RingDecomposerLib 1.0

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Contents

Chapter 1

Main Page

The RingDecomposerLib is a library for calculation of the unique ring families and related ring topology descriptions.

It is developed at the University of Hamburg, ZBH - Center for Bioinformatics by Niek Andresen, Florian Flachsenberg and Matthias Rarey.

The library is distributed under BSD New license, see the file LICENSE and BSD New.

Please cite:

Kolodzik, A.; Urbaczek, S.; Rarey, M. Unique Ring Families: A Chemically Meaningful Description of Molecular Ring Topologies. J. Chem. Inf. Model., 2012, 52, pp 2013-2021

Flachsenberg, F.; Andresen, N.; Rarey, M. RingDecomposerLib: An Open-Source Implementation of Unique Ring Families and other Cycle Bases. SUBMITTED

This package contains a C-library as well as an optional Python wrapper for the library.

These pages are the documentation of the RingDecomposerLib library and the Python wrapper.

For installation instructions see here: Installation instructions

Core library RingDecomposerLib

The documentation of the C library is available here: RingDecomposerLib.h

The testing util for the library documented is here: Test.c

A minimal example can be found here: Minimal Example

Python wrapper py_urf

The documentation of the Python wrapper can be found here: py_rdl.Calculator.Calculator, py_rdl.Graph.Graph

Example scripts that show how to use the Python wrapper together with RDKit can be found here: Minimal RDKit Example, RDKit Example

A minimal example im Python looks like this:

```
import py_rdl
data = py_rdl.Calculator.get_calculated_result([(0,1),(1,2),(2,3),(3,4),(4,5),(5,0)])
print(data.get_nof_urf())
```

Chapter 2

Minimal Example

A minimal example for the C library is:

```c
/*
 * This file is part of the RingDecomposerLib, licensed
 * under BSD New license (see LICENSE in the root directory).
 * Copyright (c) 2016
 * University of Hamburg, ZBH - Center for Bioinformatics
 * Niek Andresen, Florian Flachsenberg, Matthias Rarey
 *
 * Please cite:
 *
 * Kolodzik, A.; Urbaczek, S.; Rarey, M.
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 * of Molecular Ring Topologies.
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 *
 * Flachsenberg, F.; Andresen, N.; Rarey, M.
 * RingDecomposerLib: An Open-Source Implementation of
 * Unique Ring Families and other Cycle Bases.
 * SUBMITTED
 */

#include <assert.h>
#include <stdio.h>

#include "RingDecomposerLib.h"

int main()
{
  RDL_graph* graph;
  RDL_data* data;
  unsigned nof_urf, i;
  double nof_rc;
  const unsigned nof_edges=10, nof_nodes=8;
  unsigned edges[10][2] = {
    {0,1}, {1,2}, {2,3}, {3,4}, {4,5},
    {5,0}, {0,6}, {6,2}, {3,7}, {7,5} };
  /* step 1: prepare RDL_graph structure input graph */
  graph = RDL_initNewGraph(nof_nodes);
  for (i = 0; i < nof_edges; ++i) {
    RDL_addUEdge(graph, edges[i][0], edges[i][1]);
  }
  /* step 2: calculate URFs, RCFs */
  data = RDL_calculate(graph);
  /* check that calculation was successful */
  assert(data != NULL);
  /* step 3: how many URFs and RCs does the graph have? */
  nof_urf = RDL_getNofURF(data);
  nof_rc = RDL_getNofRC(data);

  RDL_cycle *cycle;
  RDL_cycleIterator *it = RDL_getRCyclesIterator(data);
  while(!RDL_cycleIteratorAtEnd(it)) {
    cycle = RDL_cycleIteratorGetCycle(it);
    /* <do something with the cycle> */
    RDL_deleteCycle(cycle);
    RDL_cycleIteratorNext(it);
  }
  RDL_deleteCycleIterator(it);

  /* delete data and graph */
  RDL_deleteData(data);
```

```
  printf("URFs: %d\n RCs: %.0f\n", nof_urf, nof_rc);

  return 0;
}
```

Chapter 3

Minimal RDKit Example

A minimal example for using the RingDecomposerLib together with RDKit is:

```
1 # This file is part of the RingDecomposerLib, licensed
2 # under BSD New license (see LICENSE in the root directory).
3 # Copyright (c) 2016
4 # University of Hamburg, ZBH - Center for Bioinformatics
5 # Niek Andresen, Florian Flachsenberg, Matthias Rarey
6 #
7 # Please cite:
8 #
9 # Kolodzik, A.; Urbaczek, S.; Rarey, M.
10 # Unique Ring Families: A Chemically Meaningful Description
11 # of Molecular Ring Topologies.
12 # J. Chem. Inf. Model., 2012, 52, pp 2013-2021
13 #
14 # Flachsenberg, F.; Andresen, N.; Rarey, M.
15 # RingDecomposerLib: An Open-Source Implementation of
16 # Unique Ring Families and other Cycle Bases.
17 # SUBMITTED
18
19 from __future__ import print_function
20 import py_rdl
21 import rdkit.Chem
22
23 # p-cyclophane as URF example
24 molecule = rdkit.Chem.MolFromSmiles('C1c2ccc(cc2)CCc2ccc(cc2)C1')
25
26 # calculation step
27 data = py_rdl.Calculator.get_calculated_result(
28            molecule.GetBonds(),              # pass edges
29            rdkit.Chem.Bond.GetBeginAtom,     # get first atom
30            rdkit.Chem.Bond.GetEndAtom,       # get second atom
31            rdkit.Chem.Atom.GetIdx,           # identify atom
32            rdkit.Chem.Bond.GetIdx            # identify edge
33        )
34
35 # iterate over URFs
36 for urf in data.urfs:
37     # print URF
38     print(urf)
39     # URF can be used as an index, get RCs
40     rcs = data.get_relevant_cycles_for_urf(urf)
41     # print RCs
42     for rc in rcs:
43         print(rc)
```

Chapter 4

RDKit Example

A more complex examplefor using the RingDecomposerLib together with RDKit is:

```
# This file is part of the RingDecomposerLib, licensed
# under BSD New license (see LICENSE in the root directory).
# Copyright (c) 2016
# University of Hamburg, ZBH - Center for Bioinformatics
# Niek Andresen, Florian Flachsenberg, Matthias Rarey
#
# Please cite:
#
# Kolodzik, A.; Urbaczek, S.; Rarey, M.
# Unique Ring Families: A Chemically Meaningful Description
# of Molecular Ring Topologies.
# J. Chem. Inf. Model., 2012, 52, pp 2013-2021
#
# Flachsenberg, F.; Andresen, N.; Rarey, M.
# RingDecomposerLib: An Open-Source Implementation of
# Unique Ring Families and other Cycle Bases.
# SUBMITTED

## @file rdkit_demo.py
## @brief This file containes simple demo for using the
## Python wrapper
## of the RingDecomposerLib together with RDKit.
##
## usage:
##
##     rdkit_demo.py --input <input_file> [--output]
##
## The program takes as input a molecule file
## (.smi or .sdf) and reads in every molecule and
## calculates the ring topology and prints it to stdout.
##
## The parameter `--output` is optional. If specified,
## the script will write a number of SVG images,
## where RCs are marked according to family membership.

from __future__ import absolute_import, print_function

import argparse
import os
import random
import sys

import py_rdl

import rdkit.Chem
import rdkit.Chem.AllChem
import rdkit.Chem.Draw


def analyze_molecule(molecule):
    data = py_rdl.Calculator.get_calculated_result(
                molecule.GetBonds(),              # pass edges
                rdkit.Chem.Bond.GetBeginAtom,     # get first atom
                rdkit.Chem.Bond.GetEndAtom,       # get second atom
                rdkit.Chem.Atom.GetIdx,           # identify atom
                rdkit.Chem.Bond.GetIdx            # identify edge
            )

    print('URFs')
    for urf in data:
        print(urf)
```

```
62          print(urf.weight)
63          print(urf.nodes)
64          print(urf.edges)
65          print(data.get_relevant_cycles_for_urf(urf))
66
67      print('URF for each atom')
68      for a in molecule.GetAtoms():
69          print(a.GetIdx(), data.get_urfs_for_node(a.GetIdx()))
70
71      print('URF for each bond')
72      for b in molecule.GetBonds():
73         print(b.GetIdx(), data.get_urfs_for_edge(b.GetIdx()))
74
75      print('MCB')
76      print(data.get_sssr())
77
78      return data
79
80
81  def get_rgb_from_hsv(h, s, v, a):
82      def clamp(v, minv, maxv):
83          return max(minv, min(v, maxv))
84
85      h = clamp(h, 0.0, 360.0)
86      s = clamp(s, 0.0, 1.0)
87      v = clamp(v, 0.0, 1.0)
88
89      i = int(h / 60.0)
90      r = (h % 60.0) / 60.0
91      p = v * (1.0 - s)
92      q = v * (1.0 - s * r)
93      t = v * (1.0 - s * (1.0 - r))
94
95      if i == 0 or i == 6:
96          return (v, t, p, a)
97      elif i == 1:
98          return (q, v, p, a)
99      elif i == 2:
100         return (p, v, t, a)
101     elif i == 3:
102         return (p, q, v, a)
103     elif i == 4:
104         return (t, p, v, a)
105     elif i == 5:
106         return (v, p, q, a)
107
108     raise ValueError("Internal color error")
109
110
111 def get_distinct_colors(nof_colors, h=0.0, s=0.8, v=0.4, a=1.0, variation=0.2):
112     colors = []
113
114     for i in range(nof_colors):
115         h_ = (h + i * 360.0 / nof_colors) % 360.0
116         s_ = s + variation * random.random()
117         v_ = v + variation + random.random()
118         colors.append(get_rgb_from_hsv(h_, s_, v_, a)[:-1])
119
120     return colors
121
122
123 def draw_molecule(mol, filename, higlights):
124     rdkit.Chem.AllChem.Compute2DCoords(mol)
125
126     drawer = rdkit.Chem.Draw.rdMolDraw2D.MolDraw2DSVG(200, 200)
127     drawer.DrawMolecule(mol, highlightAtoms=None, highlightBonds=highlights,
128         highlightAtomColors=None, highlightBondColors=highlights)
129
130     drawer.FinishDrawing()
131     svg = drawer.GetDrawingText().replace('svg:', '')
132
133     with open(filename, 'w') as outfile:
134         outfile.write(svg)
135
136
137 if __name__ == '__main__':
138     parser = argparse.ArgumentParser('RDKit ring family example')
139     parser.add_argument('--input', type=str, required=True,
140                         help='Input file (.smi or .sdf)')
141     parser.add_argument('--output', action='store_true',
142                         help='Write .svg output files with URFs')
143
144     args = parser.parse_args()
145
146     ext = os.path.splitext(args.input)[1]
147
148     if ext == '.smi':
```

```
149         supplier = rdkit.Chem.SmilesMolSupplier(args.input, titleLine=False)
150     elif ext == '.sdf':
151         supplier = rdkit.Chem.SDMolSupplier(args.input)
152     else:
153         raise ValueError('invalid extension: %s' % ext)
154 
155     for i, mol in enumerate(supplier):
156         print("Molecule", i)
157         if mol is None:
158             print("ERROR")
159             continue
160         if mol.HasProp("_Name"):
161             name = mol.GetProp("_Name")
162         else:
163             name = "NO_NAME"
164         print(name)
165         data = analyze_molecule(mol)
166         if args.output:
167             rcps = data.get_relevant_cycle_prototypes()
168             rcf_colors = get_distinct_colors(len(rcps))
169 
170             urf_colors = get_distinct_colors(data.get_nof_urf())
171             for j, r in enumerate(rcps):
172                 outfile_name = args.input + '_{}_rcp_{}.svg'.format(i, j)
173                 highlights = {b: rcf_colors[j] for b in r.edges}
174                 draw_molecule(mol, outfile_name, highlights)
175             for j, r in enumerate(data.get_relevant_cycles()):
176                 outfile_name = args.input + '_{}_rc_{}_rcf.svg'.format(i, j)
177                 highlights = {b: rcf_colors[r.rcf.index] for b in r.edges}
178                 draw_molecule(mol, outfile_name, highlights)
179 
180                 outfile_name = args.input + '_{}_rc_{}_urf.svg'.format(i, j)
181                 highlights = {b: urf_colors[r.urf.index] for b in r.edges}
182                 draw_molecule(mol, outfile_name, highlights)
```

