Introduction to the Phase-Field Method and Its Applications

Hands on tutorials and exercises

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MUPRO

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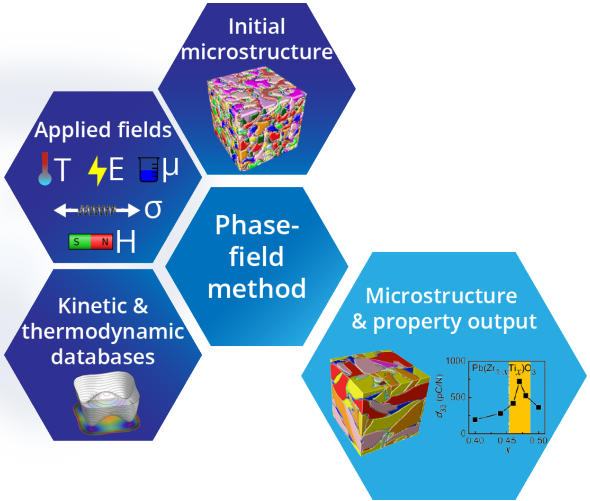
μ for Mesoscale Microstructure PROperty Professional



Part One: Tutorials

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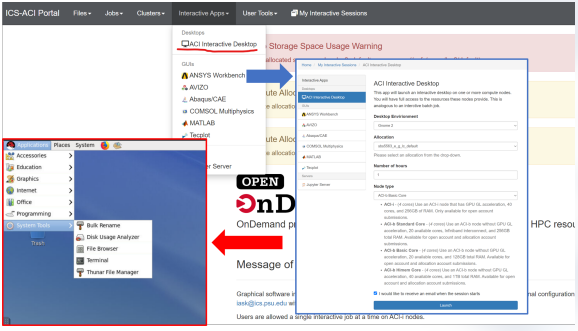
Connect to the online portal:
portal.aci.ics.psu.edu



Most used commands

ls	list directory
cd	change directory
cp	copy
mkdir	make directory
module list	loaded modules
module avail	available modules
module load	load module
qsub	submit job
qstat	status of job

Preparation

```
cd ~/scratch # Go to your scratch folder
mkdir pfm    # Create a folder for the tutorial
cd pfm       # Go into the created folder
module load python/3.6.3-anaconda5.0.1
cp -r /gpfs/group/dml129/default/matse_sc_data/lchen/doc .
```

```
cp -r /gpfs/group/dml129/default/matse_sc_data/lchen/project1 .
cd project1
ls
```

input.in	Boundary conditions and applied external field
pot.in	Thermodynamic and physical properties of the material
ferro.pbs	The PBS submission script
Ferroelectric.exe	The executable that we are using

Phase-field model

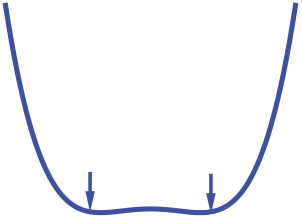
$$\frac{\partial \eta}{\partial t} = -L\frac{\delta F}{\delta \eta}$$

doi: 10.1146/annurev-matsci-071312-121634, doi: 10.1063/1.5116910, doi: 10.1002/adfm.201801725

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta F}{\delta \eta}, \quad F = \int_{\Omega} (f_{land} + f_{grad}) d\Omega$$

$$f_{land}(\boldsymbol{p}) = \alpha_i p_i^2 + \alpha_{ij} p_i^2 p_j^2 + \alpha_{ijk} p_i^2 p_j^2 p_k^2$$

$$f_{grad}(\boldsymbol{p}) = \frac{1}{2} G^{p}_{ijkl} p_{i,j} p_{k,l}$$



doi: 10.1146/annurev-matsci-071312-121634, doi: 10.1063/1.5116910, doi: 10.1002/adfm.201801725

