MUPRO MANUAL

Ferroelectric module

June 6, 2017

Contents

Preface

This MuFE manual is written for researchers who has knowledge about the basics of ferroelectrics. Programming experiences is not necessary. However, basic knowledge of LINUX operations are necessary, as currently only the linux executable is released.

This manual start with a brief introduction and a simple example to get the reader started using the program. Followed by detailed introduction of different input files, output data and pre/post processing scripts. Next all of the parameters that can be set using the input.in file is listed and explained in detail.

The book is mainly a reference guide and explains most files and control flags implemented in the code. The book also tries to give an impression on how MuFE works. However, a more complete description of the underlying algorithms and theories can be found in the recommended reference section.

The guide continues to grow as new features are added to the code. It is therefore always possible that the version you hold in your hands is outdated. Therefore, users mighht find it useful to check the online version of the MuFE guide from time to time, to learn about new features added to the code.

Chapter 1

Installation and setup

1.1 Prerequisite

MuFE is build with intel parallel studio cluster edition, and Intel mpi is required to run the program. Make sure the **$LD_LIBRARY_PATH** is correctly configured that the folder containing shared library **libmpi.so.12** and **libmpifort.so.12** must be presented.

1.2 Installation

To install the package, simply run the **install.sh** script. The script takes one argument, that is the **mupro install path**, if no argument is passed, then a default folder **/opt/MUPRO/** will be used. For example, if you execute this command

```
./install.sh /usr/local/MUPRO
```

The script will fist create the install directory **/usr/local/MUPRO**, next copy all of the contents in your current distribution folder into the install directory. And then add several lines to your **/.bashrc** to setup the environment variable **MUPROROOT**, and create alias to the executable for easier usage. The **MUPROROOT** variable should be set to place where the MUPRO license file **license.lic** is located. This is very important because if not set correctly, then the license checking process will fail.

1.3 Using the package

If worked correctly, the install.sh script should have created alias to the executable files for the MuFE package, all of the alias start with **mupro-**, you can double tab to find out available ones.

1.4 About license.lic

In order to generate a valid license file, the following information is necessary:

1. **hostname**. Be careful that this may not be the host name you used to get access to your linux server, but the host name of the login node you get connected to. For example, I can connect to the Penn State server through **ssh xuc116@aci-b.aci.ics.psu.edu**, but due to there are multiple login nodes, I'm actually connected to a node called **aci-004.aci.production.int.aci.ics.psu.edu**. This is the host name you should provide to us, rather than the **aci-b.aci.ics.psu.edu** one. If there are more than more hostname that you may get connected to you can supply us with a list of them. You can easily

obtain the hostname of your server or computer by execute **echo $HOSTNAME** in the linux terminal.

2. **username**. The user name you want to grant access to use MuFE. You can find the user name by typing **echo $USER** in the terminal. Note if you apply for the group license rather than individual one, you should provide the group name instead of user name.

3. **group name**. The group of users that you want to grant access to use MuFE. You can find all of the group you belong to by executing the **id** command in terminal.

4. **ip address**. You can obtain your server's ip address by typing **curl ipinfo.io/ip** in terminal. Same as hostname, if there are more than one ip address that you may get connected to, you can provide us with a list of them.

Chapter 2

MuFerro: an introduction

2.1 MuPro and MuFE

MuPro represents microstructure pro, which is a bundle of several phase-field based microstructure modeling programs, ranging from alloy solidification and precipitation to ferroelectric and ferromagnetic domain evolution. Different from most simulation programs, all of the programs in MuPro package is solve through spectral method rather than finite difference or finite element. MPI and FFTW3 boost our code efficiency, and empowers us to perform 3D simulations at relatively low cost.

MuFE is one of the modules in MuPro package, which can evolve ferroelectric domains structures by solving the time dependent Ginzgurg Landau equations that takes elastic and electric contribution into consideration. The equation is evoled using a semi-implicit spectral scheme in a parallel fashion. This ensured the coupled equations are solved accurately and efficiently. MuFE can be used to simulate both bulk and thin film material, and study the domain's response to external mechanical and electrical stimuli. Some interesting features of current MuFE or to be included in a near future version, includes the ability to take into account of different film orientation, inhomogeneous structure, such as superlattices and islands, flexoelectric effect, dislocations, charged defects and oxygen-octahedral rotation.

2.2 A quick tutorial

The files needed for this tutorial can be found in the MuFE example folder (usually located at mupro/install/path/MUPRO_version_number/Ferroelectric/Example).

1. Copy the following three files from the example folder to your work directory.

input.in This file is the central input file of MuFE. Each line consists of a tag, which is a predefined keyword that tells the program what to do and how to do it. It is followed by an equation sign '=' and one or several values associated with the keyword. For each keyword, a default will be used if it is not been specified in the file.

Polar.in This file contains the polarization at each grid points in a columnar fashion. An example of the file is shown in Table 2.1. The first line specify the x, y and z range of the simulation system. The first three columns represents the grid position. The 3rd to 6th columns represents the polarization components projected to the x, y, and z axis of the Catesian coordinate for claculation (global coordinate), Px, Py, Pz. The 7th to 9th columns represents the polarization components projected to the 1, 2, and 3 axis of the crytallography coordinates (local coordinate).

Table 2.1: Example of Polar.in file

10	10	10						
1	1	1	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	1	2	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	1	3	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
1	1	10	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	2	1	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	2	2	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
1	10	10	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2	10	10	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3	10	10	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
10	10	10	0.00E+00	0.0000000E	0.00E+00	0.00E+00	0.00E+00	0.00E+00

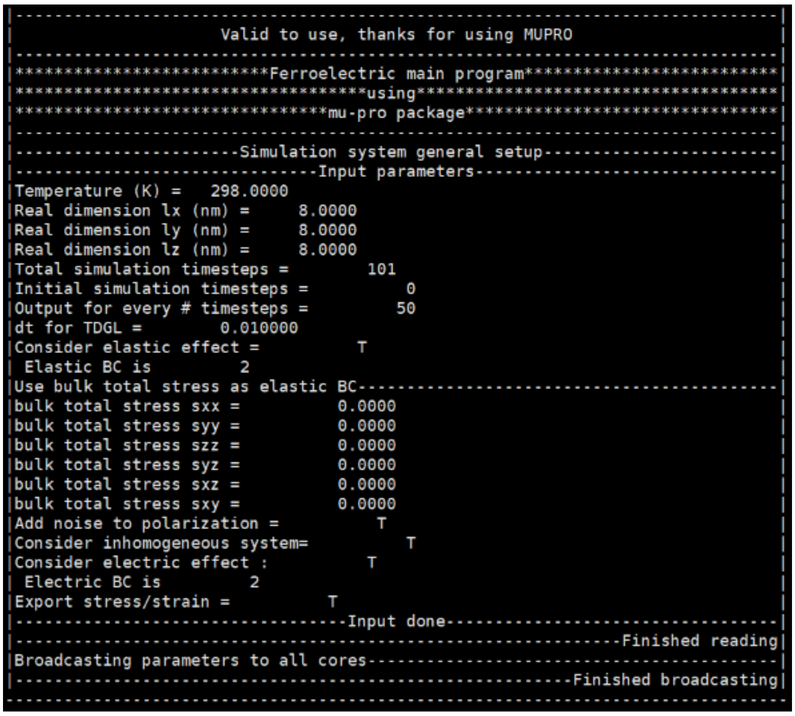
pot.in This file store the necessary thermodynamic parameters and other physical properties for the ferroelectric material you want to simulate, such as of Landau potential coefficients, elastic constants, electrostrictive coeffficents.For this quick tutorial, $BaTiO_3$ is used. The content of this pot.in is shown in Listing 2.1.