Chapter 5

Installation instructions

This document describes the installation procedure for the RingDecomposerLib library.

This package uses CMake for the build process. See the `CMake documentation` for general configuration options.

The most useful option is `-DCMAKE_INSTALL_PREFIX=<your/target/path>` for changing the install directory.

Core library

Prerequisites

For the core library the build process needs `CMake` (>= 3.1) and an ANSI-C compiler (for example gcc, clang or MSVC).

Installation Unix and macOS

Installation on Unix using `make` and the system's default C compiler.

```
mkdir build
cd build
cmake .. -DCMAKE_BUILD_TYPE=Release
make && make install
```

Test

Use the following command to test the build of the core library. Testing is strongly recommended.

```
make test
```

The program will compare the relevant cycles to the cycles present in the input file. Furthermore the URFs will be validated, i.e. calculated with an independent exponential algorithm (definition of the URFs). The SSSR will also be validated (it is checked if it's a cycle base). A number of consistency tests is executed to ensure integrity and robustness. See the file `test/README` for a descriptions of the test files.

Warning

> All tests should succeed! If any test fails, check the output. On exceptionally slow machines the failure could result from timeouts.

Installation Windows

Installation on Windows using the `Visual Studio` C compiler and `MSBuild.exe` from the command line (`cmd.exe`). Replace `Visual Studio 14 2015` by your Version.

```
mkdir build
cd build
cmake.exe -G"Visual Studio 14 2015" ..
MSBuild.exe ALL_BUILD.vcxproj /property:Configuration=Release
MSBuild.exe INSTALL.vcxproj /property:Configuration=Release
```

Use the following command to test the build of the core library.

```
MSBuild.exe RUN_TESTS.vcxproj /property:Configuration=Release
```

Python wrapper

The Python wrapper is optional.

Prerequisites

The Python wrapper needs additionally `Python` (>= 2.7 or >= 3.3), and `Cython`.

Installation Unix and macOS

On Unix use the same commands as for installation of the core library with the CMake option -DBUILD_PYTHON-_WRAPPER=ON

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_PYTHON_WRAPPER=ON
```

Depending on your system configuration you may have to specify additional options.

If your Python executable isn't in your current $PATH – or you want to use another – specify with:

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_PYTHON_WRAPPER=ON -DPYTHON_EXECUTABLE=<path/to/your/python/executa
```

Use `-DPYTHON_FLAGS` to modify the installation behaviour of the python wrapper If you can't or don't want to install the Python wrapper into the default directory, specify the target with:

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_PYTHON_WRAPPER=ON -DPYTHON_FLAGS="--user"
```

or

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_PYTHON_WRAPPER=ON -DPYTHON_FLAGS="--prefix=<python/library/install
```

Use the following command to test the core library and the Python wrapper. Testing is strongly recommended.

```
make test
```

Warning

> The Python wrapper will already be installed during `make` and not `make install`. If you don't want the wrapper to be installed, set `-DPYTHON_FLAGS="--prefix=/some/temp/folder"`. In that case the Python tests will fail.

Installation Windows

On Windows use

```
cmake.exe -G"Visual Studio 14 2015" .. -DBUILD_PYTHON_WRAPPER=ON
```

Warning

Before compiling with `MSBuild.exe` you may have to set one environment variable. This is neccessary because Python2.7 on Windows usually is built using `Visual Studio 9 2008`. Replace `VS140COMNTOOLS` by your version.

```
SET VS90COMNTOOLS=%VS140COMNTOOLS%
```

The other options are the same as for Unix.

Warning

The Python wrapper will already be installed during the build step and not the install step. If you don't want the wrapper to be installed, set `-DPYTHON_FLAGS="--prefix=/some/temp/folder"`. In that case the Python tests will fail.

C++ RDKit Benchmark

The C++ RDKit Benchmark is optional. It demonstrates the usage with RDKit and is the tool used for benchmarking the library in the paper.

Prerequisites

The C++ RDKit Benchmark needs `RDKit` (>= 2016.03.01) to be installed and an C++ compiler (g++, clang++, MSCV). Additionally the RDKit header files (for example librdkit-dev package for Debian) and the boost header files (for example libboost-dev for Debian) are needed (>= 1.45).

Installation (Unix and macOS)

Use the same commands as for Installation of the core library with the CMake option -DBUILD_RDKIT_BENCHMARK=ON

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_RDKIT_BENCHMARK=ON
```

Depending on your system configuration you may have to specify additional options.

If the boost libraries are not in the default search path, change with `-DBOOST_ROOT` (see `FindBoost` for details).

If the RDKit headers are not in a default search path, specify with:

```
cmake .. -DCMAKE_BUILD_TYPE=Release -DBUILD_RDKIT_BENCHMARK=ON -DRDKIT_INCLUDE_DIR=<path/to/your/rdkit/headers
```

Warning

Because of the complex dependencies the RDKit Benchmark is currently untested on Windows.

Chapter 6

Hierarchical Index

6.1 Class Hierarchy

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

Chapter 7

Class Index

7.1 Class List

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

Chapter 8

File Index

8.1 File List

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

Chapter 9

Class Documentation

9.1 py_rdl.Calculator.Calculator Class Reference

Public Member Functions

- def __init__
- def get_calculated_result_for_graph
- def get_calculated_result
- def set_graph
- def calculate
- def is_calculated
- def get_nof_urf
- def get_nof_rcf
- def get_nof_ringsystems
- def __len__
- def get_nodes_for_urf
- def get_nodes_for_rcf
- def get_nodes_for_ringsystem
- def get_edges_for_urf
- def get_edges_for_rcf
- def get_edges_for_ringsystem
- def get_weight_for_urf
- def get_weight_for_rcf
- def get_relevant_cycles_for_urf
- def get_relevant_cycles_for_rcf
- def get_urfs_for_node
- def get_urfs_for_edge
- def get_rcfs_for_node
- def get_rcfs_for_edge
- def get_sssr
- def get_relevant_cycles
- def get_nof_relevant_cycles
- def get_nof_relevant_cycles_for_urf
- def get_relevant_cycle_prototypes
- def __getitem__

Public Attributes

- urfs

  List of calculated URFs.
- rcfs

  List of calculated RCFs.
- ringsystems

  List of calculated ring systems.

9.1.1 Detailed Description

```
Object for representing a calculation result.
```

9.1.2 Constructor & Destructor Documentation

9.1.2.1 def py_rdl.Calculator.Calculator.__init__ (*self, graph*)

```
Initialize a new Calculator object with a Graph.

