*b1,k1);
00565
             u.update(dt*b2,k2);
00566
             u.update(dt*b3,k3);
00567
            u.update(dt*b4,k4);
t += dt;
00568
```

```
}
00570
00572
          void set_state (time_type t_, const Vector<number_type>& u_)
00573
            t = t_;
00574
00575
            u = u:
00576
00577
00579
          const Vector<number_type>& get_state () const
00580
00581
            return u;
00582
00583
00585
          time_type get_time () const
00586
00587
            return t;
00588
00589
          time_type get_dt () const
00592
          {
00593
            return dt;
00594
00595
00597
          size_type get_order () const
00598
00599
            return 4;
00600
00601
00602
        private:
         const M& model;
00603
00604
          time_type t, dt;
00605
          time_type c2,c3,c4,a21,a32,a43,b1,b2,b3,b4;
00606
          Vector<number_type> u,w;
00607
          Vector<number_type> k1,k2,k3,k4;
00608
00609
00614
        template<class M>
        class RKF45
00615
00616
00617
        public:
00619
          typedef typename M::size_type size_type;
00620
00622
          typedef typename M::time type time type;
00623
00625
          typedef typename M::number_type number_type;
00626
00628
          RKF45 (const M& model )
00629
            : model(model_), u(model.size()), w(model.size()), ww(model.size()), k1(model.size()),
              k2(model.size()), k3(model.size()), k4(model.size()), k5(model.size()), k6(model.size()),
00630
00631
              steps(0), rejected(0)
00632
00633
            TOL = time_type(0.0001);
00634
            rho = time_type(0.8);
            alpha = time_type(0.25);
beta = time_type(4.0);
dt_min = 1E-12;
00635
00636
00637
00638
00639
             c2 = time_type(1.0)/time_type(4.0);
00640
             c3 = time_type(3.0)/time_type(8.0);
00641
            c4 = time_type(12.0)/time_type(13.0);
00642
            c5 = time_type(1.0);
            c6 = time_type(1.0)/time_type(2.0);
00643
00644
00645
            a21 = time_type(1.0)/time_type(4.0);
00646
00647
            a31 = time_type(3.0)/time_type(32.0);
00648
            a32 = time_type(9.0)/time_type(32.0);
00649
00650
            a41 = time_type(1932.0)/time_type(2197.0);
             a42 = time_type(-7200.0)/time_type(2197.0);
00652
            a43 = time_type(7296.0)/time_type(2197.0);
00653
00654
             a51 = time_type(439.0)/time_type(216.0);
            a52 = time_type(-8.0);
a53 = time_type(3680.0)/time_type(513.0);
00655
00656
00657
            a54 = time_type(-845.0)/time_type(4104.0);
00658
00659
             a61 = time_type(-8.0)/time_type(27.0);
00660
            a62 = time\_type(2.0);
             a63 = time_type(-3544.0)/time_type(2565.0);
00661
            a64 = time_type(1859.0)/time_type(4104.0);
00662
            a65 = time_type(-11.0)/time_type(40.0);
00663
00664
00665
            b1 = time_type(25.0)/time_type(216.0);
            b2 = time_type(0.0);
b3 = time_type(1408.0)/time_type(2565.0);
00666
00667
00668
            b4 = time_type(2197.0)/time_type(4104.0);
```

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```
b5 = time_type(-1.0)/time_type(5.0);
00670
00671
             bb1 = time_type(16.0)/time_type(135.0);
             bb2 = time_type(0.0);
bb3 = time_type(6656.0)/time_type(12825.0);
00672
00673
             bb4 = time_type(28561.0)/time_type(56430.0);
bb5 = time_type(-9.0)/time_type(50.0);
00674
00675
00676
             bb6 = time_type(2.0)/time_type(55.0);
00677
00678
             model.initialize(t,u);
00679
             dt = 0.1;
00680
00681
00683
           void set_dt (time_type dt_)
00684
00685
             dt = dt_;
00686
00687
00689
           void set_TOL (time_type TOL_)
00690
00691
             TOL = TOL_;
00692
00693
00695
           void step ()
00696
00697
             steps++;
00698
00699
             // stage 1
00700
             model.f(t,u,k1);
00701
00702
             // stage 2
00703
             w = u;
00704
             w.update(dt*a21,k1);
00705
             model.f(t+c2*dt,w,k2);
00706
00707
             // stage 3
00708
             w = u;
00709
             w.update(dt*a31,k1);
00710
             w.update(dt*a32,k2);
00711
             model.f(t+c3*dt,w,k3);
00712
00713
             // stage 4
00714
             w = u;
00715
             w.update(dt*a41,k1);
00716
             w.update(dt*a42,k2);
00717
             w.update(dt*a43,k3);
00718
             model.f(t+c4*dt,w,k4);
00719
00720
             // stage 5
00721
             w = u;
00722
             w.update(dt*a51,k1);
00723
             w.update(dt*a52,k2);
00724
             w.update(dt*a53,k3);
00725
             w.update(dt*a54,k4);
00726
             model.f(t+c5*dt,w,k5);
00727
00728
             // stage 6
00729
             w = u;
00730
             w.update(dt*a61,k1);
00731
             w.update(dt*a62,k2);
00732
             w.update(dt*a63,k3);
00733
             w.update(dt*a64,k4);
00734
             w.update(dt*a65,k5);
00735
             model.f(t+c6*dt,w,k6);
00736
00737
             // compute order 4 approximation
             w = u;
00738
00739
             w.update(dt*b1,k1);
00740
             w.update(dt*b2,k2);
00741
             w.update(dt*b3,k3);
00742
             w.update(dt*b4,k4);
00743
             w.update(dt*b5,k5);
00744
00745
             // compute order 5 approximation
00746
             ww = u;
00747
             ww.update(dt*bb1,k1);
00748
             ww.update(dt*bb2,k2);
00749
             ww.update(dt*bb3,k3);
00750
             ww.update(dt*bb4,k4);
00751
             ww.update(dt*bb5,k5);
00752
             ww.update(dt*bb6,k6);
00753
00754
             // estimate local error
00755
             w -= ww;
00756
             time_type error(norm(w));
00757
             time_type dt_opt(dt*pow(rho*TOL/error,0.2));
dt_opt = std::min(beta*dt,std::max(alpha*dt,dt_opt));
00758
```

```
//std::cout « "est. error=" « error « " dt_opt=" « dt_opt « std::endl;
00760
00761
             if (error<=TOL)</pre>
00762
              {
                t += dt;
00763
00764
                 u = ww;
00765
                dt = dt_opt;
00766
00767
             else
00768
              {
00769
                 rejected++;
00770
                dt = dt_opt;
00771
                 if (dt>dt_min) step();
00772
00773
          }
00774
00776
           const Vector<number_type>& get_state () const
00777
            return u;
00779
00780
00782
          time_type get_time () const
00783
00784
            return t;
00785
00786
00788
           time_type get_dt () const
00789
00790
            return dt;
00791
00792
00794
           size_type get_order () const
00795
00796
            return 5;
00797
00798
00800
          void get info () const
00802
            std::cout « "RE: steps=" « steps « " rejected=" « rejected « std::endl;
00803
00804
00805
        private:
          const M& model;
00806
00807
           time_type t, dt;
00808
          time_type TOL, rho, alpha, beta, dt_min;
00809
          time_type c2,c3,c4,c5,c6;
          time_type a21,a31,a32,a41,a42,a43,a51,a52,a53,a54,a61,a62,a63,a64,a65;
00810
          time_type b1,b2,b3,b4,b5; // 4th order
time_type bb1,bb2,bb3,bb4,bb5,bb6; // 5th order
00811
00812
          Vector<number_type> u,w,ww;
Vector<number_type> k1,k2,k3,k4,k5,k6;
00813
00814
00815
          mutable size_type steps, rejected;
00816
00817
00818
00824
        template<class M, class S>
00825
        class RE
00826
00827
        public:
00829
          typedef typename M::size_type size_type;
00830
00832
          typedef typename M::time_type time_type;
00833
00835
          typedef typename M::number_type number_type;
00836
00838
          RE (const M& model_, S& solver_)
00839
            : model(model_), solver(solver_), u(model.size()),
00840
               wlow(model.size()), whigh(model.size()), ww(model.size()),
00841
               steps(0), rejected(0)
00842
            model.initialize(t,u); // initialize state
dt = 0.1; // set initial time step
00843
00844
             two_power_m = 1.0;
00845
             for (size_type i=0; i<solver.get_order(); i++)</pre>
00846
               two_power_m *= 2.0;
00847
00848
             TOL = time_type(0.0001);
00849
             rho = time_type(0.8);
            alpha = time_type(0.25);
beta = time_type(4.0);
dt_min = 1E-12;
00850
00851
00852
00853
00854
00856
           void set_dt (time_type dt_)
00857
00858
            dt = dt_;
00859
00860
```

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```
void set_TOL (time_type TOL_)
00863
             TOL = TOL_;
00864
00865
           }
00866
00868
           void step ()
00869
          {
00870
             // count steps done
            steps++;
00871
00872
00873
             // do 1 step with 2*dt
             time_type H(2.0*dt);
00874
00875
             solver.set_state(t,u);
00876
             solver.set_dt(H);
00877
             solver.step();
00878
             wlow = solver.get_state();
00879
00880
             // do 2 steps with dt
00881
             solver.set_state(t,u);
00882
             solver.set_dt(dt);
00883
             solver.step();
00884
             solver.step();
00885
             whigh = solver.get_state();
00886
00887
             // estimate local error
             ww = wlow;
00889
             ww -= whigh;
00890
             \label{time_type} \verb| error(norm(ww) / (pow(H, 1.0 + solver.get_order()) * (1.0 - 1.0 / two_power_m))); \\
             time_type dt_opt(pow(rho*TOL/error,1.0/((time_type)solver.get_order())));
dt_opt = std::min(beta*dt,std::max(alpha*dt,dt_opt));
//std::cout « "est. error=" « error « " dt_opt=" « dt_opt « std::endl;
00891
00892
00893
00894
00895
00896
               {
                 t += H;
00897
                 u = whigh;
00898
00899
                 u *= two_power_m;
00900
                 u -= wlow;
00901
                 u /= two_power_m-1.0;
00902
                 dt = dt_opt;
00903
             else
00904
00905
               {
00906
                 rejected++;
00907
                 dt = dt_opt;
00908
                  if (dt>dt_min) step();
00909
00910
00911
00913
           const Vector<number_type>& get_state () const
00914
00915
00916
00917
00919
           time_type get_time () const
00920
00921
            return t;
00922
00923
00925
           time_type get_dt () const
00926
00927
            return dt;
00928
00929
00931
           size_type get_order () const
00932
00933
            return solver.get_order()+1;
00934
00935
           void get_info () const
00938
            std::cout « "RE: steps=" « steps « " rejected=" « rejected « std::endl;
00939
00940
           }
00941
00942
        private:
00943
          const M& model;
00944
           S& solver;
00945
           time_type t, dt;
00946
           time_type two_power_m;
00947
           Vector<number type> u,wlow,whigh,ww;
00948
          time_type TOL, rho, alpha, beta, dt_min;
00949
          mutable size_type steps, rejected;
00950
00951
00952
00962
        template<class M, class S>
00963
        class IE
```

```
{
00966
          // h_n f(t_n, y_n) - y_n + y_{n-1} = 0
00967
          class NonlinearProblem
00968
          public:
00969
            typedef typename M::size_type size_type;
00971
00972
00974
            typedef typename M::number_type number_type;
00975
            NonlinearProblem (const M& model_, const Vector<number_type>& yold_,
00977
00978
                               typename M::time_type tnew_, typename M::time_type dt_)
00979
              : model(model_), yold(yold_), tnew(tnew_), dt(dt_)
00980
            { }
00981
00983
            std::size_t size () const
00984
00985
              return model.size();
00986
00987
00989
            void F (const Vector<number_type>& x, Vector<number_type>& result) const
00990
00991
              model.f(tnew,x,result);
             result *= dt;
result -= x;
00992
00993
00994
              result += yold;
00995
00996
00998
            void F_x (const Vector<number_type>& x, DenseMatrix<number_type>& result) const
00999
01000
              model.f x(tnew,x,result);
01001
              result *= dt;
01002
              for (size_type i=0; i<model.size(); i++) result[i][i] -= number_type(1.0);</pre>
01003
01004
01005
            void set_tnew_dt (typename M::time_type tnew_, typename M::time_type dt_)
01006
01007
              tnew = tnew ;
              dt = dt_;
01008
01009
01010
01011
          private:
            const M& model:
01012
01013
            const Vector<number_type>& yold;
01014
            typename M::time_type tnew;
01015
            typename M::time_type dt;
01016
01017
        public:
01018
          typedef typename M::size_type size_type;
01020
01021
01023
          typedef typename M::time_type time_type;
01024
01026
          typedef typename M::number_type number_type;
01027
01029
          IE (const M& model_, const S& newton_)
01030
           : verbosity(0), model(model_), newton(newton_), u(model.size()), unew(model.size())
01031
01032
            model.initialize(t,u);
01033
            dt = dtmax = 0.1;
01034
01035
01037
          void set_dt (time_type dt_)
01038
01039
           dt = dtmax = dt_;
01040
01041
01043
          void set_verbosity (size_type verbosity_)
01044
01045
           verbosity = verbosity :
01046
          }
01047
01049
          void step ()
01050
           if (verbosity>=2)
01051
              std::cout « "IE: step" « " t=" « t « " dt=" « dt « std::endl;
01052
01053
            NonlinearProblem nlp(model,u,t+dt,dt);
01054
            bool reduced = false;
01055
            error = false;
            while (1)
01056
01057
              {
01058
                unew = u;
01059
                newton.solve(nlp,unew);
01060
                if (newton.has_converged())
01061
01062
                    u = unew;
01063
                    t += dt;
01064
                    if (!reduced && dt<dtmax-1e-13)
```

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```
01065
                      {
01066
                        dt = std::min(2.0*dt,dtmax);
01067
                        if (verbosity>0)
                          std::cout ""IE: increasing time step to " " dt " std::endl;
01068
01069
01070
                    return:
01071
01072
                else
01073
01074
                    if (dt<1e-12)</pre>
01075
                        HDNUM_ERROR("time step too small in implicit Euler");
01076
01077
                        error = true;
01078
                        break;
01079
01080
                    dt *= 0.5;
01081
                    reduced = true;
01082
                    nlp.set_tnew_dt(t+dt,dt);
                    if (verbosity>0) std::cout « "IE: reducing time step to " « dt « std::endl;
01083
01084
                  }
01085
01086
          }
01087
01089
          bool get_error () const
01090
01091
           return error;
01092
01093
01095
          void set_state (time_type t_, const Vector<number_type>& u_)
01096
          {
01097
           t = t:
01098
           u = u_;
01099
01100
01102
          const Vector<number_type>& get_state () const
01103
01104
           return u;
01105
01106
01108
          time_type get_time () const
01109
01110
           return t;
01111
01112
01114
          time_type get_dt () const
01115
01116
           return dt;
01117
01118
01120
          size_type get_order () const
01121
         {
01122
           return 1;
01123
01124
01126
          void get_info () const
01127
01128
01129
01130
       private:
01131
         size_type verbosity;
01132
         const M& model;
01133
         const $& newton;
01134
         time_type t, dt, dtmax;
01135
         number_type reduction;
01136
          size_type linesearchsteps;
01137
         Vector<number_type> u;
         Vector<number_type> unew;
01138
01139
         mutable bool error;
01140
01141
01152
        template<class M, class S>
01153
       class DIRK
01154
       public:
01155
01156
01158
         typedef typename M::size_type size_type;
01159
01161
         typedef typename M::time_type time_type;
01162
         typedef typename M::number_type number_type;
01164
01165
01167
         typedef DenseMatrix<number_type> ButcherTableau;
01168
        private:
01169
01170
          static ButcherTableau initTableau(const std::string method)
01173
01174
```

```
if(method.find("Implicit Euler") != std::string::npos){
01176
               ButcherTableau butcher(2,2,0.0);
               butcher[1][1] = 1;
butcher[0][1] = 1;
01177
01178
               butcher[0][0] = 1;
01179
01180
01181
               return butcher;
01182
01183
             else if (method.find("Alexander") != std::string::npos) {
01184
               ButcherTableau butcher(3,3,0.0);
               const number_type alpha = 1. - sqrt(2.)/2.;
butcher[0][0] = alpha;
01185
01186
               butcher[0][1] = alpha;
01187
01188
01189
               butcher[1][0] = 1.;
               butcher[1][1] = 1. - alpha;
butcher[1][2] = alpha;
01190
01191
01192
01193
               butcher[2][1] = 1. - alpha;
               butcher[2][2] = alpha;
01194
01195
01196
               return butcher;
01197
             else if(method.find("Crouzieux") != std::string::npos){
01198
01199
               ButcherTableau butcher(3,3,0.0);
               const number_type beta = 1./2./sqrt(3);
butcher[0][0] = 0.5 + beta;
01200
01201
01202
               butcher[0][1] = 0.5 + beta;
01203
               butcher[1][0] = 0.5 - beta;
01204
01205
               butcher[1][1] = -1. / sqrt(3);
01206
               butcher[1][2] = 0.5 + beta;
01207
01208
               butcher[2][1] = 0.5;
               butcher[2][2] = 0.5;
01209
01210
01211
               return butcher;
01212
01213
             else if (method.find("Midpoint Rule") != std::string::npos) {
01214
               ButcherTableau butcher(2,2,0.0);
               butcher[0][0] = 0.5;
butcher[0][1] = 0.5;
01215
01216
               butcher[1][1] = 1;
01217
01218
01219
               return butcher;
01220
01221
             else if(method.find("Fractional Step Theta") != std::string::npos){
01222
               ButcherTableau butcher(5,5,0.0);
               const number_type theta = 1 - sqrt(2.)/2.;
const number_type alpha = 2. - sqrt(2.);
01223
01224
01225
               const number_type beta = 1. - alpha;
               butcher[1][0] = theta;
butcher[1][1] = beta * theta;
01226
01227
01228
               butcher[1][2] = alpha * theta;
01229
               butcher[2][0] = 1.-theta;
01230
               butcher[2][1] = beta * theta;
01231
               butcher[2][2] = alpha * (1.-theta);
butcher[2][3] = alpha * theta;
01232
01233
01234
               butcher[3][0] = 1.;
01235
               butcher[3][1] = beta * theta;
01236
               butcher[3][2] = alpha * (1.-theta);
butcher[3][3] = (alpha + beta) * theta;
01237
01238
               butcher[3][4] = alpha * theta;
01239
01240
01241
               butcher[4][1] = beta * theta;
               butcher[4][2] = alpha * (1.-theta);
01242
               butcher[4][3] = (alpha + beta) * theta;
01243
               butcher[4][4] = alpha * theta;
01244
01245
01246
               return butcher;
01247
             else
01248
01249
               HDNUM_ERROR("Order not available for Runge Kutta solver.");
01250
01251
01252
01253
           static int initOrder(const std::string method)
01254
01255
             if (method.find("Implicit Euler") != std::string::npos) {
01256
               return 1;
01257
01258
             else if (method.find("Alexander") != std::string::npos) {
01259
              return 2;
01260
01261
             else if(method.find("Crouzieux") != std::string::npos){
```

