

Reference Manual

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Chapter 1

TB-NumCal

1.1 Introduction

TB-NumCal is a program aimed to perform different types of numerical calculations in tight-binding models. In the core of the program we use mainly the Kernel Polynomial method to compute different spectral quantities such as the conductivity tensor, the non-equilibrium spin-density or the density of states. Although a complementary approach, the Time-Evolution method is also implemented.

The program is designed to work using both MPI and OpenMP paradigms of parallelism. Although the parallelism works different in each approach for the sake of performance. Instead of OpenMP the program can benefit from the platform CUDA for GPU calculations, which in many case result in a noticeable increasement in speed.

1.2 Installation

The installation process is very simple, however, for optimal performance some tuning must be performed. For the moment, the program is entirely tested within Intel Parallel 2016, therefore the variables INTEL_HOME, MPI_HOME, OMP_HOME and CUDA_HOME should be set in the arch_make file. For now the INTEL_HOME variable is mandatory, but if MPI_HOME, OMP_HOME or CUDA_HOME is not set, then the compilation will be performed excluding this options of parallelism, if both CUDA and OMP are set, CUDA takes priority over OMP.

Chapter 2

Namespace Index

2.1 Namespace List

Here is a list of all namespaces with brief descriptions:

custom_random	11
my	Namespace for the classes created for this project	11
NumCal	??
sparse	Defines the std::vector class	12

Chapter 3

Hierarchical Index

3.1 Class Hierarchy

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

NumCal::cerr_class	??
NumCal::cout_class	??
EigenMat	
my::SparseMatrix	23

Chapter 4

Class Index

4.1 Class List

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

NumCal::cerr_class	..	??
NumCal::cout_class	..	??
my::SparseMatrix		
The Sparse Matrix Class. Inherited from sparse::EigenMat		23

Chapter 5

File Index

5.1 File List

Here is a list of all files with brief descriptions:

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/tmp/TB-QuantumTransp/include/ lattice_geometry.h	26
/tmp/TB-QuantumTransp/include/ mpi_util.hpp	??
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Chapter 6

Namespace Documentation

6.1 custom_random Namespace Reference

Typedefs

- typedef boost::random::uniform_real_distribution< [my::real](#) > [uniform_real_dist](#)
- typedef boost::random::mt19937 [generator](#)

6.1.1 Typedef Documentation

6.1.1.1 typedef boost::random::mt19937 [custom_random::generator](#)

6.1.1.2 typedef boost::random::uniform_real_distribution<[my::real](#)> [custom_random::uniform_real_dist](#)

6.2 my Namespace Reference

Namespace for the classes created for this project.

Classes

- class [SparseMatrix](#)
The Sparse Matrix Class. Inherited from [sparse::EigenMat](#).

Typedefs

- typedef [external_real](#) [real](#)
- typedef unsigned long [size_t](#)
- typedef int [integer](#)
- typedef [external_complex](#) [complex](#)
- typedef [external_scalar](#) [scalar](#)
- typedef [external_vector](#) [vector](#)
- typedef [external_dvector](#) [dvector](#)
- typedef Eigen::SparseMatrix< [scalar](#), Eigen::RowMajor, [my::integer](#) > [SpMat](#)
- typedef Eigen::Triplet< [scalar](#) > [spEntry](#)

6.2.1 Detailed Description

Namespace for the classes created for this project.

6.2.2 Typedef Documentation

6.2.2.1 `typedef external_complex my::complex`

6.2.2.2 `typedef external_dvector my::dvector`

6.2.2.3 `typedef int my::integer`

6.2.2.4 `typedef external_real my::real`

6.2.2.5 `typedef external_scalar my::scalar`

6.2.2.6 `typedef unsigned long my::size_t`

6.2.2.7 `typedef Eigen::Triplet<scalar> my::spEntry`

6.2.2.8 `typedef Eigen::SparseMatrix< scalar, Eigen::RowMajor, my::integer > my::SpMat`

6.2.2.9 `typedef external_vector my::vector`

6.3 NumCal Namespace Reference

Classes

- class [cerr_class](#)
- class [cout_class](#)

