Contents

μ-Pro® Eff Documentation

The μ-Pro® Eff program calculates effective elastic, electric, magnetic, diffusion, and conduction, etc. properties of a given composite system with arbitrary composite structure, and the spatial distribution of mechanical, electric, and magnetic, etc. variables responsive to applied external fields.

1 Installation and setup

1.1 Prerequiste

μ-Eff is built with Intel parallel studio cluster edition, and Intel mpi is required to run the program (**libmpi.so.12** and **libmpifort.so.12** are necessary). With Intel mpi installed, if things are not working automatically, you can use the **ldd** command to check the dynamic libraries linked with the executable, and add the correct path for the missing shared library by export **$LD_LIBRARY_PATH**.

1.2 Installation

To install the package, simply run the install.sh script. The script takes one argument, that is the μ-Pro® 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 install.sh script will first create the install directory **/usr/local/MUPRO**, next copy all the contents in your current distribution folder into the install directory, and then add several lines to your **~/.bashrc** file to setup the environment variable **MUPROROOT**, and create alias to the executable for easier usage.

1.3 Using the package

If the package is installed correctly, you should have a set of customized command defined in the ~/.bashrc start with mupro- or copy-mupro-. These commands enable you to execute the program without copy the .exe around.

1.4 Activate your usage

To register your copy of the program, we need the following information:

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 one 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 μ-Mag. 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. Groupname. The group of users that you want to grant access to use μ-Mag. 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.

2 Simulation Method

The program takes the phase/domain structure and properties of each of the containing phases/domain as input. It calculates the effective properties of a multi-phase/domain composite through establishing and solving equilibrium equations in the system, including:

- Mechanical equilibrium equation
- Electrostatic equilibrium equation
- Magnetostatic equilibrium equation
- Steady-state diffusion equilibrium equation
- Steady-state heat equation
- Steady-state electrical conduction equation

The equilibrium equations are solved using the Fourier spectral iterative perturbation method.[1-6]

2.1 Elastic system

The program calculates the effective elastic stiffness **c** of a composite, and the spatial distribution of strain $\boldsymbol{\varepsilon}(\mathbf{x})$ and stress $\boldsymbol{\sigma}(\mathbf{x})$ responsive to an applied strain/stress, where **x** is the position vector. The following equation(s) are solved.

$\nabla \cdot \boldsymbol{\sigma} = 0$, where $\boldsymbol{\sigma} = \mathbf{c}\boldsymbol{\varepsilon}$

2.2 Dielectric system

The program calculates the dielectric permittivity $\boldsymbol{\kappa}_r$ of a composite, and the spatial distribution of electric field $\mathbf{E}(\mathbf{x})$, electric polarization $\mathbf{P}(\mathbf{x})$, and electric displacement $\mathbf{D}(\mathbf{x})$, responsive to an applied electric field. The following equation(s) are solved.

$\nabla \cdot \mathbf{D} = 0$, where $\mathbf{D} = \varepsilon_0 \boldsymbol{\kappa}_r \mathbf{E}$

2.3 Piezoelectric system

The program calculates the effective elastic stiffness **c**, dielectric permittivity $\boldsymbol{\kappa}_r$, and piezoelectric charge coefficient **d** of a composite, and the spatial distribution of strain $\boldsymbol{\varepsilon}(\mathbf{x})$, stress $\boldsymbol{\sigma}(\mathbf{x})$, electric field $\mathbf{E}(\mathbf{x})$, electric polarization $\mathbf{P}(\mathbf{x})$, and electric displacement $\mathbf{D}(\mathbf{x})$, responsive to applied strain/stress and/or electric field. The following equation(s) are solved. [5]

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = 0 \\ \nabla \cdot \mathbf{D} = 0 \end{cases}, \text{ where } \begin{cases} \boldsymbol{\sigma} = \mathbf{c}\left(\boldsymbol{\varepsilon} - \mathbf{d}^T \mathbf{E}\right) \\ \mathbf{D} = \varepsilon_0 \boldsymbol{\kappa}_r \mathbf{E} + \mathbf{d}\boldsymbol{\sigma} \end{cases}$$

2.4 Magnetic system

The program calculates the magnetic permeability $\boldsymbol{\mu}_r$ of a composite, and the spatial distribution of magnetic field $\mathbf{H}(\mathbf{x})$, magnetization $\mathbf{M}(\mathbf{x})$, and magnetic induction $\mathbf{B}(\mathbf{x})$, responsive to an applied magnetic field. The following equation(s) are solved.

$\nabla \cdot \mathbf{B} = 0$, where $\mathbf{B} = \mu_0 \boldsymbol{\mu}_r \mathbf{H} + \mathbf{q}\boldsymbol{\sigma}$

2.5 Piezomagnetic system

The program calculates the effective elastic stiffness **c**, magnetic permeability $\boldsymbol{\mu}_r$, and piezomagnetic coefficient **q** of a composite, and the spatial distribution of strain $\boldsymbol{\varepsilon}(\mathbf{x})$, stress $\boldsymbol{\sigma}(\mathbf{x})$, magnetic field $\mathbf{H}(\mathbf{x})$, magnetization $\mathbf{M}(\mathbf{x})$, and magnetic induction $\mathbf{B}(\mathbf{x})$, responsive to applied strain/stress and/or magnetic field. The following equation(s) are solved.