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```
01262
              return 3;
01263
01264
            else if (method.find("Midpoint Rule") != std::string::npos) {
01265
              return 2;
01266
            else if (method.find("Fractional Step Theta") != std::string::npos) {
01267
01268
              return 2;
01269
01270
            else{
01271
              HDNUM_ERROR("Order not available for Runge Kutta solver.");
01272
01273
01274
01275
01277
          // h_n f(t_n, y_n) - y_n + y_{n-1} = 0
01278
          {\tt class\ Nonlinear Problem}
01279
01280
          public:
01282
            typedef typename M::size_type size_type;
01283
01285
            typedef typename M::number_type number_type;
01286
01288
            NonlinearProblem (const M& model_, const Vector<number_type>& yold_,
                               typename M::time_type told_, typename M::time_type dt_,
const ButcherTableau & butcher_, const int rk_step_,
01289
01290
01291
                               const std::vector< Vector<number_type> > & k_)
01292
              : model(model_), yold(yold_), told(told_),
01293
                dt(dt_), butcher(butcher_), rk_step(rk_step_), k_old(model.size(),0)
01294
01295
              for(int i=0; i<rk_step; ++i)</pre>
01296
                k_old.update(butcher[rk_step][1+i] * dt, k_[i]);
01297
01298
01300
            std::size_t size () const
01301
01302
              return model.size();
01303
01304
01306
            void F (const Vector<number_type>& x, Vector<number_type>& result) const
01307
01308
              result = k_old;
01309
01310
              Vector<number type> current z(x);
01311
              current_z.update(1.,yold);
01312
01313
              const number_type tnew = told + butcher[rk_step][0] * dt;
01314
01315
              Vector<number_type> current_k (model.size(),0.);
01316
              model.f(tnew,current_z,current_k);
01317
              result.update(butcher[rk_step][rk_step+1] * dt, current_k);
01318
01319
              result.update(-1.,x);
01320
01321
01323
            void F_x (const Vector<number_type>& x, DenseMatrix<number_type>& result) const
01324
01325
              const number_type tnew = told + butcher[rk_step][0] * dt;
01326
01327
              Vector<number_type> current_z(x);
01328
              current_z.update(1.,yold);
01329
01330
              model.f x(tnew,current z,result);
01331
01332
              result *= dt * butcher[rk_step][rk_step+1];
01333
01334
              for (size_type i=0; i<model.size(); i++) result[i][i] -= number_type(1.0);</pre>
01335
01336
01337
            void set told dt (typename M::time type told , typename M::time type dt )
01338
01339
              told = told_;
01340
              dt = dt_;
01341
            }
01342
01343
          private:
            const M& model;
01344
01345
            const Vector<number_type>& yold;
01346
            typename M::time_type told;
01347
            typename M::time_type dt;
01348
            const ButcherTableau & butcher;
            const int rk_step;
01349
01350
            Vector<number_type> k_old;
01351
          };
01352
        public:
01353
01354
01357
          DIRK (const M& model , const S& newton , const ButcherTableau & butcher , const int order )
```

```
: verbosity(0), butcher(butcher_), model(model_), newton(newton_),
01359
              u(model.size()), order(order_)
01360
01361
           model.initialize(t,u);
01362
            dt = dtmax = 0.1;
01363
01364
01367
          DIRK (const M& model_, const S& newton_, const std::string method)
01368
          : verbosity(0), butcher(initTableau(method)), model(model_), newton(newton_), u(model.size()),
01369
              order(initOrder(method))
01370
01371
           model.initialize(t.u);
01372
           dt = dtmax = 0.1;
01373
01374
01375
          void set_dt (time_type dt_)
01377
01378
01379
           dt = dtmax = dt_;
01380
01381
01383
          void set_verbosity (size_type verbosity_)
01384
01385
           verbosity = verbosity ;
01386
01387
01389
          void step ()
01390
01391
01392
            const size_type R = butcher.colsize()-1;
01393
01394
           bool reduced = false;
01395
            error = false;
01396
            if (verbosity>=2)
              std::cout « "DIRK: step to" « " t+dt=" « t+dt « " dt=" « dt « std::endl;
01397
01398
01399
            while (1)
01400
01401
                bool converged = true;
01402
01403
                // Perform R Runge-Kutta steps
                std::vector< Vector<number_type> > k;
01404
01405
                for(size type i=0; i<R; ++i) {</pre>
01406
                  if (verbosity>=2)
01407
                    std::cout « "DIRK: step nr "« i « std::endl;
01408
01409
                  Vector<number_type> current_z (model.size(),0.0);
01410
                  // Set starting value of k_i
01411
01412
                  // model.f(t,u,current_k);
01413
01414
                  // Solve nonlinear problem
01415
                  NonlinearProblem nlp(model,u,t,dt,butcher,i,k);
01416
01417
                  newton.solve(nlp,current_z);
01418
01419
                  converged = converged && newton.has_converged();
01420
                  if(!converged)
01421
                    break;
01422
                  current_z.update(1., u);
const number_type t_i = t + butcher[i][0] * dt;
01423
01424
01425
                  Vector<number_type>current_k (model.size(),0.);
01426
                  model.f(t_i,current_z,current_k);
01427
01428
                  k.push_back( current_k );
01429
                }
01430
01431
                if (converged)
01432
                  {
01433
                    if(verbosity >= 2)
                       std::cout « "DIRK finished"« std::endl;
01434
01435
                    // Update to new solution
01436
                    for(size_type i=0; i<R; ++i)</pre>
01437
01438
                      u.update(dt*butcher[R][1+i],k[i]);
01439
01440
                    t += dt;
01441
                    if (!reduced && dt<dtmax-1e-13)
01442
                      {
                        dt = std::min(2.0*dt,dtmax);
01443
01444
                         if (verbosity>0)
01445
                          std::cout « "DIRK: increasing time step to " « dt « std::endl;
01446
01447
                    return;
01448
01449
                else
```

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```
01451
                    if (dt<1e-12)</pre>
01452
                        HDNUM_ERROR("time step too small in implicit Euler");
01453
01454
                        error = true;
01455
                        break:
01456
01457
                    dt *= 0.5;
01458
                    reduced = true;
01459
                    if (verbosity>0) std::cout « "DIRK: reducing time step to " « dt « std::endl;
                  }
01460
01461
             }
01462
         }
01463
01465
          bool get_error () const
01466
01467
           return error:
01468
01469
01471
          void set_state (time_type t_, const Vector<number_type>& u_)
01472
          {
           t = t_;
01473
01474
           u = u_{-};
01475
01476
01478
          const Vector<number_type>& get_state () const
01479
01480
           return u;
01481
01482
01484
          time_type get_time () const
01485
01486
           return t;
01487
01488
01490
          time_type get_dt () const
01491
          {
01492
           return dt;
01493
01494
01496
          size_type get_order () const
01497
01498
           return order;
01499
01500
01502
          void get_info () const
01503
01504
01505
01506
        private:
01507
         size_type verbosity;
01508
         const DenseMatrix<number_type> butcher;
01509
          const M& model;
01510
         const S& newton;
         time_type t, dt, dtmax;
01511
01512
         number_type reduction;
01513
          size_type linesearchsteps;
          Vector<number_type> u;
01514
01515
         int order;
01516
          mutable bool error;
01517
01518
01520
        template<class T, class N>
       inline void gnuplot (const std::string& fname, const std::vector<T> t, const std::vector<Vector<N> >
01521
01522
01523
         std::fstream f(fname.c_str(),std::ios::out);
01524
          for (typename std::vector<T>::size_type n=0; n<t.size(); n++)</pre>
01525
              f « std::scientific « std::showpoint
01527
                « std::setprecision(16) « t[n];
              for (typename Vector<N>::size_type i=0; i<u[n].size(); i++)
   f « " " « std::scientific « std::showpoint</pre>
01528
01529
                 01530
01531
              f « std::endl;
01532
01533
         f.close();
01534
01535
       template<class T, class N>
01537
       inline void gnuplot (const std::string& fname, const std::vector<T> t, const std::vector<Vector<N> >
01538
     u, const std::vector<T> dt)
01539
01540
          std::fstream f(fname.c_str(),std::ios::out);
01541
          for (typename std::vector<T>::size_type n=0; n<t.size(); n++)</pre>
01542
01543
              f « std::scientific « std::showpoint
```

```
« std::setprecision(16) « t[n];
             for (typename Vector<N>::size_type i=0; i<u[n].size(); i++)
    f « " " « std::scientific « std::showpoint</pre>
01546
             01547
01548
01549
01550
             f « std::endl;
01551
01552
        f.close();
01553 }
01554
01555 } // namespace hdnum
01556
01557 #endif
```

5.10 src/opcounter.hh File Reference

This file implements an operator counting class.

```
#include <type_traits>
#include <iostream>
#include <cmath>
#include <cstdlib>
```

Classes

- class hdnum::oc::OpCounter< F >
- struct hdnum::oc::OpCounter< F >::Counters

Struct storing the number of operations.

Functions

```
• template<typename F >
 OpCounter< F > hdnum::oc::operator- (const OpCounter< F > &a)

    template<typename F >

 OpCounter< F > hdnum::oc::operator+ (const OpCounter< F > &a, const OpCounter< F > &b)
template<typename F >
 OpCounter< F > hdnum::oc::operator+ (const OpCounter<math>< F > &a, const F &b)
• template<typename F >
 OpCounter< F > hdnum::oc::operator+ (const F &a, const OpCounter< F > &b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator+ (const
 OpCounter< F > &a, const T &b)
• template<typename F, typename T >
 std::enable if < std::is arithmetic < T >::value, OpCounter < F > >::type hdnum::oc::operator+ (const T
 &a, const OpCounter< F > \&b)
template<typename F >
 OpCounter< F > & hdnum::oc::operator+= (OpCounter<math>< F > &a, const OpCounter< F > &b)
• template<typename F >
 OpCounter< F > & hdnum::oc::operator += (OpCounter < F > &a, const F &b)
• template<typename F, typename T>
 std::enable if < std::is arithmetic < T >::value, OpCounter < F > & >::type hdnum::oc::operator+=
 (OpCounter< F > &a, const T &b)
• template<typename F >
 OpCounter< F > hdnum::oc::operator- (const OpCounter<math>< F > &a, const OpCounter< F > &b)
```

```
template<typename F >
 OpCounter< F > hdnum::oc::operator- (const OpCounter< F > &a, const F &b)
• template<typename F >
 OpCounter< F > hdnum::oc::operator- (const F &a, const OpCounter<math>< F > \&b)
• template<typename F, typename T >
 std::enable if < std::is arithmetic < T >::value, OpCounter < F > >::type hdnum::oc::operator (const
 OpCounter< F > &a, const T &b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator- (const T
 &a, const OpCounter< F > \&b)
• template<typename F >
 OpCounter< F > & hdnum::oc::operator= (OpCounter < F > &a, const OpCounter < F > &b)

    template<typename F >

 OpCounter< F > & hdnum::oc::operator= (OpCounter<math>< F > &a, const F &b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > & >::type hdnum::oc::operator-=
 (OpCounter< F > &a, const T &b)
• template<typename F >
 OpCounter < F > hdnum::oc::operator* (const OpCounter < F > &a, const OpCounter < F > &b)
• template<typename F >
 OpCounter< F > hdnum::oc::operator* (const OpCounter< F > &a, const F &b)

    template<typename F >

 OpCounter< F > hdnum::oc::operator* (const F &a, const OpCounter<math>< F > \&b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator* (const
 OpCounter< F > &a, const T &b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator* (const T
 &a, const OpCounter< F > \&b)

    template<typename F >

 OpCounter< F > & hdnum::oc::operator *= (OpCounter < F > &a, const OpCounter < F > &b)

    template<typename F >

 OpCounter< F > & hdnum::oc::operator*= (OpCounter<math>< F > &a, const F &b)
• template<typename F, typename T>
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > & >::type hdnum::oc::operator*=
 (OpCounter< F > &a, const T &b)

    template<typename F >

 OpCounter< F > hdnum::oc::operator/ (const OpCounter<math>< F > &a, const OpCounter< F > &b)
 OpCounter< F > hdnum::oc::operator/ (const OpCounter< F > &a, const F &b)

    template<typename F >

  OpCounter< F > hdnum::oc::operator/ (const F &a, const OpCounter<math>< F > \&b)
• template<typename F, typename T>
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator/ (const
 OpCounter< F > &a, const T &b)
• template<typename F , typename T >
 std::enable_if< std::is_arithmetic< T >::value, OpCounter< F > >::type hdnum::oc::operator/ (const T
 &a, const OpCounter< F > &b)
• template<typename F >
 OpCounter< F > & hdnum::oc::operator/= (OpCounter<math>< F > &a, const OpCounter< F > &b)
• template<typename F >
  OpCounter< F > & hdnum::oc::operator/= (OpCounter<math>< F > &a, const F &b)
• template<typename F , typename T >
 std::enable if < std::is arithmetic < T >::value, OpCounter < F > & >::type hdnum::oc::operator/=
 (OpCounter< F > &a, const T &b)
• template<typename F >
 bool hdnum::oc::operator< (const OpCounter< F > &a, const OpCounter< F > &b)
```

```
template<typename F >
  bool hdnum::oc::operator< (const OpCounter< F > &a, const F &b)
• template<typename F >
  bool hdnum::oc::operator< (const F &a, const OpCounter< F > &b)
• template<typename F , typename T >
  bool hdnum::oc::operator< (const OpCounter< F > &a, const T &b)
 \bullet \ \ \text{template} \! < \! \text{typename F , typename T} > 
  bool hdnum::oc::operator< (const T &a, const OpCounter< F > &b)
• template<typename F >
  bool hdnum::oc::operator< (const OpCounter< F > &a, const OpCounter< F > &b)

    template<typename F >

  bool hdnum::oc::operator<= (const OpCounter< F > &a, const F &b)
template<typename F >
  bool hdnum::oc::operator<= (const F &a, const OpCounter< F > &b)

    template<typename F, typename T >

  bool hdnum::oc::operator<= (const OpCounter< F > &a, const T &b)
• template<typename F, typename T>
  bool hdnum::oc::operator<= (const T &a, const OpCounter< F > &b)

    template<typename F >

  bool hdnum::oc::operator> (const OpCounter< F > &a, const OpCounter< F > &b)
• template<typename F >
  bool hdnum::oc::operator> (const OpCounter< F > &a, const F &b)
• template<typename F >
  bool hdnum::oc::operator> (const F &a, const OpCounter< F > &b)
• template<typename F , typename T >
  bool hdnum::oc::operator> (const OpCounter< F > &a, const T &b)

    template < typename F , typename T >

  bool hdnum::oc::operator> (const T &a, const OpCounter< F > &b)
template<typename F >
  bool hdnum::oc::operator>= (const OpCounter< F > &a, const OpCounter< F > &b)

    template<typename F >

  bool hdnum::oc::operator>= (const OpCounter< F > &a, const F &b)
• template<typename F >
  bool hdnum::oc::operator>= (const F &a, const OpCounter< F > &b)
• template<typename F, typename T>
  bool hdnum::oc::operator>= (const OpCounter< F > &a, const T &b)

    template<typename F , typename T >

  bool hdnum::oc::operator>= (const T &a, const OpCounter< F > &b)
• template<typename F >
  bool hdnum::oc::operator!= (const OpCounter< F > &a, const OpCounter< F > &b)

    template<typename F >

  bool hdnum::oc::operator!= (const OpCounter< F > &a, const F &b)

    template<typename F >

  bool hdnum::oc::operator!= (const F &a, const OpCounter< F > &b)
• template<typename F, typename T>
  bool hdnum::oc::operator!= (const OpCounter< F > &a, const T &b)

    template<typename F , typename T >

  bool hdnum::oc::operator!= (const T &a, const OpCounter< F > &b)
template<typename F >
  bool hdnum::oc::operator== (const OpCounter< F > &a, const OpCounter< F > &b)
• template<typename F >
  bool hdnum::oc::operator== (const OpCounter< F > &a, const F &b)
\bullet \;\; template {<} typename \; F >
  bool hdnum::oc::operator== (const F &a, const OpCounter< F > &b)
• template<typename F, typename T>
  bool hdnum::oc::operator== (const OpCounter< F > &a, const T &b)
```

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```
• template<typename F , typename T >
 bool hdnum::oc::operator== (const T &a, const OpCounter< F > &b)
• template<typename F >
 OpCounter< F > hdnum::oc::exp (const OpCounter<math>< F > &a)
template<typename F >
 OpCounter< F > hdnum::oc::pow (const OpCounter< F > &a, const OpCounter< F > &b)
• template<typename F >
 OpCounter< F > hdnum::oc::pow (const OpCounter< F > &a, const F &b)
• template<typename F , typename T >
 OpCounter< F > hdnum::oc::pow (const OpCounter<math>< F > &a, const T &b)
• template<typename F >
 OpCounter< F > hdnum::oc::pow (const F &a, const OpCounter<math>< F > \&b)
• template<typename F , typename T >
 OpCounter< F > hdnum::oc::pow (const T &a, const OpCounter<math>< F > \&b)
• template<typename F >
 OpCounter< F > hdnum::oc::sin (const OpCounter< F > &a)
template<typename F >
 OpCounter< F > hdnum::oc::cos (const OpCounter<math>< F > &a)
• template<typename F >
 OpCounter< F > hdnum::oc::sqrt (const OpCounter< F > &a)
template<typename F >
 OpCounter< F > hdnum::oc::abs (const OpCounter<math>< F > &a)
```

5.10.1 Detailed Description

This file implements an operator counting class.

5.11 opcounter.hh

```
Go to the documentation of this file.
```

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*-
00002 #ifndef __OPCOUNTER_
00003 #define __OPCOUNTER_
00004
00005 #include <type_traits>
00006 #include <iostream>
00007 #include <cmath>
00008 #include <cstdlib>
00009
00014 namespace hdnum {
00015
       namespace oc {
00016
        template<typename F>
00017
          class OpCounter;
00018
00019 }
00021 namespace hdnum {
00022
        namespace oc {
00028
          template<typename F>
00029
          class OpCounter
00030
00031
00032
          public:
00033
00034
            using size_type = std::size_t;
00035
00036
            using value_type = F;
00037
00038
             OpCounter()
            : _v()
{}
00039
00040
00041
00042
            template<tvpename T>
            OpCounter(const T& t, typename std::enable_if<std::is_same<T,int>::value and
00043
      !std::is_same<F,int>::value>::type* = nullptr)
```

```
00044
              : _v(t)
00045
            { }
00046
00047
            OpCounter(const F& f)
            : _v(f)
00048
00049
00050
00051
            OpCounter(F&& f)
            : _v(f)
00052
00053
00054
            explicit OpCounter(const char* s)
00055
              : _v(strtod(s,nullptr))
00056
00057
00058
00059
            OpCounter& operator=(const char* s)
00060
00061
              _v = strtod(s,nullptr);
00062
              return *this;
00063
00064
00065
            explicit operator F() const
00066
00067
              return _v;
00068
00069
00070
            OpCounter& operator=(const F& f)
00071
              _v = f;
00072
              return *this;
00073
00074
00075
00076
            OpCounter& operator=(F&& f)
00077
00078
              _v = f;
              return *this;
00079
00080
00081
00082
            friend std::ostream& operator«(std::ostream& os, const OpCounter& f)
00083
              os « "OC(" « f._v « ")";
00084
              return os;
00085
00086
00087
00088
            friend std::istringstream& operator>(std::istringstream& iss, OpCounter& f)
00089
00090
              iss » f._v;
00091
              return iss;
00092
00093
00094
            F* data()
00095
00096
              return &_v;
00097
00098
00099
            const F* data() const
00100
00101
              return &_v;
00102
00103
00104
            F _v;
00105
00107
            struct Counters {
00108
00109
              size_type addition_count;
00110
              size_type multiplication_count;
00111
              size_type division_count;
00112
              size_type exp_count;
00113
              size_type pow_count;
00114
              size_type sin_count;
00115
              size_type sqrt_count;
00116
              size_type comparison_count;
00117
00118
              Counters()
               : addition_count(0)
00119
00120
                , multiplication_count(0)
00121
                , division_count(0)
00122
               , exp_count(0)
00123
                , pow_count(0)
00124
                , sin_count(0)
00125
                , sqrt_count(0)
00126
                 , comparison_count(0)
00127
              { }
00128
00129
              void reset()
00130
00131
                addition_count = 0;
```

