**Magnetic Program Documentation**

May 11, 2016

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**1 Purpose of the program**

The program simulates the microstructure evolution of a magnet under applied external fields.

**2 Simulation Method**

**2.1 Basic design**

The total size of the simulation system is , which is evenly discretized into  cuboid grids, i.e., the size of each simulation grid is , , and .

The simulation system can be one of the following types:

Bulk, 3-D;

Bulk, 2-D;

Bulk, 1-D;

Thin film, 3-D;

Thin film, 2-D;

Island-on-substrate, 3-D;

Island-on-substrate, 2-D;

Freestanding finite-size magnet, 3-D;

Freestanding finite-size magnet, 2-D;

Freestanding finite-size magnet, 1-D.

A set of additional parameters are used to specify the system, which may include the film thickness *nf*, island (or finite-size magnet) thickness *ni*3, island (or finite-size magnet) lengths *ni*1 and *ni*2, and substrate thickness *ns*. Schematics of all types of systems and corresponding parameters are listed below. All the parameters are in the unit of grid numbers.

**Table 2.1** Types of systems

|  |  |  |
| --- | --- | --- |
| **System type and schematics** | **Parameters specifying the system** | **Value of parameters** |
| Bulk, 3-D  C:\Users\tuy123\Desktop\bulk.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | Length of the system along *x*2 direction |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | 0 |
| *ni*3 | 0 |
| Bulk, 2-D  C:\Users\tuy123\Desktop\bulk2d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | 1 |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | 0 |
| *ni*3 | 0 |
| Bulk, 1-D  C:\Users\tuy123\Desktop\bulk1d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | 1 |
| *n*3 | 1 |
| *nf* | 0 |
| *ni*3 | 0 |
| Thin film, 3-D  C:\Users\tuy123\Desktop\film.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | Length of the system along *x*2 direction |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | Thickness of the film along *x*3 direction |
| *ns* | Thickness of the substrate along *x*3 direction |
| Thin film, 2-D  C:\Users\tuy123\Desktop\film2d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | 1 |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | Thickness of the film along *x*3 direction |
| *ns* | Thickness of the substrate along *x*3 direction |
| Island(s)-on-substrate, 3-D  C:\Users\tuy123\Desktop\Picture2.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | Length of the system along *x*2 direction |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | 0 |
| *ni*3 | Thickness of the island along *x*3 direction |
| *ns* | Thickness of the substrate along *x*3 direction |
| *C*Island | 1 |
| *ni*1 | Length of the island along *x*1 direction |
| *ni*2 | Length of the island along *x*2 direction |
| Island(s)-on-substrate, 2-D  C:\Users\tuy123\Desktop\island2d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | 1 |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | 0 |
| *ni*3 | Thickness of the island along *x*3 direction |
| *ns* | Thickness of the substrate along *x*3 direction |
| *C*Island | 1 |
| *ni*1 | Length of the island along *x*1 direction |
| *ni*2 | 1 |
| Freestanding finite-size magnet, 3-D  C:\Users\tuy123\Desktop\finite.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | Length of the system along *x*2 direction |
| *n*3 | Length of the system along *x*3 direction |
| *nf* | 0 |
| *ni*3 | Thickness of the magnet along *x*3 direction |
| *ns* | 0 |
| *C*Island | 1 |
| *ni*1 | Length of the magnet along *x*1 direction |
| *ni*2 | Length of the magnet along *x*2 direction |
| Freestanding finite-size magnet, 2-D  C:\Users\tuy123\Desktop\finite2d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | Length of the system along *x*2 direction |
| *n*3 | 1 |
| *nf* | 0 |
| *ni*3 | 1 |
| *ns* | 0 |
| *C*Island | 1 |
| *ni*1 | Length of the magnet along *x*1 direction |
| *ni*2 | Length of the magnet along *x*2 direction |
| Freestanding finite-size magnet, 1-D  C:\Users\tuy123\Desktop\finite1d.png | *n*1 | Length of the system along *x*1 direction |
| *n*2 | 1 |
| *n*3 | 1 |
| *nf* | 0 |
| *ni*3 | 1 |
| *ns* | 0 |
| *C*Island | 1 |
| *ni*1 | Length of the magnet along *x*1 direction |
| *ni*2 | 1 |

