MP2 Calc

Generated by Doxygen 1.9.8

Chapter 1

Computation of the MP2 energy

This program reads the `.h5` file and computes the MP2 energy.

1.1 Theory

The MP2 energy is given by the formula:

```
E_{\text{MP2}} = E_{\text{HF}} +
 \sum_{(i,j)\in\text{occupied}}\sum_{(a,b)\in\text{virtual}}\langle ij||ab\rangle\frac{2\langle
      ij||ab\rangle-\langle ij||ba\rangle}{\varepsilon_i+\varepsilon_j-\varepsilon_a-\varepsilon_b}
```

where the E_{HF} is the Hartree-Fock energy calculated by the following formula:

```
E_{\text{HF}} = E_{NN} + 2\sum_{i=1}^{N_{\text{occ}}}\langle i|h|i\rangle +
      \sum_{i=1}^{N_{\text{occ}}}\sum_{j=1}^{N_{\text{occ}}} \left(2\langle ij||ij\rangle - \langle
      ij||ji\rangle\right)
```

1.2 Dependencies

The program depends on the `HDF5` library and `TREXIO` library.

1.2.1 HDF5

On Ubuntu, the `HDF5` library can be installed using the following command:

```
$ sudo apt-get install libhdf5-dev
```

1.2.2 TREXIO

The `TREXIO` library can be installed using the following command:

```
$ wget https://github.com/TREX-CoE/trexio/releases/download/v2.5.0/trexio-2.5.0.tar.gz
$ tar -zxvf trexio-2.5.0.tar.gz
$ cd trexio-2.5.0
$ ./configure
$ make
$ sudo make install
```

Note that when configuring the `TREXIO` library, you may need to specify the path to the `HDF5` library if it is not installed in the default location. See more information here.

1.3 Installation and usage

To install the program, run the following commands:

```
$ git clone git@github.com:vfornemo/ACT-homeworks.git
$ cd project1
$ ./compile.sh
```

The program can be run using the following command:

```
./main.o [path/to/input.h5]
```

The program will read the `input.h5` file and write the MP2 energy to the standard output.

1.4 Example

```
$ ./main.o ./data/h2o.h5
```

The output will be:

```
Reading file: ./data/h2o.h5
Nucleus repulsion energy: 9.194966
Number of up electrons: 5
Number of MOs: 24
Number of 2e integrals: 13458
h_core_sum: -123.151186
eri_sum: 37.929422
Electronic energy: -85.221764
HF energy: -76.026799
MP2 energy: -76.230759
```

Chapter 2

Installation

To install the program, run the following commands:

```
$ git clone git@github.com:vfornemo/ACT-homeworks.git
$ cd project1
$ ./compile.sh
```

The program will be available as `main.o` in the `project1` directory.

Chapter 3

Class Index

3.1 Class List

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

Chapter 4

File Index

4.1 File List

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

Chapter 5

Class Documentation

5.1 Mol Struct Reference

Mol struct contains all the information of the molecule.

`#include <mol.h>`

Public Attributes

- int32_t **mo_num**
  number of MOs
- int32_t **n_up**
  number of up electrons (or down electrons for RHF)
- int64_t **n_2e_int**
  number of 2e integrals
- energy **e_nuc**
  nucleus repulsion energy
- int32_t * **eri_index**
  2e integrals index
- energy * **eri_value**
  2e integrals values
- energy * **eri_seq**
  2e integrals in unique index sequence
- energy * **h_core**
  1e integrals
- energy * **e_mo**
  MO energies.
- energy **h_core_sum**
  sum of diagonal elements of h_core
- energy **eri_sum**
  sum of eri values
- energy **e_elec**
  electronic energy
- energy **e_hf**
  HF energy.
- energy **e_mp2**
  MP2 energy.

5.1.1 Detailed Description

Mol struct contains all the information of the molecule.