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```
multiplication_count = 0;
00133
                 division_count = 0;
00134
                 exp_count = 0;
00135
                 pow_count = 0;
                 sin_count = 0;
00136
                 sqrt_count = 0;
00137
00138
                 comparison_count = 0;
00139
00140
00142
              template<typename Stream>
00143
              void reportOperations(Stream& os, bool doReset = false)
00144
              {
00145
                 os « "additions: " « addition_count « std::endl
00146
                    « "multiplications: " « multiplication_count « std::endl
00147
                    « "divisions: " « division_count « std::endl
                    « "exp: " « exp_count « std::endl
« "pow: " « pow_count « std::endl
00148
00149
                    « "sin: " « sin_count « std::endl
00150
                    « "sqrt: " « sqrt_count « std::endl
00151
00152
                    « "comparisons: " « comparison_count « std::endl
                    « std::endl
« "total: " « addition_count + multiplication_count + division_count + exp_count +
00153
00154
     pow_count + sin_count + sqrt_count + comparison_count « std::endl;
00155
00156
                if (doReset)
00157
                  reset();
00158
00159
00161
              size_type totalOperationCount(bool doReset=false)
00162
00163
                if (doReset)
00164
                  reset();
00165
00166
                 return addition_count + multiplication_count + division_count + exp_count + pow_count +
      sin_count + sqrt_count + comparison_count;
00167
00168
00169
              Counters& operator+=(const Counters& rhs)
00170
00171
                 addition_count += rhs.addition_count;
00172
                 multiplication_count += rhs.multiplication_count;
                 division_count += rhs.division_count;
00173
00174
                 exp count += rhs.exp count;
                pow_count += rhs.pow_count;
00175
00176
                sin_count += rhs.sin_count;
                 sqrt_count += rhs.sqrt_count;
00177
00178
                 comparison_count += rhs.comparison_count;
00179
                 return *this;
              }
00180
00181
00182
              Counters operator-(const Counters& rhs)
00183
00184
00185
                 r.addition_count = addition_count - rhs.addition_count;
                 r.multiplication_count = multiplication_count - rhs.multiplication_count;
00186
                r.division_count = division_count - rhs.division_count;
00187
                r.exp_count = exp_count - rhs.exp_count;
r.pow_count = pow_count - rhs.pow_count;
00189
                 r.sin_count = sin_count - rhs.sin_count;
00190
00191
                 r.sqrt_count = sqrt_count - rhs.sqrt_count;
                 r.comparison_count = comparison_count - rhs.comparison_count;
00192
00193
                 return r;
00194
00195
00196
             };
00197
00198
             static void additions(std::size_t n)
00199
00200
              counters.addition count += n;
00201
00202
00203
             static void multiplications(std::size_t n)
00204
00205
              counters.multiplication_count += n;
00206
00207
00208
             static void divisions(std::size_t n)
00209
00210
              counters.division_count += n;
00211
00212
00213
             static void reset()
00214
00215
              counters.reset();
00216
00217
00219
            template<tvpename Stream>
```

```
static void reportOperations(Stream& os, bool doReset = false)
00221
00222
              counters.reportOperations(os, doReset);
00223
00224
00226
            static size type totalOperationCount(bool doReset=false)
00227
00228
              return counters.totalOperationCount(doReset);
00229
00230
00231
           static Counters counters:
00232
00233
          };
00234
00235
          template<typename F>
00236
          typename OpCounter<F>::Counters OpCounter<F>::counters;
00237
00238
          00239
          // negation
00240
00241
00242
          template<typename F>
00243
          OpCounter<F> operator-(const OpCounter<F>& a)
00244
00245
            ++OpCounter<F>::counters.addition_count;
00246
           return {-a._v};
00247
00248
00249
00250
          // ***********************
00251
          // addition
00252
00253
          template<typename F>
00254
00255
          OpCounter<F> operator+(const OpCounter<F>& a, const OpCounter<F>& b)
00256
00257
            ++OpCounter<F>::counters.addition count;
00258
           return {a._v + b._v};
00259
00260
00261
          template<typename F>
00262
          OpCounter<F> operator+(const OpCounter<F>& a, const F& b)
00263
00264
            ++OpCounter<F>::counters.addition_count;
00265
           return {a._v + b};
00266
00267
00268
          template<typename F>
          \label{eq:const_factor} \mbox{OpCounter} < \mbox{F} > \mbox{ operator} + (\mbox{const F\& a, const OpCounter} < \mbox{F} > \& b)
00269
00270
00271
            ++OpCounter<F>::counters.addition_count;
00272
           return {a + b._v};
00273
00274
00275
          template<typename F, typename T>
00276
         typename std::enable_if<
00277
           std::is_arithmetic<T>::value,
00278
            OpCounter<F>
00279
           >::type
00280
          operator+(const OpCounter<F>& a, const T& b)
00281
00282
            ++OpCounter<F>::counters.addition count;
00283
           return {a._v + b};
00284
00285
00286
          template<typename F, typename T>
00287
          typename std::enable_if<</pre>
00288
            std::is arithmetic<T>::value,
00289
           OpCounter<F>
00290
            >::type
00291
          operator+(const T& a, const OpCounter<F>& b)
00292
00293
            ++OpCounter<F>::counters.addition_count;
00294
           return {a + b._v};
00295
00296
00297
          template<typename F>
00298
          OpCounter<F>& operator+=(OpCounter<F>& a, const OpCounter<F>& b)
00299
00300
            ++OpCounter<F>::counters.addition count:
00301
           a._v += b._v;
00302
           return a;
00303
00304
00305
          template<typename F>
          OpCounter<F>& operator+=(OpCounter<F>& a, const F& b)
00306
00307
```

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```
00308
             ++OpCounter<F>::counters.addition_count;
00309
00310
             return a;
00311
          }
00312
           template<typename F, typename T>
00313
          typename std::enable_if<
00314
00315
             std::is_arithmetic<T>::value,
00316
             OpCounter<F>&
00317
            >::type
00318
           operator+=(OpCounter<F>& a, const T& b)
00319
00320
             ++OpCounter<F>::counters.addition count;
00321
00322
             return a;
00323
00324
00325
00326
           // subtraction
00327
00328
00329
           template<typename F>
00330
           \label{localization} \mbox{OpCounter}\mbox{<} \mbox{F}>\& \mbox{ a, const OpCounter}\mbox{<} \mbox{F}>\& \mbox{ b)}
00331
00332
             ++OpCounter<F>::counters.addition_count;
00333
             return {a._v - b._v};
00334
00335
00336
           template<typename F>
00337
           OpCounter<F> operator-(const OpCounter<F>& a, const F& b)
00338
00339
             ++OpCounter<F>::counters.addition_count;
00340
             return {a._v - b};
00341
00342
00343
           template<typename F>
00344
           OpCounter<F> operator-(const F& a, const OpCounter<F>& b)
00345
00346
             ++OpCounter<F>::counters.addition_count;
00347
             return {a - b._v};
00348
00349
00350
           template<typename F, typename T>
00351
          typename std::enable_if<
00352
             std::is_arithmetic<T>::value,
00353
             OpCounter<F>
00354
            >::type
00355
           operator-(const OpCounter<F>& a, const T& b)
00356
00357
             ++OpCounter<F>::counters.addition count;
00358
             return {a._v - b};
00359
00360
00361
           template<typename F, typename T>
00362
           typename std::enable_if<</pre>
00363
             std::is arithmetic<T>::value,
00364
             OpCounter<F>
00365
             >::type
00366
           operator-(const T& a, const OpCounter<F>& b)
00367
00368
             ++OpCounter<F>::counters.addition count;
00369
             return {a - b._v};
00370
00371
00372
           template<typename F>
00373
           \label{local_prop} \mbox{OpCounter} < \mbox{F} > \& \mbox{ operator} -= (\mbox{OpCounter} < \mbox{F} > \& \mbox{ a, const OpCounter} < \mbox{F} > \& \mbox{ b)}
00374
00375
             ++OpCounter<F>::counters.addition_count;
00376
             a._v -= b._v;
00377
             return a;
00378
00379
00380
           template<typename F>
           OpCounter<F>& operator-=(OpCounter<F>& a, const F& b)
00381
00382
00383
             ++OpCounter<F>::counters.addition_count;
00384
             a._v -= b;
00385
             return a;
00386
00387
00388
           template<typename F, typename T>
00389
           typename std::enable_if<
00390
             std::is_arithmetic<T>::value,
             OpCounter<F>&
00391
00392
             >::type
           operator -= (OpCounter <F >& a, const T& b)
00393
00394
```

```
00395
           ++OpCounter<F>::counters.addition_count;
00396
00397
           return a;
00398
         }
00399
00400
00401
                                 *****************
00402
         // multiplication
00403
                             00404
00405
         template<typename F>
00406
         OpCounter<F> operator*(const OpCounter<F>& a, const OpCounter<F>& b)
00407
00408
           ++OpCounter<F>::counters.multiplication_count;
00409
           return {a._v * b._v};
00410
00411
00412
         template<typename F>
00413
         OpCounter<F> operator*(const OpCounter<F>& a, const F& b)
00414
00415
           ++OpCounter<F>::counters.multiplication_count;
00416
           return {a._v * b};
00417
         }
00418
00419
         template<typename F>
00420
         OpCounter<F> operator*(const F& a, const OpCounter<F>& b)
00421
00422
           ++OpCounter<F>::counters.multiplication_count;
00423
           return {a * b._v};
00424
00425
00426
         template<typename F, typename T>
00427
         typename std::enable_if<
00428
           std::is_arithmetic<T>::value,
00429
           OpCounter<F>
00430
           >::type
00431
         operator* (const OpCounter<F>& a, const T& b)
00432
00433
           ++OpCounter<F>::counters.multiplication_count;
00434
           return {a._v * b};
00435
00436
         template<typename F, typename T>
00437
         typename std::enable_if<
00438
00439
           std::is_arithmetic<T>::value,
00440
           OpCounter<F>
00441
           >::type
00442
         operator*(const T& a, const OpCounter<F>& b)
00443
00444
           ++OpCounter<F>::counters.multiplication count;
00445
           return {a * b._v};
00446
00447
00448
         template<typename F>
00449
         OpCounter<F>& operator *= (OpCounter<F>& a, const OpCounter<F>& b)
00450
00451
           ++OpCounter<F>::counters.multiplication_count;
00452
           a._v *= b._v;
00453
           return a;
00454
00455
00456
         template<typename F>
00457
         OpCounter<F>& operator *= (OpCounter<F>& a, const F& b)
00458
00459
           ++OpCounter<F>::counters.multiplication_count;
00460
           a._v *= b;
00461
           return a;
00462
00463
00464
         template<typename F, typename T>
00465
         typename std::enable_if<
00466
           std::is_arithmetic<T>::value,
00467
           OpCounter<F>&
00468
           >::type
00469
         operator *= (OpCounter < F > & a, const T& b)
00470
00471
           ++OpCounter<F>::counters.multiplication_count;
00472
           a._v *= b;
00473
           return a;
00474
         }
00475
00476
00477
                            ****************
00478
         // division
00479
         00480
00481
         template<tvpename F>
```

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```
00482
         OpCounter<F> operator/(const OpCounter<F>& a, const OpCounter<F>& b)
00483
00484
            ++OpCounter<F>::counters.division_count;
00485
           return {a._v / b._v};
00486
00487
00488
          template<typename F>
00489
          OpCounter<F> operator/(const OpCounter<F>& a, const F& b)
00490
00491
            ++OpCounter<F>::counters.division_count;
00492
           return {a._v / b};
00493
00494
00495
         template<typename F>
00496
         OpCounter<F> operator/(const F& a, const OpCounter<F>& b)
00497
00498
            ++OpCounter<F>::counters.division_count;
00499
           return {a / b._v};
00500
00501
00502
         template<typename F, typename T>
00503
         typename std::enable_if<
00504
            std::is_arithmetic<T>::value,
00505
           OpCounter<F>
00506
            >::type
00507
          operator/(const OpCounter<F>& a, const T& b)
00508
00509
            ++OpCounter<F>::counters.division_count;
00510
            return {a._v / b};
00511
00512
00513
         template<typename F, typename T>
00514
         typename std::enable_if<
00515
            std::is_arithmetic<T>::value,
00516
            OpCounter<F>
00517
           >::type
00518
         operator/(const T& a, const OpCounter<F>& b)
00519
00520
            ++OpCounter<F>::counters.division_count;
00521
           return {a / b._v};
00522
00523
00524
         template<tvpename F>
00525
         OpCounter<F>& operator/=(OpCounter<F>& a, const OpCounter<F>& b)
00526
00527
            ++OpCounter<F>::counters.division_count;
00528
            a._v /= b._v;
00529
           return a;
00530
00531
00532
          template<typename F>
00533
          OpCounter<F>& operator/=(OpCounter<F>& a, const F& b)
00534
00535
            ++OpCounter<F>::counters.division_count;
00536
           a._v /= b;
00537
           return a;
00538
00539
00540
         template<typename F, typename T>
00541
         typename std::enable_if<
00542
            std::is arithmetic<T>::value,
00543
            OpCounter<F>&
00544
            >::type
00545
          operator/=(OpCounter<F>& a, const T& b)
00546
00547
            ++OpCounter<F>::counters.division_count;
00548
           a._v /= b;
           return a;
00549
00550
00551
00552
00553
00554
                                             **********
00555
          // comparisons
00556
00557
00558
00559
          // less
00560
          00561
00562
00563
          template<typename F>
00564
         bool operator<(const OpCounter<F>& a, const OpCounter<F>& b)
00565
00566
            ++OpCounter<F>::counters.comparison_count;
00567
           return {a._v < b._v};</pre>
00568
```

```
00569
         template<typename F>
00570
00571
         bool operator<(const OpCounter<F>& a, const F& b)
00572
00573
           ++OpCounter<F>::counters.comparison_count;
00574
           return {a._v < b};</pre>
00575
00576
00577
         template<typename F>
00578
         bool operator<(const F& a, const OpCounter<F>& b)
00579
           ++OpCounter<F>::counters.comparison_count;
00580
00581
           return {a < b._v};</pre>
00582
00583
00584
         template<typename F, typename T> \,
         bool operator<(const OpCounter<F>& a, const T& b)
00585
00586
00587
           ++OpCounter<F>::counters.comparison_count;
00588
           return {a._v < b};</pre>
00589
00590
         template<typename F, typename T> bool operator<(const T& a, const OpCounter<F>& b)
00591
00592
00593
00594
           ++OpCounter<F>::counters.comparison_count;
00595
           return {a < b._v};</pre>
00596
00597
00598
00599
                                 ****************
00600
          // less_or_equals
00601
                              ******
00602
00603
          template<typename F>
         bool operator <= (const OpCounter <F >& a, const OpCounter <F >& b)
00604
00605
00606
           ++OpCounter<F>::counters.comparison_count;
00607
           return {a._v <= b._v};</pre>
00608
00609
00610
         template<typename F>
00611
         bool operator <= (const OpCounter <F >& a, const F& b)
00612
00613
           ++OpCounter<F>::counters.comparison_count;
           return {a._v <= b};</pre>
00614
00615
00616
00617
         template<tvpename F>
00618
         bool operator <= (const F& a, const OpCounter <F>& b)
00619
00620
           ++OpCounter<F>::counters.comparison_count;
00621
           return {a <= b._v};</pre>
00622
         }
00623
         template<typename F, typename T>
00624
00625
         bool operator <= (const OpCounter <F >& a, const T& b)
00626
00627
           ++OpCounter<F>::counters.comparison_count;
00628
           return {a._v <= b};</pre>
00629
00630
          template<typename F, typename T>
00631
00632
         bool operator <= (const T& a, const OpCounter <F > & b)
00633
00634
           ++OpCounter<F>::counters.comparison_count;
00635
           return {a <= b._v};</pre>
00636
00637
00638
00639
          00640
         // greater
          // ****************************
00641
00642
00643
         template<typename F>
00644
         bool operator>(const OpCounter<F>& a, const OpCounter<F>& b)
00645
00646
           ++OpCounter<F>::counters.comparison_count;
00647
           return {a._v > b._v};
00648
00649
00650
          template<typename F>
00651
         bool operator>(const OpCounter<F>& a, const F& b)
00652
00653
           ++OpCounter<F>::counters.comparison_count;
00654
           return {a._v > b};
00655
          }
```

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```
00656
00657
          template<typename F>
00658
          bool operator>(const F& a, const OpCounter<F>& b)
00659
00660
            ++OpCounter<F>::counters.comparison_count;
00661
            return {a > b._v};
00662
00663
00664
          template<typename F, typename T>
00665
          bool operator>(const OpCounter<F>& a, const T& b)
00666
00667
            ++OpCounter<F>::counters.comparison_count;
00668
            return {a._v > b};
00669
00670
          template<typename F, typename T> bool operator>(const T& a, const OpCounter<F>& b)
00671
00672
00673
00674
            ++OpCounter<F>::counters.comparison_count;
00675
            return {a > b._v};
00676
00677
00678
00679
                                                **********
00680
          // greater_or_equals
00681
00682
00683
          template<typename F>
00684
          bool operator>=(const OpCounter<F>& a, const OpCounter<F>& b)
00685
00686
            ++OpCounter<F>::counters.comparison_count;
00687
            return {a._v >= b._v};
00688
00689
00690
          template<typename F>
00691
          bool operator >= (const OpCounter <F >& a, const F& b)
00692
00693
            ++OpCounter<F>::counters.comparison_count;
00694
            return {a._v >= b};
00695
00696
00697
          template<typename F>
00698
          bool operator>=(const F& a, const OpCounter<F>& b)
00699
00700
            ++OpCounter<F>::counters.comparison_count;
00701
            return {a >= b._v};
00702
00703
00704
          template<typename F, typename T>
bool operator>=(const OpCounter<F>& a, const T& b)
00705
00706
00707
            ++OpCounter<F>::counters.comparison_count;
00708
            return {a._v >= b};
00709
00710
00711
          template<typename F, typename T> bool operator>=(const T& a, const OpCounter<F>& b)
00712
00713
00714
            ++OpCounter<F>::counters.comparison_count;
00715
            return {a >= b._v};
00716
00717
00718
00719
00720
          // inequals
00721
          00722
00723
          template<typename F>
00724
          bool operator!=(const OpCounter<F>& a, const OpCounter<F>& b)
00725
00726
            ++OpCounter<F>::counters.comparison_count;
00727
            return {a._v != b._v};
00728
          }
00729
00730
          template<typename F>
00731
          bool operator!=(const OpCounter<F>& a, const F& b)
00732
00733
            ++OpCounter<F>::counters.comparison_count;
00734
            return {a._v != b};
00735
00736
00737
          template<typename F>
00738
          bool operator!=(const F& a, const OpCounter<F>& b)
00739
00740
            ++OpCounter<F>::counters.comparison_count;
00741
            return {a != b._v};
00742
```

```
00743
00744
          template<typename F, typename T>
00745
          bool operator!=(const OpCounter<F>& a, const T& b)
00746
00747
            ++OpCounter<F>::counters.comparison_count;
00748
           return {a._v != b};
00749
00750
00751
          template<typename F, typename T>
00752
          bool operator!=(const T& a, const OpCounter<F>& b)
00753
00754
            ++OpCounter<F>::counters.comparison count;
00755
           return {a != b._v};
00756
00757
00758
00759
          00760
          // equals
00761
                      ******************
00762
          template<typename F>
00763
00764
          bool operator == (const OpCounter <F >& a, const OpCounter <F >& b)
00765
00766
            ++OpCounter<F>::counters.comparison_count;
00767
           return {a._v == b._v};
00768
00769
00770
          template<typename F>
00771
          bool operator == (const OpCounter <F >& a, const F& b)
00772
00773
            ++OpCounter<F>::counters.comparison_count;
00774
           return {a._v == b};
00775
00776
00777
          template<typename F>
00778
          bool operator == (const F& a, const OpCounter < F > & b)
00779
00780
            ++OpCounter<F>::counters.comparison_count;
00781
           return {a == b._v};
00782
00783
00784
         template<typename F, typename T>
bool operator==(const OpCounter<F>& a, const T& b)
00785
00786
00787
            ++OpCounter<F>::counters.comparison_count;
            return {a._v == b};
00788
00789
00790
00791
         template<typename F, typename T>
bool operator==(const T& a, const OpCounter<F>& b)
00792
00793
00794
            ++OpCounter<F>::counters.comparison_count;
00795
            return {a == b._v};
00796
00797
00798
00799
00800
00801
          // functions
00802
          // *******
00803
00804
          template<typename F>
00805
          OpCounter<F> exp(const OpCounter<F>& a)
00806
00807
            ++OpCounter<F>::counters.exp_count;
00808
            return {std::exp(a._v)};
00809
00810
00811
          template<tvpename F>
00812
          OpCounter<F> pow(const OpCounter<F>& a, const OpCounter<F>& b)
00813
00814
            ++OpCounter<F>::counters.pow_count;
00815
           return {std::pow(a._v,b._v)};
00816
00817
00818
          template<typename F>
00819
          OpCounter<F> pow(const OpCounter<F>& a, const F& b)
00820
00821
            ++OpCounter<F>::counters.pow_count;
00822
           return {std::pow(a._v,b)};
00823
00824
00825
          template<typename F, typename T>
00826
          OpCounter<F> pow(const OpCounter<F>& a, const T& b)
00827
00828
            ++OpCounter<F>::counters.pow_count;
00829
            return {std::pow(a._v,b)};
```

```
00830
00831
00832
          template<typename F>
00833
          OpCounter<F> pow(const F& a, const OpCounter<F>& b)
00834
            ++OpCounter<F>::counters.pow_count;
00835
00836
            return {std::pow(a,b._v)};
00837
00838
00839
          template<typename F, typename T> \,
00840
          OpCounter<F> pow(const T& a, const OpCounter<F>& b)
00841
00842
            ++OpCounter<F>::counters.pow_count;
00843
            return {std::pow(a,b._v)};
00844
00845
00846
          template<typename F>
00847
          OpCounter<F> sin(const OpCounter<F>& a)
00848
00849
            ++OpCounter<F>::counters.sin_count;
00850
            return {std::sin(a._v)};
00851
00852
00853
          template<typename F>
00854
          OpCounter<F> cos(const OpCounter<F>& a)
00855
00856
            ++OpCounter<F>::counters.sin_count;
00857
            return {std::cos(a._v)};
00858
00859
00860
          template<tvpename F>
00861
          OpCounter<F> sqrt (const OpCounter<F>& a)
00862
00863
            ++OpCounter<F>::counters.sqrt_count;
00864
            return {std::sqrt(a._v)};
00865
00866
00867
          template<typename F>
00868
          OpCounter<F> abs(const OpCounter<F>& a)
00869
00870
            ++OpCounter<F>::counters.comparison_count;
00871
            return {std::abs(a._v)};
00872
00873
00874 }
00875
00876 #endif // __OPCOUNTER_
```

5.12 src/pde.hh File Reference

solvers for partial differential equations

```
#include <vector>
#include "newton.hh"
```

Classes

class hdnum::StationarySolver< M >
 Stationary problem solver. E.g. for elliptic problems.