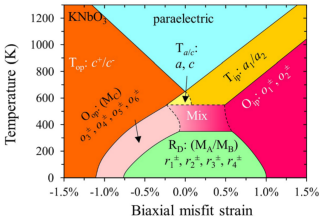
Phase-field model

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta F}{\delta \eta}, \quad F = \int_{\Omega}(f_{land} + f_{grad} + f_{elas})d\Omega$$

$$f_{land}(\boldsymbol{p}) = \alpha_i p_i^2 + \alpha_{ij} p_i^2 p_j^2 + \alpha_{ijk} p_i^2 p_j^2 p_k^2$$

$$f_{grad}(\boldsymbol{p}) = \frac{1}{2} G_{ijkl}^{p} p_{i,j} p_{k,l}$$

$$f_{elas}(\boldsymbol{p}, \boldsymbol{\epsilon}) = \frac{1}{2} C_{ijkl}(\epsilon_{ij} - \epsilon_{ij}^{0})(\epsilon_{kl} - \epsilon_{kl}^{0})$$



doi: 10.1146/annurev-matsci-071312-121634, doi: 10.1063/1.5116910, doi: 10.1002/adfm.201801725

Phase-field model

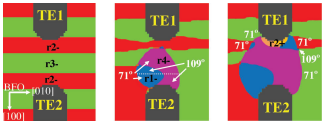
$$\frac{\partial \eta}{\partial t} = -L\frac{\delta F}{\delta \eta}, \quad F = \int_\Omega (f_{land} + f_{grad} + f_{elas} + f_{elec}) d\Omega$$

$$f_{land}(\boldsymbol{p}) = \alpha_i p_i^2 + \alpha_{ij} p_i^2 p_j^2 + \alpha_{ijk} p_i^2 p_j^2 p_k^2$$

$$f_{grad}(\boldsymbol{p}) = \frac{1}{2} G^p_{ijkl} p_{i,j} p_{k,l}$$

$$f_{elas}(\boldsymbol{p}, \boldsymbol{\epsilon}) = \frac{1}{2} C_{ijkl} (\epsilon_{ij} - \epsilon^0_{ij})(\epsilon_{kl} - \epsilon^0_{kl})$$

$$f_{elec}(\boldsymbol{p}, \boldsymbol{E}) = -\frac{1}{2}\epsilon_0 E_i E_j - E_i p_i$$



doi: 10.1146/annurev-matsci-071312-121634, doi: 10.1063/1.5116910, doi: 10.1002/adfm.201801725

Project 1: Ferroelectric – Input: pot.in

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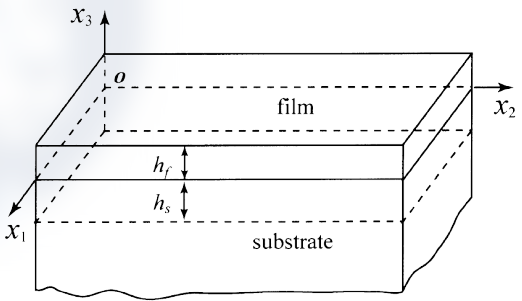
```
{
    "name": "PbTiO3",
    "Comment": "",
    "Reference": "Li Y.L. et al., Acta Materialia 2002 50(2)",
    "Prerequisite": {
        "CurieT": "752.15"
    },
    "Normalizer": {
        "P0": "0.757"
    },
    "Landau": {
        "a1": "3.8*10^5*(TEM-CurieT)",
        "a11": "-73000000",
        "a12": "7.5*10^8",
        "a111": "2.6*10^8",
        "a112": "6.1*10^8",
        "a123": "-3700000000"
    },
    "Electrostrictive": {
        "Q11": "0.089",
        "Q12": "-0.026",
        "Q44": "0.03375"
    },
    "ElasticStiffness": {
        "C11": "174600000000",
        "C12": "79370000000",
        "C44": "111100000000"
    }
}
```

pot.in is a json format input file for the MUPRO ferroelectric module, which feeds those necessary physical parameters into the program, such as the landau coefficient, the electrostrictive coefficient, the elastic stiffness, etc.

doi: 10.1146/annurev-matsci-071312-121634, doi: 10.1063/1.5116910, doi: 10.1002/adfm.201801725

```
SYSDIM = 128 128 36
REALDIM = 128 128 36
LBULK = False
FILMTHICK = 20
SUBTHICK = 12

TEM = 298

LPNOISE = T
PNOISMAG = 0.1
GRADPCON = 0.6 -0.6 0.6

TTOTAL = 50000
TSTART = 0
TOUTPUT = 10000

LELAS = t
CELASBC = 0
MISFIT = -0.005 -0.005 0.0

LELEC = t
CELECBC = 2
DIELECON = 45 45 45

LOUTELAS = T
LOUTELEC = T
```

input.in is a free format input file for the MUPRO ferroelectric module. It controls how the simulation will be executed.