Use @classmethod provided instead
(get_calculated_result_for_graph, get_calculated_result).

You can access URFs, RCFs and ring systems with the
public attributes `urfs`, `rcfs` and `ringsystems`.
The objects can be uses as indices for all functions below,
that operate on the respective ring descriptions.
```

9.1.3 Member Function Documentation

9.1.3.1 def py_rdl.Calculator.Calculator.__getitem__ (*self, item*)

```
Get the item-th URF.
item: The index of the URF
raises RDLError if calculation wasn't successful
raises IndexError if the index is out of range
returns the item-th URF.
```

9.1.3.2 def py_rdl.Calculator.Calculator.__len__ (*self*)

```
Builtin for getting the length (number of URFs).
```

9.1.3.3 def py_rdl.Calculator.Calculator.calculate (*self*)

```
Calculate results for the graph datastructure.
raises RDLError, if the calculation fails

When creating a Calculator object with the
@classmethod provided
(get_calculated_result_for_graph, get_calculated_result)
calling this function
is not necessary.
```

9.1.3.4 def py_rdl.Calculator.Calculator.get_calculated_result (*cls, edge_iterable, get_node_1 =* `operator.itemgetter(0)`, *get_node_2 =* `operator.itemgetter(1)`, *get_node_id =* `lambda x: x`, *get_edge_id =* `lambda x: x`)

```
Calculate the ring topologies and return the results.

edge_iterable: an iterable containing the edges
get_node_1: function retrieving the first node of an edge
get_node_2: function retrieving the second node of an edge
get_node_id: function for retrieving node identifier
get_edge_id: function for retrieving edge identifier
returns the calculated Calculator

This @classmethod creates a new Graph.
The edge_iterable can be any iterable (list, generator etc.).
An edge can be as simple as a pair of nodes.
The get_node function must return the respective nodes adjacent
to an edge.
The node must be hashable. If it's not, use some unique ID
instead.
The edge must be hashable. If it's not, use some unique ID
instead.
```

9.1.3.5 def py_rdl.Calculator.Calculator.get_calculated_result_for_graph (*cls, graph*)

```
Calculate the ring topologies for a Graph
and return the results.
```

9.1.3.6 def py_rdl.Calculator.Calculator.get_edges_for_rcf (*self, rcf_index*)

```
Get the edges in this RCF.
raises RDLError if calculation wasn't successful
returns list of edges in this RCF
```

9.1.3.7 def py_rdl.Calculator.Calculator.get_edges_for_ringsystem (*self, rs_index*)

```
Get the edges in this Ringsystem.
A ring system is a 2-connected component of the graph.
raises RDLError if calculation wasn't successful
returns list of edges in this Ringsystem
```

9.1.3.8 def py_rdl.Calculator.Calculator.get_edges_for_urf (*self, urf_index*)

```
Get the edges in this URF.
raises RDLError if calculation wasn't successful
returns list of edges in this URF
```

9.1.3.9 def py_rdl.Calculator.Calculator.get_nodes_for_rcf (*self, rcf_index*)

```
Get the nodes in this RCF.
raises RDLError if calculation wasn't successful
returns list of nodes in this RCF
```

9.1.3.10 def py_rdl.Calculator.Calculator.get_nodes_for_ringsystem (*self, rs_index*)

```
Get the nodes in this Ringsystem.
A ring system is a 2-connected component of the graph.
raises RDLError if calculation wasn't successful
returns list of nodes in this Ringsystem
```

9.1.3.11 def py_rdl.Calculator.Calculator.get_nodes_for_urf (*self, urf_index*)

```
Get the nodes in this URF.
raises RDLError if calculation wasn't successful
returns list of nodes in this URF
```

9.1.3.12 def py_rdl.Calculator.Calculator.get_nof_rcf (*self*)

```
Get the number of RCFs.
raises RDLError if calculation wasn't successful
```

9.1.3.13 def py_rdl.Calculator.Calculator.get_nof_relevant_cycles (*self*)

```
Get the number of relevant cycles.
raises RDLError if calculation wasn't successful
returns number of RCs
```

9.1.3.14 def py_rdl.Calculator.Calculator.get_nof_relevant_cycles_for_urf (*self, urf_index*)

```
Get the number of relevant cycles for given URF.
raises RDLError if calculation wasn't successful
returns number of RCs
```

9.1.3.15 def py_rdl.Calculator.Calculator.get_nof_ringsystems (*self*)

```
Get the number of Ringsystems.
A ring system is a 2-connected component of the graph.
raises RDLError if calculation wasn't successful
```

9.1.3.16 def py_rdl.Calculator.Calculator.get_nof_urf (*self*)

```
Get the number of URFs.
raises RDLError if calculation wasn't successful
```

9.1.3.17 def py_rdl.Calculator.Calculator.get_rcfs_for_edge (*self, edge*)

```
Get the RCFs this edge is part of.
raises RDLError if calculation wasn't successful
returns list of RCFs
```

9.1.3.18 def py_rdl.Calculator.Calculator.get_rcfs_for_node (*self, node*)

```
Get the RCFs this node is part of.
raises RDLError if calculation wasn't successful
returns a list of RCFs
```

9.1.3.19 def py_rdl.Calculator.Calculator.get_relevant_cycle_prototypes (*self*)

```
Get relevant cycle prototypes (one for each RCF).
raises RDLError if calculation wasn't successful
returns list of relevant cycle prototypes
```

9.1.3.20 def py_rdl.Calculator.Calculator.get_relevant_cycles (*self*)

```
Get relevant cycles.
raises RDLError if calculation wasn't successful
returns generator for enumerating relevant cycles
```

9.1.3.21 def py_rdl.Calculator.Calculator.get_relevant_cycles_for_rcf (*self, rcf_index*)

```
Get the cycles in this of RCF.
raises RDLError if calculation wasn't successful
returns generator for enumerating relevant cycles in this RCF
```

9.1.3.22 def py_rdl.Calculator.Calculator.get_relevant_cycles_for_urf (*self, urf_index*)

```
Get the cycles in this of URF.
raises RDLError if calculation wasn't successful
returns generator for enumerating relevant cycles in this URF
```

9.1.3.23 def py_rdl.Calculator.Calculator.get_sssr (*self*)

```
Get a minimal cycle base.
raises RDLError if calculation wasn't successful
returns list of cycles
```

9.1.3.24 def py_rdl.Calculator.Calculator.get_urfs_for_edge (*self, edge*)

```
Get the URFs this edge is part of.
raises RDLError if calculation wasn't successful
returns list of URFs
```

9.1.3.25 def py_rdl.Calculator.Calculator.get_urfs_for_node (*self, node*)

```
Get the URFs this node is part of.
raises RDLError if calculation wasn't successful
returns a list of URFs
```

9.1.3.26 def py_rdl.Calculator.Calculator.get_weight_for_rcf (*self, rcf_index*)

```
Get weight of this RCF.
raises RDLError if calculation wasn't successful
return weight for given RCF
```

9.1.3.27 def py_rdl.Calculator.Calculator.get_weight_for_urf (*self, urf_index*)

```
Get weight of this URF.
raises RDLError if calculation wasn't successful
return weight for given URF
```

9.1.3.28 def py_rdl.Calculator.Calculator.is_calculated (*self*)

```
Check calculation status.
returns True if calculation was successful, False otherwise.
```

9.1.3.29 def py_rdl.Calculator.Calculator.set_graph (*self*, *graph*)

```
Set the graph data structure.

This has to be a Graph object. See Graph
for a generic interface.
```

9.1.4 Member Data Documentation

9.1.4.1 py_rdl.Calculator.Calculator.rcfs

List of calculated RCFs.

You can access individual RCFs using this list and use the RCF objects as index to all functions below, that take an RCF as argument.

9.1.4.2 py_rdl.Calculator.Calculator.ringsystems

List of calculated ring systems.

You can access individual ring systems using this list and use the Ringsystem objects as index to all functions below, that take an ring system as argument.

9.1.4.3 py_rdl.Calculator.Calculator.urfs

List of calculated URFs.

You can access individual URFs using this list and use the URF objects as index to all functions below, that take an URF as argument.

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

- src/python/py_rdl/Calculator.py

9.2 py_rdl.wrapper.Cycle.Cycle Class Reference

Public Member Functions

- def __init__
- def weight

  Get the weight of the cycle.
- def **__str__**
- def **__repr__**

Public Attributes

- edges

  set of edges
- nodes

set of nodes

- urf

  URF this cycle belongs to.

- rcf

  RCF this cycle belongs to.

9.2.1 Detailed Description

```
This class represents an cycle by it's edges,
nodes, and the urf and rcf it is part of.
```

9.2.2 Constructor & Destructor Documentation

9.2.2.1 def py_rdl.wrapper.Cycle.Cycle.__init__ (*self, edges, nodes, urf, rcf*)