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

- src/mol.h

Chapter 6

File Documentation

6.1 src/hf.c File Reference

This module contains the functions for HF energy calculation.

```
#include <stdio.h>
#include <stdlib.h>
#include <trexio.h>
#include "reader.h"
#include "mol.h"
#include "util.h"
```

Include dependency graph for hf.c:

6.2 src/hf.h File Reference

This module contains the functions for HF energy calculation.

```
#include <stdio.h>
#include <stdlib.h>
#include "mol.h"
#include "util.h"
```

Include dependency graph for hf.h: This graph shows which files directly or indirectly include this file:

Functions

- void get_hcore_sum (Mol *const m)

  Get the core Hamiltonian sum.
- void hf_kernel (Mol *const m)

  Calculate the HF energy.
- int match_eri (int i, int j, int k, int l, Mol *const m)

  Match the ERI index HF ERI should be <ij|ij> or <ij|ji>, for <ij|kl>, check if i == k and j == l or i == l and j == k.
- void get_eri_sum (Mol *const m)

  Get sum of ERI values.

6.2.1 Detailed Description

This module contains the functions for HF energy calculation.

Author

Tianyi Gao

Version

1.0

Date

2024-11-24

Copyright

GNU Public License V3.0

6.2.2 Function Documentation

6.2.2.1 get_eri_sum()

```
void get_eri_sum (
            Mol *const m )
```

Get sum of ERI values.

Parameters

m	Mol struct

6.2.2.2 get_hcore_sum()

```
void get_hcore_sum (
            Mol *const m )
```

Get the core Hamiltonian sum.

Parameters

m	Mol struct

6.2.2.3 hf_kernel()

```
void hf_kernel (
```

```
            Mol *const m )
```

Calculate the HF energy.

Parameters

m	Mol struct

6.2.2.4 match_eri()

```
int match_eri (
            int i,
            int j,
            int k,
            int l,
            Mol *const m )
```

Match the ERI index HF ERI should be <ij|ij> or <ij|ji>, for <ij|kl>, check if i == k and j == l or i == l and j == k.

Parameters

i	
j	
k	
l	
m	

Returns

1 if i = j = k = l \

2 if i = k and j = l \

3 if i = l and j = k \

0 if none of the above

6.3 hf.h

Go to the documentation of this file.

```
00001
00011 #ifndef HF_H
00012 #define HF_H
00013
00014 #include <stdio.h>
00015 #include <stdlib.h>
00016 #include "mol.h"
00017 #include "util.h"
00018
00024 void get_hcore_sum(Mol* const m);
00025
00031 void hf_kernel(Mol* const m);
00032
00047 int match_eri(int i, int j, int k, int l, Mol* const m);
00048
00054 void get_eri_sum(Mol* const m);
00055
00056 #endif
```

6.4 src/main.c File Reference

This program reads the `.h5` file and computes the MP2 energy.

```
#include <stdio.h>
#include <stdlib.h>
#include <trexio.h>
#include "reader.h"
#include "mol.h"
#include "util.h"
#include "hf.h"
#include "mp2.h"
```

Include dependency graph for main.c:

Functions

- int **main** (int argc, char *argv[])
  Application entry.

6.4.1 Detailed Description

This program reads the `.h5` file and computes the MP2 energy.

Author

Yifan Jiang, Tianyi Gao

Version

1.0

Date

2024-11-25

Copyright

GNU Public License V3.0

6.5 src/mol.c File Reference

This module contains the functions for Mol struct.

```
#include <stdio.h>
#include <stdlib.h>
#include "mol.h"
#include "reader.h"
#include "util.h"
```

Include dependency graph for mol.c:

Functions

- void mol_init (Mol *const m, char *filename)
  initialize the Mol struct from the .h5 file
- void mol_destruct (Mol *const m)
  destruct the Mol struct
- energy get_nth_eri (int64_t n, Mol *const m)
  get the nth 2e integral value
- void gen_eri_index (Mol *const m)
  extract the 2e integral value into a 1D array, with unique index sequence
- energy get_eri_energy (Mol *const m, int32_t i, int32_t j, int32_t a, int32_t b)
  Given (ijab), return the 2e integral energy of (ia|jb)

6.5.1 Detailed Description

This module contains the functions for Mol struct.