2. Run the MuFE program. If you installed the package through the **install.sh** we provided, then you should be able to run it just by typing **mupro-Ferroelectric** in terminal. Otherwise, you need to find the **MUPRO-Ferro.exe** located in the Ferroelectric folder of our MuFE distribution and then either execute it by give the whole path to the binary, or copy it to your current working directory. You need to make sure you have all the three input files copied to the current directory, in which you're trying to run the MuFE program.

```
{
    "name"       : "BiTiO3",
    "Comment"        : "Fitted by Jian Jun Wang, the landau coefficient needs to be updated according to stress for every time step",
    "Reference"      : "JAP 108. 114105 (2010)",
    "CurieT"         : 390,
    "a0"             : 42769496,
    "p0"             : 0.26,
    "Landau"    :
        {   "a1"     : "5*10^5*160*(cosh(160/tem)/sinh(160/tem)-cosh(160/390)/sinh(160/390))",
            "a11"    : -1.154E8,
            "a12"    :  6.530E8,
            "a111"   : -2.105E9,
            "a112"   :  4.091E9,
            "a123"   : -6.688E9,
            "a1111"  :  7.590E10,
            "a1112"  : -2.193E10,
            "a1122"  : -2.221E10,
            "a1123"  :  2.416E10
        },
    "Electrostrictive"  :
        {
            "Q11"    :  0.11   ,
            "Q12"   : -0.045 ,
            "Q44"   :  0.029
        },
    "ElasticModulus"    :
        {
            "C11"   :  1.7794E11,
            "C12"   :  0.9635E11,
            "C44"   :  1.2199E11
        },
    "ElasticCompliance" :
        {
            "S11"   :  9.07E-12,
            "S12"   : -3.186E-12,
            "S44"   :  8.197E-12
        },
    "Gradient"          :
        {
            "G11"   : 5.10E-10,
            "G12"   : 0.0,
            "G44"   : 1.0E-11,
            "GM44"  : 1.0E-11
        }
}
```

Listing 2.1: pot.in file

After the program started, some information will be printed to the screen as shown in Figure 2.1.



```
|------------------------------------------------------------------------------|
|                      Valid to use, thanks for using MUPRO                    |
|------------------------------------------------------------------------------|
|**************************Ferroelectric main program**************************|
|************************************using*************************************|
|********************************mu-pro package********************************|
|------------------------------------------------------------------------------|
|-----------------------Simulation system general setup------------------------|
|-------------------------------Input parameters-------------------------------|
|Temperature (K) =   298.0000                                                  |
|Real dimension lx (nm) =     8.0000                                           |
|Real dimension ly (nm) =     8.0000                                           |
|Real dimension lz (nm) =     8.0000                                           |
|Total simulation timesteps =        101                                       |
|Initial simulation timesteps =          0                                     |
|Output for every # timesteps =         50                                     |
|dt for TDGL =        0.010000                                                 |
|Consider elastic effect =           T                                         |
| Elastic BC is          2                                                     |
|Use bulk total stress as elastic BC-------------------------------------------|
|bulk total stress sxx =          0.0000                                       |
|bulk total stress syy =          0.0000                                       |
|bulk total stress szz =          0.0000                                       |
|bulk total stress syz =          0.0000                                       |
|bulk total stress sxz =          0.0000                                       |
|bulk total stress sxy =          0.0000                                       |
|Add noise to polarization =          T                                        |
|Consider inhomogeneous system=          T                                     |
|Consider electric effect :          T                                         |
| Electric BC is          2                                                    |
|Export stress/strain =          T                                             |
|----------------------------------Input done----------------------------------|
|---------------------------------------------------------------Finished reading|
|Broadcasting parameters to all cores------------------------------------------|
|----------------------------------------------------------Finished broadcasting|
--------------------------------------------------------------------------------
```

Figure 2.1: Example screen output

After the program finished, you will get some output data files, all of which are in columnar pattern similar to the **Polar.in** file, that first three column define the position for data point, and then rest of the columns are data at each grid point. You may process the data or visualize it use the tools you're most familiar with.

We have provided several examples in out MuFE distributions including this quick tutorial files, but in the future when you are trying to prepare these files yourself, it may seems like a daunting task for beginners, that's why we have this manual and some other tools to help you out.

For the creating the **input.in** file, you should refer to the Chapter 4 and find the keyword you need for your specific case. For the **Polar.in** file, we prepared a small program called "Structure-Generator" that will help you create some commonly used or geometrically simple domain structures. And lastly, for the **pot.in** file, we are building an online database for phenomenological thermodynamic parameters, in the future you may want to download potential files from the website directly. For now, we put the thermodynamic parameters for some common materials in the "potential" folder in the ferroelectric directory of MuFE distribution. But of course, you can use your own parameters for the potential file. The **pot.in** file is in the JSON format, you are allowed to change the value (number or string after the colon), but not the keys (the string before the colon, which is the name for the parameter we used in our simulation), since once the keys are changed, we can no longer find all of the value needed for simulation, and the program may crash.

The post processing, can also be quite challenging sometimes. We also prepare some gnuplot scripts, as well as a visualization gui based on VTK+Qt to help you get started with the process, and when you have more sophisticated visualization needs, you may find the right one that suits you the most.

2.3 Structure of MuFerro package

MuFE is a Fortran 90 program. It allows for dynamic memory allocation and a single executable which can be used for any type of calculation. Generally the executables and the pseudo potentials should reside in the following directories:

```
MuPro root directory
├─license.lic
└─MUPRO_1.0.6
   ├─Ferroelectric
   │  ├─MUPRO-ferro.exe
   │  ├─Ferroelectric.pbs
   │  ├─Potential
   │  └─Example
   ├─Plot
   │  ├─Some gnuplot scripts ...
   │  └─Some bash scripts ...
   └─Structure-Generator
      ├─structureGenerator.exe
      └─Example
```

The **MuPro root directory** contains the license.lic file and the MuPro distribution of specific version, in this example is **MUPRO_1.0.6**. In the **MUPRO_1.0.6** folder there are three directories,

Ferroelectric contains the main program for MuFE phase-field simulation, an example PBS script for you to submit jobs on systems using PBS job queue system, a **Potential** folder which contains several commonly used thermodynamic potentials and physical properties that the program needs, and an **Example** folder that contains some example project for you to try out and gain experience with using the program.

Plot contains three pairs of gnuplot script and bash script, one for 1D plot, one for 2D scalar heat plot, and the third for 2D vector glyph plot.

Structure-Generator contains a tool we prepared for you to generator some simple domain structures that can be directly used as the **Polar.in** file for MuFE program.

Chapter 3

Files of MuFerro

3.1 Input files

The following input files need to be presented in your working directory.

1. input.in
2. pot.in
3. Polar.in

Some other optional input files are

- OctaTilt.in
- AFMtip.in

3.1.1 input.in

input.in file is in a free-format structure, each line of the file is made up of several parts

identifier The string that appears before "=" in each line. Identifiers are keywords that MuFE used to link the corresponding parameters in the program with values that are set in the input file. According to the values to be set, the identifiers can be classified into four types: 1. logical switch 2. choice options 3. single value 4. array values.

values The values that appears after "=" and before "#" in each line. These are numbers, booleans or string values related to the identifier.

comments The string after "#".