```
Initialize a cycle with edges, nodes and
ring families.
```

9.2.3 Member Function Documentation

9.2.3.1 def py_rdl.wrapper.Cycle.Cycle.weight (*self*)

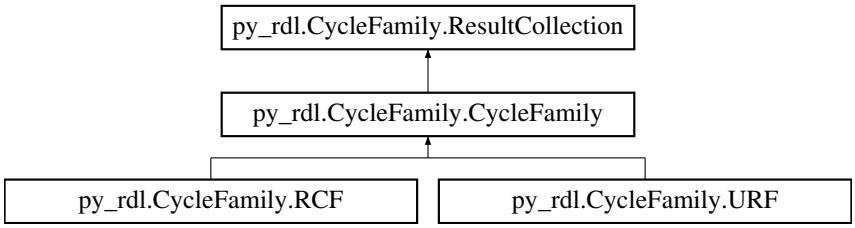
Get the weight of the cycle.

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

- src/python/py_rdl/wrapper/Cycle.py

9.3 py_rdl.CycleFamily.CycleFamily Class Reference

Inheritance diagram for py_rdl.CycleFamily.CycleFamily:



Public Member Functions

- def __init__

Public Attributes

- weight

  weight of the cycle family

9.3.1 Detailed Description

```
Object for representing a cycle family.
```

9.3.2 Constructor & Destructor Documentation

9.3.2.1 def py_rdl.CycleFamily.CycleFamily.__init__ (*self, index, nodes, edges, weight*)

```
index: index of result
nodes: list or set of nodes
edges: list or set of edges
weight: weight of the cycles in the family
```

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

- src/python/py_rdl/CycleFamily.py

9.4 py_rdl.Graph.Graph Class Reference

Public Member Functions

- def __init__
- def from_edges
- def add_edge
- def get_edge_for_indices
- def get_indices_for_edge
- def get_node_for_index
- def get_index_for_node
- def get_nof_nodes
- def get_edges

9.4.1 Detailed Description

```
Object for holding a graph for calculations.
```

9.4.2 Constructor & Destructor Documentation

9.4.2.1 def py_rdl.Graph.Graph.__init__ (*self*)

```
Create a new (empty) graph.

Use this method and add individual edges or
use from_edges instead.
```

9.4.3 Member Function Documentation

9.4.3.1 def py_rdl.Graph.Graph.add_edge (*self, edge, get_node_1* = `operator.itemgetter(0)`, *get_node_2* = `operator.itemgetter(1)`, *get_node_id* = `lambda x: x`, *get_edge_id* = `lambda x: x`)

```
Add an edge to this graph.
edge: edge to be added to the graph
get_node_1: function retrieving the first node of an edge
get_node_2: function retrieving the second node of an edge
get_node_id: fucntion for retrieving node identifier
get_edge_id: function for retrieving edge identifier
```

```
returns the edge_id if successfull, None if edge already present
(and warns in that case)

This function adds an edge to the graph.
DO NOT USE AFTER CALCULATION
```

9.4.3.2 def py_rdl.Graph.Graph.from_edges (*cls, edge_iterable, get_node_1 =* `operator.itemgetter(0)`, *get_node_2 =* `operator.itemgetter(1)`, *get_node_id =* `lambda x: x`, *get_edge_id =* `lambda x: x`)

```
Create a new Graph datastructure
edge_iterable: an iterable containing the edges
get_node_1: function retrieving the first node of an edge
get_node_2: function retrieving the second node of an edge
get_node_id: function for retrieven node identifier
get_edge_id: function for retrieving edge identifier

This classmethod creates a new Graph.
The edge_iterable can be any iterable (list, generator etc.).
An edge can be as simple as a pair of nodes.
The get_node_ function must return the respective nodes adjacent
to an edge (default: first and second element of the edge).
The node must be hashable. If it's not, use some unique ID
instead.
The edge must be hashable. If it's not, use some unique ID
instead (provided by get_edge_id).
```

9.4.3.3 def py_rdl.Graph.Graph.get_edge_for_indices (*self, node_index1, node_index2*)

```
Returns the edge which is formed by the two nodes
(as indices).
node_index1: index of the first node
node_index2: index of the second node
returns edge adjacent by two nodes
raises KeyError if the edge does not exist

This function is used internally by Calculator, you
probably won't need this function.
```

9.4.3.4 def py_rdl.Graph.Graph.get_edges (*self*)

```
Get the edges in the graph.

This function is used internally by Calculator, you
won't need this function.
```

9.4.3.5 def py_rdl.Graph.Graph.get_index_for_node (*self, node*)

```
Returns the internal index for the node.
node: node object
returns the index for the node object
raises KeyError if node does not exist

This function is used internally by Calculator, you
probably won't need this function.
```

9.4.3.6 def py_rdl.Graph.Graph.get_indices_for_edge (*self, edge*)

```
Returns the edge which is formed by the two nodes
```

```
(as indices).
edge: edge
returns edge adjacent by two nodes
raises KeyError if the edge does not exist

This function is used internally by Calculator, you
probably won't need this function.
```

9.4.3.7 def py_rdl.Graph.Graph.get_node_for_index (*self, node_index*)

```
Returns the node with the internal index.
node_index: index of the node
returns the node object with this index
raises IndexError if node does not exist

This function is used internally by Calculator, you
probably won't need this function.
```

9.4.3.8 def py_rdl.Graph.Graph.get_nof_nodes (*self*)

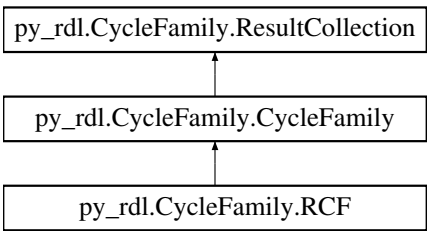
```
Get the number of nodes in the graph.
```

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

- src/python/py_rdl/Graph.py

9.5 py_rdl.CycleFamily.RCF Class Reference

Inheritance diagram for py_rdl.CycleFamily.RCF:



Public Member Functions

- def __str__
- def __init__

Additional Inherited Members

9.5.1 Detailed Description

```
Object for representing a relevant cycle family.
```

9.5.2 Constructor & Destructor Documentation

9.5.2.1 def py_rdl.CycleFamily.RCF.__init__ (*self, index, nodes, edges, weight*)

```
index: index of result
nodes: list or set of nodes
edges: list or set of edges
weight: weight of the cycles in the family
```

9.5.3 Member Function Documentation

9.5.3.1 def py_rdl.CycleFamily.RCF.__str__ (*self*)

```
to string.
```

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

- src/python/py_rdl/CycleFamily.py

9.6 RDL_cycle Struct Reference

```
#include <RingDecomposerLib.h>
```

Public Attributes

- RDL_edge * edges
- unsigned weight
- unsigned urf
- unsigned rcf

9.6.1 Detailed Description

This structure holds a cycle (or ring) in the graph. It is essentially an array of edges which are represented by pairs of nodes.

9.6.2 Member Data Documentation

9.6.2.1 RDL_edge* RDL_cycle::edges

array of RDL_edge in the cycle

9.6.2.2 unsigned RDL_cycle::rcf

RCF of the cycle

9.6.2.3 unsigned RDL_cycle::urf

URF of the cycle

9.6.2.4 unsigned RDL_cycle::weight

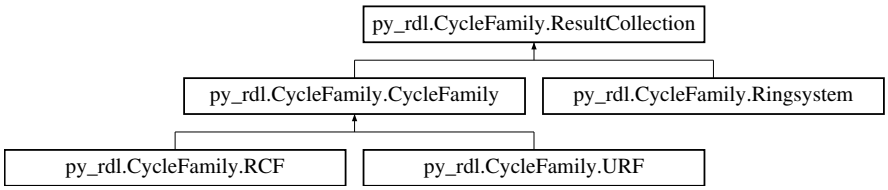
weight of the cycle (length of the array)

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

- src/RingDecomposerLib/RingDecomposerLib.h

9.7 py_rdl.CycleFamily.ResultCollection Class Reference

Inheritance diagram for py_rdl.CycleFamily.ResultCollection:



Public Member Functions

- def __init__
- def __str__
- def __repr__

Public Attributes

- index

  index of the result
- nodes

  set of nodes of the result
- edges

  set of edges of the result

9.7.1 Detailed Description

```
Object for representing a result.
```

9.7.2 Constructor & Destructor Documentation

9.7.2.1 def py_rdl.CycleFamily.ResultCollection.__init__ (*self, index, nodes, edges*)

```
index: index of result
nodes: list or set of nodes
edges: list or set of edges
```

9.7.3 Member Function Documentation

9.7.3.1 def py_rdl.CycleFamily.ResultCollection.__repr__ (*self*)

```
Representation
```

9.7.3.2 def py_rdl.CycleFamily.ResultCollection.__str__ (*self*)

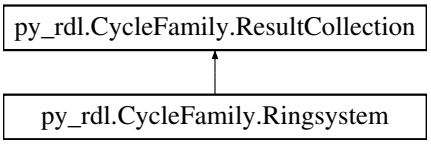
```
to string.
```

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

- src/python/py_rdl/CycleFamily.py

9.8 py_rdl.CycleFamily.Ringsystem Class Reference

Inheritance diagram for py_rdl.CycleFamily.Ringsystem:



Public Member Functions

- def __init__

Additional Inherited Members

9.8.1 Detailed Description

```
Object for representing a ringsystem.
A ring system is a 2-connected component of the graph.
```

9.8.2 Constructor & Destructor Documentation

9.8.2.1 def py_rdl.CycleFamily.Ringsystem.__init__ (*self, index, nodes, edges*)

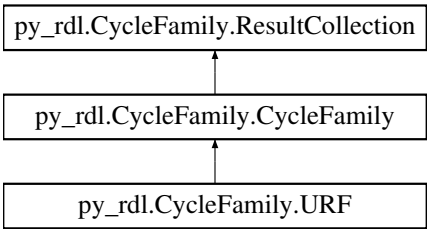
```
index: index of result
nodes: list or set of nodes
edges: list or set of edges
```

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

- src/python/py_rdl/CycleFamily.py

9.9 py_rdl.CycleFamily.URF Class Reference

Inheritance diagram for py_rdl.CycleFamily.URF:



Public Member Functions

- def __str__
- def __init__

Additional Inherited Members

9.9.1 Detailed Description

```
Object for representing a unique ring family.
```

9.9.2 Constructor & Destructor Documentation

9.9.2.1 def py_rdl.CycleFamily.URF.__init__ (*self, index, nodes, edges, weight*)

```
index: index of result
nodes: list or set of nodes
edges: list or set of edges
weight: weight of the cycles in the family
```

9.9.3 Member Function Documentation

9.9.3.1 def py_rdl.CycleFamily.URF.__str__ (*self*)

```
to string.
```

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

- src/python/py_rdl/CycleFamily.py

Chapter 10

File Documentation

10.1 src/MinimalExample/MinimalExample.c File Reference

Minimal example for the RingDecomposerLib library.