Project 1: Ferroelectric – Execution

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```
./Ferroelectric.exe # Run directly
# Or you may submit a job
```

```
qsub ferro.pbs
qstat -u [your username]
```

```
-------------------------------------------------------------------------------
                    Valid to use, thanks for using MUPRO
-------------------------------------------------------------------------------
*********************************Ferroelectric main program**********************
***********************************using*************************************
*********************************mu-pro package******************************
-------------------------------------------------------------------------------
-----------------------Simulation system general setup-------------------------
-----------------------Input parameters----------------------------------------
|Simulation dimension nx (unitless) =   128
|Simulation dimension ny (unitless) =   128
|Simulation dimension nz (unitless) =    36
|Real dimension lx (nm) =   128.0000
|Real dimension ly (nm) =   128.0000
|Real dimension lz (nm) =    36.0000
|Bulk system condition =           F
|Film thickness (unitless) =    20
|Substrate thickness (unitless) =    12
|Temperature (K) =   298.0000
|Add noise to polarization =          T
|Polarization noise magnitude =         0.100000
|Gradient coefficient g11 (unitless) =         0.600000
|Gradient coefficient g12 (unitless) =        -0.600000
|Gradient coefficient g44 (unitless) =         0.600000
|Total simulation timesteps =     50000
|Initial simulation timesteps =         0
|Output for every # timesteps =     10000
|Consider elastic effect =         T
| Elastic BC is         0
|Use thin film misfit strain as elastic BC----------------------------------
|Misfit exx =         -0.0050
|Misfit eyy =         -0.0050
|Misfit exy =          0.0000
|Consider electric effect :          T
| Electric BC is         2
|Dielectric constant epsilon11 =       45.000000
|Dielectric constant epsilon22 =       45.000000
|Dielectric constant epsilon33 =       45.000000
|Export stress/strain =        T
|Export electric related =          T
-----------------------------Input done----------------------------------------
```

```
#PBS -l nodes=1:ppn=4
#PBS -l walltime=48:00:00
#PBS -l pmem=5g
#PBS -A sbs5563_e_g_lc_default
#PBS -N lchen-p1
#PBS -j oe


module load intel
module load mkl
module load impi

cd $PBS_O_WORKDIR
echo `date`
mpirun ./Ferroelectric.exe
echo `date`
```

Project 2: Ferromagnetic – Preparation

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```
cd ..  # Go back to the pfm folder
cp -r /gpfs/group/dml129/default/matse_sc_data/lchen/project2 .
cd project2
ls
```

parameter.in	Boundary conditions and applied external field
magn.pbs	The PBS submission script
Magnetic.exe	The executable that we are using

Project 2: Ferromagnetic – Input: parameter.in

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```
# Standard Problem #3 Flower Structure
# size
REALDIM =   105.75  1   105.75
SYSDIM =    50  1   50
ISLANDTHICK =   40
ISLANDLENGTH =  40  1