Let's take a look at some examples of the four types of identifiers and their values.

logical switch All logical switch type of identifiers start with "L" representing logical type, and the acceptable values are either True or false.
Example: LELAST = True # Consider the elastic effect on ferroelectric system

choice options All choice option type of identifiers start with "C" representing choice, and the acceptable values are integers.
Example: CELASBC = 2 # Set the elastic boundary condition to be stress free for bulk simulations.

single value This type of identifiers only accept one value, and it can be either real or integer number depending on the specific identifier.
Example: TIMESTEP = 10000   # Set the maximum simulation steps to be 10000.

array value This type of identifiers accept more than one values, and it can be either real or integer number depending on the specific identifier.
Example: SYSSIZE = 128 128 40   # Set the simluation system size in x, y, z direction

3.1.2 pot.in

Like most materials simulation method, phase field simulation for ferroelectrics require an potential, the Landau potenital of ferroelectric materials. The standard potential files are provided in the potential folder of MuFE distribution. If missing, one can easily obtained the potential files from online database.

```
{
    "name"       : "BiTiO3",
    "Comment"       : "Fitted by Jian Jun Wang, the landau coefficient needs to be updated according to stress for every time step",
    "Reference"     : "JAP 108. 114105 (2010)",
    "CurieT"        : 390,
    "a0"            : 42769496,
    "p0"            : 0.26,
    "Landau"    :
        {   "a1"    : "5*10^5*160*(cosh(160/tem)/sinh(160/tem)-cosh(160/390)/sinh(160/390))",
            "a11"   : -1.154E8,
            "a12"   :  6.530E8,
            "a111"  : -2.105E9,
            "a112"  :  4.091E9,
            "a123"  : -6.688E9,
            "a1111" :  7.590E10,
            "a1112" : -2.193E10,
            "a1122" : -2.221E10,
            "a1123" :  2.416E10
        },
    "Electrostrictive"  :
        {
            "Q11"   :  0.11  ,
            "Q12"   : -0.045 ,
            "Q44"   :  0.029
        },
    "ElasticModulus"    :
        {
            "C11"   :  1.7794E11,
            "C12"   :  0.9635E11,
            "C44"   :  1.2199E11
        },
    "ElasticCompliance" :
        {
            "S11"   :  9.07E-12,
            "S12"   : -3.186E-12,
            "S44"   :  8.197E-12
        },
    "Gradient"          :
        {
            "G11"   : 5.10E-10,
            "G12"   : 0.0,
            "G44"   : 1.0E-11,
            "GM44"  : 1.0E-11
        }
}
```

3.1.3 Polar.in

Polar.in is also a mandatory input file. This stores the initial spatial distribution of polarization for calculation. It has a header line, specifing the total grid size of the system. The rest of the lines are made up of 9 columns, first three are data point positions, 4 to 6 columns are polarization under global coordinate (the lab coordinate), 7 to 9 columns are polarization in local coordinate (the crystal lattice coordinate). Be careful that the sequence of data point is z,y,x rather than x,y,z, that is the data position get update along z direction first, then y direction and in the last x direction.

Table 3.1: Example of Polar.in file

10	10	10						
1	1	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	1	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	1	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
1	1	10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	2	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1	2	2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
1	10	10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2	10	10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3	10	10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
...								
10	10	10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

3.1.4 OctaTilt.in

This file is similar to Polar.in, but store the oxygen-octahedarl rotation around three axis. Please read this reference for more information about how we consider oxygen-octahedral rotation in phase-field simulation.[Ref Xue].

3.1.5 AFMtip.in

This file is used to set the elastic/electric boundary conditions by an AFM tip, indenter, or bias electrodes. The first line of this file contains three values, the first one is the amount of changes of tip for the whole simulation, the second value is the choice of electric boundary condition, and the third value is the choice of elastic boundary condition, the meaning of different value for boundary condition can be found the in Chapter 4 for identifier of **CELASBC** and **CELECBC**.

The rest of **AFMtip.in** file are made up of 7 columns,

1. timestep that the tip parameters get changed.

2. grid position of the tip in x direciton.

3. grid position of the tip in y direction.

4. the electric potential applied to the tip.

5. the force applied by the tip to the film.

6. friction factor in x direction.

7. friction factor in y direction.

As an example, to simulate a moving AFM tip with 1V bias which writes along the path of the letter "P", one need to prepare the AFMtip.in as

```
        25     1      0
# timestep,  ntipx,  ntipy,  bias,  force,  fricx,  fricy
         1  30.00  90.00   1.00   0.00   0.0   0.0
      2001  30.00  84.00   1.00   0.00   0.0   0.0
      4001  30.00  78.00   1.00   0.00   0.0   0.0
      6001  30.00  72.00   1.00   0.00   0.0   0.0
      8001  30.00  66.00   1.00   0.00   0.0   0.0
     10001  30.00  60.00   1.00   0.00   0.0   0.0
     12001  30.00  54.00   1.00   0.00   0.0   0.0
     14001  30.00  48.00   1.00   0.00   0.0   0.0
     16001  30.00  42.00   1.00   0.00   0.0   0.0
     18001  30.00  36.00   1.00   0.00   0.0   0.0
     20001  30.00  90.00   1.00   0.00   0.0   0.0
     22001  36.00  90.00   1.00   0.00   0.0   0.0
     24001  42.00  90.00   1.00   0.00   0.0   0.0
     26001  48.00  90.00   1.00   0.00   0.0   0.0
     28001  54.00  90.00   1.00   0.00   0.0   0.0
     30001  60.00  90.00   1.00   0.00   0.0   0.0
     32001  60.00  84.00   1.00   0.00   0.0   0.0
     34001  60.00  78.00   1.00   0.00   0.0   0.0
     36001  60.00  72.00   1.00   0.00   0.0   0.0
     38001  60.00  66.00   1.00   0.00   0.0   0.0
     40001  60.00  60.00   1.00   0.00   0.0   0.0
     42001  54.00  60.00   1.00   0.00   0.0   0.0
     44001  48.00  60.00   1.00   0.00   0.0   0.0
     46001  42.00  60.00   1.00   0.00   0.0   0.0
     48001  36.00  60.00   1.00   0.00   0.0   0.0
```

Listing 3.1: PBS script

Notice the potential and force applied by tip is actually a distribution rather than uniform value. The value specified here is just one parameter used to get the distribution, you should always check the electric potential distribution and stress distribution to confirm that you get what you're expecting.

3.2 Output files

There are a few output files as listed in the table. They can be controlled by relative tags. Most of the output data files are time dependent, that is the spatial distribution of some value at a given timestep. The file name for these time dependent data have one thing in common, they are all made up of three parts separated by ".", the first one is the file name, such as "Polar", "Strain", the second one is the time step this data get output, which has a length of 8 digit, filled with 0 if the number length is less than 8, the third one is the file extension "dat". All possible data files are listed and explained in the Table 3.2.

Table 3.2: Output file list

File name	Columns	Explanation
Polar	6	Polarization in global coordinate and local coordinate
Grade_En	1	Gradient energy distribution
Grad_For	3	Gradient driving force for polarization x, y, z
Eigen_Str	6	Eigen strain distribution in voigt notation
Strain	6	Total strain distribution in voigt notation
Elast_Str	6	Elastic strain distribution in voigt notation
Stress	6	Stress distribution in voigt notation
Displace	3	Displacement x, y, z
Elast_En	1	Elastic energy
Elas_For	3	Elastic driving force for polarization x, y, z
Elect_En	1	Electric energy
Elefield	3	Electric field x, y, z
Elec_Phi	1	Electric potential
Elec_For	3	Electric driving force x, y, z
Charges	3	Bound charge, free charge, total charge
LandP_En	1	Landau energy for polarization as order parameter
LandPFor	3	Landau driving force for polarization x, y, z
Eflexo	3	Flexoelectric driving force, as known as the effective electric field, x, y, z
Gen_ForX	6	Elastic, electric, flexoelectric, landau, gradient and total driving force in x direction
Gen_ForY	6	Elastic, electric, flexoelectric, landau, gradient and total driving force in y direction
Gen_ForZ	6	Elastic, electric, flexoelectric, landau, gradient and total driving force in z direction
OctaTilt	6	Oxygen octahedral tilt around x, y, z axis
ElasQFor	3	Elastic driving force for oxygen octahedral tilt
GradQ_En	1	Gradient energy of oxygen octahedral tilt
GradQFor	3	Gradient driving force for oxygen octahedral tilt x, y, z component
LandQ_En	1	Landau energy of oxygen octahedral tilt as order parameter
LandQFor	3	Landau driving force for oxygen octahedral tilt
GenQForX	4	Elastic, landau, gradient and total driving force for oxygen octahedral tilt around x axis
GenQForY	4	Elastic, landau, gradient and total driving force for oxygen octahedral tilt around y axis
GenQForZ	4	Elastic, landau, gradient and total driving force for oxygen octahedral tilt around z axis