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = 0 \\ \nabla \cdot \mathbf{B} = 0 \end{cases}, \text{ where } \begin{cases} \boldsymbol{\sigma} = \mathbf{c}\left(\boldsymbol{\varepsilon} - \mathbf{q}^T \mathbf{H}\right) \\ \mathbf{B} = \mu_0 \boldsymbol{\mu}_r \mathbf{H} + \mathbf{q}\boldsymbol{\sigma} \end{cases}$$

2.6 Magnetoelectric system

The program calculates the effective elastic stiffness **c**, dielectric permittivity $\boldsymbol{\kappa}_r$, magnetic permeability $\boldsymbol{\mu}_r$, piezoelectric charge coefficient **d**, piezomagnetic coefficient **q**, and magnetoelectric coefficient **α** of a composite, and the spatial distribution of strain **ε**(**x**), stress **σ**(**x**), electric field **E**(**x**), electric polarization **P**(**x**), electric displacement **D**(**x**), magnetic field **H**(**x**), magnetization **M**(**x**), and magnetic induction **B**(**x**), responsive to applied strain/stress and/or magnetic field. The following equation(s) are solved. [6]

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = 0 \\ \nabla \cdot \mathbf{D} = 0 \\ \nabla \cdot \mathbf{B} = 0 \end{cases}, \text{ where } \begin{cases} \boldsymbol{\sigma} = \mathbf{c}\left(\boldsymbol{\varepsilon} - \mathbf{d}^T \mathbf{E} - \mathbf{q}^T \mathbf{H}\right) \\ \mathbf{D} = \varepsilon_0 \boldsymbol{\kappa}_r \mathbf{E} + \mathbf{d}\boldsymbol{\sigma} + \boldsymbol{\alpha}\mathbf{H} \\ \mathbf{B} = \mu_0 \boldsymbol{\mu}_r \mathbf{H} + \mathbf{q}\boldsymbol{\sigma} + \boldsymbol{\alpha}^T \mathbf{E} \end{cases}$$

2.7 Diffusion system

The program calculates the effective diffusivity **D** of a composite, and the spatial profile of concentration $c_m(\mathbf{x})$ and molar flux density $\mathbf{j}_m(\mathbf{x})$ of a steady state diffusion. The following equation(s) are solved. [4]

$$\nabla \cdot \mathbf{j}_m = 0, \text{ where } \mathbf{j}_m = \mathbf{D}\nabla c_m$$

2.8 Thermal conduction system

The program calculates the effective thermal conductivity **k** of a composite, and the spatial profile of temperature $T(\mathbf{x})$ and heat flux density $\mathbf{q}_T(\mathbf{x})$ of a steady state heat conduction. The following equation(s) are solved.

$$\nabla \cdot \mathbf{q}_T = 0, \text{ where } \mathbf{q}_T = \mathbf{k}\nabla T$$

2.9 Electrical conduction system

The program calculates the effective electrical conductivity $\boldsymbol{\sigma}_E$ of a composite, and the spatial profile of electric field **E**(**x**) and electric current $\mathbf{j}_E(\mathbf{x})$ in a steady state electric current responsive to an applied electric field. The following equation(s) are solved.

$\nabla \cdot \mathbf{j}_E = 0$, where $\mathbf{j}_E = \boldsymbol{\sigma}_E \mathbf{E}$

3 Input files

Users need to prepare two files as input:

3.1 *parameterFormatted.in* or alternatively *parameter.in*

Declares the size of the system, the type of properties considered, properties of each phase, and external fields applied. Users shall provide either *parameterFormatted.in* (fixed-format version) or *parameter.in* (free-format version). If both files are provided, only *parameter.in* will be adopted.

The format is as follows:

Table 3.1.1 Format of the input file *parameterFormatted.in*

<table>
<tr><th colspan="6">Data in the file</th><th colspan="2">Explanation</th></tr>
<tr><td></td><td></td><td></td><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td>l_1</td><td>l_2</td><td>l_3</td><td></td><td></td><td></td><td colspan="2">System real size in each direction (nm)</td></tr>
<tr><td>n_1</td><td>n_2</td><td>n_3</td><td></td><td></td><td></td><td colspan="2">Total number of simulation grids in each direction</td></tr>
<tr><td>C_S</td><td></td><td></td><td></td><td></td><td></td><td colspan="2">Choice of the system: 1-elastic; 2-dielectric; 3-piezoelectric; 4-magnetic; 5-piezomagnetic; 6-magnetoelectric; 7-diffusivity; 8-thermal conductivity; 9-electrical conductivity</td></tr>
<tr><td>N_p</td><td></td><td></td><td></td><td></td><td></td><td colspan="2">total # of phases</td></tr>
<tr><td>C_F</td><td></td><td></td><td></td><td></td><td></td><td colspan="2">Choice of the format of the input file struct.in: 1-order parameter array; 2-phase identifier (ID) array</td></tr>
<tr><td></td><td></td><td></td><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td>I_P</td><td></td><td></td><td></td><td></td><td></td><td>phase identifier (ID)</td><td rowspan="15">These lines are repeated N_p times.