```
#include <assert.h>
#include <stdio.h>
#include "RingDecomposerLib.h"
```

10.1.1 Detailed Description

Minimal example for the RingDecomposerLib library.

10.2 src/RingDecomposerLib/RingDecomposerLib.h File Reference

This file contains the API of the RingDecomposerLib library.

Classes

- struct RDL_cycle

Typedefs

- typedef struct RDL_data RDL_data
  Structure representing a calculation result.
- typedef struct RDL_graph RDL_graph
  Datastructure representing a graph for calculations.
- typedef unsigned RDL_node
  A node is represented by its index in the graph (0 to $|V|$-1).
- typedef RDL_node RDL_edge [2]
  An edge is represented by an array of size two containing the adjacent nodes.
- typedef enum RDL_ERROR_LEVEL RDL_ERROR_LEVEL
  error levels for custom logging functions
- typedef void(∗ **RDL_outputFunction**)(RDL_ERROR_LEVEL level, const char ∗m,...)
- typedef struct RDL_cycle RDL_cycle
- typedef struct RDL_cycleIterator RDL_cycleIterator
  Iterator for relevant cycles.

Enumerations

- enum RDL_ERROR_LEVEL { **RDL_DEBUG**, **RDL_WARNING**, **RDL_ERROR**, **RDL_INITIALIZE_OUTPUT** }

  error levels for custom logging functions

Functions

- RDL_API void RDL_setOutputFunction (RDL_outputFunction func)

  Set the output function for warning and error messages.
- RDL_API void RDL_writeToStderr (RDL_ERROR_LEVEL level, const char *fmt,...)

  An output function for writing everything to stderr.
- RDL_API void RDL_writeNothing (RDL_ERROR_LEVEL level, const char *fmt,...)

  No output function.
- RDL_API RDL_graph * RDL_initNewGraph (unsigned nof_nodes)

  Initializes a new RDL_graph.
- RDL_API void RDL_deleteGraph (RDL_graph *graph)

  Delete RDL_graph.
- RDL_API unsigned RDL_addUEdge (RDL_graph *graph, RDL_node node1, RDL_node node2)

  Adds an undirected edge to the graph.
- RDL_API RDL_data * RDL_calculate (RDL_graph *input_graph)

  Calculates the RDL_data structure of the given graph and returns it.
- RDL_API void RDL_deleteData (RDL_data *data)

  Deletes RDL_data from memory, including the RDL_graph.
- RDL_API unsigned RDL_getNofURF (const RDL_data *data)

  Returns the number of URFs.
- RDL_API unsigned RDL_getNofRCF (const RDL_data *data)

  Returns the number of RCFs.
- RDL_API unsigned RDL_getWeightForURF (const RDL_data *data, unsigned index)

  Returns the weight of each cycle in the URF identified by its index.
- RDL_API unsigned RDL_getWeightForRCF (const RDL_data *data, unsigned index)

  Returns the weight of each cycle in the RCF identified by its index.
- RDL_API unsigned RDL_getNodesForURF (const RDL_data *data, unsigned index, RDL_node **RDL_node_array_ptr)

  Gives the nodes of an URF identified with its index in an array of RDL_node.
- RDL_API unsigned RDL_getEdgesForURF (const RDL_data *data, unsigned index, RDL_edge **RDL_edge_array_ptr)

  Gives the edges of an URF identified with its index.
- RDL_API unsigned RDL_getNodesForRCF (const RDL_data *data, unsigned index, RDL_node **RDL_node_array_ptr)

  Gives the nodes of an RCF identified with its index in an array of RDL_node.
- RDL_API unsigned RDL_getEdgesForRCF (const RDL_data *data, unsigned index, RDL_edge **RDL_edge_array_ptr)

  Gives the edges of an RCF identified with its index.
- RDL_API unsigned RDL_getNofURFContainingNode (const RDL_data *data, RDL_node node)

  Returns the number of URFs that contain the given node.
- RDL_API unsigned RDL_getNofURFContainingEdge (const RDL_data *data, RDL_node node1, RDL_node node2)

  Returns the number of URFs that contain the RDL_edge defined by the two given nodes.
- RDL_API unsigned RDL_getNofRCFContainingNode (const RDL_data *data, RDL_node node)

  Returns the number of RCFs that contain the given node.

- RDL_API unsigned RDL_getNofRCFContainingEdge (const RDL_data *data, RDL_node node1, RDL_node node2)

  Returns the number of RCFs that contain the RDL_edge defined by the two given nodes.
- RDL_API unsigned RDL_getURFsContainingNode (const RDL_data *data, RDL_node node, unsigned **RDL_ids_ptr)

  Gives all URFs containing the node.
- RDL_API unsigned RDL_getURFsContainingEdge (const RDL_data *data, RDL_node node1, RDL_node node2, unsigned **RDL_ids_ptr)

  Gives all URFs containing the edge.
- RDL_API unsigned RDL_getRCFsContainingNode (const RDL_data *data, RDL_node node, unsigned **RDL_ids_ptr)

  Gives all RCFs containing the node.
- RDL_API unsigned RDL_getRCFsContainingEdge (const RDL_data *data, RDL_node node1, RDL_node node2, unsigned **RDL_ids_ptr)

  Gives all RCFs containing the edge.
- RDL_API void RDL_deleteCycle (RDL_cycle *cycle)

  Free memory of RDL_cycle.
- RDL_API RDL_cycleIterator * RDL_cycleIteratorNext (RDL_cycleIterator *it)

  Advance the cycle iterator by one.
- RDL_API RDL_cycle * RDL_cycleIteratorGetCycle (RDL_cycleIterator *it)

  Get the cycle as RDL_cycle.
- RDL_API int RDL_cycleIteratorAtEnd (RDL_cycleIterator *it)

  Check if iterator is at end (invalid)
- RDL_API void RDL_deleteCycleIterator (RDL_cycleIterator *it)

  Free memory of the cycle iterator.
- RDL_API unsigned RDL_getRCyclesForURF (const RDL_data *data, unsigned index, RDL_cycle ***RDL_cycle_array_ptr)

  Gives all relevant cycles of the URF with the given index.
- RDL_API RDL_cycleIterator * RDL_getRCyclesForURFIterator (const RDL_data *data, unsigned index)

  Get iterator for all relevant cycles of the URF with the given index.
- RDL_API unsigned RDL_getRCyclesForRCF (const RDL_data *data, unsigned index, RDL_cycle ***RDL_cycle_array_ptr)

  Gives all relevant cycles of the RCF with the given index.
- RDL_API RDL_cycleIterator * RDL_getRCyclesForRCFIterator (const RDL_data *data, unsigned index)

  Get iterator for all relevant cycles of the RCF with the given index.
- RDL_API unsigned RDL_getRCycles (const RDL_data *data, RDL_cycle ***RDL_cycle_array_ptr)

  Gives a list of all relevant cycles.
- RDL_API RDL_cycleIterator * RDL_getRCyclesIterator (const RDL_data *data)

  Get iterator for all relevant cycles.
- RDL_API double RDL_getNofRCForURF (const RDL_data *data, unsigned index)

  Gives the number of relevant cycles in this URF.
- RDL_API double RDL_getNofRCForRCF (const RDL_data *data, unsigned index)

  Gives the number of relevant cycles in this RCF.
- RDL_API double RDL_getNofRC (const RDL_data *data)

  Gives the number of relevant cycles.
- RDL_API unsigned RDL_getSSSR (const RDL_data *data, RDL_cycle ***RDL_cycle_array_ptr)

  Gives a set of cycles that forms a Minimal Cycle Basis of the graph.
- RDL_API unsigned RDL_getRCPrototypes (const RDL_data *data, RDL_cycle ***RDL_cycle_array_ptr)

  Gives a list of relevant cycle prototypes (one for each RCF).
- RDL_API void RDL_deleteCycles (RDL_cycle **cycles, unsigned number)

  Deallocates the structure given by RDL_getRCycles(), RDL_getSSSR(), RDL_getRCPrototypes() and RDL_getRCyclesForURF(), if called on its result and return value (the number of cycles)

- RDL_API unsigned RDL_translateCycArray (const RDL_data *data, RDL_cycle **old_array, unsigned number, char ***RDL_cycle_array_ptr)

  Translates the results of RDL_getRCycles(), RDL_getSSSR(), RDL_getRCPrototypes() and RDL_getRCyclesForURF() (arrays of RDL_cycle) into an array of cycles represented by arrays of $\{0,1\}^{|E|}$ (bitsets).
- RDL_API void RDL_deleteEdgeIdxArray (char **cycles, unsigned number)

  Deallocates the structure given by RDL_translateCycArray(), if called on its result and return value (the number of cycles).
- RDL_API unsigned RDL_getEdgeArray (const RDL_data *data, RDL_edge **RDL_edge_array_ptr)

  Gives the edges of the graph.
- RDL_API unsigned RDL_getNofEdges (const RDL_data *data)

  Get the number of edges in the graph.
- RDL_API unsigned RDL_getEdgeId (const RDL_data *data, unsigned from, unsigned to)

  Get the id of the edge.
- RDL_API unsigned RDL_getNofRingsystems (const RDL_data *data)

  Get the number of ring systems in the graph.
- RDL_API unsigned RDL_getNofNodesForRingsystem (const RDL_data *data, unsigned idx)

  Get the number of nodes in the ring system.
- RDL_API unsigned RDL_getNofEdgesForRingsystem (const RDL_data *data, unsigned idx)

  Get the number of edges in the ring system.
- RDL_API unsigned RDL_getEdgesForRingsystem (const RDL_data *data, unsigned idx, RDL_edge **edges)

  Get the edges in the ring system.
- RDL_API unsigned RDL_getNodesForRingsystem (const RDL_data *data, unsigned idx, RDL_node **nodes)

  Get the nodes in the ring system.
- RDL_API unsigned RDL_getRingsystemForEdge (const RDL_data *data, unsigned from, unsigned to)

  Get the ring system id for given edge.

Variables

- RDL_outputFunction RDL_outputFunc

  the output function for warnings and errors
- const unsigned RDL_INVALID_RESULT

  Invalid result indicator.
- const unsigned RDL_DUPLICATE_EDGE

  Duplicate edge indicator.
- const unsigned RDL_NO_RINGSYSTEM

  No ringsystem indicator.
- const double RDL_INVALID_RC_COUNT

  Invalid number of RCs.

10.2.1 Detailed Description

This file contains the API of the RingDecomposerLib library.

10.2.2 Typedef Documentation

10.2.2.1 typedef struct RDL_cycle RDL_cycle

This structure holds a cycle (or ring) in the graph. It is essentially an array of edges which are represented by pairs of nodes.

10.2.2.2 typedef struct RDL_cycleIterator RDL_cycleIterator

Iterator for relevant cycles.

Always check if the iterator is at end BEFORE incrementing or accessing it.

Example usage:

```
RDL_cycle *cycle;
RDL_cycleIterator *it = RDL_getRCyclesIterator(data);
while(!RDL_cycleIteratorAtEnd(it)) {
  cycle = RDL_cycleIteratorGetCycle(it);
  <do something with the cycle>
  RDL_deleteCycle(cycle);
  RDL_cycleIteratorNext(it);
}
RDL_deleteCycleIterator(it);
```

10.2.2.3 typedef struct RDL_data RDL_data

Structure representing a calculation result.

This is the central structure, that is used to store the calculation results. Almost all functions in this header work on it.

10.2.2.4 typedef struct RDL_graph RDL_graph

Datastructure representing a graph for calculations.

Build graph data structure that is used for the calculation. The graph is stored as an adjacency list. The vertices are numbered from 0 to |V|-1. Call the following functions:

RDL_initNewGraph(unsigned V) to initialize a new graph with V vertices (returns RDL_graph *)

RDL_addUEdge(RDL_graph *, RDL_node from, RDL_node to) to add a new (undirected) edge from the vertex with index "from" to the vertex with index "to".

Then RDL_calculate can be called on it.

10.2.3 Function Documentation

10.2.3.1 RDL_API unsigned RDL_addUEdge (RDL_graph * *graph*, RDL_node *node1*, RDL_node *node2*)

Adds an undirected edge to the graph.

Parameters

graph	pointer to the RDL_graph that the edge will to be added to
node1,node2	pair of RDL_node which the edge is going to connect

Returns

internal index of edge if successful, RDL_INVALID_RESULT on failures (invalid index, loop), RDL_DUPLICATE_EDGE if the edge was already present

10.2.3.2 RDL_API RDL_data* RDL_calculate (RDL_graph * *input_graph*)

Calculates the RDL_data structure of the given graph and returns it.

Parameters

input_graph	The graph for calculation.

Returns

pointer to the RDL_data containing the calculation result, `NULL` on failure

Note

The RDL_graph has to be an undirected graph.
Takes ownership of the RDL_graph, if calculation is successful!

10.2.3.3 RDL_API int RDL_cycleIteratorAtEnd (RDL_cycleIterator * *it*)

Check if iterator is at end (invalid)

Parameters

it	RDL_cycleIterator

Returns

0 if not at end, a non-zero value otherwise

10.2.3.4 RDL_API RDL_cycle* RDL_cycleIteratorGetCycle (RDL_cycleIterator * *it*)

Get the cycle as RDL_cycle.

Parameters

it	RDL_cycleIterator

Returns

RDL_cycle holding the cycle, `NULL` on error

Note

The RDL_cycle is constructed and returned as a pointer. You have to delete it using RDL_deleteCycle.
DO NOT call without checking RDL_cycleIteratorAtEnd

10.2.3.5 RDL_API RDL_cycleIterator* RDL_cycleIteratorNext (RDL_cycleIterator * *it*)

Advance the cycle iterator by one.

Parameters

it	RDL_cycleIterator

Returns

returns the iterator `it` itself, if successful; `NULL` on error

Note

DO NOT call without checking RDL_cycleIteratorAtEnd

10.2.3.6 RDL_API void RDL_deleteCycle (RDL_cycle * *cycle*)

Free memory of RDL_cycle.

Parameters

cycle	The RDL_cycle to delete.

10.2.3.7 RDL_API void RDL_deleteCycleIterator (RDL_cycleIterator * *it*)

Free memory of the cycle iterator.

Parameters

it	RDL_cycleIterator

10.2.3.8 RDL_API void RDL_deleteCycles (RDL_cycle ** *cycles*, unsigned *number*)

Deallocates the structure given by RDL_getRCycles(), RDL_getSSSR(), RDL_getRCPrototypes() and RDL_getRCyclesForURF(), if called on its result and return value (the number of cycles)

Parameters

cycles	The array of cycles.
number	The number of cycles in the array

10.2.3.9 RDL_API void RDL_deleteData (RDL_data * *data*)

Deletes RDL_data from memory, including the RDL_graph.

Parameters

data	pointer to the RDL_data that is going to be deleted

Note

also deletes the associated RDL_graph

10.2.3.10 RDL_API void RDL_deleteEdgeIdxArray (char ** *cycles*, unsigned *number*)

Deallocates the structure given by RDL_translateCycArray(), if called on its result and return value (the number of cycles).

Parameters

cycles	The translated array of cycles.
number	The number of cycles in the array.

10.2.3.11 RDL_API void RDL_deleteGraph (RDL_graph * *graph*)

Delete RDL_graph.

Parameters

graph	pointer to RDL_graph to delete

Note

You don't have to delete the graph after successful calculation!

10.2.3.12 RDL_API unsigned RDL_getEdgeArray (const RDL_data * *data*, RDL_edge ** *RDL_edge_array_ptr*)

Gives the edges of the graph.

Returns

the number of edges in the graph, RDL_INVALID_RESULT on error

Parameters

data	pointer to the RDL_data holding the calculation results.
RDL_edge_array_ptr	pointer that points to the result array (declare RDL_edge * and give address as parameter)

Note

Result has to be deallocated using `free(*RDL_edge_array_ptr)`

10.2.3.13 RDL_API unsigned RDL_getEdgeId (const RDL_data * *data*, unsigned *from*, unsigned *to*)

Get the id of the edge.

Parameters

data	pointer to the RDL_data holding the calculation results.
from	RDL_node starting at this edge
to	RDL_node starting at this edge

Returns

edge id, RDL_INVALID_RESULT, if not present

Note

As the graph is stored as an adjacency list, this function has linear runtime in the node degree.

10.2.3.14 RDL_API unsigned RDL_getEdgesForRCF (const RDL_data * *data*, unsigned *index*, RDL_edge ** *RDL_edge_array_ptr*)

Gives the edges of an RCF identified with its index.

Returns

the number of edges in this RCF, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results.
index	the index of the RCF
RDL_edge_array_ptr	pointer that points to the result array (declare RDL_edge * and give address as parameter)

Note

Result has to be deallocated using `free(*RDL_edge_array_ptr)` Gives an array of edges where an edge is represented by two RDL_node that it connects.

10.2.3.15 RDL_API unsigned RDL_getEdgesForRingsystem (const RDL_data * *data*, unsigned *idx*, RDL_edge ** *edges*)

Get the edges in the ring system.

Parameters

data	pointer to the RDL_data holding the calculation results.
idx	index of the ring system
edges	pointer that points to the result array (declare RDL_edge * and give address as parameter)

Note

Result has to be deallocated using `free(*edges)`

Returns

number of edges in the ring system, RDL_INVALID_RESULT on error

Note

A ring system is a 2-connected component of the graph.

10.2.3.16 RDL_API unsigned RDL_getEdgesForURF (const RDL_data * *data*, unsigned *index*, RDL_edge ** *RDL_edge_array_ptr*)

Gives the edges of an URF identified with its index.

Returns

the number of edges in this URF, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results.
index	the index of the URF
RDL_edge_array_ptr	pointer that points to the result array (declare RDL_edge * and give address as parameter)

Note

Result has to be deallocated using `free(*RDL_edge_array_ptr)` Gives an array of edges where an edge is represented by two RDL_node that it connects.

10.2.3.17 RDL_API unsigned RDL_getNodesForRCF (const RDL_data * *data*, unsigned *index*, RDL_node ** *RDL_node_array_ptr*)

Gives the nodes of an RCF identified with its index in an array of RDL_node.

Returns

the number of nodes in the RCF, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results.

index	the index of the RCF
RDL_node_array_ptr	pointer that points to the result array (declare RDL_node * and give address as parameter)

Note

result has to be deallocated using `free(*RDL_node_array_ptr)`.

10.2.3.18 RDL_API unsigned RDL_getNodesForRingsystem (const RDL_data * *data*, unsigned *idx*, RDL_node ** *nodes*)

Get the nodes in the ring system.

Parameters

data	pointer to the RDL_data holding the calculation results.
idx	index of the ring system
nodes	pointer that points to the result array (declare RDL_edge * and give address as parameter)

Note

Result has to be deallocated using `free(*nodes)`

Returns

number of nodes in the ring system, RDL_INVALID_RESULT on error

Note

A ring system is a 2-connected component of the graph.

10.2.3.19 RDL_API unsigned RDL_getNodesForURF (const RDL_data * *data*, unsigned *index*, RDL_node ** *RDL_node_array_ptr*)

Gives the nodes of an URF identified with its index in an array of RDL_node.

Returns

the number of nodes in the URF, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results.
index	the index of the URF
RDL_node_array_ptr	pointer that points to the result array (declare RDL_node * and give address as parameter)

Note

result has to be deallocated using `free(*RDL_node_array_ptr)`.

10.2.3.20 RDL_API unsigned RDL_getNofEdges (const RDL_data * *data*)

Get the number of edges in the graph.

Parameters

data	pointer to the RDL_data holding the calculation results.

Returns

number of edges in the graph, RDL_INVALID_RESULT on error

10.2.3.21 RDL_API unsigned RDL_getNofEdgesForRingsystem (const RDL_data * *data*, unsigned *idx*)

Get the number of edges in the ring system.

Parameters

data	pointer to the RDL_data holding the calculation results.
idx	index of the ring system

Returns

number of edges in the ring system, RDL_INVALID_RESULT on error

Note

A ring system is a 2-connected component of the graph.

10.2.3.22 RDL_API unsigned RDL_getNofNodesForRingsystem (const RDL_data * *data*, unsigned *idx*)

Get the number of nodes in the ring system.

Parameters

data	pointer to the RDL_data holding the calculation results.
idx	index of the ring system

Returns

number of nodes in the ring system, RDL_INVALID_RESULT on error

Note

A ring system is a 2-connected component of the graph.

10.2.3.23 RDL_API double RDL_getNofRC (const RDL_data * *data*)

Gives the number of relevant cycles.

Parameters

data	pointer to the RDL_data holding the calculation results

Returns

the number of relevant cycles RDL_INVALID_RC_COUNT if the number is too large to calculate or on failure

10.2.3.24 RDL_API unsigned RDL_getNofRCF (const RDL_data * *data*)

Returns the number of RCFs.

Parameters

data	Pointer to the RDL_data of which the number of RCF is requested

Returns

The number of RCFs, RDL_INVALID_RESULT on failure

10.2.3.25 RDL_API unsigned RDL_getNofRCFContainingEdge (const RDL_data * *data*, RDL_node *node1*, RDL_node *node2*)

Returns the number of RCFs that contain the RDL_edge defined by the two given nodes.

Parameters

data	Pointer to the RDL_data storing the calculation results.
node1,node2	pair of RDL_node connected by the edge

Returns

number of RCFs containing the edge, RDL_INVALID_RESULT on failure

Note

This functions internally enumerates all edges for each RCF. For repeated checks with different RDL_node it is recommended to enumerate them with RDL_getEdgesForRCF and check against this array.

10.2.3.26 RDL_API unsigned RDL_getNofRCFContainingNode (const RDL_data * *data*, RDL_node *node*)

Returns the number of RCFs that contain the given node.

Parameters

data	pointer to the RDL_data holding the calculation results.
node	the RDL_node to look for in the RCFs

Returns

number of RCFs containing the node, RDL_INVALID_RESULT on failure

Note

This functions internally enumerates all nodes for each RCF. For repeated checks with different RDL_node it is recommended to enumerate them with RDL_getNodesForRCF and check against this array.

10.2.3.27 RDL_API double RDL_getNofRCForRCF (const RDL_data * *data*, unsigned *index*)

Gives the number of relevant cycles in this RCF.

Parameters

data	pointer to the RDL_data holding the calculation results.
index	id of the RCF

Returns

the number of relevant cycles in the RCF or RDL_INVALID_RC_COUNT if the number is too large to calculate or on failure

10.2.3.28 RDL_API double RDL_getNofRCForURF (const RDL_data * *data*, unsigned *index*)

Gives the number of relevant cycles in this URF.

Parameters

data	pointer to the RDL_data holding the calculation results
index	the index of the URF

Returns

the number of relevant cycles in the URF or RDL_INVALID_RC_COUNT if the number is too large to calculate or on failure

10.2.3.29 RDL_API unsigned RDL_getNofRingsystems (const RDL_data * *data*)