3.3 Pre-processing files

3.3.1 PBS file for submitting tasks

Many of the linux high performance computing system are using "Portable Batch System (PBS)" to manage the queueing and allocation of jobs on the cluster. For these types of systems, a PBS script is needed for job submission.

```
#PBS -l nodes=1:ppn=2
#PBS -l walltime=24:00:00
#PBS -N Ferroelectric
#PBS -j oe
#PBS -A allocation_to_use
#PBS -M myemail@school.edu
#PBS -m ae

cd $PBS_O_WORKDIR
echo ‘date‘
mpirun MUPRO -ferroelectric.exe
echo ‘date‘
```

Listing 3.2: PBS script

3.3.2 scripts for batch tasks

From time to time you may want to run a series of jobs to see the trend of how things change. The following script gives an example that replace custom keyword in the input.in file, **nx_size** and **lx_size**, with different numbers ranging from 40 to 120, before submitting the job with PBS command.

```bash
#! /bin/bash

length=( 40 60 80 100 120 )

for interval in "${length[@]}"
do
    let nx=$interval
    let lx=($nx)
    mkdir $interval
    cd $interval
    cp ../input.in .
    sed -i "s/nx_size/${nx}/g" input.in
    sed -i "s/lx_size/${lx}/g" input.in
    qsub ferro.pbs
    cd ..
done
```

Listing 3.3: Batch submission of jobs

3.4 Post-processing files

3.4.1 GNUPlot & bash scripts

In the **Plot** folder we provide several script that enables you to quickly draw some 1D plot, 2D scalar plot and 2D vector plot for the output data MuFE program generated.

plot_1d.sh

This script helps you to draw 1D profile of a one column vs another in the data file. It takes at least 9 arguements: 1. minimum value in x direction, 2. maximum value in x direction, 3. minimum value in y direction, 4. maximum value in y direction, 5. minimum value in z direction, 6. maximum value in z direction, 7. column number of the data used for the horizontal axis of the 1D plot, 8. column number of the data used for the vertical axis of the 1D plot, 9. name of the data file.

You can actually pass more data file names as additional arguments, and the script will draw the same 1D profile for all of the data files on one figure.

An example usage of the script is shown in Listing 3.4. It means slice the **Polar.00001000.dat** file into one line, $1 \leq x \leq 128$, and $y = 40, z = 20$, then plot the figure using the first column and the fourth column of the data file, which correspond to grid position in x direction and the x component of polarization in global coordinates. The output figure has a default name of **fig1d.png**.

```
plot_1d.sh 1 128 40 40 20 20 1 4 Polar.00001000.dat
```

Listing 3.4: Example of 1D plot usage.

plot_2ds.sh

This script helps you to draw 2D heat plot for one column in the data file. It takes at 7 arguements: 1. minimum value in x direction, 2. maximum value in x direction, 3. minimum value in y direction, 4. maximum value in y direction, 5. minimum value in z direction, 6. maximum value in z direction, 7. column number of the data you want to use for the heat plot.

An example usage of the script is shown in Listing 3.5. It means slice the **Polar.00001000.dat** file into one plane, $1 \leq x \leq 128, 1 \leq y \leq 128$, and $z = 20$, then plot the figure using the fourth column of the data file, which correspond to the x component of polarization in global coordinates. The output figure has a default name of **fig2ds_Polar.png**.

```
plot_2ds.sh 1 128 1 128 20 20 4 Polar.00001000.dat
```

Listing 3.5: Example of 2D scalar plot usage.

plot_2dv.sh

This script helps you to draw 2D vector plot for two column in the data file. It takes at 8 arguements: 1. minimum value in x direction, 2. maximum value in x direction, 3. minimum value in y direction, 4. maximum value in y direction, 5. minimum value in z direction, 6. maximum value in z direction, 7. column number of the data you choose as the x component for the vector to be drawn, 8.olumn number of the data you choose as the y component for the vector to be drawn.

An example usage of the script is shown in Listing 3.6. It means slice the **Polar.00001000.dat** file into one plane, $1 \leq x \leq 128, 1 \leq y \leq 128$, and $z = 20$, then plot the figure using the fourth and fifth columns of the data file, which correspond to the x and y component of polarization in global coordinates, px is used as the x component of the 2D vector and py as the y component. The output figure has a default name of **fig2dv_Polar.png**.

```
plot_2ds.sh 1 128 1 128 20 20 4 5 Polar.00001000.dat
```

Listing 3.6: Example of 2D vector plot usage.

Chapter 4

The Input.in File

4.1 List of most important parameters

Table 4.1: Your caption here

	Tags	Class	Default	Description
System	SYSDIM	Vector	10, 10, 10	Grid points in x, y, z
	REALDIM	Vector	Same as SYSDIM	Real length along x, y, z
	SUBTHICK	Scalar	0	Grid points for substrate thickness
	FILMTHICK	Vector	0	Grid points for film thickness
	ROTANGLE	Vector	0.0, 0.0, 0.0	Euler rotation angle around z, x', z''
Time	TTOTAL	Scalar	1000	Total timesteps
	TSTART	Scalar	0	Initial timestep
	TOUT	Scalar	200	Time interval for output
	TDELTA	Scalar	0.01	Delta t of TDGL
Solvers	LINHOM	Flag	FALSE	Flag for inhomogeneous solver
	CDER	Choice	0- step-corrected FFT 1- FDM 2- normal FFT	Choices of derivative solver
Thermal	TEM	Scalar	298.0	Temperature in Kelvin
Polarization	CPOLARBC	Choice	0- natural BC 1- free BC 2- blocked BC 3- small extrapolation length 4- zero bound charge 5- large extrapolation length	Choices of boundary condition,for Px, Py, Pz
	ETRLP	Vector	0.0, 0.0, 0.0	Extrapolation length of Px, Py, Pz in nm
	LPNOISE	Flag	FALSE	Flag of polarization noise
	PNOISMAG	Scalar	0.1	Magnitude of polarization noise
	PNOISEED	Scalar	10	Seed of polarization noise
Elastic	LELAS	Flag	TRUE	Flag of elastic energy
	CELASBC	Choice	0- film 1- bulk strain 2- bulk stress	Choices of elastic boundary conditions
	MISFIT	Vector	0.0, 0.0, 0.0	Misfit strain exx, eyy, exy