# spin
SATURATION =    5.E5

# anisotropy
FLAGANI =   true
CHOICEANI = 2
ANISOTROPY =    15.708E3    0.  0.

# stray field
FLAGSTRAY = true
FLAGPERIODIC =  false

# exchange
EXCHANGE =  15.708E-12

# time
TIMESTEP =  1.E-14
NTMAX = 500000
NTOUTTABLE =    10000
NTOUTDIST = 50000
CHOICEINITMAG = 2
INITMAG =   0.  0.  1.
```

parameter.in is a free format input file for the MUPRO magnetic module. It controls the simulation program.

Project 2: Ferromagnetic – Execution

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```
./Magnetic.exe
```

```
 ------------------------------------------------------------------------------
                    Valid to use, thanks for using MUPRO
 Reading parameter.in
 ------------------------------Input parameters--------------------------------
 Real size of simulation (nm)----------------------------------------------------
     lx (nm) =    105.7500
  ---------------------------------------------------------------------------
     ly (nm) =    105.7500
  ---------------------------------------------------------------------------
     lz (nm) =    105.7500
  ---------------------------------------------------------------------------
 Simulation system dimension-----------------------------------------------------
     nx (unitless) =     50
  ---------------------------------------------------------------------------
     ny (unitless) =     50
  ---------------------------------------------------------------------------
     nz (unitless) =     50
  ---------------------------------------------------------------------------
 Island thickness (unitless) =     40
  ---------------------------------------------------------------------------
 Island dimension----------------------------------------------------------------
     grids in x :     40
  ---------------------------------------------------------------------------
     grids in y :     40
  ---------------------------------------------------------------------------
 Consider magnetocrystalline anisotropy =            T
  ---------------------------------------------------------------------------
 Type of magnetocrystalline anisotropy =      2
  ---------------------------------------------------------------------------
 Magnetocrystalline anisotropy coefficient (J/m^3) -------------------------------
     kc1 or ku1 =       15708.0000
  ---------------------------------------------------------------------------
     kc2 or ku2 =           0.0000
  ---------------------------------------------------------------------------
     kc3 =           0.0000
  ---------------------------------------------------------------------------
 Consider stray field =            T
  ---------------------------------------------------------------------------
 Consider periodic boundary =            F
  ---------------------------------------------------------------------------
 Magnetic exchange constant (J/m) =           0.0000
  ---------------------------------------------------------------------------
 Time per evolution step (s) =          0.0000
  ---------------------------------------------------------------------------
 Total simulation timesteps =      500000
  ---------------------------------------------------------------------------
 Output data table every # timesteps =       10000
  ---------------------------------------------------------------------------
```

```
qsub magn.pbs
```

```
#PBS -l nodes=1:ppn=1
#PBS -l walltime=48:00:00
#PBS -l pmem=5g
#PBS -A sbs5563_e_g_lc_default
#PBS -N lchen-p2
#PBS -j oe


module load intel
module load mkl
module load impi

cd $PBS_O_WORKDIR
echo `date`
mpirun ./Magnetic.exe
echo `date`
```

Project 3: Effective Property – Preparation

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```
cd ..  # Go back to the pfm folder
cp -r /gpfs/group/dml129/default/matse_sc_data/lchen/project3 .
cd project2
ls
```

parameter.in	Boundary conditions and applied external field
struct.in	Composite structure setup
eff.pbs	The PBS submission script
EffProperty.exe	The executable that we are using

Project 3: Effective Property – Input: parameter.in

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```
# Example with Dielectricity
# size
SYSDIM =    80  80  80
REALDIM =   300 300 300

# system
CHOICESYS = 2
NPHASES =   2
CHOICESTRUCT =  2

# distribution
OUTDIST =   t
ELECFIELD = 1.E5    0.  0.

# coefficients of phase 1
PHASEID =   1
PERMITTIVITY =  1.  1.  1.  0.  0.  0.


# coefficients of phase 2
PHASEID =   2
PERMITTIVITY =  1000.   1000.   1000.   0.  0.  0.
```

parameter.in is a free format input file for the MUPRO effective property module. It controls the simulation program.

