TeNeS Documentation

Release 0.1

Institute for Solid State Physics, University of Tokyo

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ONE

WHAT IS TENES?

1.1 Overview

TeNeS is an open-source program package for calculation of many-body quantum states based on the tensor network method. In ver. 0.1, this package calculates ground-state wavefunctions of quantum spin models, and evaluates physical quantities such as magnetization and correlation functions. For predefined models and lattices, there is a tool that makes it easy for users to generate input files. In ver. 1.0, a tool that is useful to define the own models and lattices from a simple input file will be developed. Furthermore, the Boson system will be able to be treated. This improvement will enable us to deal with various two-dimensional quantum spin and boson systems.

1.2 Developers

TeNeS is developed by the following members.

- ver 0.1
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1.3 Version information

• ver. 0.1: 2019/12/04.

1.4 License

This package is distributed under GNU General Public License version 3 (GPL v3) or later.

1.5 Copyright

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TWO

INSTALL

2.1 Download

You can download the source code for 'TeNeS' from the GitHub page . If you have git installed on your machine, type the following command to start download:

```
$ git clone https://github.com/issp-center-dev/TeNeS
```

2.2 Prerequisites

The following tools are required for building TeNeS.

- 1. C++11 compiler
- 2. CMake (>=2.8.14)
- 3. MPI and ScaLAPACK

TeNeS depends on the following libraries, but these are downloaded automatically through the build process.

- 1. mptensor
- 2. cpptoml
- 3. sanitizers-cmake

ScaLAPACK must be installed by yourself. If you use homebrew in Mac, type the following command:

```
brew install scalapack
```

For others, see the web page of ScaLAPACK.

For tenes_simple which generates the input file for tenes, the following libraries are needed.

- 1. Python (>= ver.3 is recommended)
- 2. numpy
- 3. toml

2.3 Install

1. Build TeNeS by typing the following commands:

```
$ mkdir build
$ cd build
$ cmake -DCMAKE_INSTALL_PREFIX=<path to install to> ..
$ make
```

The executable file tests will be generated in build/src directory. The default value of the <path to install to> is /usr/local.

2. Install TeNeS by typing the following commands:

```
$ make install
```

In this case, tenes is installed into the <path to install to>/bin.

Specify compiler

CMake detects your compiler automatically but sometimes this is not what you want. In this case, you can specify the compiler by the following way,

```
$ cmake -DCMAKE_CXX_COMPILER=<path to your compiler> ../
```

Use the pre-built mptensor

TeNeS is based on the parallerized tensor library mptensor. The build system of TeNeS installs this automatically, but if you want to use the specific version of the mptensor, please add the following option in cmake.

```
$ cmake -DMPTENSOR_ROOT=<path to mptensor> ../
```

4 Chapter 2. Install

THREE

USAGE

TeNeS needs to create several input files to define models, order of operations, etc. You can create and run the input file directly, but the following script is provided for ease of use:

- tenes_simple.py: A tool that generates input files for tenes by using a simple input file which specifies lattice model predefined.
- tenes_standard.py (from ver. 1.0): A tool that generates input files for tenes by using input files for generating the lattice model.

The following sections describe how to use each script, and finally how to use tenes. If you want to work with other models or grids, you can do so by creating the input file for tenes directly. See *File format* for details on the input file of tenes.

3.1 Usage of tenes_simple

tenes_simple is a tool that creates an input file of tenes for predefined models, lattices.

- Take the input file name as an argument.
- The command line options are:
 - help
 - * show help messages.
 - output
 - * output file name.
 - * default name is input.toml.
 - * Cannot have the same file name as the input file name.

3.2 Usage of tenes_simple.py

tenes_simple.py will be released at ver.1.0.