Each repetition, followed by an empty line, provides the properties of one phase.</td></tr>
<tr><td>c_{11}</td><td>c_{12}</td><td>c_{13}</td><td>c_{14}</td><td>c_{15}</td><td>c_{16}</td><td rowspan="6">(For C_S=1,3,4,6) elastic stiffness tensor c (Pa)</td></tr>
<tr><td>c_{22}</td><td>c_{23}</td><td>c_{24}</td><td>c_{25}</td><td>c_{26}</td><td></td></tr>
<tr><td>c_{33}</td><td>c_{34}</td><td>c_{35}</td><td>c_{36}</td><td></td><td></td></tr>
<tr><td>c_{44}</td><td>c_{45}</td><td>c_{46}</td><td></td><td></td><td></td></tr>
<tr><td>c_{55}</td><td>c_{56}</td><td></td><td></td><td></td><td></td></tr>
<tr><td>c_{66}</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>κ_{r11}</td><td>κ_{r22}</td><td>κ_{r33}</td><td>κ_{r23}</td><td>κ_{r13}</td><td>κ_{r12}</td><td>(For C_S=2,3,6) relative dielectric permittivity tensor $\boldsymbol{\kappa}_r$ (unitless)</td></tr>
<tr><td>d_{11}</td><td>d_{12}</td><td>d_{13}</td><td>d_{14}</td><td>d_{15}</td><td>d_{16}</td><td rowspan="3">(For C_S=3,6) piezoelectric charge coefficient tensor d (C/N)</td></tr>
<tr><td>d_{21}</td><td>d_{22}</td><td>d_{23}</td><td>d_{24}</td><td>d_{25}</td><td>d_{26}</td></tr>
<tr><td>d_{31}</td><td>d_{32}</td><td>d_{33}</td><td>d_{34}</td><td>d_{35}</td><td>d_{36}</td></tr>
<tr><td>μ_{r11}</td><td>μ_{r22}</td><td>μ_{r33}</td><td>μ_{r23}</td><td>μ_{r13}</td><td>μ_{r12}</td><td>(For C_S=4,5,6) relative magnetic permeability tensor $\boldsymbol{\mu}_r$ (unitless)</td></tr>
<tr><td>q_{11}</td><td>q_{12}</td><td>q_{13}</td><td>q_{14}</td><td>q_{15}</td><td>q_{16}</td><td rowspan="3">(For C_S=5,6) piezomagnetic coefficient tensor q (T/Pa)</td></tr>
<tr><td>q_{21}</td><td>q_{22}</td><td>q_{23}</td><td>q_{24}</td><td>q_{25}</td><td>q_{26}</td></tr>
<tr><td>q_{31}</td><td>q_{32}</td><td>q_{33}</td><td>q_{34}</td><td>q_{35}</td><td>q_{36}</td></tr>
</table>

α_{11}	α_{12}	α_{13}	α_{14}	α_{15}	α_{16}	(For C_S=6) magnetoelectric coefficient tensor **α** (C/(A·m))	
α_{21}	α_{22}	α_{23}	α_{24}	α_{25}	α_{26}		
α_{31}	α_{32}	α_{33}	α_{34}	α_{35}	α_{36}		
D_{11}	D_{22}	D_{33}	D_{23}	D_{13}	D_{12}	(For C_S=7) diffusivity tensor **D** (m^2/s)	
k_{11}	k_{22}	k_{33}	k_{23}	k_{13}	k_{12}	(For C_S=8) thermal conductivity tensor **k** (W/(m·K))	
σ_{E11}	σ_{E22}	σ_{E33}	σ_{E23}	σ_{E13}	σ_{E12}	(For C_S=9) electrical conductivity tensor $\boldsymbol{\sigma}_E$ (A/(V.m))	
F_P						Flag of whether to simulate the distribution of variables on applying an external field, in addition to the effective property calculation	
C_{EBC}						(For C_P=2, and C_S=1,3,4,6) choice of the type of elastic boundary condition: 1-applied external strain; 2-applied external stress	
ε_{11} or σ_{11}	ε_{22} or σ_{22}	ε_{33} or σ_{33}	ε_{23} or σ_{23}	ε_{13} or σ_{13}	ε_{12} or σ_{12}	(For C_P=2, and C_S=1,3,4,6) (For C_{EBC}=1) applied strain (unitless); (For C_{EBC}=2) applied stress (Pa)	
E_1	E_2	E_3				(For C_P=2, and C_S=2,3,6,9) applied electric field (V/m)	
H_1	H_2	H_3				(For C_P=2, and C_S=4,5,6) applied magnetic field (A/m)	
$\overline{\partial c_m/\partial x_1}$	$\overline{\partial c_m/\partial x_2}$	$\overline{\partial c_m/\partial x_3}$				(For C_P=2, and C_S=7) average composition gradient (mol/m^4)	
$\overline{\partial T/\partial x_1}$	$\overline{\partial T/\partial x_2}$	$\overline{\partial T/\partial x_3}$				(For C_P=2, and C_S=8) average temperature gradient (K/m)	

Table 3.1.2 Format of the input file *parameter.in*

Module	Identifier in the file	Data following the identifier in the file						Default value
Size	REALDIM	l_1	l_2	l_3				100
	SYSDIM	n_1	n_2	n_3				10
System	CHOICESYS	C_S						1
	NPHASES	N_p						2
	CHOICESTRUCT	C_F						2
The following lines can be repeated several times, with I_P = 1,2,…,N_P								
Coefficients	PHASEID	I_P						/
	STIFFNESS	c_{11}	c_{12}	c_{13}	c_{14}	c_{15}	c_{16}	0
		c_{22}	c_{23}	c_{24}	c_{25}	c_{26}		0
		c_{33}	c_{34}	c_{35}	c_{36}			0
		c_{44}	c_{45}	c_{46}				0
		c_{55}	c_{56}					0
		c_{66}						0
	PERMITTIVITY	κ_{r11}	κ_{r22}	κ_{r33}	κ_{r23}	κ_{r13}	κ_{r12}	0
	PIEZOELEC	d_{11}	d_{12}	d_{13}	d_{14}	d_{15}	d_{16}	0
		d_{21}	d_{22}	d_{23}	d_{24}	d_{25}	d_{26}	0
		d_{31}	d_{32}	d_{33}	d_{34}	d_{35}	d_{36}	0
	PERMEABILITY	μ_{r11}	μ_{r22}	μ_{r33}	μ_{r23}	μ_{r13}	μ_{r12}	0
	PIEZOMAG	q_{11}	q_{12}	q_{13}	q_{14}	q_{15}	q_{16}	0
		q_{21}	q_{22}	q_{23}	q_{24}	q_{25}	q_{26}	0
		q_{31}	q_{32}	q_{33}	q_{34}	q_{35}	q_{36}	0
	MAGELEC	α_{11}	α_{12}	α_{13}	α_{14}	α_{15}	α_{16}	0
		α_{21}	α_{22}	α_{23}	α_{24}	α_{25}	α_{26}	0
		α_{31}	α_{32}	α_{33}	α_{34}	α_{35}	α_{36}	0
	DIFFUSIVITY	D_{11}	D_{22}	D_{33}	D_{23}	D_{13}	D_{12}	0