	STRAIN	Vector	0.0, 0.0, 0.0, 0.0, 0.0, 0.0	Strain BC for bulk, exx, eyy, ezz, eyz, ezx, exy
	STRESS	Vector	0.0, 0.0, 0.0, 0.0, 0.0, 0.0	Stress BC for bulk, sxx, syy, szz, syz, szx, sxy
	TIPRAD	Scalar	50.0	Tip radius in nm
Electric	LELEC	Flag	TRUE	Flag of electric energy
	CELECBC	Choice	1- open circuit 2- short circuit 3- top open bottom short 4- top short bottom open 5- bulk	Choices of electric boundary conditions
	TIPGAMMA	Scalar	10.0	Lortenz $gamma$ for tip in nm
	SCRBOT	Scalar	0.0	Screening factor of bottom electrode
	SCRTOP	Scalar	0.0	Screening factor of top electrode
Gradient	GRADCON	Vector	0.6, 0.0, 0.3	Gradient energy tensor component g11, g12 and g44
Flexoelectric	LFLEXO	Flag	FALSE	Flag of flexoelectric energy
	FLEXOCON	Vector	5.1, 3.3, 0.045	Flexoelectric tensor component f11, f12, and f44
Oxygen Octahedral Rotation	LOCTILT	Flag	FALSE	Flag of oxygen octahedral tilt
	GRADQCON	Vector	1.0 0.0 0.5	Gradient energy tensor of OOT component v11, v12, v44
	LQNOISE	Flag	FALSE	Flag of OOT noise
	QNOISMAG	Scalar	0.1	Magnitude of OOT noise
	QNOISEED	Scalar	10	Seed of OOT noise
Outputs	LOUTLAND	Flag	FALSE	Flag of output Landau energy of polarization
	LOUTELAS	Flag	FALSE	Flag of output elastic energy
	LOUTELEC	Flag	FALSE	Flag of output elastic energy
	LOUTGRAD	Flag	FALSE	Flag of output gradient energy
	LOUTFLEX	Flag	FALSE	Flag of output flexoelectric fields
	LOUTFORC	Flag	FALSE	Flag of output driving forces

4.2 CDER

Full name: choice derivative

Type: choice

Options:
0 FFT method with step correction
1 finite difference method
2 FFT method without step correction

Description: Choose the numerical methods for taking derivatives. The places may be affected by this option include bound charges (divergence of polarization), elecric field (gradient of electric potential), and flexoelectric field/flexoelectric driving force(derivatives of stress tensors)

Notes: Do not change CDER unless following situations:

1. Flexofield calculations

4.3 CELASBC

Full name: choice elastic boundary conditions

Type: Choice

Options:

0 film boundary condition, i.e., stress-free at film surface and clamped at film bottom. (for detailed treatment please refer to micromechanics [Li 2002][Khachaturyan Chap 8?])

1 strained boundary condition for bulk, i.e., clamped boundary condition. Assign a fixed strain tensor as average strain value of bulk system. Use this combined with **STRAIN**-tag [Ref].

2 stressed boundary condition for bulk. Assign a fixed stress tensor as average stress value of bulk system. Use this combined with **STRESS**-tag [Ref].

Description: Choose the elastic boundary condition when solving for mechanical equilibrium.

Notes:

1. CELASBC = 1 and 2 only work for bulk system while CELASBC = 0 only works for film system. Please be consistent with the **LBULK** tag.

2. CELASBC = 1 is related to **STRAIN**
   CELASBC = 2 is related to **STRESS**
   CELASBC = 0 is related to **MISFIT**

4.4 CELECBC

Full name: Choice electric boundary conditions

Type: Choice

Options:

0 bulk boundary condition, i.e., given a fixed electric field to bulk system. Specify applied electric field by ELECFIELD.

1 open-circuit boundary conditions at film surface and bottom.

2 short-circuit boundary condition at film surface and bottom.

3 open-circuit boundary condition at film surface while short-circuit boundary condition at film bottom.

4 open-circuit boundary condition at film bottom while short-circuit boundary condition at film surface.

Description: Choose the electric boundary condition of electrostatic equation

Notes:

1. CELECBC = 0 only works for bulk systems while other options only work for filmsystems.

2. CELECBC = 0 is paired with ELECFIELD.

3. In experiment, even without electrode, there are still plenty of mechanisms that can compensate charges at the interface or surface, so be careful when to use the open circuit condition.

4.5 CPOLARBC

Full name: Choice polarization boundary conditions

Type: Choice

Options:

0 natural boundary condition

1 Neumann boundary condition, $\frac{dP}{dz} = 0$ at film surface and bottom.

2 Dirichlet boundary condition, $P = 0$ at film surface and bottom.

Description: Choose the boundary condition for polarization when evolving the time dependent Ginzburg Landau equation. The polarization boundary condition is related to extrapolation length in journal articles.

Notes: The boundary condition for polarization is a value that is difficult to determine, for normal calculation that focus on domain structures, you can go with the default Neumann boundary condition, which set derivative to zero. Only when you're simulating some special distribution near the interface or surface, you may want to try the other two boundary conditions.

4.6 DIELECON

Full name: Dielectric constants (background)

Type: Vector, Real

Description: To set background dielectric constant which will override the dielectric constants assigned in the pot.in file.

Notes:

1. The background dielectric constant denotes the dielectric response to applied electric field apart from the spontaneous polarization. It also represents the dielectric constant at infinite high temperature in the plot of dielectric permittivity as a function of temperature. For detailed description, please refer to [Ref. Tagantsev, Zheng & Woo]

4.7 ELECFIELD

Full name: Electric Field

Type: Vector, Real

Description: This tag sets up the electric boundary condition of bulk system using an applied electric field. It can be used to obtain the PE loop of a bulk system. Three real numbers must be specified for this tag, electric field along x, y and z direction, separated by space.

Notes:

1. The unit of assigned electric field is in V/m.

4.8 FILMTHICK

Full name: Film thickness

Type: Integer

Film thickness is the number of simulation grid points for the film. Related value is **SUBTHICK**, which is the number of simulation grid for the substrate. When the film thickness is set to 0, then the program will treat the system as a bulk simulation with periodic boundary condition in all three directions rather than a thin film simulation which is only periodic in the in-plane (x,y) direction.

Notes:

1. Set to 0 for bulk system, non 0 for thin film system.

4.9 FLEXOCON

Full name: Flexoelectric constants

Type: Vector,real

Description: This vector tag sets the three independent flexoelectric constants of cubic symmetry material, i.e., longitudinal f1111, transverse f1122, shear f1221.

Notes:

1. The unit of assigned flexoelectric constant is in V.

2. The theoretical estimation of flexoelectric constant for perovskites is within 0 20 V. The sign is usually not determined.

4.10 GRADPCON

Full name: Gradient energy constant of polarization

Type: Vector, real

Description: Gradient coefficient for polarization. Specifying this value will override the default one obtained from pot.in file. Different from the value used in pot.in, which is in SI unit, the value set by GRADPCON is in reduced unit normalized by $a_0 l_0^2$, in which a_0 is chosen to be the value of a_1, the first coefficient for landau potential, at 298k, and l_0 is the denominator for length, for ferroelectric case we use $10^{-9}m$ per grid as its value. Three values need to be specified for tag, coefficient G11, G12 and G44, as in the formular for gradient energy $\frac{G_{11}}{2}(P_{1,1}^2 + P_{2,2}^2 + P_{3,3}^2) + G_{12}(P_{1,1}P_{2,2} + P_{1,1}P_{3,3} + P_{3,3}P_{2,2}) + \frac{G_{44}}{2}[(P_{1,2} + P_{2,1})^2 + (P_{1,3} + P_{3,1})^2 + (P_{3,2} + P_{2,3})^2]$ [Phenomenological model of a 90° domain wall in BaTiO3-type ferroelectrics]PHYSICAL REVIEW B 74, 104104 2006. The default value for gradient energy coefficient is $G_{11} = 0.6$, $G_{12} = -0.6$ and $G_{44} = 0.6$. It is recommended to test the gradient energy coefficient value for your specific system, that the domain wall width should be more than 1.5 grid thick.