Project 3: Effective Property – Input: struct.in

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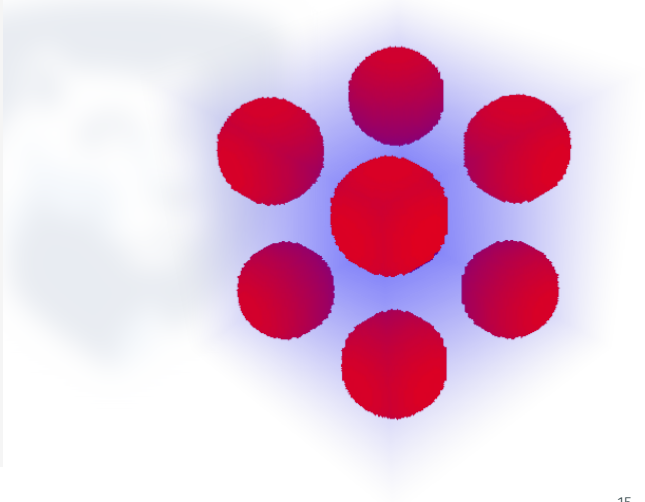
```
 1        80    80    80     ! System size
 2         1     1     1     1
 3         1     1     2     1
 4         1     1     3     1
 5         1     1     4     1
 6         1     1     5     1
 7         1     1     6     1
 8         1     1     7     1
 9         1     1     8     1
10         1     1     9     1
11         1     1    10     1
12         1     1    11     1
13         1     1    12     1
14         1     1    13     1
15         1     1    14     1
16         1     1    15     1
17         1     1    16     1
18         1     1    17     1
19         1     1    18     1
20         1     1    19     1
21         1     1    20     1
22         1     1    21     1
23         1     1    22     1
24         1     1    23     1
```

struct.in specify the composite structure.



Project 3: Effective Property – Execution

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```
./EffProperty.exe
```

```
                Valid to use, thanks for using WUPRD
Hello, I am processor   0 of  0
Reading parameter.in
------------------------------Input parameters------------------------------
Simulation dimension nx (unitless) =     80
----------------------------------------------------------------------------
Simulation dimension ny (unitless) =     80
----------------------------------------------------------------------------
Simulation dimension nz (unitless) =     80
----------------------------------------------------------------------------
Real dimension lx (nm) =    300.0000
----------------------------------------------------------------------------
Real dimension ly (nm) =    300.0000
----------------------------------------------------------------------------
Real dimension lz (nm) =    300.0000
----------------------------------------------------------------------------
 Choice of system type is      2
----------------------------------------------------------------------------
 Number of phases =      2
----------------------------------------------------------------------------
Choice of the format of the input file "struct.in" =      2
----------------------------------------------------------------------------
Flag to control whether simulate the distribution of variables=           T
----------------------------------------------------------------------------
Applied electric field ----------------------------------------------------
Applied electric field x =      100000.0000
----------------------------------------------------------------------------
 Applied electric field y =           0.0000
----------------------------------------------------------------------------
Applied electric field z =           0.0000
----------------------------------------------------------------------------
Reading Phase ID----------------------------------------------------------
Phase ID =      1
----------------------------------------------------------------------------
Reading permittivity(epsilon) of phase ID =      1
----------------------------------------------------------------------------
Reading Phase ID----------------------------------------------------------
Phase ID =      2
----------------------------------------------------------------------------
Reading permittivity(epsilon) of phase ID =      2
----------------------------------------------------------------------------
------------------------------Input done------------------------------------
```

```
qsub eff.pbs
```

```
1  #PBS -l nodes=1:ppn=1
2  #PBS -l walltime=48:00:00
3  #PBS -l pmem=5g
4  #PBS -A sbs5563_e_g_lc_default
5  #PBS -N lchen-p3
6  #PBS -j oe
7
8
9  module load intel
10 module load mkl
11 module load impi
12
13 cd $PBS_O_WORKDIR
14 echo `date`
15 mpirun ./EffProperty.exe
16 echo `date`
```

Visualization: Preparation

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```
cd ..  # Go back to the pfm folder
export PATH=/gpfs/group/dml129/default/matse_sc_data/lchen/visualize:$PATH
export PYTHONPATH=/gpfs/group/dml129/default/matse_sc_data/lchen/visualize:$PYTHONPATH
```

The second command will give you direct access to the shell scripts we put in that folder.

The third command will enable import python file from the path as a module.