	THERMCOND	k_{11}	k_{22}	k_{33}	k_{23}	k_{13}	k_{12}	0
	ELECCOND	σ_{E11}	σ_{E22}	σ_{E33}	σ_{E23}	σ_{E13}	σ_{E12}	0
Repeated lines end								
Distribution	OUTDIST	F_P						False
	CHOICEELABC	C_{EBC}						1
	STRAIN	ε_{11}	ε_{22}	ε_{33}	ε_{23}	ε_{13}	ε_{12}	0
	STRESS	σ_{11}	σ_{22}	σ_{33}	σ_{23}	σ_{13}	σ_{12}	0
	ELECFIELD	E_1	E_2	E_3				0
	MAGFIELD	H_1	H_2	H_3				0
	CONCGRAD	$\overline{\partial c_m / \partial x_1}$	$\overline{\partial c_m / \partial x_2}$	$\overline{\partial c_m / \partial x_3}$				0
	TEMGRAD	$\overline{\partial T / \partial x_1}$	$\overline{\partial T / \partial x_2}$	$\overline{\partial T / \partial x_3}$				0

Explanations of variables in Table 3.1.2 are the same as in Table 3.1.1, and are hence omitted.

3.2 *struct.in*

Contains an array describing the phase structure of the composite, arranged in a row-major order. This file has two possible formats according to C_F=1, and C_F=2, respectively, as defined in *parameter.in*. For C_F=1, it stores an array of the spatial distribution of phase concentration $o_{I_p}(\mathbf{x})$, where I_p is the phase identifier (ID), $I_p=1,2,...,N_p$. For C_F=2, it stores an array of the spatial distribution of the ID of the local dominant phase $p(\mathbf{x})$ in a composite, within a sharp phase-interface regime.

The format is as follows:

Table 3.2.1 Format of the input file *struct.in* for C_F=1

Data in the file							Explanation
n_1	n_2	n_3					Total number of simulation grids
1	1	1	$o_1(1,1,1)$	$o_2(1,1,1)$	…	$o_{N_p}(1,1,1)$	Concentration o_I of phase I ($I=1,2,…,N_p$) at grid point (1,1,1) (unitless)
⋮							⋮
1	1	n_3	$o_1(1,1,n_3)$	$o_2(1,1,n_3)$	…	$o_{N_p}(1,1,n_3)$	⋮
⋮							⋮
1	n_2	n_3	$o_1(1,n_2,n_3)$	$o_2(1,n_2,n_3)$	…	$o_{N_p}(1,n_2,n_3)$	⋮
⋮							⋮
n_1	n_2	n_3	$o_1(n_1,n_2,n_3)$	$o_2(n_1,n_2,n_3)$	…	$o_{N_p}(n_1,n_2,n_3)$	⋮

Table 3.2.2 Format of the input file *struct.in* for C_F=2

Data in the file				Explanation
n_1	n_2	n_3		Total number of simulation grids in each direction
1	1	1	$p(1,1,1)$	ID of the dominant phase at grid point (1,1,1) (unitless)
⋮				⋮
1	1	n_3	$p(1,1,n_3)$	⋮
⋮				⋮
1	n_2	n_3	$p(1,n_2,n_3)$	⋮
⋮				⋮
n_1	n_2	n_3	$p(n_1,n_2,n_3)$	⋮

4 Ouput files

effElasticStiffness.dat
Contains the effective elastic stiffness tensor **c** (Pa) of the system written in the form of a 6×6 matrix.

effDielectricPermittivity.dat
Contains the effective relative dielectric permittivity tensor $\boldsymbol{\kappa}_r$ (unitless) of the system written in the form of a 3×3 matrix.

effPiezoelectricDTensor.dat
Contains the effective piezoelectric charge coefficient tensor **d** (C/N) of the system written in the form of a 3×6 matrix.

effMagneticPermeability.dat
Contains the effective relative magnetic permeability tensor $\boldsymbol{\mu}_r$ (unitless) of the system written in the form of a 3×3 matrix.

effPiezomagneticQTensor.dat
Contains the effective piezomagnetic coefficient tensor **q** (T/Pa) of the system written in the form of a 3×6 matrix.

effMagnetoelectricTensor.dat
Contains the effective magnetoelectric coefficient tensor **α** (C/(A·m)) of the system written in the form of a 3×3 matrix.

effDiffusivity.dat
Contains the effective diffusivity tensor **D** (m^2/s) of the system written in the form of a 3×3 matrix.

effThermalConductivity.dat
Contains the effective thermal conductivity tensor **k** (W/(m·K)) of the system written in the form of a 3×3 matrix.