*C*Island on input specifies whether the in-plane (i.e., in *x*1-*x*2 plane) shape of an island or a freestanding finite-size magnet be a rectangle (*C*Island=1), an ellipse (*C*Island=2), or any other arbitrary shape (*C*Island=0), respectively. On setting *C*Island=2, *ni*1 and *ni*2 would specify the major or minor axes of the ellipse along *x*1 and *x*2 directions, respectively. On setting *C*Island=0, an arbitrary in-plane shape defined in an input file *islandShape.in* would be adopted (see Section 3 for details). Cases for *C*Island=2 and *C*Island=0 are omitted in Table 2.1.

For thin films and island(s)-on-substrate systems, the thickness of the substrate should be at least 11 grids, i.e., . At all actual surfaces of a magnet, a number of at least 4 stacking layers of vacuum is needed, if one or more of the following components is considered: (demagnetizing) stray field, magnetoelastic interaction, exchange interaction, or Dzyaloshinskii-Moriya interaction (DMI). For example, for simulating a cuboid island with a length of *ni*1 grids along *x*1 direction, *n*1 should be chosen following .

Spatial distribution of the local magnetization vector  is used to describe magnetic domain structure, where **x** is the position vector, *MS* is the spontaneous magnetization, and **m** is the normalized magnetization. The SI units are adopted in *μ*-Pro® Mag and throughout this documentation.

A set of Euler angle arrays including  are introduced to treat a polycrystal. These angle arrays rotate the system coordinate axes to the local crystallographic coordinate axes. The transformation matrix **a** from the system coordinates to the local crystallographic coordinates is

 (1)

For example, transformation of a vector **v** from the system coordinates to local crystallographic coordinates follows  (*i*,*j*=1,2,3). Here a prime (‘) in a subscript following an index 1, 2, or 3 indicates a component of a vector or a tensor in the local crystalline coordinate, e.g., *m*1’(**x**) is the component of **m**(**x**) along the local crystallographic coordinate axis  at position **x**. Note that Einstein summation convention is adopted throughout the documentation.

**2.2 Magnetization dynamics**

Temporal evolution of **m** is governed by the Landau-Lifshitz-Gilbert (LLG) equation, i.e.,

 (2)

where *t* is the time,  is the total torque, *α* is the damping constant, *γ*0 is the gyromagnetic ratio in . **H**eff is the effective magnetic field given by

. (3)

where  is the vacuum permeability, and *F*[**M**] is the Helmholtz free energy of the system, as a functional of the magnetization distribution. **H**eff includes the following contributions:

* External field **H**ext;
* Magnetic stray field or demagnetizing field **H**d;
* Magnetocrystalline anisotropy field **H**anis;
* Magnetoelastic field **H**elas;
* Exchange interaction field **H**exch;
* Dzyaloshinskii-Moriya interaction (DMI) field **H**DMI;
* Thermal fluctuation field **H**therm;
* Effective field from spin-transfer torque or spin-orbit torque **H**ST,

as below,

. (4)

*μ*-Pro® Mag provides two numerical methods for solving the LLG equation:

* IGS, implicit Gauss-Seidel projection method[1] implemented with Fourier-Spectral approach[2][3]. Contribution of the short-range interaction  is implicitly considered, while other contributions to **H**eff are explicitly evaluated.
* RK4, the Runge-Kutta method. All contributions to **H**eff are explicitly evaluated.

The time during magnetization evolution is discretized into time steps with a fixed duration , i.e.,  where  is the step number. The recommended range for the value of  is, for numerical stability and accuracy.