Functions

template < class N , class G >
 void hdnum::pde_gnuplot2d (const std::string &fname, const Vector < N > solution, const G &grid)
 gnuplot output for stationary state

5.12.1 Detailed Description

solvers for partial differential equations

5.13 pde.hh

Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*- 00002 #ifndef HDNUM_PDE_HH
00003 #define HDNUM PDE HH
00004
00005 #include<vector>
00006 #include "newton.hh"
00007
00012 namespace hdnum {
00013
00022
        template<class M>
00023
        class StationarySolver
00024
00025
00027
          typedef typename M::size_type size_type;
00028
00030
          typedef typename M::time_type time_type;
00031
00033
           typedef typename M::number_type number_type;
00034
00036
           StationarySolver (const M& model_)
00037
             : model(model_), x(model.size())
00038
00039
00040
00042
           void solve ()
00043
00044
             const size_t n_dofs = model.size();
00045
00046
             DenseMatrix<number_type> A(n_dofs, n_dofs, 0.);
00047
             Vector<number_type> b(n_dofs,0.);
00048
00049
             Vector<number_type> s(n_dofs);
                                                              // scaling factors
                                                          // row permutations
// column permutations
             Vector<size_t> p(n_dofs);
Vector<size_t> q(n_dofs);
00050
00051
00052
00053
             number_type t = 0.;
00054
00055
             x = 0.;
00056
             model.f_x(t, x, A);
00057
00058
             model.f(t, x, b);
00059
00060
00061
00062
             row_equilibrate(A,s);
                                                                 // equilibrate rows
                                                                 // LR decomposition of {\tt A}
00063
             lr_fullpivot(A,p,q);
             apply_equilibrate(s,b);
permute_forward(p,b);
00064
                                                                // equilibration of right hand side
// permutation of right hand side
00065
00066
             solveL(A, b, b);
                                                                 // forward substitution
00067
             solveR(A, x, b);
                                                                 // backward substitution
00068
             permute_backward(q,x);
                                                                 // backward permutation
00069
00070
00072
           const Vector<number_type>& get_state () const
00074
00075
00076
00078
           size_type get_order () const
00079
08000
             return 2;
00081
00082
00083
        private:
00084
          const M& model:
00085
           Vector<number_type> x;
00086
00087
00088
00090
        template<class N, class G>
00091
        inline void pde_gnuplot2d (const std::string& fname, const Vector<N> solution,
00092
                                       const G & grid)
```

```
00093
       {
00094
00095
          const std::vector<Vector<N> > coords = grid.getNodeCoordinates();
00096
         Vector<typename G::size_type> gsize = grid.getGridSize();
00097
00098
         std::fstream f(fname.c_str(), std::ios::out);
         // f « "set dgrid3d ";
00100
00101
          // f « gsize[0] « "," « gsize[1] « std::endl;
00102
          // f « "set hidden3d" « std::endl;
00103
         f « "set ticslevel 0" « std::endl;
00104
          f « "splot \"-\" using 1:2:3 with points" « std::endl;
00105
00106
         f « "#" « std::endl;
00107
         for (typename Vector<N>::size_type n=0; n<solution.size(); n++)</pre>
00108
             for (typename Vector<N>::size_type d=0; d<coords[n].size(); d++){</pre>
00109
00110
               f « std::scientific « std::showpoint
                  « std::setprecision(16) « coords[n][d] « " ";
00111
00112
00113
00114
             f « std::scientific « std::showpoint
               « std::setprecision(solution.precision()) « solution[n];
00115
00116
00117
             f « std::endl;
00118
00119
         f « "end" « std::endl;
         f « "pause -1" « std::endl;
00120
00121
         f.close();
00122
00123
00124
00125 }
00126 #endif
```

5.14 src/precision.hh File Reference

find machine precision for given float type

Functions

template<typename X > int hdnum::precision (X &eps)

5.14.1 Detailed Description

find machine precision for given float type

5.15 precision.hh

Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*- 00002 #ifndef HDNUM_PRECISION_HH
00003 #define HDNUM_PRECISION_HH
00004
00009 namespace hdnum {
00010
00011
        // find largest eps such that 0.5 + eps > 0.5
00012
         template<typename X>
00013
        int precision (X& eps)
00014
00015
                X x, large, largex, two;
00016
               large = 0.5;
two = 2.0;
x = 0.5;
00017
00018
00019
                largex = large+x;
```

```
int i(0);
00021
           while (largex>large)
00022
00023
                 eps = x;
00024
                 i = i+1;
                              00025
00026
00027
                 x = x/two;
00028
                 largex = large+x;
00029
00030
           return i:
00031
00032
00033 } // namespace hdnum
00034
00035 #endif
```

5.16 src/qr.hh File Reference

This file implements QR decomposition using Gram-Schmidt method.

```
#include <cmath>
#include <utility>
#include "densematrix.hh"
#include "vector.hh"
```

Functions

```
• template<class T >
  DenseMatrix< T > hdnum::gram_schmidt (const DenseMatrix< T > &A)
     computes orthonormal basis of Im(A) using classical Gram-Schmidt
template < class T >
  DenseMatrix< T > hdnum::modified gram schmidt (const DenseMatrix< T > &A)
     computes orthonormal basis of Im(A) using modified Gram-Schmidt
template < class T >
  DenseMatrix< T > hdnum::qr gram schmidt simple (DenseMatrix< T > &Q)
     computes gr decomposition using modified Gram-Schmidt - works only with small (m>n) and square matrices
• template<class T >
  DenseMatrix< T > hdnum::qr_gram_schmidt (DenseMatrix< T > &Q)
     computes qr decomposition using modified Gram-Schmidt - works only with small (m>n) and square matrices
  DenseMatrix< T> hdnum::gr gram schmidt pivoting (DenseMatrix< T> &Q, Vector< int > &p, int &rank,
  T threshold=0.0000000001)
     computes qr decomposition using modified Gram-Schmidt and pivoting - works with all types of matrices
template<typename T >
  void hdnum::permute_forward (DenseMatrix< T > &A, Vector< int > &p)
     applies a permutation vector to a matrix
```

5.16.1 Detailed Description

This file implements QR decomposition using Gram-Schmidt method.

5.16.2 Function Documentation

5.16.2.1 gram_schmidt()

computes orthonormal basis of Im(A) using classical Gram-Schmidt

Template Parameters

```
hdnum::DenseMatrix<T> A
```

Example:

Output:

5.16.2.2 modified_gram_schmidt()

computes orthonormal basis of Im(A) using modified Gram-Schmidt

Template Parameters

```
hdnum::DenseMatrix<T> A
```

Example:

```
hdnum::DenseMatrix<double> A({{2, 9}, {1, -5}});
hdnum::DenseMatrix<double> Q(hdnum::modified_gram_schmidt(A));
std::cout « "A = " « A « std::endl;
std::cout « "Q = " « Q « std::endl;
```

Output:

```
A = 0 1 0 1 0 2.000e+00 9.000e+00 1 1.000e+00 -5.000e+00 Q = 0 1 0 8.944e-01 4.472e-01 1 4.472e-01 -8.944e-01
```

5.16.2.3 permute_forward()

applies a permutation vector to a matrix

Template Parameters

```
hdnum::DenseMatrix<T> A
```

Parameters

```
hdnum::Vector<int> p
```

Example:

Output:

```
A = 0 1
0 9.000e+00 2.000e+00
1 -5.000e+00 1.000e+00

p = [0] 0
[1] 1
```

5.16.2.4 qr_gram_schmidt()

computes qr decomposition using modified Gram-Schmidt - works only with small (m>n) and square matrices

Template Parameters

```
hdnum::DenseMatrix<T> Q
```

Example:

Output:

```
A =
                0
                           1
         2.000e+00 9.000e+00
      0
        1.000e+00 -5.000e+00
      1
Q =
                0
        8.944e-01 4.472e-01
      0
      1
         4.472e-01 -8.944e-01
R =
                 0
         2.236e+00 5.814e+00
     0
         0.000e+00 8.497e+00
QR =
         2.000e+00 9.000e+00
     0
         1.000e+00 -5.000e+00
```

5.16.2.5 qr_gram_schmidt_pivoting()

computes qr decomposition using modified Gram-Schmidt and pivoting - works with all types of matrices

Template Parameters

hdnum::DenseMatrix <t></t>	Q
T	threshold (optional)

Parameters

hdnum::Vector <int></int>	р
int	rank

Example:

Output:

```
A =
                 0
                            1
         5.000e+00 2.000e+00 3.000e+00
      Ω
      1
         1.100e+01 9.000e+00 2.000e+00
Q =
                 0
         4.138e-01 -9.104e-01
      Ω
      1
          9.104e-01 4.138e-01
R =
                 0
      0
         1.208e+01 9.021e+00 3.062e+00
          0.000e+00 1.903e+00 -1.903e+00
      1
OR =
                 0
                           1
          5.000e+00 2.000e+00 3.000e+00
          1.100e+01 9.000e+00 2.000e+00
```

5.16.2.6 qr_gram_schmidt_simple()

computes qr decomposition using modified Gram-Schmidt - works only with small (m>n) and square matrices

Template Parameters

```
hdnum::DenseMatrix<T> Q
```

Example:

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```
hdnum::DenseMatrix<double> R(hdnum::qr_gram_schmidt_simple(Q));
std::cout « "A = " « A « std::endl;
std::cout « "Q = " « Q « std::endl;
std::cout « "R = " « R « std::endl;
std::cout « "QR = " « Q*R « std::endl;
Output:
```

```
A =
                 Ω
      0
         2.000e+00 9.000e+00
         1.000e+00 -5.000e+00
                 0
                            1
         8.944e-01 4.472e-01
      0
         4.472e-01 -8.944e-01
R =
                 0
      0
         2.236e+00 5.814e+00
      1
          0.000e+00 8.497e+00
OR =
                 0
                            1
          2.000e+00 9.000e+00
      0
      1
          1.000e+00 -5.000e+00
```

5.17 qr.hh

Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil; c-basic-offset: 2 -*-
00002 /*
00003 * File: qr.hh
00004 * Author: Raphael Vogt <cx238@stud.uni-heidelberg.de>
00005 *
00006 * Created on August 30, 2020 00007 */
80000
00009 #ifndef HDNUM_QR_HH
00010 #define HDNUM_QR_HH
00011
00012 #include <cmath>
00013 #include <utility>
00014
00015 #include "densematrix.hh"
00016 #include "vector.hh"
00017
00022 namespace hdnum {
00023
00052 template <class T>
00053 DenseMatrix<T> gram_schmidt(const DenseMatrix<T>& A) {
00054 DenseMatrix<T> Q(A);
00055
00056
           // for all columns except the first
00057
           for (int k = 1; k < Q.colsize(); k++) {
00058
                \label{eq:column_k} \mbox{\it against all previous}
                for (int j = 0; j < k; j++) {
    // compute factor</pre>
00059
00060
00061
                    T sum_nom(0.0);
00062
                    T sum_denom(0.0);
00063
                    for (int i = 0; i < Q.rowsize(); i++) {</pre>
00064
                         sum\_nom += A[i][k] * Q[i][j];
                         sum\_denom += Q[i][j] * Q[i][j];
00065
00066
                    // modify
T alpha = sum_nom / sum_denom;
00067
00068
00069
                    for (int i = 0; i < Q.rowsize(); i++) Q[i][k] -= alpha * Q[i][j];
00070
               }
00071
           for (int j = 0; j < Q.colsize(); j++) {
00072
               // compute norm of column j
00073
00074
                T sum(0.0);
00075
                for (int i = 0; i < Q.rowsize(); i++) sum += Q[i][j] * Q[i][j];</pre>
```

```
sum = sqrt(sum);
00077
                for (int i = 0; i < Q.rowsize(); i++) Q[i][j] = Q[i][j] / sum;</pre>
00078
00079
08000
           return O;
00081 }
00111 template <class T>
00112 DenseMatrix<T> modified_gram_schmidt(const DenseMatrix<T>& A) {
00113
           DenseMatrix<T> O(A);
00114
           for (int k = 0; k < Q.colsize(); k++) {
    // modify all later columns with column k
    for (int j = k + 1; j < Q.colsize(); j++) {</pre>
00115
00116
00117
00118
                     // compute factor
00119
                     T sum_nom(0.0);
00120
                     T sum_denom(0.0);
                    for (int i = 0; i < Q.rowsize(); i++) {
    sum_nom += Q[i][j] * Q[i][k];</pre>
00121
                         sum\_denom += Q[i][k] * Q[i][k];
00123
00124
                     // modify
00125
                     T alpha = sum_nom / sum_denom;
for (int i = 0; i < Q.rowsize(); i++) Q[i][j] -= alpha * Q[i][k];</pre>
00126
00127
00128
                }
00129
00130
           for (int j = 0; j < Q.colsize(); j++) {
                // compute norm of column j
T sum(0.0);
for (int i = 0; i < Q.rowsize(); i++) sum += Q[i][j] * Q[i][j];
00131
00132
00133
00134
                sum = sqrt(sum);
00135
                // scale
00136
                for (int i = 0; i < Q.rowsize(); i++) Q[i][j] = Q[i][j] / sum;</pre>
00137
00138
           return Q;
00139 }
00140
00182 template <class T>
00183 DenseMatrix<T> qr_gram_schmidt_simple(DenseMatrix<T>& Q) {
00184
            // save matrix A, before it's replaced with Q
00185
           DenseMatrix<T> A(Q);
00186
00187
           // create matrix R
00188
           DenseMatrix<T> R(Q.colsize(), Q.colsize());
00189
00190
           // start orthogonalizing
00191
           for (int k = 0; k < Q.colsize(); k++) {
                // modify all later columns with column \boldsymbol{k}
00192
00193
                for (int j = k + 1; j < Q.colsize(); j++) {
                    // compute factor
00194
00195
                     T sum_nom(0.0);
00196
                     T sum_denom(0.0);
00197
                     for (int i = 0; i < Q.rowsize(); i++) {</pre>
                         sum_nom += Q(i, j) * Q(i, k);

sum_denom += Q(i, k) * Q(i, k);
00198
00199
00200
                     }
00201
00202
                     T alpha = sum_nom / sum_denom;
00203
                     for (int i = 0; i < Q.rowsize(); i++) Q(i, j) -= alpha * Q(i, k);
00204
                }
00205
           }
00206
00207
           // add values to R, except main diagonal
           for (int i = 1; i < R.colsize(); i++) {
    for (int j = 0; j < i; j++) {</pre>
00208
00209
00210
                    T sum_nom(0.0);
00211
                     T sum_12nom(0.0);
                     for (int k = 0; k < Q.rowsize(); k++) {
    sum_nom += A(k, i) * Q(k, j);
00212
00213
                         sum_12nom += Q(k, j) * Q(k, j);
00214
00215
00216
                     sum_12nom = sqrt(sum_12nom);
00217
                     // add element
00218
                     R(j, i) = sum_nom / sum_12nom;
00219
                }
00220
00221
00222
           \ensuremath{//} add missing values and scale
00223
           for (int j = 0; j < Q.colsize(); j++) {</pre>
                // compute norm of column j
00224
                T sum(0.0);

for (int i = 0; i < Q.rowsize(); i++) sum += Q(i, j) * Q(i, j);
00225
00226
00227
                sum = sqrt(sum);
00228
                // add main diagonal to R
00229
                R(j, j) = sum;
                // scale Q for (int i = 0; i < Q.rowsize(); i++) Q(i, j) = Q(i, j) / sum;
00230
00231
```

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```
00232
00233
           return R;
00234 }
00235
00277 template <class T>
00278 DenseMatrix<T> qr_gram_schmidt(DenseMatrix<T>& Q) {
           // create matrix R
00280
           DenseMatrix<T> R(Q.colsize(), Q.colsize());
00281
00282
           // start orthogonalizing
           for (int k = 0; k < Q.colsize(); k++) {
00283
               // compute norm of column k
00284
00285
                T sum_denom(0.0);
00286
                for (int i = 0; i < Q.rowsize(); i++) {</pre>
00287
                    sum\_denom += Q(i, k) * Q(i, k);
00288
00289
               // fill the main diagonal of R with elements
00290
00291
               sum_denom = sqrt(sum_denom);
00292
               R(k, k) = sum\_denom;
00293
00294
                \ensuremath{//} scale column k to the main diagonal
               for (int i = 0; i < Q.rowsize(); i++) {
   Q(i, k) /= R(k, k);</pre>
00295
00296
00297
00298
00299
                \//\ modify all later columns with column k
               for (int j = k + 1; j < Q.colsize(); j++) {
    // compute norm of column j</pre>
00300
00301
00302
                    T sum nom(0.0);
00303
                    for (int i = 0; i < Q.rowsize(); i++) {</pre>
00304
                        sum\_nom += Q(i, k) * Q(i, j);
00305
                    ^{\prime\prime} insert missing elements to R
00306
00307
                    R(k, j) = sum_nom;
00308
                    // orthogonalize column j
for (int i = 0; i < Q.rowsize(); i++) {</pre>
00309
00310
00311
                        Q(i, j) = Q(i, k) * R(k, j);
00312
00313
               }
00314
           return R:
00315
00316 }
00317
00381 template <class T>
00382 DenseMatrix<T> qr_gram_schmidt_pivoting(DenseMatrix<T>& Q, Vector<int>& p, int& rank, T
      threshold=0.00000000001) {
00383
           \ensuremath{//} check if permutation vector has the right size
00384
           if (p.size() != Q.colsize()) {
00385
               HDNUM_ERROR("Permutation Vector incompatible with Matrix!");
00386
00387
00388
           // initialize permutation vector
           for (int i = 0; i < p.size(); i++) {
   p[i] = i;</pre>
00389
00390
00391
00392
00393
           // initialize rank
00394
           rank = 0:
00395
00396
           // save matrix A, before it's replaced with Q
00397
           DenseMatrix<T> A(Q);
00398
00399
           // create Matrix R
00400
           hdnum::DenseMatrix<T> R(A.colsize(), A.colsize());
00401
00402
           // start orthogonalizing
           for (int k = 0; k < Q.colsize(); k++) {</pre>
00403
               // find column with highest norm
00404
00405
                // compute norm of column k
00406
                T norm_k(0.0);
               for (int r = 0; r < Q.rowsize(); r++) {
    norm_k += Q(r, k) * Q(r, k);
00407
00408
00409
00410
               norm_k = sqrt(norm_k);
00411
00412
                // compare norm of column \boldsymbol{k} to the following column norms
00413
                for (int c = k+1; c < Q.colsize(); c++) {
                    T norm(0.0);
00414
                    for (int r = 0; r < Q.rowsize(); r++) {</pre>
00415
                        norm += Q(r, c) * Q(r, c);
00416
00417
00418
                    norm = sqrt(norm);
00419
                    // store permutation
                    if (norm > norm_k) {
   p[k] = c;
00420
00421
```