avElasticVariables.dat
Contains the average values of the stress and strain fields $\overline{\sigma_{11}}$, $\overline{\sigma_{22}}$, $\overline{\sigma_{33}}$, $\overline{\sigma_{23}}$, $\overline{\sigma_{13}}$, $\overline{\sigma_{12}}$, $\overline{\varepsilon_{11}}$, $\overline{\varepsilon_{22}}$, $\overline{\varepsilon_{33}}$, $\overline{\varepsilon_{23}}$, $\overline{\varepsilon_{13}}$, and $\overline{\varepsilon_{12}}$ in the system.

avElectricVariables.dat

Contains the average values of the electric field, electric polarization, and electric displacement $\overline{E_1}$, $\overline{E_2}$, $\overline{E_3}$, $\overline{P_1}$, $\overline{P_2}$, $\overline{P_3}$, $\overline{D_1}$, $\overline{D_2}$, and $\overline{D_3}$ in the system.

avMagneticVariables.dat
Contains the average values of the magnetic field, magnetization, and magnetic induction $\overline{H_1}$, $\overline{H_2}$, $\overline{H_3}$, $\overline{M_1}$, $\overline{M_2}$, $\overline{M_3}$, $\overline{B_1}$, $\overline{B_2}$, and $\overline{B_3}$ in the system.

avMolarFlux.dat
Contains the average values of the concentration gradient and molar flux density $\overline{\partial c_m(\mathbf{x})/\partial x_1}$, $\overline{\partial c_m(\mathbf{x})/\partial x_2}$, $\overline{\partial c_m(\mathbf{x})/\partial x_3}$, $\overline{\mathbf{j}_{m1}}$, $\overline{\mathbf{j}_{m2}}$, and $\overline{\mathbf{j}_{m3}}$ in the system.

avThermalFlux.dat
Contains the average values of the temperature gradient and heat flux density $\overline{\partial T(\mathbf{x})/\partial x_1}$, $\overline{\partial T(\mathbf{x})/\partial x_2}$, $\overline{\partial T(\mathbf{x})/\partial x_3}$, $\overline{\mathbf{q}_{T1}}$, $\overline{\mathbf{q}_{T2}}$, and $\overline{\mathbf{q}_{T3}}$ in the system.

strain.00000000.dat
Contains an array of $\varepsilon_{11}(\mathbf{x})$, $\varepsilon_{22}(\mathbf{x})$, $\varepsilon_{33}(\mathbf{x})$, $\varepsilon_{23}(\mathbf{x})$, $\varepsilon_{13}(\mathbf{x})$, and $\varepsilon_{12}(\mathbf{x})$ (unitless), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

stress.00000000.dat
Contains an array of $\sigma_{11}(\mathbf{x})$, $\sigma_{22}(\mathbf{x})$, $\sigma_{33}(\mathbf{x})$, $\sigma_{23}(\mathbf{x})$, $\sigma_{13}(\mathbf{x})$, and $\sigma_{12}(\mathbf{x})$ (Pa), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

elePtntl.00000000.dat
Contains an array of the electric potential $\varphi(\mathbf{x})$ (V), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

eleField.00000000.dat
Contains an array of $E_1(\mathbf{x})$, $E_2(\mathbf{x})$, and $E_3(\mathbf{x})$ (V/m), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

elePlrz.00000000.dat
Contains an array of $P_1(\mathbf{x})$, $P_2(\mathbf{x})$, and $P_3(\mathbf{x})$ (C/m^2), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

eleDspl.00000000.dat
Contains an array of $D_1(\mathbf{x})$, $D_2(\mathbf{x})$, and $D_3(\mathbf{x})$ (C/m^2), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

magField.00000000.dat

Contains an array of $H_1(\mathbf{x})$, $H_2(\mathbf{x})$, and $H_3(\mathbf{x})$ (A/m), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

magnetiz.00000000.dat
Contains an array of $M_1(\mathbf{x})$, $M_2(\mathbf{x})$, and $M_3(\mathbf{x})$ (A/m), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

magIndc.00000000.dat
Contains an array of $B_1(\mathbf{x})$, $B_2(\mathbf{x})$, and $B_3(\mathbf{x})$ (T), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

concentr.00000000.dat
Contains an array of $c_m(\mathbf{x})$ (mol/m^3), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

concGrad.00000000.dat
Contains an array of $\partial c_m(\mathbf{x})/\partial x_1$, $\partial c_m(\mathbf{x})/\partial x_2$, and $\partial c_m(\mathbf{x})/\partial x_3$ (mol/m^4), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

molFlux.00000000.dat
Contains an array of $j_{m1}(\mathbf{x})$, $j_{m2}(\mathbf{x})$, and $j_{m3}(\mathbf{x})$ (mol/(m^2·s)), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

temperat.00000000.dat
Contains an array of $T(\mathbf{x})$ (K), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

tempGrad.00000000.dat
Contains an array of $\partial T(\mathbf{x})/\partial x_1$, $\partial T(\mathbf{x})/\partial x_2$, and $\partial T(\mathbf{x})/\partial x_3$ (K/m), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

heatFlux.00000000.dat
Contains an array of $\mathbf{q}_{T1}(\mathbf{x})$, $\mathbf{q}_{T2}(\mathbf{x})$, and $\mathbf{q}_{T3}(\mathbf{x})$ (W/m^2), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

elecCurr.00000000.dat
Contains an array of $\mathbf{j}_{E1}(\mathbf{x})$, $\mathbf{j}_{E2}(\mathbf{x})$, and $\mathbf{j}_{E3}(\mathbf{x})$ (A/m^2), arranged in a row-major order. The data follow a similar format with those in *struct.in*.