Author

Yifan Jiang, Tianyi Gao

Version

1.0

Date

2024-11-25

Copyright

GNU Public License V3.0

6.5.2 Function Documentation

6.5.2.1 gen_eri_index()

```
void gen_eri_index (
            Mol *const m )
```

extract the 2e integral value into a 1D array, with unique index sequence

Parameters

m	

6.5.2.2 get_eri_energy()

```
energy get_eri_energy (
            Mol *const m,
            int32_t i,
            int32_t j,
            int32_t a,
            int32_t b )  [inline]
```

Given (ijab), return the 2e integral energy of (ia|jb)

Parameters

m	Mol struct
i,j,a,b	indices of the 2e integral

Returns

2e integral of (ia|jb)

6.5.2.3 get_nth_eri()

```
energy get_nth_eri (
            int64_t n,
            Mol *const m )
```

get the nth 2e integral value

Parameters

n	index of the 2e integral
m	Mol struct

Returns

nth 2e integral value

6.5.2.4 mol_destruct()

```
void mol_destruct (
            Mol *const m )
```

destruct the Mol struct

Parameters

m	Mol struct

6.5.2.5 mol_init()

```
void mol_init (
            Mol *const m,
            char * filename )
```

initialize the Mol struct from the .h5 file

Parameters

m	Mol struct
filename	path to the .h5 file

6.6 src/mol.h File Reference

This module contains the Mol struct and functions for Mol struct.

```
#include <stdio.h>
#include <stdlib.h>
#include <stdint.h>
```

Include dependency graph for mol.h: This graph shows which files directly or indirectly include this file:

Classes

- struct Mol

  Mol struct contains all the information of the molecule.

Typedefs

- typedef double **energy**

Functions

- void mol_init (Mol *const m, char *filename)

  initialize the Mol struct from the .h5 file
- void mol_destruct (Mol *const m)

  destruct the Mol struct
- energy get_nth_eri (int64_t n, Mol *const m)

  get the nth 2e integral value
- void gen_eri_index (Mol *const m)

  extract the 2e integral value into a 1D array, with unique index sequence
- energy get_eri_energy (Mol *const m, int32_t i, int32_t j, int32_t a, int32_t b)

  Given (ijab), return the 2e integral energy of (ia|jb)

6.6.1 Detailed Description

This module contains the Mol struct and functions for Mol struct.

Author

Yifan Jiang, Tianyi Gao

Version

1.0

Date

2024-11-23

Copyright

GNU Public License V3.0

6.6.2 Function Documentation

6.6.2.1 gen_eri_index()

```
void gen_eri_index (
            Mol *const m )
```

extract the 2e integral value into a 1D array, with unique index sequence

Parameters

m	

6.6.2.2 get_eri_energy()

```
energy get_eri_energy (
            Mol *const m,
            int32_t i,
            int32_t j,
            int32_t a,
            int32_t b )  [inline]
```

Given (ijab), return the 2e integral energy of (ia|jb)

Parameters

m	Mol struct
i,j,a,b	indices of the 2e integral

Returns

2e integral of (ia|jb)

6.6.2.3 get_nth_eri()

```
energy get_nth_eri (
            int64_t n,
            Mol *const m )
```

get the nth 2e integral value

Parameters

n	index of the 2e integral
m	Mol struct

Returns

nth 2e integral value

6.6.2.4 mol_destruct()

```
void mol_destruct (
            Mol *const m )
```

destruct the Mol struct

Parameters

m	Mol struct

6.6.2.5 mol_init()

```
void mol_init (
            Mol *const m,
            char * filename )
```