```
00422
                      }
00423
                 }
00424
                 // swap columns if necessary
00425
00426
                 if (p[k] > k) {
    for (int r = 0; r < Q.rowsize(); r++) {</pre>
00427
                          T temp_Q = Q(r, k);
Q(r, k) = Q(r, p[k]);
00429
00430
                          Q(r, p[k]) = temp_Q;
00431
                      p[p[k]] = k;
00432
00433
00434
                      // compute norm of the new column k
                      norm_k = 0;
for (int i = 0; i < Q.rowsize(); i++) {</pre>
00435
00436
00437
                         norm_k += Q(i, k) * Q(i, k);
00438
00439
                      norm_k = sqrt(norm_k);
00440
                }
00441
00442
                 // if norm of column k > threshold \rightarrow column k is linear independent
00443
                 if (norm_k > threshold) {
00444
                      rank++;
00445
                 } else {
00446
                      break;
00447
00448
00449
                 // modify all later columns with column \boldsymbol{k}
                 for (int j = k + 1; j < Q.colsize(); j++) {
    // compute factor</pre>
00450
00451
00452
                      T sum_nom(0.0);
00453
                      T sum_denom(0.0);
00454
                      for (int i = 0; i < Q.rowsize(); i++) {</pre>
00455
                           sum\_nom += Q(i, j) * Q(i, k);
00456
                           sum\_denom += Q(i, k) * Q(i, k);
00457
00458
00459
                      T alpha = sum_nom / sum_denom;
00460
                      for (int i = 0; i < Q.rowsize(); i++) Q(i, j) -= alpha * Q(i, k);
00461
00462
            }
00463
            // add values to R, except main diagonal
for (int i = 1; i < R.colsize(); i++) {
    for (int j = 0; j < i; j++) {</pre>
00464
00465
00466
00467
                      T sum_nom(0.0);
00468
                      T sum_12nom(0.0);
                      for (int k = 0; k < Q.rowsize(); k++) {
    sum_nom += A(k, p[i]) * Q(k, j);
    sum_12nom += Q(k, j) * Q(k, j);</pre>
00469
00470
00471
00472
00473
                      sum_12nom = sqrt(sum_12nom);
00474
                      // add element
00475
                      R(j, i) = sum_nom / sum_12nom;
00476
                }
00477
            }
00478
00479
            // add missing values and scale
00480
            for (int j = 0; j < Q.colsize(); j++) {</pre>
                 // compute norm of column j
T sum(0.0);
00481
00482
                 for (int i = 0; i < Q.rowsize(); i++) sum += Q(i, j) * Q(i, j);
00483
00484
                 sum = sqrt(sum);
00485
                 // add main diagonal to R
00486
                 R(j, j) = sum;
00487
                 // scale Q
                 for (int i = 0; i < Q.rowsize(); i++) Q(i, j) = Q(i, j) / sum;
00488
00489
            }
00490
00491
            return R;
00492 }
00493
00524 template<typename T>
00525 void permute_forward(DenseMatrix<T>& A, Vector<int>& p) {
00526    // check if permutation vector has the right size
00527
            if (p.size() != A.colsize()) {
00528
                 HDNUM_ERROR("Permutation Vector incompatible with Matrix!");
00529
00530
            \ensuremath{//} permutate the columns
00531
            for (int k = 0; k < p.size(); k++) {
   if (p[k] != k) {</pre>
00532
00534
                      // swap column
00535
                      for (int j=0; j < A.rowsize(); j++) {</pre>
                          T temp_A = A(j, k);

A(j, k) = A(j, p[k]);

A(j, p[k]) = temp_A;
00536
00537
00538
```

```
00540
                  // swap inside permutation vector
00541
                  int temp_p = p[k];
                  p[k] = p[temp_p];
00542
00543
                  p[temp_p] = temp_p;
00544
00545
         }
00546 }
00547
00548 } // namespace hdnum
00549
00550 #endif
```

5.18 src/qrhousholder.hh File Reference

This file implements QR decomposition using housholder transformation.

```
#include <cmath>
#include <cstdlib>
#include <fstream>
#include <iomanip>
#include <iostream>
#include <sstream>
#include <string>
#include "densematrix.hh"
#include "vector.hh"
```

Functions

```
    template < class REAL >
        DenseMatrix < REAL > hdnum::creat_I_matrix (size_t n)
    template < typename REAL >
        size_t hdnum::sgn (REAL val)
```

Function that return the sign of a number.

template < class REAL > void hdnum::qrhousholder (DenseMatrix < REAL > &A, hdnum::Vector < REAL > &v)

Funktion that calculate the QR decoposition in place the elements of A will be replaced with the elements of v_{\leftarrow} {i}vectors and the upper diagonals elements of R and the diagonal elements of R will be saved in vectro v.

template < class REAL >
 DenseMatrix < REAL > hdnum::qrhousholderexplizitQ (DenseMatrix < REAL > &A, hdnum::Vector < REAL > &v, bool show_Hi=false)

Funktion that calculate the QR decoposition in place and return Q the elements of A will be replaced with the elements of v_{ij} vectors and the upper diagonals elements of R and the diagonal elements of R will be saved in vectro v_{ij} .

5.18.1 Detailed Description

This file implements QR decomposition using housholder transformation.

5.18.2 Function Documentation

5.18.2.1 qrhousholder()

Funktion that calculate the QR decoposition in place the elements of A will be replaced with the elements of v_{\leftarrow} {i}vectors and the upper diagonals elements of R and the diagonal elements of R will be saved in vectro v.

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Template Parameters

Α	the Matrix
V	oa vector of hdnum::Vector

5.18.2.2 qrhousholderexplizitQ()

Funktion that calculate the QR decoposition in place and return Q the elements of A will be replaced with the elements of v_{i} vectors and the upper diagonals elements of R and the diagonal elements of R will be saved in vectro v.

Template Parameters

Α	the Matrix	
V	oa vector of hdnum::Vector	

Returns

Q matrix

5.19 qrhousholder.hh

Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil; c-basic-offset: 2 -*-
00002 /*
00003 * File: qrhousholder
00004 * Author: Ahmad Fadl <abohmaid@windowslive.com>
00005
00003 *
00006 * Created on August 25, 2020
00007 */
80000
00009 #ifndef HDNUM_QRHOUSHOLDER_HH
00010 #define HDNUM_QRHOUSHOLDER_HH
00011 #include <cmath>
00012 #include <cstdlib>
00013 #include <fstream>
00014 #include <iomanip>
00015 #include <iostream>
00016 #include <sstream>
00017 #include <string>
00018
00019 #include "densematrix.hh"
00020 #include "vector.hh"
00024 namespace hdnum {
00025 template <class REAL>
00026 DenseMatrix<REAL> creat_I_matrix(size_t n) {
          DenseMatrix<REAL> res(n, n, 0);
for (size_t i = 0; i < n; i++) {
   res(i, i) = 1;</pre>
00027
00028
00029
00030
00031
           return res;
00032 }
00033
00036 template <typename REAL>
00037 size_t sgn(REAL val) {
           return (REAL(0) < val) - (val < REAL(0));</pre>
```

```
00049 template <class REAL>
00050 void grhousholder(DenseMatrix<REAL>& A, hdnum::Vector<REAL>& v) {
            auto m = A.rowsize();
auto n = A.colsize();
00051
00052
             for (size_t j = 0; j < n; j++) {
    REAL s = 0;</pre>
00053
00054
00055
                   for (size_t i = j; i < m; i++) {</pre>
00056
                       s = s + pow(A(i, j), 2);
00057
00058
                   s = sqrt(s);
                   s = sqt(s);

v[j] = (-1.0) * sgn(A(j, j)) * s;

REAL fak = sqrt(s * (s + std::abs(A(j, j))));

A(j, j) = A(j, j) - v[j];

for (size_t k = j; k < m; k++) {
00059
00060
00061
00062
                       A(k, j) = A(k, j) / fak;
00063
00064
00065
                   for (size_t i = j + 1; i < n; i++) {</pre>
                        s = 0;
00067
                         for (size_t k = j; k < m; k++) {</pre>
00068
                            s = s + (A(k, j) * A(k, i));
00069
                        for (size_t k = j; k < m; k++) {
A(k, i) = A(k, i) - (A(k, j) * s);
00070
00071
00072
00073
00074
                   // normalize the vi vectors again
                   for (size_t i = m; i >= 0; i--) {
   A(i, j) = A(i, j) * fak;
   if (i == j) {
00075
00076
00077
00078
                             break:
00079
                        }
00080
00081
             }
00082 }
00093 template <class REAL>
00094 DenseMatrix<REAL> qrhousholderexplizitQ(DenseMatrix<REAL>& A,
                                                               hdnum::Vector<REAL>& v,
00096
                                                               bool show_Hi = false) {
             auto m = A.rowsize();
auto n = A.colsize();
00097
00098
             auto I = creat_I_matrix<REAL>(std::max(m, n));
00099
00100
             DenseMatrix<REAL> Q(m, m, 0);
00101
             for (size_t j = 0; j < n; j++) {
   REAL s = 0;
   for (size_t i = j; i < m; i++) {</pre>
00102
00103
00104
00105
                        s = s + pow(A(i, j), 2);
00106
                   }
00107
                   s = sqrt(s);
                   s = sqrt(s);
v[j] = (-1.0) * sqn(A(j, j)) * s;
REAL fak = sqrt(s * (s + std::abs(A(j, j))));
A(j, j) = A(j, j) - v[j];
for (size_t k = j; k < m; k++) {
    A(k, j) = A(k, j) / fak;
}</pre>
00108
00109
00110
00111
00112
00113
                   for (size_t i = j + 1; i < n; i++) {</pre>
00115
                         for (size_t k = j; k < m; k++) {
 s = s + (A(k, j) * A(k, i));
00116
00117
00118
                        for (size_t k = j; k < m; k++) {
    A(k, i) = A(k, i) - (A(k, j) * s);
00119
00120
00121
00122
00123
                   // normalize the vi vectors again
                   for (size_t i = m; i >= 0; i--) {
   A(i, j) = A(i, j) * fak;
   if (i == j) {
00124
00125
00126
                             break;
00127
00128
00129
                   }
00130
             // create qi and multiply them
00131
00132
             if (m >= n) {
                   for (size_t j = 0; j < n; j++) {
00133
00134
                        DenseMatrix<REAL> TempQ(m, m, 0.0);
                        DenseMatrix<REAL> v1(m, 1, 0.0);
DenseMatrix<REAL> v1t(1, m, 0.0);
00135
00136
                        hdnum::Vector<double> v__i(m, 0);
00137
                        for (size_t i = 0; i < m; i++) {
    if (i < j) {
00138
00140
                                   v1(i, 0) = 0;
00141
00142
                                   v_{i[i]} = 0;
00143
                                   continue;
00144
```

```
00145
                         v1(i, 0) = A(i, j);
00146
00147
                         v_{i[i]} = A(i, j);
00148
                    v1t = v1.transpose();
00149
00150
                    TempQ = (v1 * v1t);
00151
00152
00153
                    TempQ \star = (-2.0);
00154
00155
                    TempQ /= v__i.two_norm_2();
00156
00157
                    TempO += I;
00158
                    if (show_Hi) {
00159
                         std::cout « "H[" « j + 1 « "]" « TempQ;
00160
                     if (j == 0) {
00161
                         Q = TempQ;
00162
00163
00164
                    if (j > 0) {
00165
                         Q = Q * TempQ;
00166
00167
               }
00168
00169
           if (n > m) {
00170
               for (size_t j = 0; j < m; j++) {</pre>
                    DenseMatrix<REAL> TempQ(m, m, 0.0);
DenseMatrix<REAL> v1(m, 1, 0.0);
DenseMatrix<REAL> v1t(1, m, 0.0);
00171
00172
00173
                    hdnum::Vector<double> v__i(m, 0);
00174
                    for (size_t i = 0; i < m; i++) {
    if (i < j) {
       v1(i, 0) = 0;
    }
00175
00176
00177
00178
00179
                             v_{i[i]} = 0;
00180
                             continue;
00181
00182
                         v1(i, 0) = A(i, j);
00183
00184
                         v__i[i] = A(i, j);
00185
                    v1t = v1.transpose();
00186
00187
00188
                    TempQ = (v1 * v1t);
00189
00190
                    TempQ \star= (-2.0);
00191
                    TempQ /= v__i.two_norm_2();
00192
00193
00194
                    TempO += I:
00195
                    if (show_Hi) {
00196
                         std::cout « "H[" « j + 1 « "]" « TempQ;
00197
00198
                    if (j == 0) {
                         Q = TempQ;
00199
00200
00201
                    if (j > 0) {
00202
                         Q = Q * TempQ;
00203
00204
               }
00205
00206
           return O;
00207 }
00208 }
         // namespace hdnum
00209 #endif
```

5.20 src/rungekutta.hh File Reference

```
#include "vector.hh"
#include "newton.hh"
```

Classes

class hdnum::ImplicitRungeKuttaStepProblem< M >

Nonlinear problem we need to solve to do one step of an implicit Runge Kutta method.

class hdnum::RungeKutta< M, S >

classical Runge-Kutta method (order n with n stages)

Functions

template < class M , class S >
 void hdnum::ordertest (const M &model, S solver, typename M::number_type T, typename M::number_type h_0, int I)

Test convergence order of an ODE solver applied to a model problem.

5.20.1 Detailed Description

@general Runge-Kutta solver

5.20.2 Function Documentation

5.20.2.1 ordertest()

Test convergence order of an ODE solver applied to a model problem.

Template Parameters

М	Type of model
S	Type of ODE solver

Parameters

model	Model problem
solver	ODE solver
T	Solve to time T
dt	Roughest time step size
1	Number of different time step sizes dt, dt/2, dt/4,

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Go to the documentation of this file.

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil -*-
00002 #ifndef HDNUM_RUNGEKUTTA_HH
00003 #define HDNUM_RUNGEKUTTA_HH
00004
00005 #include "vector.hh"
00006 #include "newton.hh"
00007
00012 namespace hdnum {
00015 template<class M>
```

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```
class ImplicitRungeKuttaStepProblem
00017
        public:
00018
00020
          typedef typename M::size_type size_type;
00021
00023
          typedef typename M::time type time type;
00026
          typedef typename M::number_type number_type;
00027
          ImplicitRungeKuttaStepProblem (const M& model_,
00029
                                           DenseMatrix<number_type> A_,
00030
00031
                                           Vector<number_type> b_,
00032
                                           Vector<number_type> c_,
00033
                                           time_type t_,
00034
                                           Vector<number_type> u_,
00035
                                           time_type dt_)
00036
              : model(model_) , u(model.size())
            {
00037
              A = A_{;}
00038
00039
              b = b_{,}
              c = c_;
00040
00041
              s = A_.rowsize ();
              dt = dt;
00042
              n = model.size();
00043
00044
              t = t_;
00045
              u = u_;
00046
00047
00049
          std::size_t size () const
00050
00051
            return n*s:
00052
00053
00055
          void F (const Vector<number_type>& x, Vector<number_type>& result) const
00056
            Vector<Vector<number_type> > xx (s);
00057
00058
            for (int i = 0; i < s; i++)
00059
00060
              xx[i].resize(n,number_type(0));
00061
              for (int k = 0; k < n; k++)
00062
00063
                xx[i][k] = x[i*n + k];
00064
              }
00065
00066
            Vector<Vector<number_type> > f (s);
00067
            for (int i = 0; i < s; i++)
00068
00069
              f[i].resize(n, number_type(0));
00070
              model.f(t + c[i] * dt, u + xx[i], f[i]);
00071
00072
            Vector<Vector<number_type> > hr (s);
00073
            for (int i = 0; i < s; i++)
00074
00075
              hr[i].resize(n, number_type(0));
00076
00077
            for (int i = 0; i < s; i++)
00078
00079
              Vector<number_type> sum (n, number_type(0));
00080
              for (int j = 0; j < s; j++)
00081
00082
                sum.update(dt*A[i][j], f[j]);
00083
00084
              hr[i] = xx[i] - sum;
00085
00086
             //translating hr into result
00087
            for (int i = 0; i < s; i++)
00088
00089
              for (int j = 0; j < n; j++)
00090
              {
00091
                result[i*n + j] = hr[i][j];
00092
00093
            }
00094
          }
00095
00097
          void F x (const Vector<number type>& x, DenseMatrix<number type>& result) const
00098
00099
            Vector<Vector<number_type> > xx (s);
00100
            for (int i = 0; i < s; i++)
00101
00102
              xx[i].resize(n);
00103
              for (int k = 0; k < n; k++)
00104
00105
                xx[i][k] = x[i*n + k];
00106
              }
00107
            DenseMatrix<number_type> I (n, n, 0.0);
for (int i = 0; i < n; i++)</pre>
00108
00109
```

```
00110
             {
00111
              I[i][i] = 1.0;
00112
             for (int i = 0; i < s; i++)
00113
00114
00115
               for (int j = 0; j < s; j++)
00116
00117
                 DenseMatrix<number_type> J (n, n, number_type(0));
                 DenseMatrix<number_type> H (n, n, number_type(0));
model.f_x(t+c[j]*dt, u + xx[j],H);
J.update(-dt*A[i][j],H);
00118
00119
00120
                 <u>if(i==j)</u>
00121
                                                            //add I on diagonal
00122
                 {
00123
                   J+=I;
00124
00125
                 for (int k = 0; k < n; k++)
00126
00127
                   for (int 1 = 0; 1 < n; 1++)
00128
00129
                     result[n * i + k][n * j + 1] = J[k][1];
00130
00131
00132
              }
00133
            }
00134
          }
00135
00136
        private:
00137
          const M& model;
00138
          time_type t, dt;
00139
          Vector<number_type> u;
00140
                                                                       // dimension of matrix A and model.size
          int n. s:
00141
          DenseMatrix<number_type> A;
                                                                   // A, b, c as in the butcher tableau
00142
          Vector<number_type> b;
00143
          Vector<number_type> c;
00144
00145
00146
00156
        template<class M, class S = Newton>
00157
        class RungeKutta
00158
        public:
00159
          typedef typename M::size_type size_type;
00161
00162
00164
          typedef typename M::time_type time_type;
00165
          typedef typename M::number_type number_type;
00167
00168
00170
          RungeKutta (const M& model_,
00171
                       DenseMatrix<number_type> A_,
                       Vector<number_type> b_,
Vector<number_type> c_)
00172
00173
00174
             : model(model_), u(model.size()), w(model.size()), K(A_.rowsize ())
00175
            A = A_{;}
00176
            b = b_;
00177
00178
            c = c_;
            s = A_.rowsize ();
00180
            n = model.size();
00181
             model.initialize(t,u);
00182
             dt = 0.1;
             for (int i = 0; i < s; i++)
00183
00184
00185
              K[i].resize(n, number_type(0));
00186
00187
             sigma = 0.01;
00188
             verbosity = 0;
00189
             if (A_.rowsize()!=A_.colsize())
00190
             HDNUM_ERROR("need square and nonempty matrix");
00191
00192
             if (A_.rowsize()!=b_.size())
00193
             HDNUM_ERROR("vector incompatible with matrix");
00194
             if (A_.colsize()!=c_.size())
             {\tt HDNUM\_ERROR\,("vector incompatible with matrix")\,;}
00195
00196
00197
00199
         RungeKutta (const M& model_,
00200
                      DenseMatrix<number_type> A_,
00201
                      Vector<number_type> b_,
00202
                      Vector<number_type> c_,
00203
                      number_type sigma_)
00204
            : model(model_), u(model.size()), w(model.size()), K(A_.rowsize ())
00205
         {
00206
00207
           b = b_{;}
00208
           c = c_;
           s = A_.rowsize ();
00209
00210
           n = model.size();
```