5 Examples

5.1 Thermal conduction in matrix-inclusion system

This example considers the steady-state thermal conduction and thermal conductivity in a two-phase system with high-conductivity elliptical inclusions inside a low-conductivity matrix. The following material constants are adopted:

l_1 = 1mm
l_2 = 0.4mm
l_3 = 1mm
Inclusions: $k_{11} = k_{22} = k_{33}$ = 200 W/(m·K)
Matrix: $k_{11} = k_{22} = k_{33}$ = 0.2 W/(m·K)
The two-phase structure is shown below.

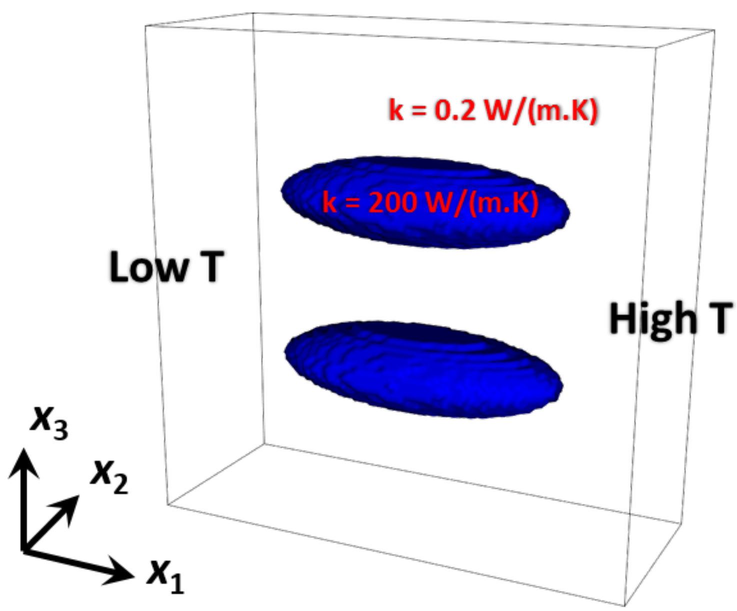

Figure 5.1.1 Schematics of the example of thermal conduction in a matrix-inclusion system.

The calculated effective thermal conductivity is

$$\mathbf{k} = \begin{pmatrix} 0.285 & 0.000 & 0.000 \\ 0.000 & 0.246 & 0.000 \\ 0.000 & 0.000 & 0.225 \end{pmatrix} \mathrm{W/(m \cdot K)}$$

The simulated temperature profile (average temperature within the system used as reference) on applying an external temperature gradient $\overline{\partial T(\mathbf{x}) / \partial x_1} = 1 \times 10^4 \,\mathrm{K/m}$ is shown below.

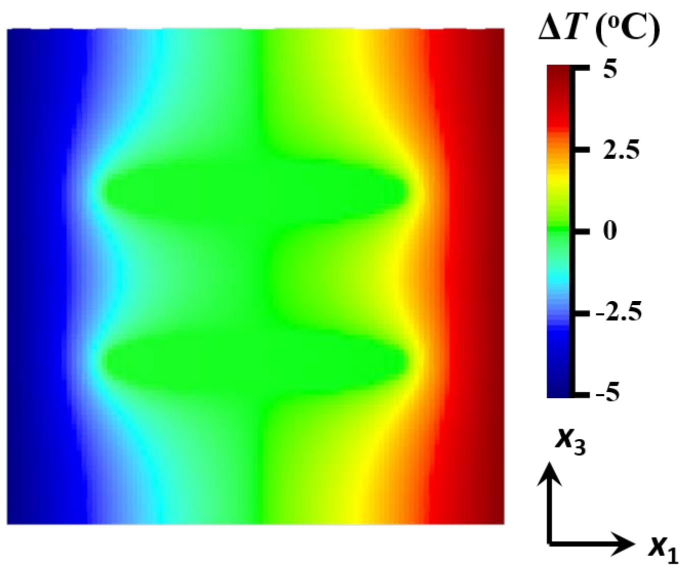

Figure 5.1.2 Temperature profile on applying an external temperature gradient.

5.2 Stress concentration in solid-gas system

This example considers the elastic property of a homogeneous solid plate with a circular hole in the center. An expansive stress σ_{11} = 100 MPa is applied. The following material constants are adopted:

$c_{11} = c_{22} = c_{33}$ = 90 GPa
$c_{12} = c_{13} = c_{23}$ = 30 GPa
$c_{44} = c_{55} = c_{66}$ = 30 GPa
The structure is shown below.

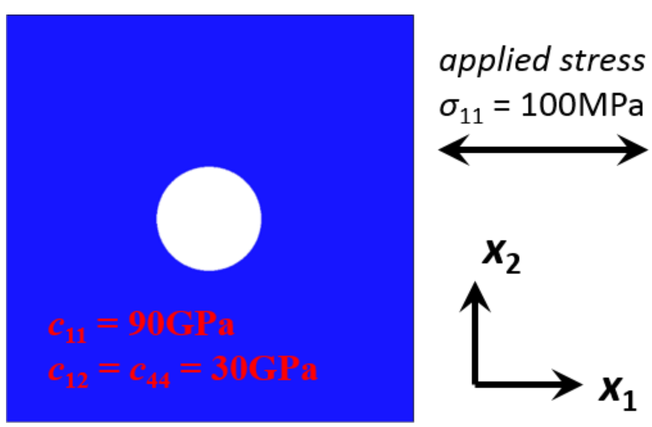

Figure 5.2.1 Schematics of the example of stress concentration in solid-gas system.