initialize the Mol struct from the .h5 file

Parameters

m	Mol struct
filename	path to the .h5 file

6.7 mol.h

Go to the documentation of this file.

```
00001
00011 #ifndef MOL_H
00012 #define MOL_H
00013
00014 #include <stdio.h>
00015 #include <stdlib.h>
00016 #include <stdint.h>
00017
00018 typedef double energy;
00019
00023 typedef struct {
00024     int32_t mo_num;
00025     int32_t n_up;
00026     int64_t n_2e_int;
00027     energy e_nuc;
00028     int32_t* eri_index;
00029     energy* eri_value;
00030     energy* eri_seq;
00031     energy* h_core;
00032     energy* e_mo;
00033     energy h_core_sum;
00034     energy eri_sum;
00035     energy e_elec;
00036     energy e_hf;
00037     energy e_mp2;
00038 } Mol;
00039
00046 void mol_init(Mol* const m, char* filename);
00047
00053 void mol_destruct(Mol* const m);
00054
00062 energy get_nth_eri(int64_t n, Mol* const m);
00063
00069 void gen_eri_index(Mol* const m);
00070
00078 energy get_eri_energy(Mol* const m, int32_t i, int32_t j, int32_t a, int32_t b);
00079
00080
00081 #endif
00082
```

6.8 src/mp2.c File Reference

This module contains the functions for MP2 energy calculation.

`#include "mp2.h"`
Include dependency graph for mp2.c:

Functions

- void cal_mp2_correlation (Mol *const m)

  Calculate the MP2 correlation energy.

6.8.1 Detailed Description

This module contains the functions for MP2 energy calculation.

Author

Yifan Jiang

Version

1.0

Date

2024-11-25

Copyright

GNU Public License V3.0

6.8.2 Function Documentation

6.8.2.1 cal_mp2_correlation()

```
void cal_mp2_correlation (
            Mol *const m )
```

Calculate the MP2 correlation energy.

Parameters

m	Mol struct

6.9 src/mp2.h File Reference

This module contains the functions for MP2 energy calculation.

```
#include "mol.h"
```

Include dependency graph for mp2.h: This graph shows which files directly or indirectly include this file:

Functions

- void cal_mp2_correlation (Mol *const m)

  Calculate the MP2 correlation energy.

6.9.1 Detailed Description

This module contains the functions for MP2 energy calculation.

Author

Yifan Jiang

Version

1.0

Date

2024-11-25

Copyright

GNU Public License V3.0

6.9.2 Function Documentation

6.9.2.1 cal_mp2_correlation()

```
void cal_mp2_correlation (
            Mol *const m )
```

Calculate the MP2 correlation energy.

Parameters

m	Mol struct

6.10 mp2.h

Go to the documentation of this file.

```
00001
00011 #ifndef MP2_H
00012 #define MP2_H
00013
00014 #include "mol.h"
00015
00021 void cal_mp2_correlation(Mol* const m);
00022
00023 #endif
```

6.11 src/reader.c File Reference

This module contains the functions for reading the trexio file.

```
#include <stdio.h>
#include <stdlib.h>
#include <trexio.h>
#include "reader.h"
#include "mol.h"
#include "util.h"
```

Include dependency graph for reader.c:

Functions

- void read_nucleus_repulsion (trexio_t ∗const trexio_file, Mol ∗const m)
  read the nucleus repulsion energy from the trexio file
- void read_electron_up_num (trexio_t ∗const trexio_file, Mol ∗const m)
  read the number of up electrons from the trexio file
- void read_mo_num (trexio_t ∗const trexio_file, Mol ∗const m)
  read the number of MOs from the trexio file
- void read_mo_1e_int_h_core (trexio_t ∗const trexio_file, Mol ∗const m)
  read the 1e integrals from the trexio file
- void read_mo_2e_int_eri_size (trexio_t ∗const trexio_file, Mol ∗const m)
  read the size of 2e integrals from the trexio file
- void read_mo_2e_int_eri (trexio_t ∗const trexio_file, Mol ∗const m)
  read the 2e integrals from the trexio file
- void read_mo_energy (trexio_t ∗const trexio_file, Mol ∗const m)
  read the MO energies from the trexio file

6.11.1 Detailed Description

This module contains the functions for reading the trexio file.