Notes:

1. Default value for gradient energy coefficient is $G_{11} = 0.6$, $G_{12} = -0.6$ and $G_{44} = 0.6$.

4.11 GRADQCON

Full name: Gradient energy contant of oxygen octahedral rotation

Type: Vector, real

Description: Gradient coefficient for oxygen octahedral rotation. Specifying this value will override the default one obtained from pot.in file. Different from the value used in pot.in, which is in SI unit, the value set by GRADQCON is in reduced unit normalized by $b_0 l_0^2$, in which b_0 is chosen to be the value of b_1, the first coefficient for landau potential, at 298k, and l_0 is the denominator for length, for ferroelectric case we use $10^{-9}m$ per grid as its value. Three values need to be specified for tag, coefficient G11, G12 and G44, as in the formular for gradient energy $\frac{v_{11}}{2}(q_{1,1}^2 + q_{2,2}^2 + q_{3,3}^2) + v_{12}(q_{1,1}q_{2,2} + q_{1,1}q_{3,3} + q_{3,3}q_{2,2}) + \frac{v_{44}}{2}[(q_{1,2} + q_{2,1})^2 + (q_{1,3} + q_{3,1})^2 + (q_{3,2} + q_{2,3})^2]$. The default value for gradient energy coefficient is $v_{11} = 1$, $v_{12} = -1$ and $v_{44} = 1$.

Notes:

1. Default value for gradient energy coefficient is $v_{11} = 1$, $v_{12} = -1$ and $v_{44} = 1$.

4.12 LAFMTIP

Full name: Flag of AFM tip

Type: logic

Description: This flag controls whether to include an AFM tip (or time-variant electric bias for film systems) into the system or not. When turning on, it requires an extra input file, **AFMtip.in**, which specifies the moving paths, electric bias and mechanical load of an AFM tip. For the format of **AFMtip.in**, please refer to Section 8.1.5.

Notes:

4.13 LELAS

Full name: Flag of elasticity

Type: logic

Description: This flag controls whether to consider the elastic effect or not. It is recommended to turn it on for normal ferroelectric simulations, since all ferroelectrics are ferroelastic materials, elastic effect plays a key role in determining the equilibrium domain structure. When LELAS is turned on, a mechanical equilibrium equation $\sigma_{ij,i} = 0$ is solved using spectral method, and the elastic driving force for polarization can be obtained based on the calculated stress distribution. In the thin film cases, the boundary condition is periodic in the x-y (in-plane) direction, traction (stress components that are related to the z direction, σ_{33}, σ_{13}, σ_{23}) free for the film surface, and displacement free at the some distance into the substrate, and such distance is given by the **SUBTHICK**. In the bulk cases, average stress or strain can be specified.[yulan li 2002]

Notes:

4.14 LELEC

Full name: Flag of electricity

Type: Logic

Description: This flag controls whether to consider the electric effect or not. It is recommended to turn it on for all kinds of ferroelectric simulaitons, because electric field can have a significant influence on polarization. When turned on, a Poisson equation is solved using the spectral method. In the thin film case, there is periodic boundary condition in the in-plane (x-y) direction, and short or open circuit boundary condition for the film normal direction. In the bulk cases, the average electric field can be specified.[yulan li 2002]

Notes:

4.15 LFLEXO

Full name: Flag of flexoelectricity

Type: Logic

Description: This flag controls whether to consider the flexoelectric effect or not.

Notes:

4.16 LINHOM

Full name: Flag of inhomogeneous system

Type: Logic

Description: This flag controls whether your want your simulated system to be considered as homogeneous or not. The homogeneous is not in the sense of different phases but in terms of material properties, such as elastic constant or dielectric constant. Inhomogeneous system require material properties to be set pointwise in the form of an array rather than a single constant, which will lead to significantly more memory usage. So only turn this flag on when necessary.

Notes:

1. Only use this flag when necessary, it will significantly increase both the calculation time and memory usage.

4.17 LOCTILT

Full name: Flag of oxygen octahedral rotation

Type: Logic

Description: This flag controls whether you want to evolve the oxygen octahedral tilt/rotation in the simulation system. Oxygen octahedral tilt is a second set of order parameter, and it is coupled with elasticity and polarization. [Fei paper]

Notes:

4.18 LOUTELAS

Full name: Flag of output elasticity

Type: Logic

Description: This flag controls whether output of elastic related data files are allowed. Files include **Displace**, **Eigen_St**, **stress**, **strain**, **ElastEn**, **Elas_For**, for more details, please see Section 3.2.

Notes:

4.19 LOUTELEC

Full name: Flag of output electricity

Type: Logic

Description: This flag controls whether output of electric related data files are allowed. Files include **Elefield**, **Elec_Phi**, **Charges**, **Elec_For**, for more details, please see Section 3.2.

Notes:

4.20 LOUTFLEX

Full name: Flag of output flexoelectric field

Type: Logic

Description: This flag controls whether output of flexoelectric are allowed. Files include **Eflexo**, for more details, please see Section 3.2.

Notes:

4.21 LOUTFORC

Full name: Flag of output all driving forces

Type: Logic

Description: This flag controls whether output of driving force is allowed. Files include **Gen_ForX**, **Gen_ForY**, **Gen_ForZ**, for more details, please see Section 3.2.

Notes:

4.22 LOUTGRAD

Full name: Flag of output gradient energy

Type: Logic

Description: This flag controls whether output of gradient energy is allowed. Files include **Grade_En**, **Grad_For**, for more details, please see Section 3.2.

Notes:

4.23 LOUTLAND

Full name: Flag of output Landau energy

Type: Logic

Description: This flag controls whether output of landau energy is allowed. Files include **LandP_En**, **LandPFor**, for more details, please see Section 3.2.

Notes:

4.24 LPNOISE

Full name: Flag of initial noise of polarization

Type: Logic

Description: This flag controls whether initial noise for polarization is added or not. The noise is a uniform distribution generated using the fortran subroutine RANDOM. The random seed is set with **PNOISEED**.

Notes:

4.25 LQNOISE

Full name: Flag of initial noise of oxygen octahedral rotation

Type: Logic

Description: This flag control whether initial noise for oxygen octahedral tilt is added or not. The noise is a uniform distribution generated using the fortran subroutine RANDOM. The random seed is set with **QNOISEED**.

Notes:

4.26 MISFIT

Full name: Misfit strain

Type: Vector,real

Description: Misfit strain that is due to the lattice mismatch between film and substrate, calculated by $\frac{a_s-a_f}{a_s}$, in which a_s is the lattice parameter for substrate and a_f is the lattice parameter for thin film. Three values need to set for this tag, they are (ϵ_{11} ϵ_{22} ϵ_{12}).

Notes:

4.27 PNOISEED

Full name: Seed for polarization noise

Type: Integer

Description: Set the seed value for the polarization noise generated with RANDOM subroutine. This is the value used in fortran subroutine RANDOM_SEED

Notes:

4.28 PNOISMAG

Full name: Noise magnitude for polarization

Type: Real

Description: Set the magnitude for polarization noise.

Notes:

4.29 QNOISEED

Full name: Seed for oxygen octahedral rotation

Type: Integer

Description: Set the seed value for the oxygen octahedral rotation noise generated with random subroutine. This is the value used in fortran subroutine RANDOM_SEED.

Notes: :

4.30 QNOISMAG

Full name: Noise magnitude for oxygen octahedral rotation

Type: Real

Description: Set the magnitude for oxygen octahedral rotation noise.

Notes: :

4.31 REALDIM

Full name: Real dimension

Type: Vector, real

Description: REALDIM is a 3 dimension vector specifying the real size of the simulated system in x, y and z direction with an unit of nanometer. Different from the SYSDIM value, REALDIM is real number rather than integer. In order to get a more reasonable simulation result, it is recommended that the width of domain walls no thinner than 1.5 simulation grid point. In other word, if you know the domain wall thickness for your simulated system is 1.5 nm, then each grid point (set with SYSDIM) in your system should be fine representing 1 nm, leading to REALDIM=1nm*SYSDIM.