The simulated stress distribution is shown below. Stress concentration around the hole is demonstrated.

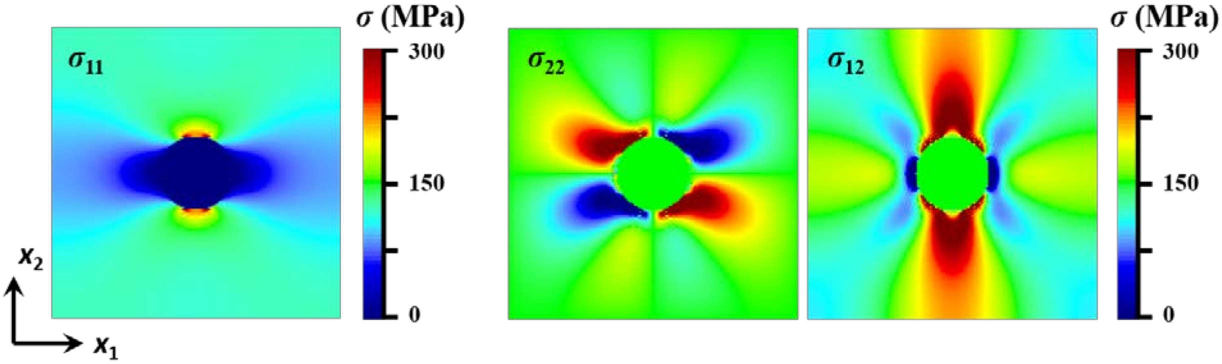

Figure 5.2.2 Stress distribution on applying an external stress σ_{11} = 100MPa.

5.3 Dielectric particles in vacuum

This example considers the electrostatic problem of within a system with periodically aligned dielectric particles inside the vacuum on applying an external electric field. The dielectric permittivity of the dielectric particles is set as $\kappa_{r11} = \kappa_{r22} = \kappa_{r33} = 1000$. An external electric field E_1 = 100 MV/m is applied. The structure is shown below.

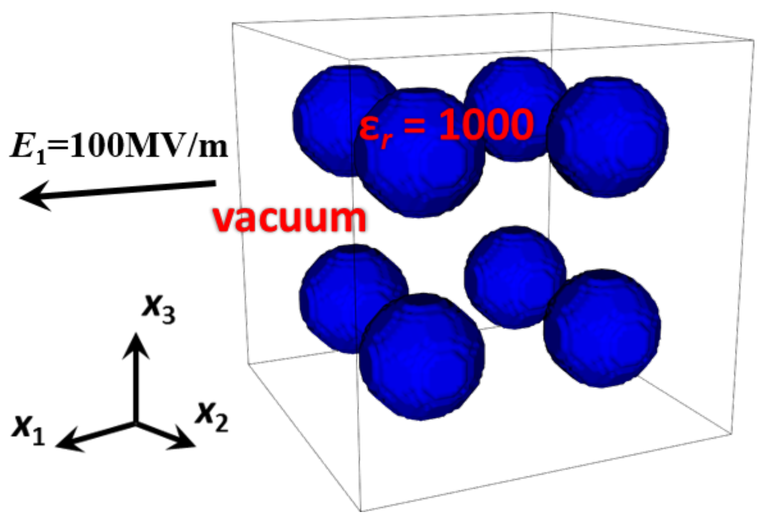

Figure 5.3.1 Schematics of the example of dielectric particles in vacuum.

The simulated electric field distribution is shown below.

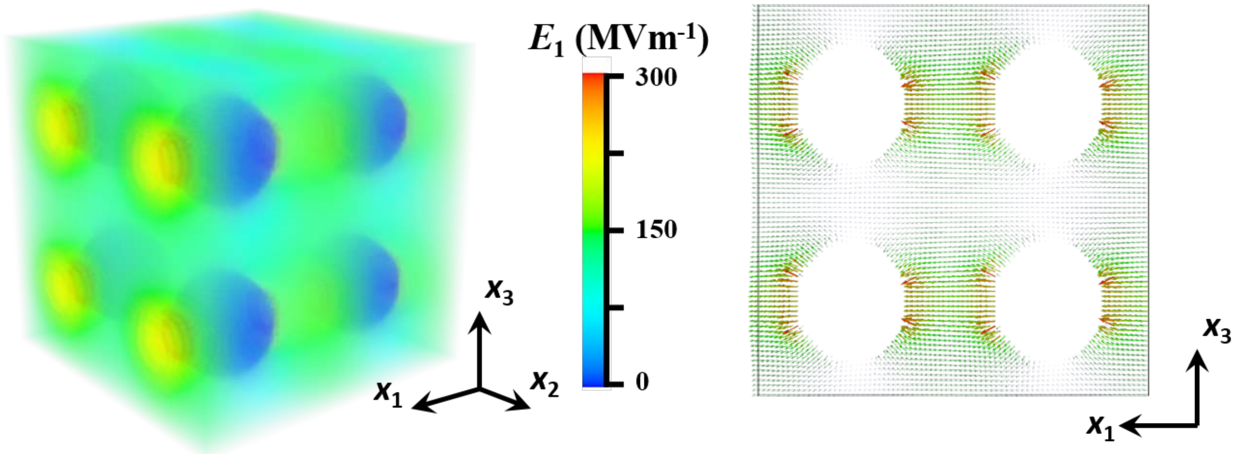

Figure 5.3.2 Electric field distribution on applying an external electric field E_1 = 100 MV/m. (Left) heat plot of E_1; (right) vector plot of E in the cross-section through the center of the dielectric particles.