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```
00211
           model.initialize(t,u);
00212
           dt = 0.1;
           for (int i = 0; i < s; i++)</pre>
00213
00214
00215
             K[i].resize(n, number_type(0));
00216
00217
           sigma = sigma_;
00218
           verbosity = 0;
00219
            if (A_.rowsize()!=A_.colsize())
00220
           HDNUM_ERROR("need square and nonempty matrix");
           if (A_.rowsize()!=b_.size())
00221
           HDNUM_ERROR("vector incompatible with matrix");
00222
00223
              (A_.colsize()!=c_.size())
00224
           HDNUM_ERROR("vector incompatible with matrix");
00225
00226
        void set_dt (time_type dt_)
00228
00229
00230
          dt = dt_{;}
00231
00232
00234
        bool check_explicit ()
00235
00236
          bool is_explicit = true;
00237
          for (int i = 0; i < s; i++)
00238
00239
            for (int j = i; j < s; j++)
00240
              if (A[i][j] != 0.0)
00241
00242
00243
                is_explicit = false;
00244
00245
00246
00247
          return is_explicit;
00248
00249
00251
        void step ()
00252
00253
          if (check_explicit())
00254
            // compute k_1
00255
00256
            w = 11:
00257
            model.f(t, w, K[0]);
00258
            for (int i = 0; i < s; i++)
00259
00260
              Vector<number_type> sum (K[0].size(), 0.0);
00261
              sum.update(b[0], K[0]);
00262
              //compute k_i
for (int j = 0; j < i+1; j++)
00263
00264
              {
00265
                sum.update(A[i][j],K[j]);
00266
00267
              Vector<number_type> wert = w.update(dt,sum);
00268
              model.f(t + c[i]*dt, wert, K[i]);
00269
              u.update(dt *b[i], K[i]);
00270
00271
00272
           if (not check_explicit())
00273
            \ensuremath{//} In the implicit case we need to solve a nonlinear problem
00274
00275
            // to do a time step.
00276
            ImplicitRungeKuttaStepProblem<M> problem(model, A, b, c, t, u, dt);
00277
            bool last_row_eq_b = true;
00278
            for (int i = 0; i < s; i++)
00279
00280
              if (A[s-1][i] != b[i])
00281
              {
00282
                last row eg b = false;
00283
00284
00285
00286
            // Solve nonlinear problem and determine coefficients
00287
            S solver:
00288
            solver.set_maxit(2000);
00289
            solver.set_verbosity(verbosity);
00290
            solver.set_reduction(1e-10);
00291
            solver.set_abslimit(1e-10);
00292
            solver.set_linesearchsteps(10);
00293
            solver.set_sigma(0.01);
00294
            Vector<number_type> zij (s*n,0.0);
00295
            solver.solve(problem, zij);
00296
00297
00298
            DenseMatrix<number_type> Ainv (s,s,number_type(0));
00299
            if (not last_row_eq_b)
00300
```

```
00301
               // Compute LR decomposition of A
00302
               Vector<number_type> w (s, number_type(0));
              Vector<number_type> x (s, number_type(0));
00303
              Vector<number_type> z (s, number_type(0));
00304
              Vector<std::size_t> p(s);
Vector<std::size_t> q(s);
00305
00306
00307
              DenseMatrix<number_type> Temp (s,s,0.0);
00308
               Temp = A;
               row_equilibrate(Temp,w);
00309
00310
              lr_fullpivot(Temp,p,q);
00311
00312
               // Use LR decomposition to calculate inverse of A
00313
               for (int i=0; i<s; i++)</pre>
00314
00315
                Vector<number_type> e (s, number_type(0));
00316
                e[i]=number_type(1);
                apply_equilibrate(w,e);
00317
00318
                permute_forward(p,e);
                solveL(Temp,e,e);
00319
00320
                solveR(Temp, z, e);
00321
                permute_backward(q, z);
00322
                 for (int j = 0; j < s; j++)
00323
                {
                      Ainv[j][i] = z[j];
00324
00325
                }
00326
              }
00327
00328
00329
            Vector<Vector<number_type> > Z (s, 0.0);
00330
            for (int i=0; i < s; i++)
00331
00332
              Vector<number_type> zero(n,number_type(0));
00333
              Z[i] = zero;
              for (int j = 0; j < n; j++)
00334
00335
              {
                Z[i][j] = zij[i*n+j];
00336
00337
              }
00338
00339
            if (last_row_eq_b)
00340
00341
              u += Z[s-1];
00342
00343
            else
00344
00345
               // compute ki
00346
              Vector<number_type> zero(n, number_type(0));
00347
              for (int i = 0; i < s; i++)
00348
              {
00349
                K[i] = zero;
00350
                for (int j=0; j < s; j++)
00351
                {
00352
                  K[i].update(Ainv[i][j], Z[j]);
00353
00354
                K[i] *= (1.0/dt);
00355
00356
                 // compute u
00357
                u.update(dt*b[i], K[i]);
00358
00359
            }
00360
          }
00361
            t = t + dt:
00362
         }
00363
00365
         void set_state (time_type t_, const Vector<number_type>& u_)
00366
           t = t_;
00367
00368
           u = u_;
00369
00370
00372
         const Vector<number_type>& get_state () const
00373
           return u;
00374
00375
         }
00376
00378
         time type get time () const
00379
00380
           return t;
00381
00382
00384
         time_type get_dt () const
00385
00386
           return dt;
00387
00388
00390
         void set_verbosity(int verbosity_)
00391
00392
           verbosity = verbosity :
```

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```
00393
          }
00394
00395
        private:
           const M& model;
00396
           time_type t, dt;
Vector<number_type> u;
Vector<number_type> w;
00397
00398
00399
00400
           Vector<Vector<number_type> > K;
                                                                     // save ki
00401
           int n;
                                                                                                                        11
      dimension of matrix A
00402
           int s;
00403
           DenseMatrix<number type> A:
                                                                                   // A. b. c as in the butcher
      tableau
               Vector<number_type> b;
00404
               Vector<number_type> c;
00405
00406
           number_type sigma;
00407
           int verbosity;
00408
        };
00409
00410
00422
         template<class M, class S>
00423
         void ordertest (const M& model,
00424
                          S solver,
                          typename M::number_type T,
00425
00426
                          typename M::number_type h_0,
00427
                          int 1)
00428
           // Get types
00429
           typedef typename M::time_type time_type;
typedef typename M::number_type number_type;
00430
00431
00432
00433
           // error_array[i] = ||u(T)-u_i(T)||
00434
           number_type error_array[1];
00435
00436
           Vector<number_type> exact_solution;
           model.exact_solution(T, exact_solution);
00437
00438
00439
           for (int i=0; i<1; i++)</pre>
00440
           {
00441
             // Set initial time and value
00442
             time_type t_start;
00443
             Vector<number_type> initial_solution(1);
             model.initialize(t_start, initial_solution);
solver.set_state(t_start, initial_solution);
00444
00445
00446
00447
             // Initial time step
00448
             time_type dt = h_0/pow(2,i);
00449
             solver.set_dt(dt);
00450
00451
             // Time loop
00452
             while (solver.get_time() <T-2*solver.get_dt())</pre>
00453
00454
                solver.step();
00455
00456
00457
             // Last steps
00458
             if (solver.get_time() <T-solver.get_dt())</pre>
00459
00460
                solver.set_dt((T-solver.get_time())/2.0);
00461
                for (int i=0; i<2; i++)
00462
                {
00463
                 solver.step();
00464
               }
00465
00466
             else
00467
00468
               solver.set_dt(T-solver.get_time());
00469
               solver.step();
00470
00471
00472
             // Error
00473
             Vector<number_type> state = solver.get_state();
             error_array[i] = norm(exact_solution-state);
00474
00475
00476
             if(i==0)
00477
00478
                std::cout « "dt: "
00479
                           « std::scientific « std::showpoint « std::setprecision(8)
                           « c
« dt
" "
00480
00481
                           « "Error: "
00482
00483
                           « error_array[0] « std::endl;
00484
00485
             <u>if(i</u>>0)
00486
               number_type rate = log(error_array[i-1]/error_array[i])/log(2);
std::cout « "dt: "
00487
00488
```

```
« std::scientific « std::showpoint « std::setprecision(8)
00490
00491
                         « "Error: "
00492
00493
                        « error_array[i]
« " "
00494
00495
                         « "Rate: "
00496
                         « rate « std::endl;
00497
       }
00498
00499
00500
00501 } // namespace hdnum
00502
00503 #endif
```

5.22 sgrid.hh

```
00001 #ifndef HDNUM_SGRID_HH
00002 #define HDNUM_SGRID_HH
00003 #include <limits>
00004 #include <assert.h>
00005
00006 namespace hdnum {
00013
        template<class N, class DF, int dimension>
00014
        class SGrid
00015
        public:
00016
00017
00019
          typedef std::size_t size_type;
00020
00022
           typedef N number_type;
00025
           typedef DF DomainFunction;
00026
00027
           enum { dim = dimension };
00028
00030
           static const int positive = 1;
00031
           static const int negative = -1;
00032
00033
        private:
00034
00035
00036
           const Vector<number_type> extent;
00037
           const Vector<size_type>
                                        size;
00038
           const DomainFunction & df;
00039
           Vector<number_type> h;
00040
           Vector<size_type> offsets;
           std::vector<size_type> node_map;
std::vector<size_type> grid_map;
std::vector<bool> inside_map;
00041
00042
00043
00044
           std::vector<bool> boundary_map;
00045
00046
           size_t n_nodes;
00047
00048
           inline Vector<size_type> index2grid(size_type index) const
00049
00050
             Vector<size_type> c(dim);
             for(int d=dim-1; d>=0; --d) {
  c[d] = index / offsets[d];
  index -= c[d] * offsets[d];
00051
00052
00053
00054
00055
             return c;
00056
00057
00058
           inline Vector<number_type> grid2world(const Vector<size_type> & c) const
00059
             Vector<number_type> w(dim);
for(int d=dim-1; d>=0; --d)
00060
00061
               w[d] = c[d] * h[d];
00062
00063
             return w;
00064
00065
00066
           inline Vector<number_type> index2world(size_type index) const
00067
00068
             Vector<number_type> w(dim);
00069
             Vector<size_type> c = index2grid(index);
00070
             return grid2world(c);
00071
00072
00073
00074
        public:
```

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```
const size_type invalid_node;
00078
00093
           SGrid(const Vector<number_type> extent_,
00094
                  const Vector<size_type> size_,
00095
                  const DomainFunction & df_)
00096
             : extent(extent_), size(size_), df(df_),
               h(dim), offsets(dim),
00098
                invalid_node(std::numeric_limits<size_type>::max())
00099
00100
             \ensuremath{//} Determine total number of nodes, increment offsets, and cell
00101
             // widths.
00102
             n \text{ nodes} = 1:
00103
             offsets.resize(dim);
00104
             h.resize(dim);
00105
             for (int d=0; d < dim; ++d) {
               n_nodes *= size[d];
offsets[d] = d==0 ? 1 : size[d-1] * offsets[d-1];
h[d] = extent[d] / number_type(size[d]-1);
00106
00107
00108
00109
00110
             // Initialize maps.
00111
00112
             node_map.resize(0);
00113
             inside_map.resize(n_nodes);
00114
             grid_map.resize(n_nodes);
00115
             boundary_map.resize(0);
00116
             boundary_map.resize(n_nodes, false);
00117
00118
             for(size_type n=0; n<n_nodes; ++n){</pre>
               Vector<size_type> c = index2grid(n);
Vector<number_type> x = grid2world(c);
00119
00120
00121
00122
               inside_map[n] = df.evaluate(x);
00123
               if(inside_map[n]){
00124
                  node_map.push_back(n);
00125
                  grid_map[n] = node_map.size()-1;
00126
00127
               else
00128
                 grid_map[n] = invalid_node;
00129
00130
00131
             // Find boundary nodes
             for(size_type n=0; n<node_map.size(); ++n){</pre>
00132
               for(int d=0; d<dim; ++d) {
  for(int s=0; s<2; ++s) {</pre>
00133
00134
00135
                   const int side = s*2-1;
00136
                    const size_type neighbor = getNeighborIndex(n,d,side,1);
00137
                    if(neighbor == invalid_node)
                      boundary_map[node_map[n]] = true;
00138
00139
                 }
00140
               }
00141
             }
00142
00143
00144
           size_type getNeighborIndex(const size_type ln, const size_type n_dim, const int n_side, const int
00164
      k = 1) const
00165
00166
             const size_type n = node_map[ln];
00167
             const Vector<size_type> c = index2grid(n);
             size_type neighbors[2];
neighbors[0] = c[n_dim];
neighbors[1] = size[n_dim]-c[n_dim]-1;
00168
00169
00170
00171
00172
             assert(n_side == 1 || n_side == -1);
00173
             if(size_type(k) > neighbors[(n_side+1)/2])
00174
               return invalid_node;
00175
00176
             const size_type neighbor = n + offsets[n_dim] * n_side * k;
00177
00178
             if(!inside_map[neighbor])
00179
               return invalid_node;
00180
00181
             return grid_map[neighbor];
00182
00183
00187
           bool isBoundaryNode(const size_type ln) const
00188
00189
             return boundary_map[node_map[ln]];
00190
00191
00195
           size_type getNumberOfNodes() const
00196
00197
             return node_map.size();
00198
00199
00200
           Vector<size_type> getGridSize() const
00201
```

```
00202
            return size;
00203
00204
00207
          Vector<number_type> getCellWidth() const
00208
00209
            return h;
00210
00211
00215
          Vector<number_type> getCoordinates(const size_type ln) const
00216
00217
            return index2world(node_map[ln]);
00218
00219
00220
          std::vector<Vector<number_type> > getNodeCoordinates() const
00221
00222
            std::vector<Vector<number_type> > coords;
00223
            for(size_type n=0; n<node_map.size(); ++n){</pre>
              coords.push_back(Vector<number_type>(dim));
00224
              coords.back() = index2world(node_map[n]);
00226
00227
            return coords;
00228
          }
00229
00230
        };
00231
00232 }
00233
00234 #endif // HDNUM_SGRID_HH
```

5.23 sparsematrix.hh

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil; c-basic-offset: 2 -*-
00002 /*
00003 * File:
                  sparsematrix.hh
00004 * Author: Christian Heusel <christian@heusel.eu>
00005 \star 00006 \star Created on August 25, 2020 00007 \star/
80000
00009 #ifndef SPARSEMATRIX_HH
00010 #define SPARSEMATRIX_HH
00011
00012 #include <algorithm>
00013 #include <complex>
00014 #include <functional>
00015 #include <iomanip>
00016 #include <iostream>
00017 #include <map>
00018 #include <numeric>
00019 #include <string>
00020 #include <type_traits>
00021 #include <vector>
00022
00023 #include "densematrix.hh"
00024 #include "vector.hh"
00025
00026 namespace hdnum {
00027
00030 template <typename REAL>
00031 class SparseMatrix {
00032 public:
00034
           using size_type = std::size_t;
00035
           using column_iterator = typename std::vector<REAL>::iterator;
00039
           using const_column_iterator = typename std::vector<REAL>::const_iterator;
00040
00041 private:
           // Matrix data is stored in an STL vector!
std::vector<REAL> _data;
00042
00043
00044
00045
            // The non-null indices are stored in STL vectors with the size_type!
           // Explanation on how the mapping works can be found here:
// https://de.wikipedia.org/wiki/Compressed_Row_Storage
00046
00047
           std::vector<size_type> _colIndices;
std::vector<size_type> _rowPtr;
00048
00049
00050
           size_type m_rows = 0;  // Number of Matrix rows
size_type m_cols = 0;  // Number of Matrix columns
00051
00052
00053
00054
           static bool bScientific:
00055
           static size_type nIndexWidth;
00056
           static size_type nValueWidth;
           static size_type nValuePrecision;
```

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```
00058
          static const REAL _zero;
00059
00060
          // !function that converts container contents into
00061
          // { 1, 2, 3, 4 }
00062
          template <typename T>
          [[nodiscard]] std::string comma_fold(T container) const {
    return "{ " +
00063
00064
00065
                      std::accumulate(
00066
                          std::next(container.cbegin()), container.cend(),
                          std::to_string(container[0]), // start with first element
[](const std::string &a, REAL b) {
00067
00068
                              return a + ", " + std::to_string(b);
00069
00070
00071
00072
00073
00074
          // This code was copied from StackOverflow to gerneralize a check whether a
00075
          // template is a specialization i.e. for std::complex
// https://stackoverflow.com/questions/31762958/check-if-class-is-a-template-specialization
00076
00077
          template <class T, template <class...> class Template>
00078
          struct is_specialization : std::false_type {};
00079
00080
          template <template <class...> class Template, class... Args>
00081
          struct is_specialization<Template<Args...>, Template> : std::true_type {};
00082
00083
          bool checkIfAccessIsInBounds(const size_type row_index,
                                         const size_type col_index) const {
00084
00085
               if (not (row_index < m_rows)) {</pre>
00086
                   {\tt HDNUM\_ERROR}("{\tt Out}\ {\tt of}\ {\tt bounds}\ {\tt access:}\ {\tt row}\ {\tt too}\ {\tt big!}\ -{\!\!\!>}\ "\ +
                               std::to_string(row_index) + " is not < " +
00087
00088
                                std::to_string(m_rows));
00089
                   return false;
00090
00091
               if (not (col_index < m_cols)) {</pre>
                   00092
00093
00094
                                std::to_string(m_cols));
00095
                   return false;
00096
00097
               return true;
00098
          }
00099
00100 public:
00116
          SparseMatrix() = default;
00117
          SparseMatrix(const size_type _rows, const size_type _cols)
00119
00120
               : _rowPtr(_rows + 1), m_rows(_rows), m_cols(_cols) {}
00121
00138
          [[nodiscard]] size_type rowsize() const { return m_rows; }
00139
00155
           [[nodiscard]] size_type colsize() const { return m_cols; }
00156
00158
          [[nodiscard]] bool scientific() const { return bScientific; }
00159
          class column_index_iterator {
00160
00161
          public:
00162
              using self_type = column_index_iterator;
00163
00164
               // conform to the iterator traits
               // https://en.cppreference.com/w/cpp/iterator/iterator_traits
00165
               using difference_type = std::ptrdiff_t;
00166
00167
               using value_type = std::pair<REAL &, size_type const &>;
00168
               using pointer = value_type *;
00169
               using reference = value_type &;
00170
               using iterator_category = std::bidirectional_iterator_tag;
00171
00172
               column_index_iterator(typename std::vector<REAL>::iterator valIter,
                                      std::vector<size_type>::iterator colIndicesIter)
00173
00174
                   : _valIter(valIter), _colIndicesIter(colIndicesIter) {}
00175
00176
               // prefix
00177
               self_type &operator++() {
                  _valIter++;
00178
                   _colIndicesIter++;
00179
00180
                   return *this;
00181
00182
00183
               // postfix
00184
               self_type &operator++(int junk) {
00185
                  self type cached = *this;
                   _valIter++;
00186
00187
                   _colIndicesIter++;
00188
                   return cached;
00189
00190
               [[nodiscard]] value_type operator*() {
00191
00192
                   return std::make_pair(std::ref(*_valIter),
```