Get the number of ring systems in the graph.

Parameters

data	pointer to the RDL_data holding the calculation results.

Returns

number of ring systems in the graph, RDL_INVALID_RESULT on error

10.2.3.30 RDL_API unsigned RDL_getNofURF (const RDL_data * *data*)

Returns the number of URFs.

Parameters

data	Pointer to the RDL_data of which the number of URF is requested

Returns

The number of URFs, RDL_INVALID_RESULT on failure

10.2.3.31 RDL_API unsigned RDL_getNofURFContainingEdge (const RDL_data * *data*, RDL_node *node1*, RDL_node *node2*)

Returns the number of URFs that contain the RDL_edge defined by the two given nodes.

Parameters

data	Pointer to the RDL_data storing the calculation results.
node1,node2	pair of RDL_node connected by the edge

Returns

number of URFs containing the edge, RDL_INVALID_RESULT on failure

Note

This functions internally enumerates all edges for each URF. For repeated checks with different RDL_node it is recommended to enumerate them with RDL_getEdgesForURF and check against this array.

10.2.3.32 RDL_API unsigned RDL_getNofURFContainingNode (const RDL_data * *data*, RDL_node *node*)

Returns the number of URFs that contain the given node.

Parameters

data	pointer to the RDL_data holding the calculation results.
node	the RDL_node to look for in the URFs

Returns

number of URFs containing the node, RDL_INVALID_RESULT on failure

Note

This functions internally enumerates all nodes for each URF. For repeated checks with different RDL_node it is recommended to enumerate them with RDL_getNodesForURF and check against this array.

10.2.3.33 RDL_API unsigned RDL_getRCFsContainingEdge (const RDL_data * *data*, RDL_node *node1*, RDL_node *node2*, unsigned ** *RDL_ids_ptr*)

Gives all RCFs containing the edge.

Returns

the number of RCFs containing the edge, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
node1	the first RDL_node of the edge
node2	the the second RDL_node of the edge
RDL_ids_ptr	pointer that points to the result array of integers containing all indices of RCFs containing the edge. (declare `unsigned *` and give address as parameter)

Note

The array RDL_ids_ptr has to be to be deallocated with `free(*RDL_ids_ptr)`
This functions internally enumerates all edges for each RCF. For repeated queries with different RDL_node it is recommended to enumerate them with RDL_getEdgesForRCF once and use this array.

10.2.3.34 RDL_API unsigned RDL_getRCFsContainingNode (const RDL_data * *data*, RDL_node *node*, unsigned ** *RDL_ids_ptr*)

Gives all RCFs containing the node.

Returns

the number of RCFs containing the node, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
node	the RDL_node
RDL_ids_ptr	pointer that points to the result array of integers containing all indices of URFs containing the node. (declare `unsigned *` and give address as parameter)

Note

The array RDL_ids_ptr has to be to be deallocated with `free(*RDL_ids_ptr)`
This functions internally enumerates all nodes for each RCF. For repeated queries with different RDL_node it is recommended to enumerate them with RDL_getNodesForRCF once and use this array.

10.2.3.35 RDL_API unsigned RDL_getRCPrototypes (const RDL_data * *data*, RDL_cycle *** *RDL_cycle_array_ptr*)

Gives a list of relevant cycle prototypes (one for each RCF).

Returns

the number of prototypes, RDL_INVALID_RESULT on error

Parameters

data	pointer to the RDL_data holding the calculation results
RDL_cycle_array_ptr	pointer to the result array (declare RDL_cycle ** and give address as parameter) The result is an array of cycles.

Note

Result has to be deallocated using RDL_deleteCycles(RDL_cycle **cycles, unsigned number)

10.2.3.36 RDL_API unsigned RDL_getRCycles (const RDL_data * *data*, RDL_cycle *** *RDL_cycle_array_ptr*)

Gives a list of all relevant cycles.

Returns

the number of cycles, RDL_INVALID_RESULT on error

Parameters

data	pointer to the RDL_data holding the calculation results
RDL_cycle_array_ptr	pointer to the result array (declare RDL_cycle ** and give address as parameter) The result is an array of cycles.

Note

Result has to be deallocated using RDL_deleteCycles(RDL_cycle **cycles, unsigned number)
Consider using RDL_getRCyclesIterator instead

10.2.3.37 RDL_API unsigned RDL_getRCyclesForRCF (const RDL_data * *data*, unsigned *index*, RDL_cycle *** *RDL_cycle_array_ptr*)

Gives all relevant cycles of the RCF with the given index.

Returns

the number of cycles found, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
index	the index of the RCF
RDL_cycle_-array_ptr	pointer that points to the result array of cycles (declare RDL_cycle ** and give address as parameter)

Note

RDL_cycle_array_ptr has to be deallocated using RDL_deleteCycles(RDL_cycle **cycles, unsigned number)
Consider using RDL_getRCyclesForRCFIterator instead

10.2.3.38 RDL_API RDL_cycleIterator* RDL_getRCyclesForRCFIterator (const RDL_data * *data*, unsigned *index*)

Get iterator for all relevant cycles of the RCF with the given index.

Returns

RDL_cycleIterator, NULL on failure

Parameters

data	pointer to the RDL_data holding the calculation results
index	the index of the RCF

Note

See RDL_cycleIterator for an example.

10.2.3.39 RDL_API unsigned RDL_getRCyclesForURF (const RDL_data * *data*, unsigned *index*, RDL_cycle *** *RDL_cycle_array_ptr*)

Gives all relevant cycles of the URF with the given index.

Returns

the number of cycles found, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
index	the index of the URF
RDL_cycle_-array_ptr	pointer that points to the result array of cycles (declare RDL_cycle ** and give address as parameter)

Note

RDL_cycle_array_ptr has to be deallocated using RDL_deleteCycles(RDL_cycle **cycles, unsigned number)
Consider using RDL_getRCyclesForURFIterator instead

10.2.3.40 RDL_API RDL_cycleIterator* RDL_getRCyclesForURFIterator (const RDL_data * *data*, unsigned *index*)

Get iterator for all relevant cycles of the URF with the given index.

Returns

RDL_cycleIterator, NULL on failure

Parameters

data	pointer to the RDL_data holding the calculation results
index	the index of the URF

Note

See RDL_cycleIterator for an example.

10.2.3.41 RDL_API RDL_cycleIterator* RDL_getRCyclesIterator (const RDL_data * *data*)

Get iterator for all relevant cycles.

Returns

RDL_cycleIterator, NULL on failure

Parameters

data	pointer to the RDL_data holding the calculation results

Note

See RDL_cycleIterator for an example.

10.2.3.42 RDL_API unsigned RDL_getRingsystemForEdge (const RDL_data * *data*, unsigned *from*, unsigned *to*)

Get the ring system id for given edge.

Parameters

data	pointer to the RDL_data holding the calculation results.
from	RDL_node starting at this edge
to	RDL_node starting at this edge

Returns

number of edges in the ring system, RDL_INVALID_RESULT on error RDL_NO_RINGSYSTEM if edge is not part of a ring system

Note

A ring system is a 2-connected component of the graph.

10.2.3.43 RDL_API unsigned RDL_getSSSR (const RDL_data * *data*, RDL_cycle *** *RDL_cycle_array_ptr*)

Gives a set of cycles that forms a Minimal Cycle Basis of the graph.

Returns

the number of cycles returned ($|E|-|V|+1$ for connected graphs), RDL_INVALID_RESULT on error

Parameters

data	pointer to the RDL_data holding the calculation results
RDL_cycle_-array_ptr	pointer that points to the result array (declare RDL_cycle ** and give address as parameter)

Note

Result has to be deallocated using RDL_deleteCycles(RDL_cycle **cycles, unsigned number) The result is an array of cycles.

10.2.3.44 RDL_API unsigned RDL_getURFsContainingEdge (const RDL_data * *data*, RDL_node *node1*, RDL_node *node2*, unsigned ** *RDL_ids_ptr*)

Gives all URFs containing the edge.

Returns

the number of URFs containing the edge, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
node1	the first RDL_node of the edge
node2	the the second RDL_node of the edge
RDL_ids_ptr	pointer that points to the result array of integers containing all indices of URFs containing the edge. (declare `unsigned *` and give address as parameter)

Note

The array RDL_ids_ptr has to be to be deallocated with `free(*RDL_ids_ptr)`
This functions internally enumerates all edges for each URF. For repeated queries with different RDL_node it is recommended to enumerate them with RDL_getEdgesForURF once and use this array.

10.2.3.45 RDL_API unsigned RDL_getURFsContainingNode (const RDL_data * *data*, RDL_node *node*, unsigned ** *RDL_ids_ptr*)

Gives all URFs containing the node.

Returns

the number of URFs containing the node, RDL_INVALID_RESULT on failure

Parameters

data	pointer to the RDL_data holding the calculation results
node	the RDL_node
RDL_ids_ptr	pointer that points to the result array of integers containing all indices of URFs containing the node. (declare `unsigned *` and give address as parameter)

Note

The array RDL_ids_ptr has to be to be deallocated with `free(*RDL_ids_ptr)`
This functions internally enumerates all nodes for each URF. For repeated queries with different RDL_node it is recommended to enumerate them with RDL_getNodesForURF once and use this array.

10.2.3.46 RDL_API unsigned RDL_getWeightForRCF (const RDL_data * *data*, unsigned *index*)

Returns the weight of each cycle in the RCF identified by its index.

Parameters

data	pointer to the RDL_data holding the URFs
index	the index of the RCF

Returns

the weight of the RCF, RDL_INVALID_RESULT on failure (if `index` is out of range)

10.2.3.47 RDL_API unsigned RDL_getWeightForURF (const RDL_data * *data*, unsigned *index*)

Returns the weight of each cycle in the URF identified by its index.

Parameters

data	pointer to the RDL_data holding the URFs
index	the index of the URF

Returns

the weight of the URF, RDL_INVALID_RESULT on failure (if `index` is out of range)

10.2.3.48 RDL_API RDL_graph* RDL_initNewGraph (unsigned *nof_nodes*)

Initializes a new RDL_graph.

Parameters

nof_nodes	the number of nodes in the graph

Returns

pointer to the new RDL_graph structure.

10.2.3.49 RDL_API void RDL_setOutputFunction (RDL_outputFunction *func*)

Set the output function for warning and error messages.

Parameters

func,:	callback function for errors and warnings

Warning

This function sets a `static` variable. When using multiple threads, only one thread should set the output function and the output function should be thread-safe.

Default is no output at all (RDL_writeNothing). Call `RDL_setOutputFunction(RDL_writeToStderr)` to enable output of warning and error messages to `stderr`.

10.2.3.50 RDL_API unsigned RDL_translateCycArray (const RDL_data * *data*, RDL_cycle ** *old_array*, unsigned *number*, char *** *RDL_cycle_array_ptr*)

Translates the results of RDL_getRCycles(), RDL_getSSSR(), RDL_getRCPrototypes() and RDL_getRCyclesForURF() (arrays of RDL_cycle) into an array of cycles represented by arrays of $\{0,1\}^{|E|}$ (bitsets).

Parameters

data	pointer to the RDL_data holding the calculation results.
old_array	The resulting structure of the functions named above
number	The return value of the functions named above (the number of cycles given)
RDL_cycle_array_ptr	pointer to the result array (declare char ** and give address as parameter)

Returns

The number of cycles given (same as the parameter 'number'), RDL_INVALID_RESULT on failure

Note

The initial structure still exists afterwards and still has to be deleted.

The resulting array has a 1 at position i if edge i is part of the cycle or 0 otherwise. An edge is identified by the position at which it was added to the graph starting at 0 (the return value of RDL_addUEdge()).

10.3 src/Test/Test.c File Reference

Demo and validation tool for the RingDecomposerLib library.

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include "RDLtesting.h"
#include "TestDemo.h"
#include "TestValidate.h"
```