Typedefs

- typedef [external_real](#) [real](#)
- typedef unsigned long [size_t](#)
- typedef int [integer](#)
- typedef [external_complex](#) [complex](#)
- typedef [external_scalar](#) [scalar](#)
- typedef [external_vector](#) [vector](#)
- typedef [external_dvector](#) [dvector](#)
- typedef Eigen::SparseMatrix< [scalar](#), Eigen::RowMajor, [my::integer](#) > [SpMat](#)
- typedef Eigen::Triplet< [scalar](#) > [spEntry](#)

6.3.1 Typedef Documentation

6.3.1.1 `typedef external_complex NumCal::complex`

6.3.1.2 `typedef external_dvector NumCal::dvector`

6.3.1.3 `typedef int NumCal::integer`

6.3.1.4 `typedef external_real NumCal::real`

6.3.1.5 `typedef external_scalar NumCal::scalar`

6.3.1.6 `typedef unsigned long NumCal::size_t`

6.3.1.7 `typedef Eigen::Triplet<scalar> NumCal::spEntry`

6.3.1.8 `typedef Eigen::SparseMatrix< scalar,Eigen::RowMajor, my::integer > NumCal::SpMat`

6.3.1.9 `typedef external_vector NumCal::vector`

6.4 sparse Namespace Reference

Defines the `std::vector` class.

Typedefs

- `typedef Eigen::SparseMatrix< my::scalar, Eigen::RowMajor, my::integer > EigenMat`
- `typedef Eigen::Triplet< my::scalar > Entry`

6.4.1 Detailed Description

Defines the `std::vector` class.

Defines the `Eigen::SparseMatrix` and `Eigen::Triplet` classes Define the different types of the program Namespace for the alias given to some of the objects of the `EigenClass`

6.4.2 Typedef Documentation

6.4.2.1 `typedef Eigen::SparseMatrix< my::scalar, Eigen::RowMajor, my::integer > sparse::EigenMat`

6.4.2.2 `typedef Eigen::Triplet<my::scalar> sparse::Entry`

Chapter 7

Class Documentation

7.1 NumCal::cerr_class Class Reference

```
#include <mpi_util.hpp>
```

Public Member Functions

- [cerr_class](#) ()
- [cerr_class](#) (const std::string _init_message)
- template<typename T >
[cerr_class](#) & [operator<<](#) (const T &v)

7.1.1 Constructor & Destructor Documentation

7.1.1.1 NumCal::cerr_class::cerr_class () [inline]

7.1.1.2 NumCal::cerr_class::cerr_class (const std::string *_init_message*) [inline]

7.1.2 Member Function Documentation

7.1.2.1 template<typename T > cerr_class& NumCal::cerr_class::operator<< (const T & v) [inline]

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

- /tmp/TB-QuantumTransp/include/[mpi_util.hpp](#)

7.2 NumCal::cout_class Class Reference

```
#include <mpi_util.hpp>
```

Public Member Functions

- [cout_class](#) ()
- [cout_class](#) (const std::string _init_message)
- template<typename T >
[cout_class](#) & [operator<<](#) (const T &v)

7.2.1 Constructor & Destructor Documentation

7.2.1.1 [NumCal::cout_class::cout_class](#) () [inline]

7.2.1.2 [NumCal::cout_class::cout_class](#) (const std::string _init_message) [inline]

7.2.2 Member Function Documentation

7.2.2.1 template<typename T > [cout_class](#)& [NumCal::cout_class::operator<<](#) (const T & v) [inline]

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

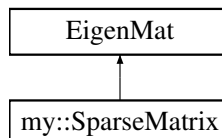
- /tmp/TB-QuantumTransp/include/[mpi_util.hpp](#)

7.3 my::SparseMatrix Class Reference

The Sparse Matrix Class. Inherited from [sparse::EigenMat](#).

```
#include <sparse_matrix.hpp>
```

Inheritance diagram for my::SparseMatrix:



Public Member Functions

- [SparseMatrix](#) ()
The Null constructor.
- [SparseMatrix](#) (const [my::integer](#) _ncol, const [my::integer](#) _nrow)
The Default constructor.
- void [Reserve](#) (const [my::integer](#) _size)
Reserve an estimated ammount of memory for the sparse matrix.
- [my::integer](#) [NumRawEntries](#) () const
Returns the total number of raw entries in the matrix.
- void [AddNewRawEntry](#) (const [sparse::Entry](#) _triplet)
Add a new Raw entry in the matrix.
- void [SetFromRawEntries](#) ()
Set the sparse matrix using the raw_entries.
- [sparse::Entry](#) [RawEntry](#) (const [my::integer](#) _idx) const
- [sparse::Entry](#) & [RawEntry](#) (const [my::integer](#) _idx)
- bool [IsSet](#) () const

Private Attributes

- `std::vector< sparse::Entry > matEntry_`
- `bool matrix_is_set`

7.3.1 Detailed Description

The Sparse Matrix Class. Inherited from [sparse::EigenMat](#).

7.3.2 Constructor & Destructor Documentation

7.3.2.1 `my::SparseMatrix::SparseMatrix ()` `[inline]`

The Null constructor.

7.3.2.2 `my::SparseMatrix::SparseMatrix (const my::integer _ncol, const my::integer _nrow)` `[inline]`

The Default constructor.

7.3.3 Member Function Documentation

7.3.3.1 `void my::SparseMatrix::AddNewRawEntry (const sparse::Entry _triplet)` `[inline]`

Add a new Raw entry in the matrix.

This method will append a new entry to the entry list, not making any check on the previous entries

7.3.3.2 `bool my::SparseMatrix::IsSet () const` `[inline]`

7.3.3.3 `my::integer my::SparseMatrix::NumRawEntries () const` `[inline]`

Returns the total number of raw entries in the matrix.

Returns the total number of raw entries in the matrix. This method will count repeated and non-zero entries

7.3.3.4 `sparse::Entry my::SparseMatrix::RawEntry (const my::integer _idx) const` `[inline]`

7.3.3.5 `sparse::Entry& my::SparseMatrix::RawEntry (const my::integer _idx)` `[inline]`

7.3.3.6 `void my::SparseMatrix::Reserve (const my::integer _size)` `[inline]`

Reserve an estimated amount of memory for the sparse matrix.

7.3.3.7 `void my::SparseMatrix::SetFromRawEntries () [inline]`

Set the sparse matrix using the raw_entries.

The list of entries after this operation is destroyed

7.3.4 Member Data Documentation

7.3.4.1 `std::vector<sparse::Entry> my::SparseMatrix::matEntry_ [private]`

7.3.4.2 `bool my::SparseMatrix::matrix_is_set_ [private]`

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

- [/tmp/TB-QuantumTransp/include/sparse_matrix.hpp](#)

Chapter 8

File Documentation

8.1 homepage.dox File Reference

8.2 /tmp/TB-QuantumTransp/include/custom_random.hpp File Reference

```
#include <boost/random/mersenne_twister.hpp>
#include <boost/random/uniform_real_distribution.hpp>
```

Namespaces

- [custom_random](#)

Typedefs

- typedef boost::random::uniform_real_distribution< [my::real](#) > [custom_random::uniform_real_dist](#)
- typedef boost::random::mt19937 [custom_random::generator](#)

8.3 /tmp/TB-QuantumTransp/include/efficient_mod.hpp File Reference

```
#include "types_definitions.hpp"
```

Functions

- [my::integer EffMod](#) ([my::integer](#) i, [my::integer](#) size)

8.3.1 Function Documentation

8.3.1.1 `my::integer EffMod (my::integer i, my::integer size)` `[inline]`

8.4 /tmp/TB-QuantumTransp/include/lattice_geometry.h File Reference

```
#include "types_definitions.hpp"
```

8.5 /tmp/TB-QuantumTransp/include/mpi_util.hpp File Reference

```
#include "mpi.h"
#include <cmath>
#include <iostream>
#include <string>
```

Classes

- class [NumCal::cout_class](#)
- class [NumCal::cerr_class](#)

Namespaces

- [NumCal](#)

Macros

- `#define NUMCAL_MPI_INIT()` `MPI::Init ()`
- `#define NUMCAL_MPI_FINALIZE()` `MPI::Finalize ()`
- `#define NUMCAL_MPI_GETRANK()` `MPI::COMM_WORLD.Get_rank ()`
- `#define NUMCAL_MPI_GETPROC()` `MPI::COMM_WORLD.Get_size ()`