Notes:

4.32 ROTANGLE

Full name: Rotation Euler angles

Type: Vector

Description: Rotation angle determines the crystallography orientation of the material, it is a 3 dimensional vector of real number that correspond the the three euler angle. We used a very common proper euler angle, z-x-z, which means first angle is the rotation around z axis, second angle is the rotation around y axis in the new coordinate system, and the third value is the rotation angle around z axis in the new system.

Notes:

4.33 SCREENTOP

Full name: Screening factor at film top

Type: Real

Description: This value is used for setting the screening percentage of top surface charges under open circuit electric boundary conditions. It can only be used for the thin film type of system, and for open circuit conditions, for which the electric displacement is fixed.

Notes:

4.34 SCREENBOT

Full name: Screening factor at film bottom

Type: Real

Description: This value is used for setting the screening percentage of film/substrate interface charges under open circuit electric boundary conditions. It can only be used for the thin film type of system, and for open circuit conditions, for which the electric displacement is fixed.

Notes:

4.35 STRAIN

Full name: Applied strain

Type: Vector, Real

Description: This value is a 6 dimension vector, (ϵ_{11}, ϵ_{22}, ϵ_{33}, ϵ_{23}, ϵ_{13}, ϵ_{12}), specifying the applied strain for bulk system.

Notes:

4.36 STRESS

Full name: Applied stress

Type: Vector, Real

Description: This value is a 6 dimension vector, (σ_{11}, σ_{22}, σ_{33}, σ_{23}, σ_{13}, σ_{12}), specifying the applied stress for bulk system.

Notes:

4.37 SUBTHICK

Full name: Substrate thickness

Type: Scalar, integer

Description: The integer value set the thickness of the substrate, which is only meaningful for the thin film case. The **SUBTHICK** is in terms of simulation grid point rather than in real world unit, such as nanometer. This value actually means the thickness of substrate lattice that is been distorted due to the mismatch between film and substrate material. And at such substrate thickness away from the interface, the no displacement, or fully clamped elastic boundary condition is applied. For example, if you set **SUBTHICK** to be 10, and in your simulation system 1 grid equals 1nm, then its physical meaning is you consider the substrate lattice not affected by the thin film, if deeper than 10 nm away from the interface.

Notes:

4.38 SYSDIM

Full name: System dimension

Type: Vector(3), real

Description: This 3 dimensional vector holds the dimension in x, y and z direction of the simulation system in real world unit of nanometer.

Notes:

4.39 TDELTA

Full name: Increment time step

Type: Real

Description: This value controls the size of marching step when we evolve the TDGL equation to minimize total free energy. Larger timestep can leads to shorter simulation time, but may also easily leads to inconvergency. Recommended values are 0.01 or 0.02 .

Notes:

4.40 TEM

Full name: Temperature

Type: Real

Description: The value set the current temperature of the simulation system. Default value is room temperature of 298k, since most experiments are carried out under such conditions.

Notes:

4.41 TIPGAMMA

Full name: AFM tip gamma

Type: Real

Description:

This value defines the gamma coefficient γ in a Lorentz distribution to describe the electric potential distribution on top of the film surface, i.e.,

$$\phi(x,y) = \frac{\gamma^2}{(x - x_{tip})^2 + (y - y_{tip})^2 + \gamma^2} \tag{4.1}$$

Notes:

1. The unit of assigned gamma is in nm.

4.42 TIPRAD

Full name: AFM tip radius

Type: Real

Description: This value defines the AFM tip radius (assuming spherical). Then the contact radius will be calculated according to Hertz contact model of a spherical indenter.[**?**]

Notes:

1. The unit of assigned tip radius is in nm.

2. The common value of a tip radius is around 30 - 100 nm.

4.43 TOUTPUT

Full name: Interval timestep for output

Type: Integer

Description: This value set the interval for output all output data files in Secition 3.2.

Notes:

4.44 TSTART

Full name: Start timestep

Type: Integer

Description: This value set the starting timestep of the simulation. Default value is 0, which is the case if you're running a new simulation. But when you are restarting from a previous output, then you may want to set this TSTART value to be where you stopped before, and then it won't create confusion in the naming of output data.

Notes:

4.45 TTOTAL

Full name: Total timesteps

Type: Integer

Description: This value set the total amount of timesteps that you want to run. For example, if the TSTART value is 10000, and the TTOTAL is 10000, then as long as you have enough wall time to finish the simulation, the program will stop at step 20000.

Notes:

Chapter 5

Examples

5.1 Equilibrium domain structure of $BaTiO_3$ single crystal

This example is about calculating the equilibrium domain structure for bulk single crystal $BaTiO_3$, at room temperature, under stress free boundary conditions.

The **input.in** file is listed in Listing 5.1, with meaning of each line explained in the comment.

```
# BTO bulk

SIMDIM = 64 64 64                      # Set the system's grid size to be nx=64, ny=64, nz=64
REALDIM = 64 64 64                     # Set the system's real size to be lx=64nm, ly=64nm, lz=64nm
LBULK = True                           # Set the simulation type to be bulk, rather than film

TEM = 298                              # Set the system temperature to be 298k,

LPNOISE = T                            # Choose to add noise to polarization for initial structure
PNOISMAG = 0.1                         # Set the magnitude for polarization noise to be 0.1
GRADPCON = 0.6 -0.6 0.6                # Set normalized gradient constant, G11=0.6, G12=-0.6, G44=0.6

TTOTAL = 50000                         # Set the maximum time step to be 50000
TSTART = 0                             # Set the initial time step to be 0
TOUTPUT = 10000                        # Set the output interval to 10000 steps

LELAS = t                              # Choose to consider the elastic contribution
CELASBC = 2                            # Use stress boundary condition
STRESS = 0.0 0.0 0.0 0.0 0.0 0.0       # Stress 11,22,33,23,13,12 components

LELEC = t                              # Choose to consider the electric contribution
CELECBC = 0                            # Choose the electric boundary condition to be bulk
DIELECON = 45 45 45                    # Set the background dielectric constant epsilon 11,22,33
ELECFIELD = 0 0 0                      # Set the bulk electric field boundary condition x,y,z

LOUTELAS = T                           # Choose to enable elastic related output
LOUTELEC = T                           # Choose to enable electric related output
```

Listing 5.1: input.in file

The **pot.in** file is listed as in Listing 5.2

```
{
    "name"       : "BaTiO3",
    "Comment"       : "Fitted by Jian Jun Wang, the landau coefficient needs to be updated according to stress for every time step",
    "Reference"     : "JAP 108. 114105 (2010)",
    "CurieT"        : 390,
    "a0"             : 42769496,
    "p0"             : 0.26,
    "Landau"    :
        {   "a1"    : "5*10^5*160*(cosh(160/tem)/sinh(160/tem)-cosh(160/390)/sinh(160/390))",
            "a11"   : -1.154E8,
            "a12"   :  6.530E8,
            "a111"  : -2.106E9,
            "a112"  :  4.091E9,
            "a123"  : -6.688E9,
            "a1111" :  7.590E10,
            "a1112" : -2.193E10,
            "a1122" : -2.221E10,
            "a1123" :  2.416E10
        },
    "Electrostrictive"  :
        {
            "Q11"   :  0.11  ,
            "Q12"   : -0.045 ,
            "Q44"   :  0.029
        },
    "ElasticModulus"    :
        {
            "C11"   :  1.7794E11,
            "C12"   :  0.9635E11,
            "C44"   :  1.2199E11
        },
    "Gradient"          :
        {
      "Reference" : "Hlinka & Marton, PRB 74, 104104(2006)",
            "G11"   : 51.0E-11,
            "G12"   : 2.0E-11,
            "G44"   : 2.0E-11,
        }
}
```