```
std::cref(*_colIndicesIter));
00194
00195
              // [[nodiscard]] value_type operator->()
                     return std::make_pair(std::ref(*_valIter),
00196
              11
00197
                                           std::cref(*_colIndicesIter));
00198
              // }
00199
00200
              [[nodiscard]] typename value_type::first_type value() {
00201
                return std::ref(*_valIter);
00202
00203
00204
              [[nodiscard]] typename value_type::second_type index() {
00205
                  return std::cref(*_colIndicesIter);
00206
00207
00208
              [[nodiscard]] bool operator==(const self_type &other) {
                  00209
00210
00211
00212
              [[nodiscard]] bool operator!=(const self_type &other) {
00213
                  return not (*this == other);
00214
00215
          private:
00216
00217
              typename std::vector<REAL>::iterator _valIter;
              std::vector<size_type>::iterator _colIndicesIter;
00218
00219
00220
00221
          class const_column_index_iterator {
00222
          public:
00223
              using self type = const column index iterator;
00224
00225
              // conform to the iterator traits
00226
              // https://en.cppreference.com/w/cpp/iterator/iterator_traits
00227
              using difference_type = std::ptrdiff_t;
              using value_type = std::pair<REAL const &, size_type const &>;
00228
              using pointer = value_type *;
00229
              using reference = value_type &;
00231
              using iterator_category = std::bidirectional_iterator_tag;
00232
00233
              const_column_index_iterator(
                  typename std::vector<REAL>::const_iterator valIter,
00234
                  std::vector<size_type>::const_iterator colIndicesIter)
00235
                  : _valIter(valIter), _colIndicesIter(colIndicesIter) {}
00236
00237
00238
              // prefix
00239
              self_type &operator++() {
                 _valIter++;
00240
                  _colIndicesIter++;
00241
00242
                  return *this:
00243
              }
00244
00245
              // postfix
              self_type operator++(int junk) {
    self_type cached = *this;
00246
00247
                  _valIter++;
00248
00249
                  _colIndicesIter++;
00250
                  return cached;
00251
00252
              [[nodiscard]] value_type operator*() {
00253
00254
                  return std::make_pair(std::ref(*_valIter),
00255
                                        std::cref(*_colIndicesIter));
00256
00257
              // TODO: This is wrong
00258
              // [[nodiscard]] value_type operator->() {
00259
              11
                     return std::make_pair(*_valIter, *_colIndicesIter);
              // }
00260
00261
00262
              [[nodiscard]] typename value_type::first_type value() {
00263
                 return std::ref(*_valIter);
00264
00265
00266
              [[nodiscard]] typename value_type::second_type index() {
00267
                  return std::cref(*_colIndicesIter);
00268
00269
00270
              [[nodiscard]] bool operator==(const self_type &other) {
00271
                  return (_valIter == other._valIter) and
00272
                         (_colIndicesIter == other._colIndicesIter);
00273
00274
              [[nodiscard]] bool operator!=(const self_type &other) {
00275
                  return not (*this == other);
00276
              }
00277
00278
          private:
00279
              typename std::vector<REAL>::const iterator valIter;
```

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```
00280
              std::vector<size_type>::const_iterator _colIndicesIter;
00281
00282
00283
          class row_iterator {
00284
          public:
00285
              using self_type = row_iterator;
00287
              // conform to the iterator traits
00288
               // https://en.cppreference.com/w/cpp/iterator/iterator_traits
00289
              using difference_type = std::ptrdiff_t;
              using value_type = self_type;
using pointer = self_type *;
using reference = self_type &;
00290
00291
00292
00293
              using iterator_category = std::random_access_iterator_tag;
00294
00295
              row_iterator(std::vector<size_type>::iterator rowPtrIter,
00296
                            std::vector<size_type>::iterator colIndicesIter,
                            typename std::vector<REAL>::iterator valIter)
00297
                  : _rowPtrIter(rowPtrIter), _colIndicesIter(colIndicesIter),
00298
00299
                    _valIter(valIter) {}
00300
00301
              [[nodiscard]] column_iterator begin() {
00302
                  return column_iterator((_valIter + *_rowPtrIter));
00303
00304
              [[nodiscard]] column_iterator end() {
00305
                  return column_iterator((_valIter + *(_rowPtrIter + 1)));
00306
00307
00308
              [[nodiscard]] column_index_iterator ibegin() {
00309
                  return column_index_iterator((_valIter + *_rowPtrIter),
00310
                                                 ( colIndicesIter + * rowPtrIter));
00311
00312
              [[nodiscard]] column_index_iterator iend() {
00313
                  return column_index_iterator(
00314
                       (_valIter + *(_rowPtrIter + 1)),
                       (_colIndicesIter + *(_rowPtrIter + 1)));
00315
00316
              }
00318
              // prefix
00319
              self_type &operator++() {
                  _rowPtrIter++;
00320
00321
                  return *this;
00322
00323
00324
              // postfix
00325
              self_type operator++(int junk) {
00326
                 self_type cached = *this;
                  _rowPtrIter++;
00327
00328
                  return cached;
00329
00330
00331
              self_type &operator+=(difference_type offset) {
                  _rowPtrIter += offset;
00332
00333
                   return *this;
00334
00335
00336
              self_type &operator==(difference_type offset) {
00337
                  _rowPtrIter -= offset;
00338
                  return *this;
00339
00340
00341
              // iter - n
00342
              self_type operator-(difference_type offset) {
00343
                self_type cache(*this);
cache -= offset;
00344
00345
                  return cache;
00346
              }
00347
00348
              // iter + n
              self_type operator+(difference_type offset) {
00350
                self_type cache(*this);
00351
                  cache += offset;
00352
                  return cache;
00353
00354
               // n + iter
00355
              friend self_type operator+(const difference_type &offset,
00356
                                          const self_type &sec) {
00357
                   self_type cache(sec);
00358
                  cache += offset;
00359
                  return cache:
00360
00361
00362
              reference operator[](difference_type offset) {
00363
                   return *(*this + offset);
00364
00365
00366
              bool operator<(const self type &other) {
```

```
return other - (*this) > 0; //
00368
00369
00370
              bool operator>(const self_type &other) {
                  return other < (*this);</pre>
00371
00372
00373
00374
              [[nodiscard]] self_type &operator*() { return *this; }
00375
              // [[nodiscard]] self_type &operator->() { return *this; }
00376
00377
              [[nodiscard]] bool operator == (const self_type &rhs) {
00378
                  return rowPtrIter == rhs. rowPtrIter;
00379
00380
              [[nodiscard]] bool operator!=(const self_type &rhs) {
00381
                  return _rowPtrIter != rhs._rowPtrIter;
00382
00383
00384
          private:
00385
              std::vector<size_type>::iterator _rowPtrIter;
00386
              std::vector<size_type>::iterator _colIndicesIter;
00387
              typename std::vector<REAL>::iterator _valIter;
00388
00389
00390
          class const_row_iterator {
00391
          public:
00392
              using self_type = const_row_iterator;
00393
00394
               // conform to the iterator traits
              // https://en.cppreference.com/w/cpp/iterator/iterator_traits
00395
00396
              using difference_type = std::ptrdiff_t;
              using value_type = self_type;
using pointer = self_type *;
using reference = self_type &;
00397
00398
00399
00400
              using iterator_category = std::bidirectional_iterator_tag;
00401
00402
              const row iterator(
00403
                  std::vector<size_type>::const_iterator rowPtrIter,
                  std::vector<size_type>::const_iterator colIndicesIter,
00405
                  typename std::vector<REAL>::const_iterator valIter)
00406
                   : _rowPtrIter(rowPtrIter), _colIndicesIter(colIndicesIter),
00407
                     _valIter(valIter) {}
00408
00409
              [[nodiscard]] const column iterator begin() const {
00410
                  return const_column_iterator((_valIter + *_rowPtrIter));
00411
00412
               [[nodiscard]] const_column_iterator end() const {
00413
                  return const_column_iterator((_valIter + *(_rowPtrIter + 1)));
00414
              }
00415
00416
              [[nodiscard]] const column index iterator ibegin() const {
                  return const_column_index_iterator(
00418
                       (_valIter + *_rowPtrIter), (_colIndicesIter + *_rowPtrIter));
00419
00420
               [[nodiscard]] const_column_index_iterator iend() const {
00421
                  return const_column_index_iterator(
00422
                      (_valIter + *(_rowPtrIter + 1)),
                       (_colIndicesIter + *(_rowPtrIter + 1)));
00423
00424
              }
00425
00426
              [[nodiscard]] const_column_iterator cbegin() const {
00427
                  return this->begin();
00428
00429
              [[nodiscard]] const_column_iterator cend() const {
00430
                  return this->end(); //
00431
              }
00432
              // prefix
00433
              self_type &operator++() {
00434
                  _rowPtrIter++;
00435
00436
                  return *this;
00437
00438
00439
              // postfix
              self_type &operator++(int junk) {
    self_type cached = *this;
00440
00441
                  _rowPtrIter++;
00442
00443
                  return cached;
00444
00445
              self_type &operator+=(difference_type offset) {
00446
                  _rowPtrIter += offset;
00447
00448
                   return *this;
00449
00450
00451
              self_type &operator==(difference_type offset) {
                  _rowPtrIter -= offset;
00452
00453
                  return *this:
```

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```
00454
              }
00455
00456
              // iter - n
              self_type operator-(difference_type offset) {
00457
00458
                 self_type cache(*this);
cache -= offset;
00459
00460
                  return cache;
00461
00462
              // iter + n
00463
              self_type operator+(difference_type offset) {
00464
00465
                self_type cache(*this);
cache += offset;
00466
00467
                  return cache;
00468
              // n + iter
00469
              friend self_type operator+(const difference_type &offset,
00470
00471
                                          const self_type &sec) {
00472
                  self_type cache(sec);
00473
                  cache += offset;
00474
                  return cache;
00475
              }
00476
00477
              reference operator[](difference_type offset) {
00478
                  return *(*this + offset);
00479
00480
00481
              bool operator<(const self_type &other) {</pre>
00482
                return other - (*this) > 0; //
00483
00484
00485
              bool operator>(const self_type &other) {
00486
                 return other < (*this); //</pre>
00487
00488
              [[nodiscard]] self_type &operator*() { return *this; }
00489
00490
              // [[nodiscard]] self_type &operator->() { return this; }
00492
              [[nodiscard]] bool operator==(const self_type &rhs) {
00493
                 return _rowPtrIter == rhs._rowPtrIter;
00494
00495
              [[nodiscard]] bool operator!=(const self_type &rhs) {
00496
                  return _rowPtrIter != rhs._rowPtrIter;
00497
00498
00499
          private:
00500
             std::vector<size_type>::const_iterator _rowPtrIter;
00501
              std::vector<size_type>::const_iterator _colIndicesIter;
00502
              typename std::vector<REAL>::const_iterator _valIter;
00503
00504
00523
          [[nodiscard]] row_iterator begin() {
00524
             return row_iterator(_rowPtr.begin(), _colIndices.begin(),
00525
                                  _data.begin());
00526
00527
00546
          [[nodiscard]] row_iterator end() {
00547
              return row_iterator(_rowPtr.end() - 1, _colIndices.begin(),
00548
                                  _data.begin());
00549
00550
          [[nodiscard]] const_row_iterator cbegin() const {
00556
00557
              return const_row_iterator(_rowPtr.cbegin(), _colIndices.cbegin(),
00558
                                        _data.cbegin());
00559
00560
00566
          [[nodiscard]] const_row_iterator cend() const {
00567
              return const_row_iterator(_rowPtr.cend() - 1, _colIndices.cbeqin(),
00568
                                         data.cbegin());
00569
00570
00572
          [[nodiscard]] const_row_iterator begin() const { return this->cbegin(); }
00574
          [[nodiscard]] const_row_iterator end() const { return this->cend(); }
00575
00600
          void scientific(bool b) const { bScientific = b; }
00601
          size_type iwidth() const { return nIndexWidth; }
00603
00604
00606
          size_type width() const { return nValueWidth; }
00607
00609
          size type precision() const { return nValuePrecision; }
00610
00612
          void iwidth(size_type i) const { nIndexWidth = i; }
00613
00615
          void width(size_type i) const { nValueWidth = i; }
00616
00618
          void precision(size type i) const { nValuePrecision = i; }
```

```
column_iterator find(const size_type row_index,
00620
00621
                                const size_type col_index) const {
00622
              checkIfAccessIsInBounds(row_index, col_index);
00623
00624
              using value_pair = typename const_column_index_iterator::value_type;
              auto row = const_row_iterator(_rowPtr.begin() + row_index,
00626
                                              _colIndices.begin(), _data.begin());
00627
              return std::find_if(row.ibegin(), row.iend(),
00628
                                    [col_index] (value_pair el) {
                                        \ensuremath{//} only care for the index here since the value
00629
                                        // is unknown
00630
00631
                                       return el.second == col_index;
00632
                                   });
00633
00634
00635
          bool exists(const size_type row_index, const size_type col_index) const {
              auto row = const_row_iterator(_rowPtr.begin() + row_index,
00636
                                              _colIndices.begin(), _data.begin());
00637
00638
              return find(row_index, col_index) != row.iend();
00639
00640
00642
          REAL &get(const size_type row_index, const size_type col_index) {
00643
              checkIfAccessIsInBounds(row_index, col_index);
00644
              // look for the entry
              using value_pair = typename const_column_index_iterator::value_type;
00646
              auto row = row_iterator(_rowPtr.begin() + row_index,
00647
                                       _colIndices.begin(), _data.begin());
00648
              auto result =
                  std::find_if(row.ibegin(), row.iend(), [col_index](value_pair el) {
00649
00650
                      // only care for the index here
00651
                       // since the value is unknown
00652
                       // anyways
00653
                      return el.second == col_index;
00654
                  });
              // we found something within the right row
00655
00656
              if (result != row.iend()) {
                  return result.value();
00658
00659
              throw std::out_of_range(
00660
                   "There is no non-zero element for these given indicies!");
00661
         }
00662
00664
          const REAL &operator()(const size_type row_index,
                                  const size_type col_index) const {
00665
00666
              checkIfAccessIsInBounds(row_index, col_index);
00667
00668
              using value_pair = typename const_column_index_iterator::value_type;
              auto row = const_row_iterator(_rowPtr.begin() + row_index,
00669
00670
                                              _colIndices.begin(), _data.begin());
              auto result =
00671
00672
                  std::find_if(row.ibegin(), row.iend(), [col_index](value_pair el) {
00673
                      \ensuremath{//} only care for the index here since the value is \ensuremath{\mathsf{unknown}}
00674
                       return el.second == col_index;
00675
                  });
00676
              // we found something within the right row
00677
              if (result != row.iend()) {
00678
                  return result.value();
00679
00680
              return _zero;
00681
          }
00682
00684
          [[nodiscard]] bool operator==(const SparseMatrix &other) const {
             return (_data == other._data) and
00685
00686
                      (_rowPtr == other._rowPtr) and
00687
                      (_colIndices == other._colIndices) and
00688
                      (m_cols == other.m_cols) and
                      (m_rows == other.m_rows);
00689
00690
          }
00693
          [[nodiscard]] bool operator!=(const SparseMatrix &other) const {
00694
              return not (*this == other);
00695
00696
00697
          // delete all the invalid comparisons
          bool operator<(const SparseMatrix &other) = delete;
00698
00699
          bool operator>(const SparseMatrix &other) = delete;
00700
          bool operator<=(const SparseMatrix &other) = delete;</pre>
          bool operator>=(const SparseMatrix &other) = delete;
00701
00702
00703
          SparseMatrix transpose() const {
              // TODO: remove / find bug here!
SparseMatrix::builder builder(m_cols, m_rows);
00704
00705
00706
              SparseMatrix::size_type curr_row = 0;
              for (auto &row : (*this)) {
    for (auto it = row.ibegin(); it != row.iend(); it++) {
00707
00708
                      builder.addEntry(it.index(), curr_row, it.value());
00709
```

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```
00710
00711
                    curr_row++;
00712
               }
00713
00714
                return builder.build();
00715
           }
00716
00719
           [[nodiscard]] SparseMatrix operator*=(const REAL scalar) {
00720
                // This could also be done out of order
                00721
00722
00723
00724
00727
           [[nodiscard]] SparseMatrix operator/=(const REAL scalar) {
00728
                \ensuremath{//} This could also be done out of order
                00729
00730
00731
00741
           template <class V>
00742
           void mv(Vector<V> &result, const Vector<V> &x) const {
00743
               static_assert(std::is_convertible<V, REAL>::value,
00744
                                "The types in the Matrix vector multiplication cant be "
00745
                                "converted properly!");
00746
00747
                if (result.size() != this->colsize()) {
00748
                    HDNUM_ERROR (
                         (std::string("The result vector has the wrong dimension! ") +
  "Vector dimension " + std::to_string(result.size()) +
  " != " + std::to_string(this->colsize()) + " colsize"));
00749
00750
00751
00752
                }
00753
00754
                if (x.size() != this->colsize()) {
00755
                    HDNUM_ERROR (
                         (std::string("The input vector has the wrong dimension! ") +
  "Vector dimension " + std::to_string(x.size()) +
  " != " + std::to_string(this->colsize()) + " colsize"));
00756
00757
00758
00759
               }
00760
00761
                size_type curr_row = 0;
00762
                for (auto row : (*this)) {
                   result[curr_row] = std::accumulate(
  row.ibegin(), row.iend(), V {}, [&](V result, auto el) -> V {
00763
00764
                             return result + (x[el.second] * el.first);
00765
00766
                        });
00767
                    curr_row++;
00768
               }
00769
           }
00770
00778
           [[nodiscard]] Vector<REAL> operator*(const Vector<REAL> &x) const {
00779
                hdnum::Vector<REAL> result(this->colsize(), 0);
00780
                this->mv(result, x);
00781
                return result;
00782
           }
00783
00792
           template <class V>
00793
           void umv(Vector<V> &result, const Vector<V> &x) const {
               static_assert(std::is_convertible<V, REAL>::value,
00794
00795
                                "The types in the Matrix vector multiplication cant be "
                                "converted properly!");
00796
00797
00798
                if (result.size() != this->colsize()) {
00799
                    HDNUM_ERROR (
00800
                        (std::string("The result vector has the wrong dimension! ") +
00801
                          "Vector dimension " + std::to_string(result.size()) +
                          "!= " + std::to_string(this->colsize()) + " colsize"));
00802
00803
                }
00804
00805
                if (x.size() != this->colsize()) {
00806
                    HDNUM_ERROR (
00807
                        (std::string("The input vector has the wrong dimension! ") +
                          "Vector dimension " + std::to_string(result.size()) +
" != " + std::to_string(this->colsize()) + " colsize"));
00808
00809
00810
               }
00811
00812
                size_type curr_row {};
00813
                for (auto row : (*this)) {
                    result[curr_row] += std::accumulate(
   row.ibegin(), row.iend(), V {}, [&](V result, auto el) -> V {
      return result + (x[el.second] * el.first);
00814
00815
00816
                        });
00817
00818
                    curr_row++;
00819
               }
00820
           }
00821
00822 private:
00823
           template <typename norm type>
```

```
norm_type norm_infty_impl() const {
             norm_type norm {};
00825
00826
              for (auto row : *this) {
00827
                 norm_type rowsum =
                      00828
00829
00831
00832
                  if (norm < rowsum) {</pre>
                      norm = rowsum;
00833
00834
                  }
00835
00836
              return norm;
00837
00838
00839 public:
         auto norm_infty() const {
   if constexpr (is_specialization<REAL, std::complex> {}) {
00847
00848
                  return norm_infty_impl<double>();
00850
              } else {
00851
                 return norm_infty_impl<REAL>();
00852
              }
00853
          }
00854
00855
          [[nodiscard]] std::string to_string() const noexcept {
            00856
00857
00858
00859
          }
00860
00861
          void print() const noexcept { std::cout « *this; }
00862
00886
          static SparseMatrix identity(const size_type dimN) {
00887
              auto builder = typename SparseMatrix<REAL>::builder(dimN, dimN);
              for (typename SparseMatrix<REAL>::size_type i = 0; i < dimN; ++i) {</pre>
00888
00889
                  builder.addEntry(i, i, REAL {1});
00890
              return builder.build();
00892
00893
00918
          SparseMatrix<REAL> matchingIdentity() const { return identity(m_cols); }
00919
00920
          class builder {
              size_type m_rows {}; // Number of Matrix rows, 0 by default
size_type m_cols {}; // Number of Matrix columns, 0 by default
00921
00922
00923
              std::vector<std::map<size_type, REAL» _rows;</pre>
00924
00925
          public:
              builder(size_type new_m_rows, size_type new_m_cols)
00926
00927
                  : m_rows {new_m_rows}, m_cols {new_m_cols}, _rows {m_rows} {}
00928
00929
              builder(const std::initializer_list<std::initializer_list<REAL» &v)</pre>
00930
                  : m_rows {v.size()}, m_cols {v.begin()->size()}, _rows(m_rows) {
00931
                  size_type i = 0;
                  for (auto &row : v) {
    size_type j = 0;
    for (const REAL &element : row) {
00932
00933
00934
00935
                           addEntry(i, j, element);
00936
                           j++;
00937
00938
                       i++:
00939
                  }
00940
              }
00941
00942
              builder() = default;
00943
00944
              std::pair<typename std::map<size_type, REAL>::iterator, bool> addEntry(
00945
                  size_type i, size_type j, REAL value) {
return _rows.at(i).emplace(j, value);
00946
00947
00948
00949
              std::pair<typename std::map<size_type, REAL>::iterator, bool> addEntry(
                  size_type i, size_type j) {
return addEntry(i, j, REAL {});
00950
00951
00952
00953
00954
              [[nodiscard]] bool operator==(
00955
                  const SparseMatrix::builder &other) const {
                  00956
00957
                         (_rows == other._rows);
00958
              }
00960
00961
               [[nodiscard]] bool operator!=(
00962
                  const SparseMatrix::builder &other) const {
00963
                  return not (*this == other);
00964
              }
```