Visualization: Domain

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```
cd project1
plot_domain.sh 1 128 1 1 1 36 0.1 0.1 0.1 Polar.00050000.dat
```

1,2 Minimum and maximum in X direction of the plotting region

3,4 Minimum and maximum in Y direction of the plotting region

5,6 Minimum and maximum in Z direction of the plotting region

7,8,9 Threshold for vector to be considered as valid polarization

10 Data file name

```
display Apersp_P_Polar.00050000.png
```

Visualization: 2D

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```
cd ../project3
plot_2ds.sh 1 80 20 20 1 80 3 eleField.00000000.dat
```

1,2 Minimum and maximum in X direction of the plotting region

3,4 Minimum and maximum in Y direction of the plotting region

5,6 Minimum and maximum in Z direction of the plotting region

7 The column of the data file to be plotted

8 Data file name

```
display fig2ds_eleField.00000000_4_80.png
```

```
cd ../project2
python
```

Now in the python console, type the following commands

```
import nt_vtk  # a module for data conversion
data = nt_vtk.Data("magnt.00500000.dat",nt_vtk.SCALAR)
data.get_vtk_file('magnt.00500000.vtk')
# You can also convert to numpy array using data.get_np_array()
```

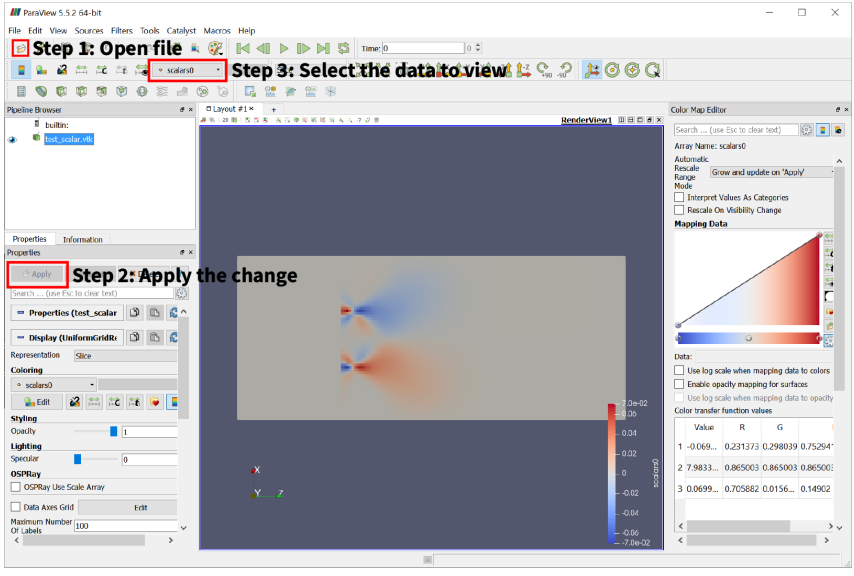
Or you may put the above commands into a file, such as data.py run it as below

```
python data.py
```

Next, we will use Paraview to visualize the vtk file.

```
module load paraview
paraview
```

Visualization: VTK



Part Two: Exercises

Get the doc


```
cd ..  # Go back to the pfm folder
cd doc
xpdf [the pdf name you want to open]
```

Read the documentation for information of the **keywords** you may use for each program.

Exercise 1: Ferroelectric

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In project 1, we have a thin film setup with 0 misfit strain. Please modify the input.in file and run simulations with compressive (-0.5%) and tensile (0.5%) biaxial misfit strain.

Change **MISFIT**.

Exercise 2: Ferromagnetic

In project 2, we have got a flower structure. For exercise 2, please modify the parameter.in file to obtain a vortex structure.

Set **CHOICEINITMAG** to be **3**, **INITMAG** to be **0 -1 0**

In project 3, we have computed the effective dielectric permittivity. For exercise 3, please modify the parameter.in file to calculate the effective thermal conductivity, for the following setup.

- **CHOICESYS** set to **8**
- **TEMGRAD** set to **1.E4 0 0**
- **THERMCOND** of phase 1 to **0.2 0.2 0.2 0 0 0**
- **THERMCOND** of phase 2 to **200 200 200 0 0 0**