Listing 5.2: pot.in file

Always remember to check the **const.dat** file whether the values for flags, choices and parameters are the same as your expectation.

```
--------------------------------------------------------------------------------
********************Flags and choices for the simualtion*******************
--------------------------------------------------------------------------------
| choice_material          :          BaTiO3
| flag_noise_p             :     T  |  output_landau          :     F  |
| flag_elastic             :     T  |  output_elastic         :     T  |
| flag_electric            :     T  |  output_electric        :     T  |
| flag_AFMtip              :     F  |  output_gradient        :     F  |
| flag_flexo               :     F  |  output_flexo           :     F  |
| output_driving_force     :     F  |  output_time_depend     :        |
| output_driving_force     :     F  |  output_time_depend     :        |
| flag_bulk                :     T  |  flag_inhomo            :     F  |
| choice_elas_BC           :     2  |  choice_elec_BC         :     2  |
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
********************The real constants in SI units*************************
--------------------------------------------------------------------------------
```

```
| a0    =    4.27695E+07 | p0     =        0.26000 | g110 =    4.27695E-11 |
| xf    =        1.00000 | tem    =      298.00000 |                       |
-------------------------------------------------------------------------------
| a1    =   -4.27695E+07 | a11    =   -1.15400E+08 | a12  =    6.53000E+08 |
| a111  =   -2.10600E+09 | a112   =    4.09100E+09 | a123 =   -6.68800E+09 |
| a1111 =    7.59000E+10 | a1112  =   -2.19300E+10 | a1122=   -2.22100E+10 |
| a1123 =    2.41600E+10 |                         |                       |
| c11   =    1.77940E+11 | c12    =    9.63500E+10 | c44  =    1.21990E+11 |
| s11   =    9.07028E-12 | s12    =   -3.18612E-12 | s44  =    8.19739E-12 |
| Q11   =    1.10000E-01 | Q12    =   -4.50000E-02 | Q44  =    2.90000E-02 |
| eps1  =    4.50000E+01 | eps2   =    4.50000E+01 | eps3 =    4.50000E+01 |
| g11   =    2.56617E-11 | g12    =   -2.56617E-11 | g44  =    2.56617E-11 |
-------------------------------------------------------------------------------

-------------------------------------------------------------------------------
************************Dimensionless material constants*********************
-------------------------------------------------------------------------------
| a1     =       -1.00000 | a11    =       -0.18240 | a12     =       1.03211 |
| a111   =       -0.22502 | a112   =        0.43711 | a123    =      -0.71459 |
| a1111  =        0.54821 | a1112  =       -0.15840 | a1122   =      -0.16042 |
| a1123  =        0.17450 |                         |                         |
| c11    =    61544.99741 | c12    =    33325.05620 | c44     =   42193.29119 |
| s11    =        0.00003 | s12    =       -0.00001 | s44     =       0.00002 |
| Q11    =        0.00744 | Q12    =       -0.00304 | Q44     =       0.00196 |
| eps1   =        0.01704 | eps2   =        0.01704 | eps3    =       0.01704 |
| g11    =        0.60000 | g12    =       -0.60000 | g44(m)  =       0.60000 |
-------------------------------------------------------------------------------

-------------------------------------------------------------------------------
******************************Some other parameters**************************
-------------------------------------------------------------------------------
| Lx        =      64.000 | Ly        =      64.000 | Lz        =      64.000 |
| nx        =          64 | ny        =          64 | nz        =          64 |
| flim_grid =           0 | sub_grid  =           0 |
| dx        =       1.000 | dy        =       1.000 | dz        =       1.000 |
-------------------------------------------------------------------------------
```

Listing 5.3: const.dat file

If the parameters looks fine to you, usually you should take a quick look at the **energy.out** file, which contains energy summation for all system grid point of each time step. The beginning of the file is shown in Listing 5.4.

```
        step              Elastic Energy    Electric Energy      Landau Energy  Gradient P Energy       Total Energy
kt:        1 energy:   0.1032848345E+04   0.9398782304E+05  -0.3734208495E+05   0.2823160738E+05   0.8591019382E+05
kt:        2 energy:   0.8158606020E+03   0.1585332232E+05  -0.3530906729E+05   0.1840756288E+05  -0.2323214885E+03
kt:        3 energy:   0.7559950332E+03   0.2787724738E+04  -0.3547078752E+05   0.1542340774E+05  -0.1650366000E+05
kt:        4 energy:   0.7218784418E+03   0.5508686643E+03  -0.3606537342E+05   0.1371553289E+05  -0.2107709343E+05
kt:        5 energy:   0.6943022941E+03   0.1439256013E+03  -0.3679505762E+05   0.1236344560E+05  -0.2359338413E+05
kt:        6 energy:   0.6702223019E+03   0.5705124401E+02  -0.3760617678E+05   0.1119703888E+05  -0.2568186435E+05
kt:        7 energy:   0.6489871593E+03   0.3148713822E+02  -0.3848642736E+05   0.1017104049E+05  -0.2763491257E+05
kt:        8 energy:   0.6302753569E+03   0.2045260631E+02  -0.3943099878E+05   0.9263263637E+04  -0.2951700718E+05
kt:        9 energy:   0.6138202820E+03   0.1428600937E+02  -0.4043680075E+05   0.8457551773E+04  -0.3135114269E+05
kt:       10 energy:   0.5993845920E+03   0.1038491475E+02  -0.4150140340E+05   0.7740588714E+04  -0.3315104517E+05
```

Listing 5.4: Energy summation for each time step

5.2 Domain structure of $BaTiO_3$ thin film under different substrate mismatch strain

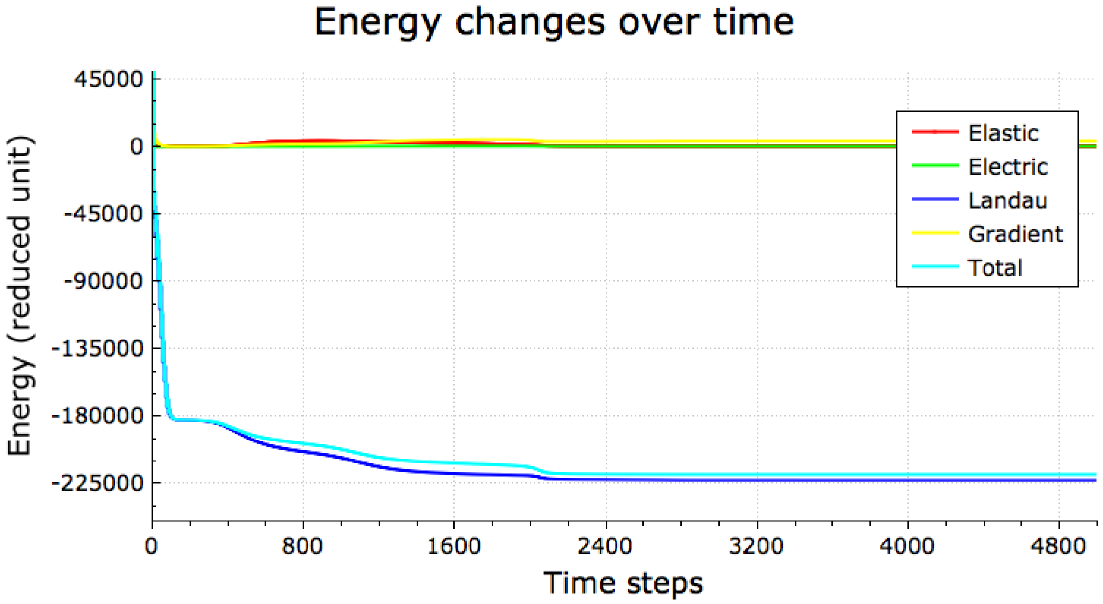


Figure 5.1: How energy components vary with time