3.3 Usage of tenes

If you prepare input files of tenes by yourself, You can directry run tenes as follows:

- Take the input file name as an argument.
- The command line options are:
 - help Show help messages.
 - version Show the version number.
 - quiet Do not print any messages to the standard output.

tnsolve input.toml

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TUTORIAL

4.1 Ising model with transverse magnetic field

This section presents an example of calculation when the transverse magnetic field is applied to the Ising model. By changing the variable G in the input file, the magnitude of the transverse magnetic field will be modified. For example, when the transverse magnetic field is 0, the input file becomes

```
[parameter]
[parameter.tensor]
       # tensor_dim
D = 2
CHI = 10 \# env\_dim
[parameter.simple_update]
num\_step = 1000
tau = 0.01
[parameter.ctm]
iteration_max = 10
[lattice]
type = "square lattice"
L_sub = [2,2]
[model]
type = "spin"
Jz = -1.0
Jx = 0.0
Jy = 0.0
G = 0.0
```

In this case, since Jz = -1.0, the ferro magnetic state becomes the ground state at G=0. When the input file name is simple.toml, type the following commands to execute tenes:

```
$ tenes_simple simple.toml
$ tenes input.toml
```

Then, the following logs are output to the standard output.

```
Start simple update
Start calculating observables
Start updating environment
Start calculating local operators
Save site observables to output/site_obs.dat
```

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```
Start calculating energy
Save energy to output/energy.dat
Start calculating NN correlation
Save NN correlation to output/neighbor_obs.dat
Save elapsed times to output/time.dat

Energy = -0.5
Local operator 0 = 0.5
Local operator 1 = 1.90794709356e-11

time simple update = 3.21127
time full update = 0
time environmnent = 0.875561
time observable = 0.132412
```

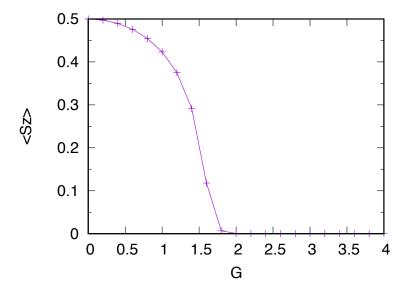
The execution status of each process is displayed first. After finishing the calculation, Energy and the local operators Local operator 0 << Sz>, Local operator 1 << Sx>) are outputted, respectively. Finally, time is printed to show the calculation time (Time unit is seconds). In the output folder, energy.dat, parameters.dat, time.dat, neighbor_obs.dat, site_obs.dat are outputted. For details about each output file, see the file formats. The value of < Sz> can be extracted from the value following the 0 0 component of site_obs.dat or the Local operator 0 in the standard output. By changing G in increments of 0.1 from 0 to 2.0 and running tenes_simple and tenes, the following result is obtained.

As an example of the sample script, tutorial_example.py , tutorial_read.py are prepared in the sample/01_transverse_field_ising directory. The calculation will be done by typing the following command:

```
$ python tutorial_example.py
```

For MacBook2017 (1.4 GHz Intel Core i7), the calculation was finished in a few minutes. By typing the following command, G, energy, <Sz> and <Sx> are oututted in the standard output:

```
$ python tutorial_read.py
```



As you can see from the figure, with increasing G, the <Sz> decreases gradually from 0.5 to 0.

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FILE FORMAT

5.1 Input file for tense_simple

- File format is TOML format.
- \bullet The input file has five sections: model, parameter, lattice, observable, correlation .
- In future, the file will be split by specifying a file name.

5.1.1 parameter section

The contents of the parameter section are copied directly to the parameter section of the input file of tenes. You can also specify the imaginary time step size for the imaginary time evolution operator in simple and full updates in the subsections simple_update, full_update.

Name	Description	Туре	Default
tau	imaginary time step in the imaginary	Real	0.01
	time evolution operator		

The following parameters are common to the tenes input file.

parameter.tensor

Name	Description	Type	Default
D	The virtual bond dimensions of the cen-	Integer	2
	tral tensor		
CHI	The virtual bond dimensions of the angu-	Integer	4
	lar transfer matrix		
save_dir	Directory to write optimized tensors	Str	6677
load_dir	Directory to read initial tensor	Str	6677

- save_dir Store optimized tensors below this directory. When it is empty, the tensors are not saved.
- load_dir Read various tensors from below this directory. Must be the same degree of parallelism as when saved. Not read if it is empty.

parameter.simple_update

Name	Description	Туре	Default
num_step	Number of simple updates	Integer	0
lambda_cutoff	cutoff of the mean field to be considered	Real	1e-12
	zero in the simple update		

parameter.full_update

Name	Description	Туре	Default
num_step	Number of full updates	Integer	0
env_cutoff	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing environ-		
	ment through full updates		
inverse_precision	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing the pseu-		
	doinverse matrix with full update		
convergence_epsilon	Convergence criteria for truncation opti-	Real	1e-12
	mization with full update		
iteration_max	Maximum iteration number for trunca-	Integer	1000
	tion optimization on full updates		
gauge_fix	Whether the tensor gauge is fixed	Boolean	true
fastfullupdate	Whether the Fast full update is adopted	Boolean	true

parameter.ctm

Name	Description	Туре	Default
projector_cutoff	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing CTM pro-		
	jectors		
convergence_epsilon	CTM convergence criteria	Real	1e-10
iteration_max	Maximum iteration number of conver-	Integer	100
	gence for CTM		
projector_corner	Whether to use only the 1/4 corner tensor	Boolean	true
	in the CTM projector calculation		
use_rsvd	Whether to replace SVD with Random	Boolean	false
	SVD		
rsvd_oversampling_factor	Ratio of the number of the oversampled	Real	2.0
	elements to that of the obtained elements		
	in the Random SVD method		

parameter.random

Name	Description	Туре	Default
seed	Seed of the pseudo-random number gen-	Integer	11
	erator used to initialize the tensor		

Each MPI process has the own seed as seed plus the process ID (MPI rank).

Example