8.5.1 Macro Definition Documentation

8.5.1.1 `#define NUMCAL_MPI_FINALIZE()` `MPI::Finalize ()`

8.5.1.2 `#define NUMCAL_MPI_GETPROC()` `MPI::COMM_WORLD.Get_size ()`

8.5.1.3 `#define NUMCAL_MPI_GETRANK()` `MPI::COMM_WORLD.Get_rank ()`

8.5.1.4 `#define NUMCAL_MPI_INIT()` `MPI::Init ()`

8.6 /tmp/TB-QuantumTransp/include/sparse_matrix.hpp File Reference

```
#include <vector>
#include "Eigen/Sparse"
#include "types_definitions.hpp"
```

Classes

- class [my::SparseMatrix](#)

The Sparse Matrix Class. Inherited from [sparse::EigenMat](#).

Namespaces

- [sparse](#)

Defines the `std::vector` class.

- [my](#)

Namespace for the classes created for this project.

Typedefs

- typedef `Eigen::SparseMatrix< my::scalar, Eigen::RowMajor, my::integer > sparse::EigenMat`
- typedef `Eigen::Triplet< my::scalar > sparse::Entry`

8.7 /tmp/TB-QuantumTransp/include/timing.hpp File Reference

```
#include <ctime>
#include <cstdio>
```

8.8 /tmp/TB-QuantumTransp/include/types_definitions.hpp File Reference

```
#include "Eigen/Sparse"
#include <complex>
#include <vector>
```

Namespaces

- [my](#)

Namespace for the classes created for this project.

- [NumCal](#)

Typedefs

- typedef float [external_real](#)
- typedef std::complex< [external_real](#) > [external_complex](#)
- typedef std::complex< [external_real](#) > [external_scalar](#)
- typedef std::vector< [external_scalar](#) > [external_vector](#)
- typedef std::vector< [external_scalar](#) > [external_dvector](#)
- typedef [external_real](#) [my::real](#)
- typedef unsigned long [my::size_t](#)
- typedef int [my::integer](#)
- typedef [external_complex](#) [my::complex](#)
- typedef [external_scalar](#) [my::scalar](#)
- typedef [external_vector](#) [my::vector](#)
- typedef [external_dvector](#) [my::dvector](#)
- typedef Eigen::SparseMatrix< scalar, Eigen::RowMajor, [my::integer](#) > [my::SpMat](#)
- typedef Eigen::Triplet< scalar > [my::spEntry](#)
- typedef [external_real](#) [NumCal::real](#)
- typedef unsigned long [NumCal::size_t](#)
- typedef int [NumCal::integer](#)
- typedef [external_complex](#) [NumCal::complex](#)
- typedef [external_scalar](#) [NumCal::scalar](#)
- typedef [external_vector](#) [NumCal::vector](#)
- typedef [external_dvector](#) [NumCal::dvector](#)
- typedef Eigen::SparseMatrix< scalar, Eigen::RowMajor, [my::integer](#) > [NumCal::SpMat](#)
- typedef Eigen::Triplet< scalar > [NumCal::spEntry](#)

8.8.1 Typedef Documentation

8.8.1.1 typedef std::complex< [external_real](#) > [external_complex](#)

8.8.1.2 typedef std::vector< [external_scalar](#) > [external_dvector](#)

8.8.1.3 typedef float [external_real](#)

8.8.1.4 typedef std::complex< [external_real](#) > [external_scalar](#)

8.8.1.5 typedef std::vector< [external_scalar](#) > [external_vector](#)

8.9 /tmp/TB-QuantumTransp/src/TB-QuantumTransp.cpp File Reference

```
#include <string>
#include <iostream>
#include <fstream>
#include "types_definitions.hpp"
#include "lattice.hpp"
#include "kpm.hpp"
#include "kpm_parallel.hpp"
#include "onsite_disorder.hpp"
#include <sys/time.h>
```


Functions

- int `main` (int argc, char **argv)

8.9.1 Function Documentation

8.9.1.1 int main (int *argc*, char ** *argv*)

Parameters of the irregular part of the hamiltonian

Look for the line kpm_infor

Setting the irregular Irregular Hamiltonian

The first Calculation will be a density of states

if(id==0)