Author

Tianyi Gao, Yifan Jiang

Version

1.0

Date

2024-11-25

Copyright

GNU Public License V3.0

6.11.2 Function Documentation

6.11.2.1 read_electron_up_num()

```
void read_electron_up_num (
            trexio_t *const trexio_file,
            Mol *const m )
```

read the number of up electrons from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.2 read_mo_1e_int_h_core()

```
void read_mo_1e_int_h_core (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the 1e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.3 read_mo_2e_int_eri()

```
void read_mo_2e_int_eri (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the 2e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.4 read_mo_2e_int_eri_size()

```
void read_mo_2e_int_eri_size (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the size of 2e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.5 read_mo_energy()

```
void read_mo_energy (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the MO energies from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.6 read_mo_num()

```
void read_mo_num (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the number of MOs from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.11.2.7 read_nucleus_repulsion()

```
void read_nucleus_repulsion (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the nucleus repulsion energy from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12 src/reader.h File Reference

This module contains the functions for reading the trexio file.

```
#include <stdio.h>
#include <trexio.h>
#include "mol.h"
```

Include dependency graph for reader.h: This graph shows which files directly or indirectly include this file:

Functions

- void read_nucleus_repulsion (trexio_t ∗const trexio_file, Mol ∗const m)
  read the nucleus repulsion energy from the trexio file
- void read_electron_up_num (trexio_t ∗const trexio_file, Mol ∗const m)
  read the number of up electrons from the trexio file
- void read_mo_num (trexio_t ∗const trexio_file, Mol ∗const m)
  read the number of MOs from the trexio file
- void read_mo_1e_int_h_core (trexio_t ∗const trexio_file, Mol ∗const m)
  read the 1e integrals from the trexio file
- void read_mo_2e_int_eri_size (trexio_t ∗const trexio_file, Mol ∗const m)
  read the size of 2e integrals from the trexio file
- void read_mo_2e_int_eri (trexio_t ∗const trexio_file, Mol ∗const m)
  read the 2e integrals from the trexio file
- void read_mo_energy (trexio_t ∗const trexio_file, Mol ∗const m)
  read the MO energies from the trexio file

6.12.1 Detailed Description

This module contains the functions for reading the trexio file.

Author

Tianyi Gao, Yifan Jiang

Version

1.0

Date

2024-11-23

Copyright

GNU Public License V3.0

6.12.2 Function Documentation

6.12.2.1 read_electron_up_num()

```
void read_electron_up_num (
            trexio_t *const trexio_file,
            Mol *const m )
```

read the number of up electrons from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.2 read_mo_1e_int_h_core()

```
void read_mo_1e_int_h_core (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the 1e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.3 read_mo_2e_int_eri()

```
void read_mo_2e_int_eri (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the 2e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.4 read_mo_2e_int_eri_size()

```
void read_mo_2e_int_eri_size (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the size of 2e integrals from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.5 read_mo_energy()

```
void read_mo_energy (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the MO energies from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.6 read_mo_num()

```
void read_mo_num (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the number of MOs from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.12.2.7 read_nucleus_repulsion()

```
void read_nucleus_repulsion (
             trexio_t *const trexio_file,
             Mol *const m )
```

read the nucleus repulsion energy from the trexio file

Parameters

trexio_file	trexio file handler
m	Mol struct

6.13 reader.h

Go to the documentation of this file.

```
00001
00011 #ifndef READER_H
00012 #define READER_H
00013
00014 #include <stdio.h>
00015 #include <trexio.h>
00016 #include "mol.h"
```

```
00017
00024 void read_nucleus_repulsion(trexio_t* const trexio_file, Mol* const m);
00025
00032 void read_electron_up_num(trexio_t* const trexio_file, Mol* const m);
00033
00040 void read_mo_num(trexio_t* const trexio_file, Mol* const m);
00041
00048 void read_mo_1e_int_h_core(trexio_t* const trexio_file, Mol* const m);
00049
00056 void read_mo_2e_int_eri_size(trexio_t* const trexio_file, Mol* const m);
00057
00064 void read_mo_2e_int_eri(trexio_t* const trexio_file, Mol* const m);
00065
00072 void read_mo_energy(trexio_t* const trexio_file, Mol* const m);
00073
00074 #endif
```

6.14 src/util.c File Reference

This module contains the utility functions.