```
[parameter]
[parameter.tensor]
D = 4  # tensor_dim
CHI = 16  # env_dim

[parameter.simple_update]
num_step = 1000

[parameter.full_update]
num_step = 1

[parameter.ctm]
iteration_max = 5
```

5.1.2 lattice section

Specify the lattice information. Square lattice and honeycomb lattice are defined as lattice types.

Name	Description	Type
type	Lattice name (square lattice or honey-	Str
	comb lattice)	
L_sub	Unit cell size	An integer or a list of two
		integers

When a list of two integers is passed as L_sub , the first element gives the value of Lx and the second one does Ly. If L_sub is an integer, Both Lx and Ly will have the same value. A list of three or more elements causes an error.

Sites in a unit cell are indexed starting from 0. These are arranged in order from the x direction.

Sites in a unit cell of $L_sub = [2, 3]$ are arranged as follows:

```
Y

^ 4 5

| 2 3

.->x 0 1
```

Square lattice

There are two types of bond, horizontal (0) and vertical (1) (corresponding to – and | in the below figure).

The unit cell for $L_sub = 2$ is given as follows:

```
0 1
| | |
2 - 3 - 2
| | |
0 - 1 - 0
```

Honeycomb lattice

Unit cell size (Each element of L_sub) must be an even number.

There are 3 types of bonds: x, y, and z (corresponding to -, \sim , | in the below figure). Each site with an even index has a rightward (x), a leftward (y), and an upward (z) bonds and each site with an odd index has a leftward (x), a rightward (y), and a bottomward (z) bonds.

The unit cell for $L_sub = 2$ is given as follows:

```
0 1
| 2 ~ 3 - 2
| 0 - 1 ~ 0
```

5.1.3 model section

Specify the type of the model. Only the Spin system can be spcified in ver. 0.1.

Name	Description	Type
type	The type of the model	Str

Spin system

Spin system

$$\mathcal{H} = \sum_{\langle ij \rangle} \left[\sum_{\alpha}^{x,y,z} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha} + B \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \right] - \sum_i \left[h S_i^z + \Gamma S_i^x - D \left(S_i^z \right)^2 \right]$$

Table 1: :header: "Name", "Description", "Type", "Default" :widths: 30, 30, 10, 10

S	Magnituide of the local spin	Real	0.5
Jx	The x component of the exchange interaction J	Real or a list of Real	1.0
Jy	The y component of the exchange interaction J	Real or a list of Real	1.0
Jz	The z component of the exchange interaction J	Real or a list of Real	1.0
BQ	Biquadratic interaction B	Real or a list of Real	0.0
h	longitudinal magnetic field h	Real	0.0
G	Transverse magnetic field Γ	Real	0.0
D	On-site spin anisotropy D	Real	0.0

By providing a list of exchange and biquadratic interactions, we can vary the magnitude of the interaction for each type of lattice bond. If the number of elements in the list is less than the type of lattice bond, the remainder is filled in with the last element specified.

5.1.4 observable section

By default, the local physical quantities used for physical quantities measurements: S^z and S^x . Measurements of more detailed physical quantities can be made by overwriting the format common to the input file of tenes. For details, See observable section *Input file for tenes*.

5.1.5 correlation section

For tenes_simple , correlation functions $C=\langle A(0)B(r)\rangle$ are not calculated by default. For calculating correlation functions, they have to be specified in the same file format as the input file of tenes. For details, See correlation section *Input file for tenes*.

5.2 Input file for tenes

- File format is TOML format.
- The input file has five sections: parameter, lattice, evolution, observable, correlation
 - In the future we will be able to split it by specifying the file name.

5.2.1 parameter section

Various parameters such as the number of updates are specified in this section. Only the parameters in this section have default values. This section has five sub sections, tensor, simple_update, full_update, ctm, random.

parameter.tensor

Name	Description	Туре	Default
D	The virtual bond dimensions of the cen-	Integer	2
	tral tensor		
CHI	The virtual bond dimensions of the angu-	Integer	4
	lar transfer matrix		
save_dir	Directory to write optimized tensors	Str	<i>د</i> >>دد>
load_dir	Directory to read initial tensor	Str	، ۲۶۶٬۰۰۰

- save_dir Store optimized tensors below this directory. When it is empty, the tensors are not saved.
- load_dir Read various tensors from below this directory. Must be same degree of parallelism as when saved. Not read if it is empty.

parameter.simple_update

Name	Description	Туре	Default
num_step	Number of simple updates	Integer	0
lambda_cutoff	cutoff of the mean field to be considered	Real	1e-12
	zero in the simple update		

parameter.full_update

Name	Description	Type	Default
num_step	Number of full updates	Integer	0
env_cutoff	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing environ-		
	ment through full updates		
inverse_precision	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing the pseu-		
	doinverse matrix with full update		
convergence_epsilon	Convergence criteria for truncation opti-	Real	1e-12
	mization with full update		
iteration_max	Maximum iteration number for trunca-	Integer	1000
	tion optimization on full updates		
gauge_fix	Whether the tensor gauge is fixed	Boolean	true
fastfullupdate	Whether the Fast full update is adopted	Boolean	true

parameter.ctm

Name	Description	Туре	Default
projector_cutoff	Cutoff of singular values to be consid-	Real	1e-12
	ered as zero when computing CTM pro-		
	jectors		
convergence_epsilon	CTM convergence criteria	Real	1e-10
iteration_max	Maximum iteration number of conver-	Integer	100
	gence for CTM		
projector_corner	Whether to use only the 1/4 corner tensor	Boolean	true
	in the CTM projector calculation		
use_rsvd	Whether to replace SVD with Random	Boolean	false
	SVD		
rsvd_oversampling_factor	Ratio of the number of the oversampled	Real	2.0
	elements to that of the obtained elements		
	in the Random SVD method		

$\verb"parameter.random"$

Name	Description	Туре	Default
seed	Seed of the pseudo-random number gen-	Integer	11
	erator used to initialize the tensor		

Each MPI process has the own seed as seed plus the process ID (MPI rank).

Example

```
[parameter]
[parameter.tensor]
D = 4  # tensor_dim
```

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```
CHI = 16  # env_dim
[parameter.simple_update]
num_step = 1000

[parameter.full_update]
num_step = 1

[parameter.ctm]
iteration_max = 5
```

5.2.2 lattice section

Specify the unit cell information. Unit cell has a shape of a rectangular with the size of Lx times Ly.

Name	Description	Туре
L_sub	Unit cell size	An integer or a list of integer

When a list of two integers is passed as L_sub , the first element gives the value of Lx and the second one does Ly. If L_sub is an integer, Both Lx and Ly will have the same value. A list of three or more elements causes an error.

Sites in a unit cell are indexed starting from 0. These are arranged in order from the x direction.