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```
00965
00966
                [[nodiscard]] size_type colsize() const noexcept { return m_cols; }
00967
                [[nodiscard]] size_type rowsize() const noexcept { return m_rows; }
00968
00969
                size_type setNumCols(size_type new_m_cols) noexcept {
00970
                    m cols = new m cols;
00971
                    return m_cols;
00972
                size_type setNumRows(size_type new_m_rows) {
00973
00974
                    m_rows = new_m_rows;
00975
                    _rows.resize(m_cols);
00976
                     return m_rows;
00977
                }
00978
00979
                void clear() noexcept {
                    for (auto &row : _rows) {
00980
00981
                         row.clear():
00982
00983
00984
                [[nodiscard]] std::string to_string() const {
00985
                    std::string output;
for (std::size_t i = 0; i < _rows.size(); i++) {</pre>
00986
00987
                         for (const auto &indexpair : _rows[i]) {
   output += std::to_string(i) + ", " +
00988
00989
                                         std::to_string(indexpair.first) + " => " +
00990
00991
                                          std::to_string(indexpair.second) + "\n";
00992
00993
                     }
00994
                     return output:
00995
00996
00997
                [[nodiscard]] SparseMatrix build() {
00998
                     auto result = SparseMatrix<REAL>(m_rows, m_cols);
00999
                     for (std::size_t i = 0; i < _rows.size(); i++) {
    result._rowPtr[i + 1] = result._rowPtr[i];
    for (const auto &indexpair : _rows[i]) {</pre>
01000
01001
01003
                             result._colIndices.push_back(indexpair.first);
01004
                              result._data.push_back(indexpair.second);
01005
                              result._rowPtr[i + 1]++;
01006
                         }
01007
                     }
01008
                     return result;
01009
                }
01010
           };
01011 };
01012
01013 template <typename REAL>
01014 bool SparseMatrix<REAL>::bScientific = true;
01015 template <typename REAL>
01016 std::size_t SparseMatrix<REAL>::nIndexWidth = 10;
01017 template <typename REAL>
01018 std::size_t SparseMatrix<REAL>::nValueWidth = 10;
01019 template <typename REAL>
01020 std::size_t SparseMatrix<REAL>::nValuePrecision = 3;
01021 template <typename REAL>
01022 const REAL SparseMatrix<REAL>::_zero {};
01023
01024 template <typename REAL>
01025 std::ostream &operator«(std::ostream &s, const SparseMatrix<REAL> &A) {
01026
           using size_type = typename SparseMatrix<REAL>::size_type;
01027
01028
           s « std::endl;
           s « " " « std::setw(A.iwidth()) « " " « " ";
01029
01030
           for (size_type j = 0; j < A.colsize(); ++j) {
    s « std::setw(A.width()) « j « " ";</pre>
01031
01032
01033
           s « std::endl;
01035
           for (size_type i = 0; i < A.rowsize(); ++i) {
    s « " " « std::setw(A.iwidth()) « i « " ";</pre>
01036
01037
                for (size_type j = 0; j < A.colsize(); ++j) {</pre>
01038
                     if (A.scientific()) {
01039
01040
                         s « std::setw(A.width()) « std::scientific « std::showpoint
01041
                           « std::setprecision(A.precision()) « A(i, j) « " ";
01042
                     } else {
01043
                         s 	ext{ w std::setw(A.width()) } 	ext{ w std::fixed } 	ext{ w std::showpoint }
01044
                           « std::setprecision(A.precision()) « A(i, j) «
01045
                    }
01046
01047
                s « std::endl;
01048
           }
01049
           return s;
01050 }
01051
```

```
01053 template <typename REAL>
01054 inline void zero(SparseMatrix<REAL> &A) {
01055
           A = SparseMatrix<REAL>(A.rowsize(), A.colsize());
01056 }
01057
01091 template <class REAL>
01092 inline void identity(SparseMatrix<REAL> &A) {
01093
          if (A.rowsize() != A.colsize()) {
01094
               HDNUM_ERROR("Will not overwrite A since Dimensions are not equal!");
01095
01096
           A = SparseMatrix<REAL>::identity(A.colsize());
01097 }
01098
01099 template <typename REAL>
01100 inline void readMatrixFromFile(const std::string &filename,
01101
                                         SparseMatrix<REAL> &A) {
           // Format taken from here:
01102
           // https://math.nist.gov/MatrixMarket/formats.html#coord
01103
01104
01105
           using size_type = typename SparseMatrix<REAL>::size_type;
01106
           std::string buffer;
01107
           std::ifstream fin(filename);
           size_type i = 0;
size_type j = 0;
01108
01109
01110
           size_type non_zeros = 0;
01111
           if (fin.is_open()) {
01112
               // ignore all comments from the file (starting with %) while (fin.peek() == '%') fin.ignore(2048, '\n');
01113
01114
01115
               std::getline(fin, buffer);
std::istringstream first_line(buffer);
01116
01117
01118
               first_line » i » j » non_zeros;
01119
01120
               auto builder = typename SparseMatrix<REAL>::builder(i, j);
01121
               while (std::getline(fin, buffer)) {
01122
01123
                   std::istringstream iss(buffer);
01124
01125
                    REAL value {};
                   iss » i » j » value; // i-1, j-1, because matrix market does not use zero based indexing builder.addEntry(i - 1, j - 1, value);
01126
01127
01128
01129
01130
               A = builder.build();
01131
               fin.close();
01132
          } else
               HDNUM_ERROR(("Could not osspen file! \"" + filename + "\""));
01133
           }
01134
01135 }
01136
01137 } // namespace hdnum
01138
01139 #endif // SPARSEMATRIX HH
```

5.24 src/timer.hh File Reference

A simple timing class.

```
#include <sys/resource.h>
#include <ctime>
#include <cstring>
#include <cerrno>
#include "exceptions.hh"
```

Classes

· class hdnum::TimerError

Exception thrown by the Timer class

· class hdnum::Timer

A simple stop watch.

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5.24.1 Detailed Description

A simple timing class.

5.25 timer.hh

Go to the documentation of this file.

```
00001 #ifndef DUNE_TIMER_HH
00002 #define DUNE_TIMER_HH
00003
00004 #ifndef TIMER_USE_STD_CLOCK
00005 // headers for getrusage(2)
00006 #include <sys/resource.h>
00007 #endif
80000
00009 #include <ctime>
00010
00011 // headers for stderror(3)
00012 #include <cstring>
00013
00014 // access to errno in C++ \,
00015 #include <cerrno>
00016
00017 #include "exceptions.hh"
00018
00019 namespace hdnum {
00020
00026 class TimerError : public SystemError {};
00027
00028
00041 class Timer
00042 {
00043 public:
00045
              Timer ()
00046
00047
                reset();
00048
00049
00051
               void reset()
00052
00053 #ifdef TIMER_USE_STD_CLOCK
00054
               cstart = std::clock();
00055 #else
00056
                rusage ru;
00057
               if (getrusage(RUSAGE_SELF, &ru))
00058
                  HDNUM_THROW(TimerError, strerror(errno));
00059
                cstart = ru.ru_utime;
00060 #endif
00061
              }
00064
               double elapsed () const
00065
00066 #ifdef TIMER_USE_STD_CLOCK
               return (std::clock()-cstart) / static_cast<double>(CLOCKS_PER_SEC);
00067
00068 #else
00069
               if (getrusage(RUSAGE_SELF, &ru))
HDNUM_THROW(TimerError, strerror(errno));
00070
00071
00072
                 return 1.0 * (ru.ru_utime.tv_sec - cstart.tv_sec) + (ru.ru_utime.tv_usec - cstart.tv_usec) /
      (1000.0 * 1000.0);
00073 #endif
00074
00075
00076 private:
00077 #ifdef TIMER_USE_STD_CLOCK
00078 std::clock_t cstart;
        std::clock_t cstart;
00079 #else
08000
       struct timeval cstart;
00081 #endif
00082 }; // end class Timer
00083
00084 \} // end namespace
00085
00086 #endif
```

5.26 vector.hh

```
00001 // -*- tab-width: 4; indent-tabs-mode: nil; c-basic-offset: 2 -*-
00002 /*
00003 * File: vect
00004 * Author: ngo
               vector.hh
00005 *
00006 * Created on April 14th, 2011
00007 */
00008
00009 #ifndef _VECTOR_HH
00010 #define _VECTOR_HH
00012 #include <assert.h>
00013
00014 #include <cmath>
00015 #include <cstdlib>
00016 #include <fstream>
00017 #include <iomanip>
00018 #include <iostream>
00019 #include <sstream>
00020 #include <vector>
00021
00022 #include "exceptions.hh"
00023
00024 namespace hdnum {
00025
00029
       template<typename REAL>
00030
       class Vector : public std::vector<REAL> // inherit from the STL vector
00031
00032
       public:
         typedef std::size_t size_type;
00035
00036
       private:
       static bool bScientific;
static std::size_t nIndexWidth;
00037
00038
00039
         static std::size t nValueWidth;
00040
         static std::size_t nValuePrecision;
00041
       public:
00042
00043
00045
          Vector() : std::vector<REAL>()
00046
00047
00048
                  00050
          Vector( const size_t size,
00051
00052
00053
            : std::vector<REAL>( size, defaultvalue_ )
00054
00055
00056
00058
          Vector (const std::initializer_list<REAL> &v)
00059
00060
           for (auto elem : v) this->push back(elem);
00061
00062
00063
00064
00086
          Vector& operator=( const REAL value )
00087
00088
            const size t s = this->size();
            Vector & self = *this;
00089
00090
           for (size_t i=0; i<s; ++i)</pre>
00091
              self[i] = value;
00092
            return *this;
00093
          }
00094
00104
          Vector sub (size_type i, size_type m)
00105
00106
            Vector v(m);
           Vector &self = *this;
00107
00108
            size_type k=0;
           for (size_type j=i; j<i+m; j++) {
   v[k]=self[j];
   k++;</pre>
00109
00110
00111
00112
00113
            return v;
00114
          }
00115
00116
00117
00118 #ifdef DOXYGEN
00150
          Vector& operator=( const Vector& y )
00151
            // It is already implemented in the STL vector class itself!
00152
00153
```

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```
00154 #endif
00155
00156
00157
           Vector& operator*=( const REAL value )
00159
00160
             Vector &self = *this;
for (size_t i = 0; i < this->size(); ++i)
  self[i] *= value;
00161
00162
00163
00164
             return *this;
           }
00165
00166
00167
00169
           Vector& operator/=( const REAL value )
00170
            Vector &self = *this;
for (size_t i = 0; i < this->size(); ++i)
   self[i] /= value;
return *this;
00171
00172
00173
00174
00175
00176
00177
00179
           Vector& operator+=( const Vector & y )
00180
00181
             assert( this->size() == y.size());
00182
             Vector &self = *this;
for (size_t i = 0; i < this->size(); ++i)
00183
00184
              self[i] += y[i];
00185
             return *this;
00186
00187
00188
00190
           Vector& operator==( const Vector & y )
00191
00192
             assert( this->size() == y.size());
             Vector &self = *this;
for (size_t i = 0; i < this->size(); ++i)
00193
00194
              self[i] -= y[i];
00195
00196
             return *this;
00197
00198
00199
00201
           Vector & update(const REAL alpha, const Vector & v)
00202
00203
             assert( this->size() == y.size());
00204
             Vector &self = *this;
             for (size_t i = 0; i < this->size(); ++i)
  self[i] += alpha * y[i];
00205
00206
             return *this;
00207
00208
00209
00210
00242
           REAL operator*(Vector & x) const
00243
             assert( x.size() == this->size() ); // checks if the dimensions of the two vectors are equal
00244
00245
             REAL sum(0);
00246
             const Vector & self = *this;
00247
             for( size_t i = 0; i < this->size(); ++i )
00248
              sum += self[i] * x[i];
00249
             return sum;
00250
00251
00252
00253
00254
00287
           Vector operator+(Vector & x) const
00288
00289
             assert(x.size() == this->size()); // checks if the dimensions of the two vectors are equal
00290
             Vector sum( *this );
00291
             sum += x;
00292
             return sum;
00293
00294
00295
00296
00329
           Vector operator-(Vector & x) const
00330
00331
             assert(\ x.size() == this -> size()); // checks if the dimensions of the two vectors are equal
            Vector sum( *this );
sum -= x;
00332
00333
00334
             return sum;
00335
00336
00337
00338
00340
           REAL two_norm_2() const
00341
```

```
00342
            REAL sum(0);
            const Vector & self = *this;
for (size_t i = 0; i < (size_t) this->size(); ++i)
  sum += self[i] * self[i];
00343
00344
00345
00346
            return sum;
00347
00348
00373
          REAL two_norm() const
00374
00375
            return sqrt(two_norm_2());
00376
00377
00379
          bool scientific() const
00380
00381
            return bScientific;
00382
00383
00411
          void scientific (bool b) const
00412
00413
            bScientific=b;
00414
00415
00417
          std::size_t iwidth () const
00418
00419
            return nIndexWidth;
00420
00421
00423
          std::size_t width () const
00424
00425
            return nValueWidth;
00426
00427
00429
          std::size_t precision () const
00430
00431
            return nValuePrecision;
00432
00433
00435
          void iwidth (std::size_t i) const
00436
00437
            nIndexWidth=i;
00438
00439
00441
          void width (std::size t i) const
00442
00443
            nValueWidth=i;
00444
00445
00447
          void precision (std::size_t i) const
00448
00449
            nValuePrecision=i:
00450
00451
00452
00453
00454
00455
00456
        template<typename REAL>
00457
        bool Vector<REAL>::bScientific = true;
00458
00459
        template<typename REAL>
        std::size_t Vector<REAL>::nIndexWidth = 2;
00460
00461
00462
        template<typename REAL>
00463
        std::size_t Vector<REAL>::nValueWidth = 15;
00464
00465
        template<typename REAL>
00466
        std::size_t Vector<REAL>::nValuePrecision = 7;
00467
00468
00490
        template <typename REAL>
00491
        inline std::ostream & operator «(std::ostream & os, const Vector<REAL> & x)
00492
00493
          os « std::endl;
00494
00495
          for (size_t r = 0; r < x.size(); ++r)
00496
00497
               if( x.scientific() )
00498
                   os « "["
00499
00500
                      « std::setw(x.iwidth())
00501
                     « r
« "]"
00502
00503
                      « std::scientific
00504
                      « std::showpoint
00505
                      « std::setw( x.width() )
00506
                      « std::setprecision( x.precision() )
00507
                     « x[r]
```

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```
« std::endl;
00509
00510
              else
00511
                {
                  os « "["
00512
00513
                     « std::setw(x.iwidth())
00514
                      « r
« "]"
00515
00516
                      « std::fixed
00517
                      « std::showpoint
                      « std::setw( x.width() )
00518
00519
                      « std::setprecision( x.precision() )
00520
                      « x[r]
00521
                      « std::endl;
00522
                }
00523
00524
          return os:
00525
        }
00526
00527
00528
00551
        template<typename REAL>
00552
        inline void gnuplot(
                             const std::string& fname,
const Vector<REAL> x
00553
00554
00555
00556
00557
          std::fstream f(fname.c_str(),std::ios::out);
00558
          for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00559
00560
              if( x.scientific() )
00561
00562
                   f « std::setw(x.width())
00563
                     « i
00564
                     « std::scientific
00565
                     « std::showpoint
00566
                     « std::setw( x.width() )
00567
                     « std::setprecision( x.precision() )
00568
                     « x[i]
00569
                     « std::endl;
00570
                }
00571
              else
00572
                {
00573
                   f « std::setw(x.width())
00574
00575
                     « std::fixed
00576
                     « std::showpoint
                     « std::setw( x.width() )
00577
00578
                     « std::setprecision( x.precision() )
00579
                     « x[i]
00580
                     « std::endl;
00581
                }
00582
00583
          f.close();
00584
00585
00586
        template<typename REAL>
00587
        inline void gnuplot(
00588
                              const std::string& fname,
00589
                             const std::vector<std::string>& t,
00590
                             const Vector<REAL> x
00591
00592
00593
          std::fstream f(fname.c_str(),std::ios::out);
00594
          for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00595
              if( x.scientific() )
00596
00597
                  f « t[i] « " "
00598
00599
                     « std::scientific
00600
                     « std::showpoint
00601
                     « std::setw( x.width() )
00602
                     « std::setprecision( x.precision() )
00603
                     « x[i]
00604
                     « std::endl;
00605
                }
00606
              else
00607
                  f « t[i] « " "
00608
00609
                     « std::fixed
00610
                     « std::showpoint
                     « std::setw( x.width() )
00611
00612
                     « std::setprecision( x.precision() )
00613
                     « x[i]
00614
                     « std::endl;
00615
                }
00616
```

```
00617
          f.close();
00618
00619
00621
        template<typename REAL>
00622
        inline void gnuplot (
00623
                             const std::string& fname,
00624
                             const Vector<REAL> x,
00625
                             const Vector<REAL> y
00626
00627
          std::fstream f(fname.c_str(),std::ios::out);
00628
          for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00629
00630
00631
              if( x.scientific() )
00632
00633
                   f « std::setw(x.width())
00634
                     « i
00635
                     « std::scientific
00636
                     « std::showpoint
00637
                     « std::setw( x.width() )
00638
                     « std::setprecision( x.precision() )
                     « x[i]
« " "
00639
00640
                     « std::setw( x.width() )
00641
00642
                     « std::setprecision( x.precision() )
00643
                     « y[i]
00644
                     « std::endl;
00645
              else
00646
00647
                {
00648
                  f « std::setw(x.width())
00649
                     « i
00650
                     « std::fixed
00651
                     « std::showpoint
00652
                     00653
                     « std::setprecision( x.precision() )
00654
                    « x[i]
« " "
00655
00656
                     « std::setw( x.width() )
00657
                     « std::setprecision( x.precision() )
00658
                     « y[i]
00659
                     « std::endl;
00660
                }
00661
00662
00663
          f.close();
00664
       }
00665
00666
00667
00696
        template<typename REAL>
00697
        inline void readVectorFromFile (const std::string& filename, Vector<REAL> &vector)
00698
          std::string buffer;
std::ifstream fin( filename.c_str() );
00699
00700
00701
          if( fin.is_open() ){
00702
            while(fin){
00703
              std::string sub;
00704
              fin » sub;
              //std::cout « " sub = " « sub.c_str() « ": ";
00705
              if( sub.length()>0 ){
00706
00707
               REAL a = atof(sub.c_str());
00708
                //std::cout « std::fixed « std::setw(10) « std::setprecision(5) « a;
00709
                vector.push_back(a);
00710
00711
00712
            fin.close();
00713
00714
          else{
00715
            HDNUM_ERROR("Could not open file!");
00716
00717
00718
00719
00721
        template<class REAL>
00722
        inline void zero (Vector<REAL>& x)
00723
00724
         for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00725
            x[i] = REAL(0);
00726
00727
00729
        template<class REAL>
00730
        inline REAL norm (Vector<REAL> x)
00731
          REAL sum(0.0);
for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)
  sum += x[i]*x[i];</pre>
00732
00733
00734
```

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```
00735
          return sqrt(sum);
00736
00737
00739
        template<class REAL>
00740
        inline void fill (Vector<REAL>& x, const REAL t)
00741
00742
        for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00743
            x[i] = t;
00744
00745
00768
        template<class REAL>
00769
        inline void fill (Vector<REAL>& x, const REAL& t, const REAL& dt)
00770
00771
         REAL myt(t);
          for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00772
           x[i] = myt;
myt += dt;
}
00773
00774
00775
00776
00777
        }
00778
00779
00802
        template<class REAL>
        inline void unitvector (Vector<REAL> & x, std::size_t j)
00803
00804
00805
         for (typename Vector<REAL>::size_type i=0; i<x.size(); i++)</pre>
00806
             x[i] = REAL(1);
00807
00808
            else
00809
             x[i] = REAL(0);
00810
       }
00811
00812
00813 } // end of namespace hdnum
00814
00815 #endif /* _VECTOR_HH */
```

Index

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