**2.3 External field, stray field, and magnetostatic boundary condition**

The magnetic field **H** consists of external field and magnetostatic stray field, i.e., . In *μ*-Pro® Mag, the external field **H**ext is considered spatially uniform in the simulation system, in the unit of A/m. The volume density of external field energy is given by

. (5)

*μ*-Pro® Mag provides an option of choosing **H**ext on input as a combination of a DC and an AC component, i.e., 

The magnetostatic stray field energy is given by

 (6)

The energy density is written as

. (7)

**H**stray is obtained at each evolution step by solving the magnetostatic equilibrium equation

 (8)

Two types of boundary condition are used for **H**stray. In a period boundary condition, the simulation system is considered as a building block that appears repeatedly appear in 3-D space, and the stray field is expressed as , where *ϕ* is the magnetic scalar potential with a periodic boundary condition solved using the Fourier spectral method, as given in Ref. [3], the 3×3 symmetric matrix **N***D* is the demagnetizing factor which depends only on the macroscopic shape of the actual sample (not the shape of the simulation system, e.g., see Table 2.2), and  is the average magnetization of the simulation system. In a finite-size boundary condition, space outside the simulation system is considered to be filled by vacuum without magnetization, electric charge, or current etc., and the stray field is solved based on convolution theorem accelerated by FFT[4], without explicitly utilizing demagnetizing factors. Table 2.2 lists the recommended stray field boundary conditions and (when applicable) demagnetizing factors for typical types of systems.

**Table 2.2** Recommended stray field boundary condition and demagnetizing factor

|  |  |  |
| --- | --- | --- |
| **System type** | **Boundary condition** | **(ND1, ND2, ND3)** |
| Bulk (periodic) | Periodic | (0, 0, 0) or (1/3, 1/3, 1/3), or calculated based on the macroscopic shape of the sample |
| Thin film (periodic in-plane) | Periodic | (0, 0, 1) |
| Island(s)-on-substrate arrays (periodic in-plane) | Periodic | (0, 0, 1) |
| Single group of island(s)-on-substrate | Finite-size | / |
| Freestanding finite-size magnet | Finite-size | / |

**2.4 Magnetocrystalline anisotropy**

Two types of magnetocrystalline anisotropy are considered, the cubic anisotropy with magnetic easy axes along <100>, <110>, or <111> crystal axes, and the uniaxial anisotropy in ultra-thin films with a magnetic easy/hard axis perpendicular to the film plane. The volume density of magnetocrystalline anisotropy energy is given by

Cubic anisotropy

 (9A)

Uniaxial anisotropy

 (9B)

where **K** is the magnetocrystalline anisotropy coefficient.

The anisotropy effective field is calculated as

 (10)

**2.5 Magneto-Elastic interaction**

The elastic energy density is given by

 (11)

where **c** is the elastic stiffness tensor, **ε** is the strain, and **ε**0 is the stress-free strain calculated as

 (12)

where *λ*100 and *λ*111 are saturation magnetostriction along <100> and <111> crystalline axes, respectively.

The magnetoelastic effective field is written as

 (13)

where **σ** is the stress field given by .

Assuming that the elastic equilibrium condition holds at each evolution step, the strain and stress are obtained at each evolution step through solving the mechanical equilibrium equation

 (14)

using a Fourier spectral method[5][6] based on Khachaturyan’s elasticity theory[7]. Table 2.3 summarizes the boundary conditions implemented in typical types of systems. Examples showing the influence of elastic boundary condition on the magnetic domain structure can be found in Ref.[8].

**Table 2.3** Elastic boundary conditions

|  |  |
| --- | --- |
| **System type** | **Boundary condition** |
| Bulk (periodic) | 3-d periodic, with specified applied strain **ε***a* or applied stress **σ***a* |
| Thin film (periodic in-plane) | Thin film boundary condition (see Ref. [5] for details), with specified in-plane substrate strain **ε***a* (i.e., , , and ) |
| Island(s)-on-substrate | Periodic in-plane, stress-free island surfaces, with specified in-plane substrate strain **ε***a* (i.e., , , and ) |
| Freestanding finite-size magnet | Stress-free |

An iterative Fourier-Spectral method is used (see details in Ref. [6]) to solve equation (14) in elastically inhomogeneous systems (that is, spatially variant **c**), including:

* Island-on-substrate system
* freestanding finite-size systems
* Polycrystals
* Film-on-substrate system where the magnet and substrate have different elastic stiffness.