Sites in a unit cell of $L_sub = [2, 3]$ are arranged as follows:

```
y
^ 4 5
| 2 3
.->x 0 1
```

Information of bonds is given in the evolution and the observable sections.

5.2.3 evolution section

Define the imaginary time evolution opetrators used in simple and full updates.

Name	Description	Type
matrix	Matrix representation about the imaginary time	A list of string
	evolution opetrators	
simple_update	The order of the bonds that act on the index of the	A list of string
	imaginary time evolution operator in simple update	
full_update	The order of the bonds that act on the index of the	A list of string
	imaginary time evolution operator in full update	

matrix

- One matrix is defined by a list of string.
- Columns are separated by one or more blanks, and rows are separated by one or more newlines.
- The order defined corresponds exactly to the number of the matrix. This order numbers are used to specify simple_update and full_update (0-origin).

simple_update and full_update

- One row represents one operator action.
- Each line consists of four fields: int int string int.
 - 1. A site to which bond connects
 - 2. A site to which bond connects
 - 3. Horizontal (h) or Vertical (v)
 - 4. Operator number (0-origin)

Example

```
[evolution]
simple_update = """
0 1 h 0
3 2 h 0
2 3 h 0
1 0 h 0
0 2 v 0
3 1 v 0
2 0 v 0
1 3 v 0
full_update = """
0 1 h 0
3 2 h 0
2 3 h 0
1 0 h 0
0 2 v 0
3 1 v 0
2 0 v 0
1 3 v 0
matrix = [
0.9975031223974601 0.0 0.0 0.0
0.0 1.0025156589209967 -0.005012536523536887 0.0
0.0 -0.005012536523536888 1.0025156589209967 0.0
0.0 0.0 0.0 0.9975031223974601
.....
]
```

5.2.4 observable section

In this section, the information about physical quantities to be observed is specified.

Name	Description	Туре
local_operator	Site opertor (ex. Sz)	A list of string
hamiltonian	Bond hamiltonian	A list of string
hamiltonian_bonds	Type of bond Hamiltonian and the set of bonds that	string
	act	

local_operator, hamiltonian

Same as evolution.matrix. The order you define corresponds exactly to the index of the operator Hamiltonian.

hamiltonian_bonds

Same as evolution.simple_update.

Example

```
[observable]
local_operator = [
 0.5 0.0
0.0 -0.5
" " "
 0.0 0.5
 0.5 0.0
""",
hamiltonian_bonds = """
0 1 h 0
3 2 h 0
2 3 h 0
1 0 h 0
0 2 v 0
3 1 v 0
2 0 v 0
1 3 v 0
" " "
hamiltonian = [
                    0.0
 0.25 0.0 0.0
 0.0 -0.25 0.5
                     0.0
      0.5 - 0.25
                    0.0
 0.0
        0.0 0.0
 0.0
                    0.25
""",
```

5.2.5 correlation section

In the following, the parameters about the correlation function $C = \langle A(0)B(r) \rangle$ is described.

Name	Description	Type
r_max	Maximum distance r of the correlation function	Integer
operators	Numbers of operators A and B that measure corre-	A list for Integer
	lation functions	

The operators defined in the observable section are used.

Example

```
[correlation]
r_max = 5
operators = [[0,0], [0,1], [1,1]]
```

5.3 Output files

Output files are generated in the output directry.

5.3.1 parameters.dat

Paramters in the parameter and lattice sections defined in the input file are outputted.

5.3.2 energy.dat

The energy of each site is output.

5.3.3 site_obs.dat

- The expected values of the site operator are outputted.
- Each row consists of four columns.
 - 1. Index of the operator
 - 2. Index of the sites
 - 3. Real part of the expected value
 - 4. Imaginary part of the expected value