10.3.1 Detailed Description

Demo and validation tool for the RingDecomposerLib library. This tool can be used for demo output and for testing/validation.

Demo output

Start the tool with

```
Test demo <filename>
```

The program will output the ring topology calculated by the library. The input file must be in DIMACS format as described below.

Validation

Start the tool with

```
Test validate <filename> [<timeout>]
```

The program will compare the relevant cycles to the cycles present in the input file. Furthermore the URFs will be validated, i.e. calculated with an independent exponential algorithm (definition of the URFs). The same procedure is applied to the SSSR (verify it's a cycle base). A number of consistency tests is executed to ensure integrity and robustness. See the file `test/README` for a descriptions of the test files.

The input file must be in DIMACS format as described below. A number of interesting example graphs are in the folder `test`.

The parameter `timeout` is optional and specifies a timeout in seconds for the exponential URF validation and the SSSR validation algorithm. (Timeouts are failures!)

File format

The input file format is a (modified) DIMACS graph format. See folder `test` for example files. Graph format specification:

First line:

```
p <number of nodes> <number of edges> [<nof cycles>]
```

with `<nof cycles>` optional.

Then the edges of the graph follow

```
e <node1> <node2>
```

If `<nof cycles>` was specified, then the relevant cycles of the graph are listed:

```
r <ring id> <ring size> <node1> <node2>
```

`<ring id>` and `<ring size>` are repeated for each edge of the graph as specified by `<node1>` and `<node2>`.

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