A convergence of the iterative approximation is claimed when the difference of total elastic energy between adjacent recursion loops is within a tolerance value Δe (arbitrary unit), i.e., , where  is the total elastic energy of the *n*-th iterative approximation. If convergence is not reached after the allowed maximum number nRecurs of recursion loops, the program claims to fail to solve the mechanical equilibrium equation and stops. An output file *fort.72* will be generated and updated on solving the mechanical equilibrium equation with inhomogeneous elasticity, containing the total elastic energy (arbitrary unit) in every recursion loop. Both nRecurs and Δe are user adjustable (see Section 3) with recommended range of 100~2000 and 10-5~10-3, respectively.

**2.6 Magnetic exchange interaction**

The density of magnetic exchange energy is given by

 (15)

where *A* is the exchange constant in the unit of J/m.

The exchange field is expressed as

 (16)

**2.7 Dzyaloshinskii-Moriya interaction (DMI)**

The DMI module in *μ*-Pro® Mag belongs to the interface type[9], which can be invoked when simulating an ultrathin magnetic thin film or island with perpendicular magnetic anisotropy. Consider a homogenous effective DMI constant *D*, the interface DMI energy density is given by

 (17)

The effective magnetic field due to DMI is therefore expressed as

 (18)

where **e**3 is the unit vector along the *x*3 direction.

**2.8 Thermal fluctuation**

The thermal fluctuation field is given by

 (19)

where  is the Boltzmann constant, *T* is the Kelvin temperature,  is the volume of a grid, and **η** is a random vector with three independent components *η*1, *η*2, and *η*3 all obeying standard normal distribution. Values of these three components are independent at each evolution step.

**2.9 Spin torque**

The spin-orbit torque and Slonczewski spin-transfer torque are given by

 (20)

where  is the normalized fixed-layer magnetization in the case of spin-transfer torque, while represents the direction of spin current generated through Spin Hall Effect; and the pre-factor depends on the type of the spin torque.

For spin-orbit torque[10],

 (21)

where  is the Bohr magneton, *J* is the electric current density,  is the spin Hall angle,  is the elementary charge. *d* is the thickness of the free magnetization layer, as defined with the type of the system (see Table 2.1).

For Slonczewski spin-transfer torque[11][12],

 (22)

where  is the spin polarization constant.

The effective field corresponding to spin-orbit torque or Slonczewski spin-transfer torque is given by

 (23)

The Zhang-Li spin-transfer torque is given by[13]

 (24)

where  is the degree of non-adiabaticity.

The effective field corresponding to a Zhang-Li spin-transfer torque is given by

 (25)

**3 Input files**

Users need to prepare one to five files as input:

***parameter.in***

Declares the size of the system, the type of properties considered, properties of each phase, and external fields applied. This file can be written using the GUI provided in *μ*-Pro® package.

The format is as follows:

**Table 3.1** Format of the input file *parameter.in*

|  |  |  |  |
| --- | --- | --- | --- |
| Data in the file | | | Explanation |
| l1 | l2 | l3 | System real size along x1, x2, and x3 directions (nm) |
| n1 | n2 | n3 | Total number of simulation grids along x1, x2, and x3 directions |
| ns | nf |  | See Section 2.1 |
| CIsland |  |  | See Section 2.1 |
| ni1 | ni2 | ni3 | See Section 2.1 |
| CGrain |  |  | Choice of input type of crystalline grain structure: 0-Euler angles φ, θ, and ψ (°) array read from file *eulerAng.in*; 1-single crystal with specified Euler angles |
| φC | θC | ψC | (For CGrain=1) Euler angles φ, θ, and ψ (°) of the single crystal orientation |
| MS | γ | α | MS – saturation magnetization (A/m);  γ – electron gyromagnetic ratio (m/(A.s));  α – damping constant (unitless) |
| FlAnis |  |  | Flag of whether to consider magnetocrystalline anisotropy |
| CAnis |  |  | (For FlAnis=true) Choice of type of magnetocrystalline anisotropy: 1-cubic; 2-uniaxial |
| K1 | K2 | K3 | (For FlAnis=true and CAnis=1) K1, K2, K3 – cubic magnetocrystalline anisotropy coefficient **K** (J/m3);  (For FlAnis=true and CAnis=2) K1, K2 – uniaxial magnetocrystalline anisotropy coefficient **K** (J/m3) |
| FlStray |  |  | Flag of whether to consider stray field |
| FlPer |  |  | (For FlStray=true) Flag of the magnetostatic boundary condition: whether to use a periodic (or otherwise finite-size) boundary |
| ND11 | ND22 | ND33 | (For FlStray=true and FlPer=true) demagnetizing factor **N**D (unitless) |
| ND23 | ND13 | ND12 |
| CHext |  |  | Choice of input type of external magnetic field: 0-an array of field sequence read from file *hExt.in* with possible linear interpolations; 1-DC and AC components defined in following lines, i.e., |
| HDC1 | HDC2 | HDC3 | (For CHext=1) DC component of external magnetic field **H**DC (A/m) |
| HAC1 | HAC2 | HAC3 | (For CHext=1) magnitude of AC component of external magnetic field **H**AC (A/m) |
| fAC |  |  | (For CHext=1) frequency of AC component of external magnetic field (Hz) |
| A |  |  | Magnetic exchange energy coefficient (J/m) |
| FlElas |  |  | Flag of whether to consider magnetoelastic effect |
| λ100 | λ111 |  | (For FlElas=true) Saturation magnetostriction **λ** (unitless) |
| c1’1’ | c1’2’ | c4’4’ | (For FlElas=true) Elastic stiffness **c** of the magnet in Voigt notation (Pa) |
| cs1’1’ | cs1’2’ | cs4’4’ | (For film or island, and FlElas=true) Elastic stiffness **c**s of the substrate in Voigt notation (Pa) |
| FlStrain |  |  | (For bulk and FlElas=true) Flag of the mechanical boundary condition: whether to use an applied strain (or otherwise an applied stress) |
| () | () | () | (For film or island, and FElas=true) in-plane substrate strain **ε***a*;  (For bulk, FlElas=true, and FlStrain=true) in-plane components of applied strains **ε***a* (unitless);  (For bulk, FlElas=true, and FlStrain=false) in-plane components of applied stress **σ***a* (Pa) |
| () | () | () | (For bulk, FlElas=true, and FlStrain=true) out-of-plane components of applied strains **ε***a* (unitless);  (For bulk, FlElas=true, and FlStrain=false) out-of-plane components of applied stress **σ***a* (Pa) |
| nRecurs | Δe |  | (For FlElas=true, and with inhomogeneous elastic stiffness in the system) nRecurs – maximum number of recursion loops for elastic solver;  (For FlElas=true, and with inhomogeneous elastic stiffness in the system) Δe – maximum error for elastic solver |
| FST |  |  | Flag of whether to consider spin torque |
| CST |  |  | (For FlST=true) type of spin torque: 1-spin-orbit torque 2-Slonczewski spin-transfer torque 3-Zhang-Li spin-transfer-torque |
| θSH |  |  | (For FlST=true, and CST=1) spin Hall angle in a spin-orbit torque |
| ηSP |  |  | (For FlST=true, and CST=2) spin polarization constant in a Slonczewski spin-transfer torque |
| ξSTT |  |  | (For FlST=true, and CST=3) degree of non-adiabaticity in a Zhang-Li spin-transfer torque |
| J1 | J2 | J3 | (For FlST=true, and CST=1 or 2) J3 – spin-polarized electric current density along x3 direction  For FlST=true, and CST=3) J1, J2, J3 – spin-polarized electric current density **J** |
|  |  |  | (For FlST=true, and CST=1 or 2) normalized magnetization **m***P* in the fixed layer in a spin torque structure (unitless) |
| FlDMI |  |  | Flag of whether to consider Dzyaloshinskii-Moriya interaction (DMI) |
| D |  |  | (For FlDMI=true) continuous effective DMI constant |
| FlTherm |  |  | Flag of whether to consider thermal fluctuation field |
| T |  |  | (For FlTherm=true) temperature (K) |
| CLLG |  |  | Type of LLG numerical solver: 1-implicit Gauss-Seidel using Fourier spectral 2-explicit RK4 |
| Δt |  |  | Time per evolution step (s) |
| kt0 | ktMax |  | kt0 – number of the starting evolution step;  ktMax – number of the finishing evolution step |
| ktTable | ktDist |  | ktTable – output step interval for data table;  ktDist – output step interval for spatial distribution |
| CInitialM |  |  | Choice of input type of initial magnetization distribution: 0-an array of magnetization distribution read from file *Magnt.in*; 1-random orientation; 2-specified uniform orientation; 3-specified vortex domain |
| a1 | a2 | a3 | (For CInitialM=2) axis of **a** uniform orientation of the initial magnetization;  (For CInitialM=3) axis of **a** vortex of the initial magnetization |
| FlOutH | FlOutE |  | FlOutH – flag of whether to output distribution of effective fields  FlOutE – flag of whether to output distribution of energy densities |
| FlOutS |  |  | (For FlElas=true) flag of whether to output distribution of eigenstrain, strain, and stress |