Example

5.3.4 neighbor_obs.dat

- Nearest neighbor correlations for site operations are outputted.
- Each row consists of five columns.
 - 1. Index of the operator
 - 2. Index of the sites
 - 3. Index of the sites
 - 4. Real part of the expected value
 - 5. Imaginary part of the expected value

```
# $1: op_index
# $2: source_site
# $3: target_site
# $4: real
# $5: imag
0 0 1 -7.05927615064968900e-02 0.0000000000000000e+00
0 0 2 -7.27068456430051274e-02 0.0000000000000000e+00
0 1 0 -7.13284385957392297e-02 0.0000000000000000e+00
0 1 3 -7.19523349256113581e-02 0.0000000000000000e+00
0 2 3 -7.12610364895483045e-02 0.0000000000000000e+00
0 2 0 -7.19731507561011952e-02 0.0000000000000000e+00
0 3 2 -7.05633558230210067e-02 0.0000000000000000e+00
0 3 1 -7.26803750807340498e-02 0.0000000000000000e+00
1 0 1 -1.85942869237103348e-01 0.00000000000000000e+00
1 0 2 -1.87164731677545187e-01 0.00000000000000000e+00
1 1 0 -1.86360382550076586e-01 0.00000000000000000e+00
1 1 3 -1.86768451086366694e-01 0.00000000000000000e+00
1 2 3 -1.86384181909805935e-01 0.00000000000000000e+00
1 2 0 -1.86747576732693515e-01 0.0000000000000000e+00
1 3 2 -1.85975089525013598e-01 0.00000000000000000e+00
1 3 1 -1.87196522916879049e-01 0.00000000000000000e+00
```

5.3.5 correlation.dat

- Correlation functions are outputted.
- Each row consists of eight columns.
 - 1. Index of the left operator
 - 2. Site index of the left operator
 - 3. Index of the right operator
 - 4. Site index of the right operator
 - 5. Unit cell offset of the right operator (x)
 - 6. Unit cell offset of the right operator (y)
 - 7. Real part of the expected value
 - 8. Imaginary part of the expected value

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Example

```
# $1: left_op
# $2: left_site
# $3: right_op
# $4: right_site
# $5: offset_x
# $6: offset_y
# $7: real
# $8: imag
0 0 0 1 0 0 -7.05927615064967928e-02 0.00000000000000000e+00
0 0 0 0 1 0 1.19668843226761017e-02 0.00000000000000000e+00
0 0 0 1 1 0 -2.43086229320005863e-03 0.00000000000000000e+00
0 0 0 0 2 0 7.42729194528496308e-04 0.0000000000000000e+00
0\ 0\ 0\ 1\ 2\ 0\ -4.38794819416885419e-04\ 0.000000000000000000e+00
0\ 0\ 0\ 2\ 0\ 0\ -7.27068456430051135e - 02\ 0.000000000000000000e + 00
0 0 0 0 1 1.23339845746621279e-02 0.0000000000000000e+00
0 0 0 2 0 1 -2.50111186244407349e-03 0.00000000000000000e+00
0 0 0 0 0 2 7.54607806587391516e-04 0.0000000000000000e+00
0 0 0 2 0 2 -4.47734559969679546e-04 0.00000000000000000e+00
1 0 1 1 0 0 -1.85942869237103237e-01 0.00000000000000000e+00
1 3 1 1 0 3 -1.65874245891461547e-01 0.00000000000000000e+00
```

5.3.6 time.dat

The calculation time is outputted.

REFERENCES

Please see the following documents if you want to know the algorithms used in TeNeS.

- Lecture slides and video
 - Slide: https://www.issp.u-tokyo.ac.jp/public/caqmp2019/slides/808L_Okubo.pdf
 - youtube: https://www.youtube.com/watch?v=EL9iGwoqZes&list=PLyL_XwLqTTm6roebw6MgIK0ljrN8cSQUX
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CONTACTS

• About Bugs

Please report all problems and bugs on the github Issues page

To resolve bugs early, follow these guidelines when reporting:

- Please specify the version of TeNeS you are using.
- If there are problems for installation, please inform us about your operating system and the compiler, and include the input / output and CMakeCache.txt when you run cmake and make.
- If a problem occurs during execution, enter the input file used for execution and its output.

Thank you for your cooperation.

• Others

If you have any questions about topics related to your research that are difficult to consult at Issues on GitHub, please contact the following contact information.

 $E\text{-mail:} \ \texttt{tenes-dev} \underline{\quad} \texttt{at} \underline{\quad} \texttt{issp.u-tokyo.ac.jp} \ (\texttt{replace} \ \underline{\quad} \texttt{at} \underline{\quad} \texttt{by} \ @)$