5.4 Piezoelectric particles in a dielectric matrix

This example considers the piezoelectric property of a system with periodically aligned piezoelectric squares in a dielectric matrix. The following material constants are adopted:
Inclusions:
$\kappa_{r11} = \kappa_{r22} = \kappa_{r33} = 100$
$c_{11} = c_{22} = c_{33} = 45$ GPa
$c_{12} = c_{13} = c_{23} = 15$ GPa
$c_{44} = c_{55} = c_{66} = 15$ GPa
$d_{31} = d_{32} = -30$ nC/N
$d_{33} = 100$ nC/N
$d_{15} = d_{24} = 80$ nC/N
Matrix:
$\kappa_{r11} = \kappa_{r22} = \kappa_{r33} = 100$
$c_{11} = c_{22} = c_{33} = 90$ GPa
$c_{12} = c_{13} = c_{23} = 30$ GPa
$c_{44} = c_{55} = c_{66} = 30$ GPa
The two-phase structure is shown below.

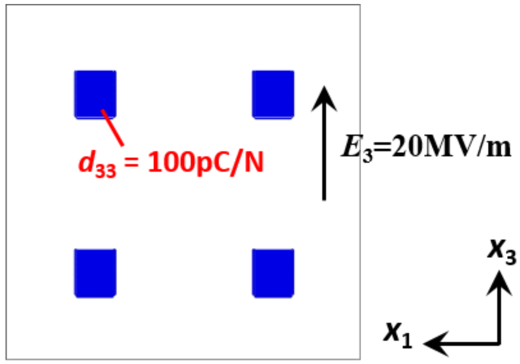

Figure 5.4.1 Schematics of the example of piezoelectric particles in a dielectric matrix.

The calculated effective elastic stiffness **c**, dielectric permittivity $\boldsymbol{\kappa}_r$, and piezoelectric coefficient **d** of the system is

$$\mathbf{c} = \begin{pmatrix} 85.9 & 28.6 & 28.5 & 0.0 & 0.0 & 0.0 \\ 28.6 & 87.0 & 28.7 & 0.0 & 0.0 & 0.0 \\ 28.5 & 28.7 & 87.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 28.8 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 28.7 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 28.8 \end{pmatrix} \text{GPa}$$

$$\boldsymbol{\kappa}_r = \begin{pmatrix} 100 & 0 & 0 \\ 0 & 100 & 0 \\ 0 & 0 & 98 \end{pmatrix}$$

$$\mathbf{d} = \begin{pmatrix} 0.00 & 0.00 & 0.00 & 0.00 & 4.13 & 0.00 \\ 0.00 & 0.00 & 0.00 & 3.38 & 0.00 & 0.00 \\ -1.56 & -1.08 & 4.99 & 0.00 & 0.00 & 0.00 \end{pmatrix} \text{nC/N}$$

The simulated spatial distribution of strain and stress on applying an external electric field of E_3 = 20 MV/m is shown below.

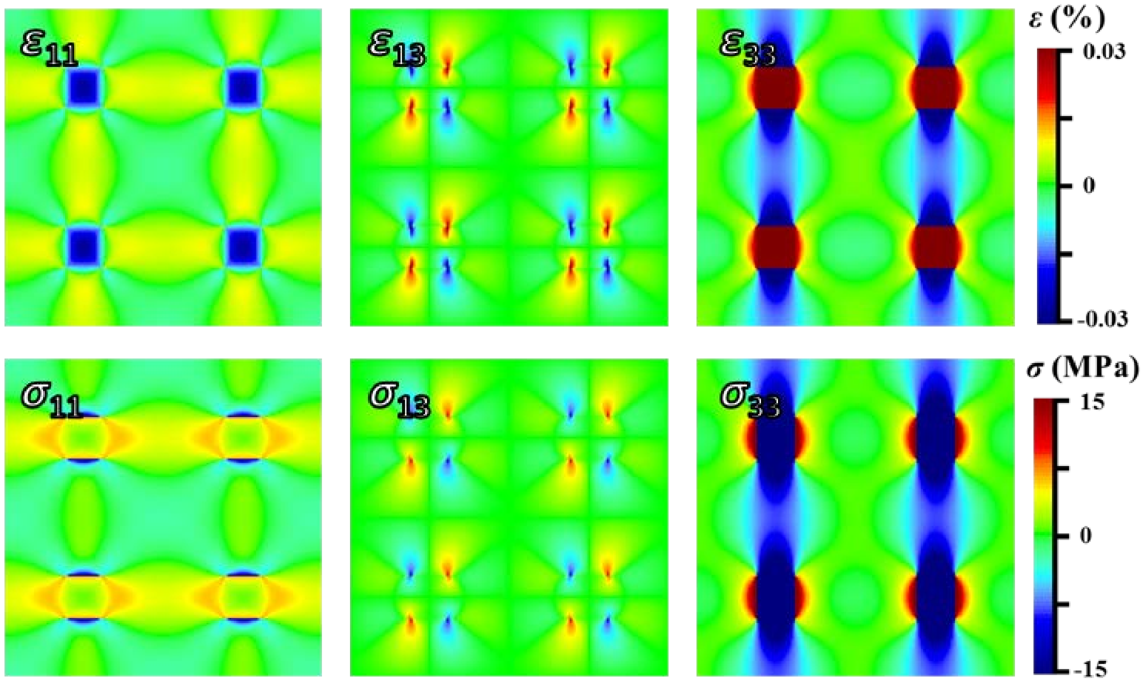

Figure 5.4.2 Spatial distribution of strain and stress on applying an external electric field of E_3 = 20 MV/m.

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