***islandShape.in* (optional)**

Contains an array  describing the 2-d in-plane shape of a magnetic island. This file is used only in an island-on-substrate or a finite-size magnet system with CIsland=0, as defined in the file *parameter.in*.

The format is as follows:

**Table 3.2** Format of the input file *islndShape.in*

|  |  |  |  |
| --- | --- | --- | --- |
| Data in the file | | | Explanation |
| 1 | 1 | om2d(1, 1) | If om2d(1, 1)=1, grid points (1, 1, k) where k is within the thickness of the island are considered within the magnetic island, i.e., om(1, 1, k)=1.  If om2d(1, 1)=0, grid points (1, 1, k) where k is within the thickness of the island are considered vacuum, i.e., om(1, 1, k)=0. |
|  |  |  |  |
| 1 | n2 | om2d (1, n2) |  |
|  |  |  |  |
| n1 | n2 | om2d (n1, n2) |  |

***eulerAng.in* (optional)**

Contains an array of the distribution of the Euler angles  of grains in polycrystals, arranged in a row-major order. This file is used only with CGrain=0, as defined in the file *parameter.in*.

The format is as follows:

**Table 3.3** Format of the input file *eulerAng.in*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Data in the file** | | | | | | **Explanation** |
| n1 | n2 | n3 |  |  |  | Total number of simulation grids in each direction |
| 1 | 1 | 1 | φ(1, 1, 1) | θ(1, 1, 1) | ψ(1, 1, 1) | φ, θ, ψ – Euler angles of the grain containing the grid point (1, 1, 1) (°) |
|  | | | | | |  |
| 1 | 1 | n3 | φ(1, 1, n3) | θ(1, 1, n3) | ψ(1, 1, n3) |  |
|  | | | | | |  |
| 1 | n2 | n3 | φ(1, n2, n3) | θ(1, n2, n3) | ψ(1, n2, n3) |  |
|  | | | | | |  |
| n1 | n2 | n3 | φ(n1, n2, n3) | θ(n1, n2, n3) | ψ(n1, n2, n3) |  |

***hExt.in* (optional)**

Contains an array of the external magnetic field sequence . This file is used only with CHext=0, as defined in the file *parameter.in*.