```
#include <stdio.h>
#include <stdlib.h>
#include "util.h"
#include "mol.h"
```

Include dependency graph for util.c:

Functions

- void print_matrix (double *const m, int row, int col)
  print a double array in matrix format
- double sum_diag (double *const m, int n, int order)
  sum to nth diagonal elements of a square matrix
- int32_t index_2e (int i, int j, int k, int l, int n)
  calculates unique index of given (ijkl) for 2e integrals

6.14.1 Detailed Description

This module contains the utility functions.

Author

Tianyi Gao

Version

1.0

Date

2024-11-23

Copyright

GNU Public License V3.0

6.14.2 Function Documentation

6.14.2.1 index_2e()

```
int32_t index_2e (
            int i,
            int j,
            int k,
            int l,
            int n )  [inline]
```

calculates unique index of given (ijkl) for 2e integrals

Note

0 <= i, j, k, l < n

i <= j, k <= l, i <= k

if i == k, then j <= l

Parameters

i,j,k,l	indices of the 2e integrals
n	number of MOs

Returns

unique index

6.14.2.2 print_matrix()

```
void print_matrix (
            double *const m,
            int row,
            int col )
```

print a double array in matrix format

Parameters

m	array to be printed
row	number of rows
col	number of columns

6.14.2.3 sum_diag()

```
double sum_diag (
            double *const m,
```

```
            int n,
            int order )
```

sum to nth diagonal elements of a square matrix

Parameters

m	1D matrix data array
n	sum up to nth diagonal elements
order	order of the matrix (row = col)

Returns

sum of the diagonal elements

6.15 src/util.h File Reference

This module contains the utility functions.

```
#include <stdio.h>
#include <stdlib.h>
#include "mol.h"
```

Include dependency graph for util.h: This graph shows which files directly or indirectly include this file:

Functions

- void print_matrix (double *const m, int row, int col)
  print a double array in matrix format
- double sum_diag (double *const m, int n, int order)
  sum to nth diagonal elements of a square matrix
- int32_t index_2e (int i, int j, int k, int l, int n)
  calculates unique index of given (ijkl) for 2e integrals

6.15.1 Detailed Description

This module contains the utility functions.

Author

Tianyi Gao

Version

1.0

Date

2024-11-23

Copyright

GNU Public License V3.0

6.15.2 Function Documentation

6.15.2.1 index_2e()

```
int32_t index_2e (
             int i,
             int j,
             int k,
             int l,
             int n )  [inline]
```

calculates unique index of given (ijkl) for 2e integrals

Note

0 <= i, j, k, l < n

i <= j, k <= l, i <= k

if i == k, then j <= l

Parameters

i,j,k,l	indices of the 2e integrals
n	number of MOs

Returns

unique index

6.15.2.2 print_matrix()

```
void print_matrix (
             double *const m,
             int row,
             int col )
```

print a double array in matrix format

Parameters

m	array to be printed
row	number of rows
col	number of columns

6.15.2.3 sum_diag()

```
double sum_diag (
             double *const m,
```

```
            int n,
            int order )
```

sum to nth diagonal elements of a square matrix

Parameters

m	1D matrix data array
n	sum up to nth diagonal elements
order	order of the matrix (row = col)

Returns

sum of the diagonal elements

6.16 util.h

Go to the documentation of this file.

```
00001
00012 #ifndef UTIL_H
00013 #define UTIL_H
00014 #include <stdio.h>
00015 #include <stdlib.h>
00016 #include "mol.h"
00017
00025 void print_matrix(double* const m, int row, int col);
00034 double sum_diag(double* const m, int n, int order);
00035
00045 int32_t index_2e(int i, int j, int k, int l, int n);
00046
00047 #endif
```

Index