The format is as follows:

**Table 3.4** Format of the input file *hExt.in*

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Data in the file** | | | | **Explanation** |
| kt1 | Hext1(kt1) | Hext2(kt1) | Hext3(kt1) | Hext1(kt1), Hext2(kt1), and Hext3(kt1) – external magnetic field **H**ext at the kt1-th evolution step (A/m) |
| kt2 | Hext1(kt2) | Hext2(kt2) | Hext3(kt2) |  |
|  |  |  |  |  |
| ktn | Hext1(ktn) | Hext2(ktn) | Hext3(ktn) |  |

In obtaining  at all evolution steps kt, the program considers linear interpolations of  between adjacent evolution steps kt provided in this file.

***magnt.in* (optional)**

Contains an array of the distribution of initial magnetization , arranged in a row-major order. This file is used only with CInitialM=0, as defined in the file *parameter.in*.

The format is as follows:

**Table 3.5** Format of the input file *magnt.in*

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Data in the file** | | | | | | **Explanation** |
| n1 | n2 | n3 |  |  |  | Total number of simulation grids in each direction |
| 1 | 1 | 1 | m1(1, 1, 1) | m2(1, 1, 1) | m3(1, 1, 1) | m1, m2, m3 – normalized initial magnetization **m** at grid point (1,1,1) (unitless) |
|  | | | | | |  |
| 1 | 1 | n3 | m1(1, 1, n3) | m2(1, 1, n3) | m3(1, 1, n3) |  |
|  | | | | | |  |
| 1 | n2 | n3 | m1(1, n2, n3) | m2(1, n2, n3) | m3(1, n2, n3) |  |
|  | | | | | |  |
| n1 | n2 | n3 | m1(n1, n2, n3) | m2(n1, n2, n3) | m3(n1, n2, n3) |  |

**4 Ouput files**

**4.1 Files generated before doing evolution**

***oMag.00000000.dat***

Contains an array of  (unitless), arranged in a row-major order. The data follow a similar format with those in *magnt.in*. The file is generated before simulating evolution steps.

***cGlob.00000000.dat* (optional)**

Contains an array of  (Pa) in Voigt notation, arranged in a row-major order. The data follow a similar format with those in *magnt.in*. The file is generated before simulating evolution steps and only under FlElas=true.

***hExt.dat***

Contains an array of the external magnetic field sequence  (A/m) at all evolution steps. The data follow a similar format with those in *hExt.in*. The file is generated before simulating evolution steps.

**4.2 Files generated during evolution steps**

***avMagntz.dat***

Contains an array of average values of the normalized magnetization (unitless) inside the magnet at every ktTable evolution steps. The data follow a similar format with those in *hExt.in*. The file is updated every ktTable steps.

***avHEff.dat***

Contains an array of average values of the effective fields (A/m) inside the magnet at every ktTable evolution steps. The data follow a similar format with those in *hExt.in*. The file is updated every ktTable steps.

***avStrain.dat* (optional)**

Contains an array of average values of the strain and eigenstrain  (unitless) inside the magnet at every ktTable evolution steps. The data follow a similar format with those in *hExt.in*. The file is updated every ktTable steps, and only under FlElas=true.

***avStress.dat* (optional)**

Contains an array of average values of the stress , and  (Pa) inside the magnet at every ktTable evolution steps. The data follow a similar format with those in *hExt.in*. The file is updated every ktTable steps, and only under FlElas=true.

***magnt.\*\*.dat***

Contains an array of  (unitless) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps.

***hEff.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true.

***hStra.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true and FlStray=true.

***hAnis.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true and FlAnis=true.

***hElas.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true and FlElas=true.

***hST.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true and FlST=true.

***hTher.\*\*.dat* (optional)**

Contains an array of  (A/m) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutH=true and FlTherm=true.

***eigStn.\*\*.dat* (optional)**

Contains an array of  (unitless) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutS=true and FlElas=true.

***strain.\*\*.dat* (optional)**

Contains an array of  (unitless) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutS=true and FlElas=true.

***stress.\*\*.dat* (optional)**

Contains an array of  (Pa) at a certain evolution step, arranged in a row-major order, where \*\* represents the 8-digit evolution step number. The data follow a similar format with those in *magnt.in*. A file is generated every ktDist steps and only under FlOutS=true and FlElas=true.

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